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Mathematical Expression and Reasoning for Computer Science

Lecture Notes for CSC165 (Version 0.4)

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 $A\ new\ domain:\ number\ theory$

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Prologue: what is this course about, and why should I care?

In CSC165, we will be talking about how to express statements precisely using the language of mathematical logic. This gives a way to communicate ideas without any ambiguity, which is an essential skill for any discipline. For example, the English statement "Some people like David" can be interpreted as saying that at least one person likes David, or that few, many, or even all people like David. What about "You can get cake or ice cream"? Does this mean that you may enjoy both cake and ice cream, or that you must choose between the two? Another example is the English expression "If you are a Pittsburgh Pens fan, then you are not a Philadelphia Flyers fan." Its meaning is clear enough if you meet a Pens fan, but what does this mean, if anything, for someone who *isn't* a Pittsburgh Pens fan? Does the same reasoning apply to the statement "If you can solve any problem in this course, then you will get an A"? Mathematical expressions in formal logic, on the other hand, have only one meaning. They remove all ambiguity so that only one interpretation is possible.

The second major theme of the course is developing methods to give rigorous mathematical proofs or disproofs of mathematical statements. We don't just want to be able to express ideas, we want to be able to argue—to both ourselves and others—that these ideas are correct. Mathematical proofs are a way to convince someone of something in an absolute sense, without worrying about biases, rhetoric, feelings, or alternate interpretations. The beauty of mathematics is that unlike other vast areas of human knowledge, it is possible to prove that a mathematical statement is true with one-hundred percent certainty. Without a rigorous mathematical proof, we can be easily fooled by our intuition and preconceptions. We will see throughout the course that some statements that seem perfectly reasonable turn out to be wrong, and others turn out to be true in surprising ways. Sometimes our intuition is valid and a proof seems like a mere formality; but often our intuition is incorrect, and going through the process of a rigorous mathematic proof is the only way that we discover the truth!

Why mathematical expression and reasoning in computer science?

So many reasons! Perhaps the most basic one is program correctness. Say your friend has written a complicated program that she says does something truly remarkable. How do you know it is correct? You can test it on some inputs, but how do you know that your tests are thorough enough? Programmers often

¹ What does it *mean* for a program to "be correct?" How can you *prove* that a program is correct?

rely on a combination of tests and their own intuition to convince themselves that their programs are correct, but neither of these are guarantees. A correctness proof will convince you that without a shadow of a doubt, the algorithm is correct on all possible inputs. Not only that, but the practice of proving the correctness of algorithms will refine your own intuitions, making you a better programmer overall.

But wait. Maybe her program does what she claims, but what if on some inputs it takes an extremely long time to run?² A worst-case complexity analysis is a formal way to convince you that no matter what the input is, her program will run in some guaranteed number of time steps, independent of which computer or programming language is used to write and run this program.

These are two fundamental computer science areas where formal mathematical expression is required to precisely define concepts, and mathematical reasoning is required to prove statements about those concepts. Throughout this course we will follow this two-step process of defining and then proving things very explicitly, and we will practice on many examples. There are many other applications of mathematical expression and reasoning in computer science, some of which we list below. In all cases, mathematical expression allows us to precisely define our claims about the system in question, and mathematical proofs give us a mechanism to convince others with certainty that our system is working as we specified.

- Program verification. This is essentially program correctness mentioned above, and is in fact an entire subarea of computer science. Formal verification is the use of mathematical expression and reasoning in order to argue that a given software or hardware system is correct. Again, you need mathematical expression in order to specify without ambiguity both what the system is and what it means for the system to be correct. Then you need proofs in order to prove or disprove the correctness of the system.
- Cryptography. Cryptography is the science of developing techniques to communicate information in a way that is secure even in the presence of adversaries. The most basic cryptographic task is to send an encrypted message across the Internet to a particular person so that the intended receiver is able to decrypt the message, while ensuring that other agents, for whom the message is not intended, are not able to modify the message or to decrypt it. The area of cryptography is now quite sophisticated, and there are extremely clever protocols that allow us to perform many tasks, such as public-key cryptography, digital signatures, and data authentication. Mathematical expression is required in order to even define precisely what we mean by "secure." Then proofs are needed in order to show that our cryptographic techniques are indeed secure.
- Privacy. Issues of privacy are abundant. How do we manage the massive amount of data that is available through the web, while at the same time keep sensitive information private? In order to study this question, one first needs a formal definition of what is even meant by privacy. Intuitively, we want such a definition to capture the idea that data can be used for the benefit of society—such as to discover correlations between behaviour, symptoms and diseases—but so that the privacy of any particular person is not compromised. Once the definition is in place, the job then becomes to develop protocols and mechanisms that do useful things while maintaining a privacy guarantee. Again, one needs mathematical expression in order to state the definition of privacy, and proofs in order to show that the mechanisms satisfy the privacy definition.

² What does it mean for a program to "take a long time to run?" How can you prove that a program takes a long (or short) time to run?

³ You can think about it, but it is not at all obvious what such a definition should say. In fact, there are many definitions of security and other cryptographic notions used in theory and practice, depending on the context.

⁴ As with "security," there are many definitions out there for what is meant by "privacy," including the notion of differential privacy that has lately been in the news.

- Artificial intelligence. Many problems in artificial intelligence and machine learning involve logic. For example, in order to navigate a robot through a room, it helps to have a precise description of the room, as well as a plan for how to move through the room. Practically all problems in artificial intelligence involve mathematical expression and reasoning, including: natural language processing, image recognition, learning and planning.
- Complexity theory. Complexity theory is about whether important problems that we want solve can be carried out efficiently with respect to costly resources. Common resources considered are time, computer memory, and randomness.⁵ This study requires formal definitions of what we mean by efficient; research in this area aims to invent proofs that certain problems can or cannot be solved efficiently.

Course overview

In our first few weeks of this course, we will discuss mathematical expressions. That is, you will learn a new language and how to express precise statements in this language. It may seem daunting to pick up a new language in a few short weeks, but in fact you probably have been using this language since you were born. What we will do is formalize your intuitive understanding of logic so that it is as clear as possible what constitutes a legal mathematical statement and what doesn't.

After learning how to express our statements in this language of mathematical logic, we will discuss ways of reasoning about the truth (or falsehood) of these statements. You will both read and write proofs, learning how to construct airtight arguments and communicate them to others, and how to poke holes in flawed proofs. To practice the dual skills of expression and reasoning in computer science domains, we will introduce several new domains to serve as the foundations for our mathematical statements: number theory, combinations and permutations, program runtime, and graphs.6

⁵ The idea of "randomness" as a resource may be a surprising one, but is in fact the heart of one of the biggest open questions in complexity theory: If a problem can be solved by an efficient randomized algorithm, can it be solved by an efficient algorithm which has no randomness?

⁶ Of course, we are not introducing these domains just for the sake of having a few new definitions to play around with. Each of the domains we will study in this course serve a vital role in many areas of computer science, which we will only scratch the surface of in this course.

1 Mathematical Expression

As a starting point for formalizing our intuition of logic, we will define two mathematical notions that we will use repeatedly throughout the course: sets and functions. Much of the terminology here may be review for you (or at least appear vaguely familiar), but please pay careful attention to the **bolded terms**, as we will make heavy use of each of them throughout the course. Each of these terms has a specific technical meaning (given by our definition) that may be subtly different from your intuitive understanding. As we will stress again and again, *definitions* are precise statements about the meaning of a term or symbol; whenever we define something, it will be your responsibility to understand that definition so that you can understand—and later, reason about—statements using these terms at any point in the rest of this course and beyond.

Sets

Definition 1.1. A set is a collection of distinct objects, which we call elements of the set. A set can have a finite number of elements, or infinitely many elements. The size of a finite set A is the number of elements in the set, and is denoted by |A|. The empty set (the set consisting of zero elements) is denoted by \emptyset .

Before moving on, let us see some concrete examples of sets. These examples illustrate not just the versatility of what sets can represent, but also illustrate various ways of *defining* sets.

Example 1.1. A finite set can be described by explicitly listing all its elements between curly brackets, such as $\{a, b, c, d\}$ or $\{2, 4, -10, 3000\}$.

Example 1.2. A set of records of all people that work for a small company. Each record contains the person's name, salary, and age. For example:

{(Ava Doe, \$70000, 53), (Donald Dunn, \$67000, 30), (Mary Smith, \$65000, 25), (John Monet, \$70000, 40)}.

Example 1.3. Here are some familiar *infinite* sets of numbers. Note that we use the ... to indicate the continuation of a pattern of numbers.

- The set of natural numbers, $\mathbb{N} = \{0, 1, 2, \dots\}^{1}$
- The set of integers, $\mathbb{Z} = \{\dots, -2, -1, 0, 1, 2, \dots\}$.
- The set of positive integers, $\mathbb{Z}^+ = \{1, 2, \dots\}$.
- The set of rational numbers, Q.
- The set of real numbers, \mathbb{R} .
- The set of non-negative real numbers, $\mathbb{R}^{\geq 0}$.

¹ By convention in computer science, 0 is a natural number.

Example 1.4. The set of all finite strings over 0, 1. A finite string over 0, 1 is a finite sequence $b_1b_2b_3 b_k$, where k is some positive integer (called its length)² and each of b_1 , b_2 , etc. is either 0 or 1. The string of length 0 is called the *empty string*, and is typically denoted by the symbol ϵ .

Note that we have defined this set without explicitly listing all of its elements, but instead by describing exactly what properties its elements have. For example, using our definition, we can say that this set contains the element 01101000, but does not contain the element 012345.³

Example 1.5. A set can also be described as in this example:

$$\{x \mid x \in \mathbb{N} \text{ and } x \geq 5\}.$$

This is the set of all natural numbers which are greater than or equal to 5. The left part (before the |) describes the elements in the set in terms of a variable x, and right part states the *condition* on this variable that must be satisfied.⁴

As a more complex example, we can define the set of rational numbers as:

$$\mathbb{Q}=\left\{rac{p}{q}\,\middle|\, p,q\in\mathbb{Z} ext{ and } q
eq 0
ight\}$$

We have only scratched the surface of the kinds of objects we can represent using sets. Later on in the course, we will enrich our set of examples by studying sets of computer programs, sequences of numbers, and graphs.

Operations on sets

We have already seen one set operation: the size operator, |A|. In this subsection, we'll list other common set operations that we will use in this course.

The following *boolean* set operations return either True or False. We only describe when these operations return True; they return False in all other cases.

- $x \in A$: returns True when x is an element of A; $y \notin A$ returns True when y is not an element of A.
- $A \subseteq B$: returns True if every element of A is also in B. We say in this case that A is a subset of B.

A set A is a subset of itself, and the empty set is a subset of every set: $A \subseteq A$ and $\emptyset \subseteq A$ are always True.

• A = B: returns True if $A \subseteq B$ and $B \subseteq A$. In this case, A and B contain the exact same elements.

The following operations return sets:

- $A \cup B$, the union of A and B. Returns the set consisting of all elements that occur in A, in B, or in both.
- $A \cap B$, the intersection of A and B. Returns the set consisting of all elements that occur in both A and B.

² For example, the length of the string 10100101 is eight.

³ Food for thought: how would you generate a list of all finite strings over 0, 1?

⁴ Tip: The | can be read as "where".

- $A \setminus B$, the difference of A and B. Returns the set consisting of all elements that are in A but that are not in B.
- A × B, the (Cartesian) product of A and B. Returns the set consisting of all pairs (a, b) where a is an element of A and b is an element of B.
- $\mathcal{P}(A)$, the power set of A, returns the set consisting of all subsets of A.⁵ For example, if $A = \{1, 2, 3\}$, then

$$\mathcal{P}(A) = \{\emptyset, \{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}, \{1, 2, 3\}\}.$$

⁵ Food for thought: what is the relationship between |A| and $|\mathcal{P}(A)|$?

Functions

Definition 1.2. Let A and B be sets. A function $f:A\to B$ is a mapping from elements in A to elements in B. A is called the domain of the function, and B is called the codomain of the function. For example, if A and B are both the set of integers, then the (predecessor) function $Pred: \mathbb{Z} \to \mathbb{Z}$, defined by Pred(x) = x - 1, is the function that maps each integer x to the integer before it.

A more formal definition of the term "mapping" above is a subset of the Cartesian product $A \times B$, where every element of A appears exactly once. For example, we can define the *Pred* function as the following set:

$$\{\ldots, (-2, -3), (-1, -2), (0, -1), (1, 0), (2, 1), \ldots\}$$

Functions can have more than one input. For sets A_1, A_2, \ldots, A_k and B, a k-ary function $f: A_1 \times A_2 \times \cdots \times A_k \to B$ is a function that takes k arguments, where for each i between 1 and k, the i-th argument of f must be an element of A_i , and where f returns an element of B. We have common English terms for small values of k: unary, binary, and ternary functions take one, two, and three inputs, respectively. For example, the addition operator $+: \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a binary function that takes two real numbers and returns their sum. For readability, we usually write this function as x + y instead of +(x, y).

A predicate is a function whose codomain is {True, False}.6 For example, we can define the predicate $Odd: \mathbb{N} \to \{\text{True}, \text{False}\}$ by mapping all even numbers to False, and all odd numbers to True. Given a predicate P and element x of its domain, we say that x satisfies P when P(x) is True.

Predicates and sets have a natural equivalence that we will sometimes make use of in this course. Given a predicate $P:A\to \{\text{True}, \text{False}\}$, we can define the set $\{x \mid x \in A \text{ and } P(x) = \text{True}\}$, i.e., the set of elements of A which satisfy P. On the flip side, given a subset $S \subseteq A$, we can define the predicate $P: A \to \{\text{True}, \text{False}\}$ by $P(x) = \text{True if } x \in S$, and $P(x) = \text{False if } x \notin S$. For example, consider the predicate $Even: \mathbb{N} \to \{\text{True}, \text{False}\}$ that is True exactly when its argument is even. This predicate corresponds to the set of natural numbers $\{0, 2, 4, \dots\}$.

Summation and product notation

When performing calculations, we'll often end up writing sums of terms, where each term follows a pattern. For example:

$$\frac{1+1^2}{3+1} + \frac{2+2^2}{3+2} + \frac{3+3^2}{3+3} + \dots + \frac{100+100^2}{3+100}$$

⁶ In other courses, you may see True and False represented as the numbers 1 and 0, respectively.

We will often use *summation notation* to express such sums concisely. We could rewrite the previous example simply as:

$$\sum_{i=1}^{100} \frac{i+i^2}{3+i}.$$

In this example, i is called the *index of summation*, and 1 and 100 are the *lower* and *upper bounds* of the summation, respectively. A bit more generally, for any pair of integers j and k, and any function $f: \mathbb{Z} \to \mathbb{R}$, we can use summation notation in the following way:

$$\sum_{i=j}^{k} f(i) = f(j) + f(j+1) + f(j+2) + \dots + f(k).$$

We can similarly use product notation to abbreviate multiplication:⁷

$$\prod_{i=j}^{k} f(i) = f(j) \times f(j+1) \times f(j+2) \times \cdots \times f(k).$$

It is sometimes useful (e.g., in certain formulas) to allow a summation or product's lower bound to be greater than its upper bound. In this case, we say the summation or product is *empty*, and define their values as follows:⁸

- When j > k, $\sum_{i=j}^{k} f(i) = 0$.
- When j > k, $\prod_{i=j}^{k} f(i) = 1$.

 7 Fun fact: the Greek letter Σ (sigma) corresponds to the first letter of "sum," and the Greek letter Π (pi) corresponds to the first letter of "product."

⁸ These particular values are chosen so that adding an empty summation and multiplying by an empty product do not change the value of an expression.

Exercise Break!

- 1.1 Use summation/product notation to express each of the following quantities:
 - (a) The sum of the numbers from 148 to 165, inclusive.
 - (b) The product of the first n positive integers (1, 2, ..., n).
 - (c) The sum of the first n even natural numbers (0, 2, ..., 2(n-1)).
 - (d) The product of the first n odd natural numbers (1, 3, ..., 2n 1).

Inequalities

Finally, in this course we will deal heavily with the manipulation of *inequalities*. While many of these operations are very similar to manipulating equalities, there are enough differences to warrant a comprehensive list.

Theorem 1.1. For all real numbers a, b, and c, the following are true:

- (a) If $a \leq b$ and $b \leq c$, then $a \leq c$.
- (b) If $a \leq b$, then $a + c \leq b + c$.
- (c) If $a \le b$ and c > 0, then $ac \le bc$.

- (d) If $a \leq b$ and c < 0, then $ac \geq bc$.
- (e) If $0 < a \le b$, then $\frac{1}{a} \ge \frac{1}{b}$. (f) If $a \le b < 0$, then $\frac{1}{a} \ge \frac{1}{b}$.

Moreover, if we replace any of the "if" inequalities with a strict inequality (i.e., change \leq to <), then the corresponding "then" inequality is also strict.

The previous theorem tells us that basic operations like adding a number or multiplying by a positive number preserves inequalities. However, other operations like multiplying by a negative number or taking reciprocals reverses the direction of the inequality, which is something we didn't have to worry about when dealing with equalities. But it turns out that, at least for non-negative numbers, most of our familiar functions preserve inequalities.

Definition 1.3. Let $f: \mathbb{R}^{\geq 0} \to \mathbb{R}^{\geq 0}$. We say that f is strictly increasing when for all $x, y \in \mathbb{R}^{\geq 0}$, if x < y then f(x) < f(y).

Most common functions are strictly increasing:

- Raising to a positive power, e.g., $f(x) = x^2$ or $f(x) = x^{3.14}$.
- Logarithms with a base greater than one, e.g., $f(x) = \log_3(x+1)$.
- Exponential functions with a base greater than one, e.g., $f(x) = 2^x$.

Moreover, adding two strictly increasing functions, or multiplying a strictly increasing function by a positive constant or another strictly increasing function, results in another strictly increasing function. So for example, we know that $f(x) = 300x^2 + x \log_3 x + 2^{x+100}$ is also strictly increasing.

It should be clear from this definition that the following property holds, which enables us to manipulate inequalities using a host of common functions.

Theorem 1.2. For all non-negative real numbers a and b, and all strictly increasing functions $f: \mathbb{R}^{\geq 0} \to \mathbb{R}^{\geq 0}$, if $a \leq b$, then $f(a) \leq f(b)$.

Moreover, if a < b, then f(a) < f(b).

Propositional logic

We are now ready to begin our study of the formal language of logic. We will start with propositional logic, an elementary system of logic that is a crucial building block underlying other, more expressive systems of logic that we will need in this course.

Definition 1.4. A proposition is a statement that is either True or False. Examples of propositions are:

- 2 + 4 = 6
- 3-5>0
- Every even integer greater than 2 is the sum of two prime numbers.
- Python's implementation of list.sort is correct on every input list.

⁹ For example, the following is true: "If a < b, then a + c < b + c."

We use propositional variables to represent propositions; by convention, propositional variable names are lowercase letters starting at p.¹⁰

A propositional/logical operator is a predicate whose arguments must all be either True or False. Finally, a propositional formula is an expression that is built up from propositional variables by applying these operators.

In the following sections, we describe the various operators we will use in this course. It is important to keep in mind when reading that these operators inform both the structure of formulas (what they look like) as well as the truth value of these formulas (what they mean: whether the formula is True or False based on the truth values of the individual propositional variables).

The basic operators NOT, AND, OR

The unary operator **NOT** (also called "negation") is denoted by the symbol ¬. It negates the truth value of its input. So if p is True, then $\neg p$ is False, and vice versa. This is shown in the truth table at the side.

The binary operator AND (also called "conjunction") is denoted by the symbol ∧. It returns True when both its arguments are True.

The binary operator OR (also called "disjunction") is denoted by the symbol \vee , and returns True if one or both of its arguments are True.

The truth tables for AND and NOT agree with the popular English usage of the terms; however, the operator OR may seem somewhat different from your intuition, because the word "or" has two different meanings to most English speakers. Consider the English statement "You can have cake or ice cream." From a nutritionist, this might be an exclusive or: you can have cake or you can have ice cream, but not both. But from a kindly relative at a family reunion, this might be an inclusive or: you can have both cake and ice cream if you want! The study of mathematical logic is meant to eliminate the ambiguity by picking one meaning of OR and sticking with it. In our case, we will always use OR to mean the inclusive or, as illustrated in the last row of its truth table. 11

AND and OR are similar in that they are both binary operators on propositional variables. However, the distinction between AND and OR is very important. Consider for example a rental agreement that reads "first and last months' rent and a \$1000 deposit" versus a rental agreement that reads "first and last months' rent or a \$1000 deposit." The second contract is fulfilled with much less money down than the first contract.

The implication operator

One of the most subtle and powerful relationships between two propositions is *implication*, which is represented by the symbol \Rightarrow . The implication $p \Rightarrow q$ asserts that whenever p is True, q must also be True. An example of logical implication in English is the statement: "If you push that button, then the fire alarm will go off."12 Implications are so important that the parts have been given names. The statement p is called the hypothesis of the implication and the statement q is called the *conclusion* of the implication.

¹⁰ The concept of a propositional variable is different from other forms of variables you have seen before, and even ones that we will see later in this chapter. Here's a rule of thumb: if you read an expression involving a propositional variable p, you should be able to replace p with the statement "CSC165 is cool" and still have the expression make sense.

p	$\neg p$
False	True
True	False

q	$p \wedge q$
False	False
True	False
False	False
True	True
	False True False

p	q	$p \lor q$
False	False	False
False	True	True
True	False	True
True	True	True

¹¹ The symbol ⊕ is often used to represent the exclusive or operator, but we will not use it in this course.

¹² In some contexts, we think of logical implication as the temporal relationship that q is inevitable if p occurs. But this is not always the case! Be careful not to confuse implication with causation.

How should the truth table be defined for $p \Rightarrow q$? First, when both p and q are True, then $p \Rightarrow q$ should be True, since when p occurs, q also occurs. Similarly, it is clear that when p is True and q is False, then $p \Rightarrow q$ is False (since then q is not inevitably True when p is True). But what about the other two cases, when p is False and q is either True or False? This is another case where our intuition from both English language it a little unclear. Perhaps somewhat surprisingly, in both of these remaining cases, we will still define $p \Rightarrow q$ to be True.

The two cases when p is False but $p \Rightarrow q$ is True are called the vacuous truth cases. How do we justify this assignment of truth values? The key intuition is that because the statement doesn't say anything about whether or not q should occur when p is False, it cannot be disproven when p is False. In our example above, if the alarm button is not pushed, then the statement is not saying anything about whether or not the fire alarm will go off. It is entirely consistent with this statement that if the button is not pushed, the fire alarm can still go off, or may not go off.

The formula $p \Rightarrow q$ has two equivalent 13 formulas which are often useful. To make this concrete, we'll use our example "If you are a Pittsburgh Pens fan, then you are not a Flyers fan" from the introduction.

The following two formulas are equivalent to $p \Rightarrow q$:

- $\neg p \lor q$. On our example: "You are not a Pittsburgh Pens fan, or you are not a Flyers fan." This makes use of the vacuous truth cases of implication, in that if p is False then $p \Rightarrow q$ is True, and if p is True then q must be True as well.
- $\neg q \Rightarrow \neg p$. On our example: "If you are a Flyers fan, then you are not a Pittsburgh Pens fan." Intuitively, this says that if q doesn't occur, then p cannot have occurred either.

This equivalent formula is in fact so common that we give it a special name: the contrapositive of the implication $p \Rightarrow q$.

There is one more related formula that we will discuss before moving on. If we take $p \Rightarrow q$ and switch the hypothesis and conclusion, we obtain the implication $q \Rightarrow p$, which is called the **converse** of the original implication.

Unlike the two formulas in the list above, the converse of an implication is not logically equivalent to the original implication. Consider the statement "If you can solve any problem in this course, then you will get an A." Its converse is "If you will get an A, then you can solve any problem in this course." These two statements certainly don't mean the same thing!

Biconditional

The final logical operator that we will consider is the biconditional, denoted by $p \Leftrightarrow q$. This operator returns True when the implication $p \Rightarrow q$ and its converse $q \Rightarrow p$ are both True.

In other words, $p \Leftrightarrow q$ is an abbreviation for $(p \Rightarrow q) \land (q \Rightarrow p)$. A nice way of thinking about the biconditional is that it asserts that its two arguments have the same truth value.

p	q	$p \Rightarrow q$
False	False	True
False	True	True
True	False	False
True	True	True

p	q	$p \Leftrightarrow q$
alse	False	True
alse	True	False
True	False	False
Γrue	True	True

¹³ Here, "equivalent" means that the two formulas have the same truth values; for any setting of their propositional variables to True and False, the formulas will either both be True or both be False.

While we could use the natural translation of \Rightarrow and \land into English to also translate \Leftrightarrow , the result is a little clunky: $p \Leftrightarrow q$ becomes "if p then q, and if q then p." Instead, we often shorten this using a quite nice turn of phrase: "p if and only if q," which is abbreviated to "p iff q."

Summary

We have now seen all five propositional operators that we will use in this course. Now is an excellent time to review these and make sure you understand the notation, meaning, and English words used to indicate each one.

operator	notation	English
NOT	eg p	p is not true
AND	$p \wedge q$	p and q
OR	$p \vee q$	p or q (or both!)
implication	$p\Rightarrow q$	if p , then q
bi-implication	$p \Leftrightarrow q$	p if and only if q

Exercise Break!

1.2 A tautology is a formula that is True for every possible assignment of values to its propositional variables. Decide if each of the following propositional formulas are tautologies.

```
a) ((p \Rightarrow q) \land (p \Rightarrow r)) \Leftrightarrow (p \Rightarrow (q \land r))
```

- b) $(p \Rightarrow q) \Leftrightarrow (\neg p \lor q)$
- c) $(\neg(p \lor q)) \Leftrightarrow (\neg p \land \neg q)$

Predicate logic

While propositional logic is a good starting point, most interesting statements in mathematics contain variables over domains larger than simply {True, False}. For example, the statement "x is a power of 2" is not a proposition because its truth value depends on the value of x. It is only after we *substitute* a value for x that we may determine whether the resulting statement is True or False. For example, if x = 8, then the statement becomes "8 is a power of 2", which is True. But if x = 7, then the statement becomes "7 is a power of 2", which is False.

A statement whose truth value depends on one or more variables from any set is a predicate: a function whose codomain is $\{\text{True}, \text{False}\}$. We typically use uppercase letters starting from P to represent predicates, differentiating them from propositional variables. For example, if P(x) is defined to be the statement "x is a power of 2", then P(8) is True and P(7) is False. Thus a predicate is like a proposition except that it contains one or more variables; when we substitute particular values for the variables, we obtain a proposition.

As with all functions, predicates can depend on more than one variable. For example, if we define the predicate Q(x,y) to mean " $x^2 = y$," then Q(5,25) is True since $5^2 = 25$, but Q(5, 24) is False. ¹⁴

We usually define a predicate by giving the statement that involves the variables, e.g., "P(x) is the statement 'x is a power of 2." However, there is another component which is crucial to the definition of a predicate: the domain that each of the predicate's variable(s) belong to. You must always give the domain of a predicate as part of its definition. So we would complete the definition of P(x) as follows:

$$P(x)$$
: "x is a power of 2," where $x \in \mathbb{N}$.

Quantification of variables

Unlike propositional formulas, a predicate by itself does not have a truth value: as we discussed earlier, "x is a power of 2" is neither True nor False, since we don't know the value of x. We have seen one way to obtain a truth value in substituting a concrete element of the predicate's domain for its input, e.g., setting x=8 in the statement "x is a power of 2," which is now True.

However, we often don't care about whether a specific value satisfies a predicate, but rather some aggregation of the predicate's truth values over all elements of its domain. For example, the statement "every real number x satisfies the inequality $x^2 - 2x + 1 \ge 0$ " doesn't make a claim about a specific real number like 5 or π , but rather all possible values of x!

There are two types of "truth value aggregation" we want to express; each type is represented by a quantifier that modifies a predicate by specifying how a certain variable should be interpreted.

Definition 1.5. The existential quantifier is written as \exists , and represents the concept of "there exists an element in the domain that satisfies the given predicate."

Example 1.6. For example, the statement $\exists x \in \mathbb{N}, x > 0$ can be translated as "there exists a natural number x that is greater than or equal to zero." This statement is True since (for example) when x = 1, we know that $x \ge 0$.

Note that there are many more natural numbers that are greater than or equal to 0. The existential quantifier says only that there has to be at least one element of the domain satisfying the predicate, but it doesn't say exactly how many elements do so.

One should think of $\exists x \in S$ as an abbreviation for a big **OR** that runs through all possible values for x from the domain S. For the previous example, we can expand it by substituting all possible natural numbers for x^{15}

$$(0 \ge 0) \lor (1 \ge 0) \lor (2 \ge 0) \lor (3 \ge 0) \lor \cdots$$

Definition 1.6. The universal quantifier is written as \forall , and represents the concept that "every element in the domain satisfies the given predicate."

Example 1.7. For example, the statement $\forall x \in \mathbb{N}, x > 0$ can be translated as "every natural number x is greater than or equal to zero." This statement is True since

¹⁴ Just as how common arithmetic operators like + are really binary functions, the common comparison operators like = and < are binary predicates, taking two numbers and returning True or False.

¹⁵ In this case, the OR expression is technically infinite, since there are infinitely many natural numbers.

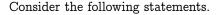
the smallest natural number is zero itself. However, the statement $\forall x \in \mathbb{N}, x \geq 10$ is False, since not every natural number is greater than or equal to 10.

One should think of $\forall x \in S$ as an abbreviation for a big **AND** that runs through all possible values of x from S. Thus, $\forall x \in \mathbb{N}, x > 0$ is the same as

$$(0 \ge 0) \land (1 \ge 0) \land (2 \ge 0) \land (3 \ge 0) \land \cdots$$

Example 1.8. Let us look at a simple example of these quantifiers. Suppose we define Loves(a, b) to be a binary predicate that is True whenever person a loves person b.

For example, the diagram on the right defines the relation "Loves" for two collections of people: $A = \{ \text{Ella, Patrick, Malena, Breanna} \}$, and $B = \{ \text{Laura, Stanley, Thelonious, Sophia} \}$. A line between two people indicates that the person on the left loves the person on the right.



- $\exists a \in A, \ Loves(a, \text{Thelonious}), \text{ which means "there exists someone in } A \text{ who loves Thelonious."}$ This is True since Malena loves Thelonious. 16
- $\exists a \in A$, Loves(a, Sophia), which means "there exists someone in A who loves Sophia." This is False since no one loves Sophia.
- $\forall a \in A$, Loves(a, Stanley), which means "every person in A loves Stanley." This is True, since all four people in A love Stanley.
- $\forall a \in A, \ Loves(a, \text{Thelonious}), \text{ which means "every person in } A \text{ loves Thelonious."}$ This is False, since Ella does not love Thelonius.

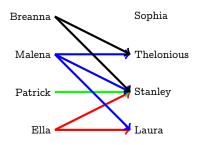
Understanding multiple quantifiers

It is usually straightforward to understand logical formulas with just a single quantifier, since they can generally be translated into English as either "there exists an element x of set S that satisfies P(x)" or "every element x of set S satisfies P(x)." However, we will often have situations where there are multiple variables that are quantified, and we need to pay special attention to what such statements are actually saying. For example, our Loves predicate is binary—what if we wanted to quantify both of its inputs? For example, consider the formula

$$\forall a \in A, \ \forall b \in B, \ Loves(a,b).$$

We translate this as "for every person a in A, for every person b in B, a loves b." After some thought, we notice that the order in which we quantified a and b doesn't matter; the statement "for every person b in B, for every person a in A, a loves b" means exactly the same thing! In both cases, we are considering all possible pairs of people (one from A and one from B).

So in general when we have two consecutive universal quantifiers the order does not matter. The following two formulas are equivalent:¹⁷



¹⁶ We could also have said here that Breanna loves Thelonious.

[•] $\forall x \in S_1, \forall y \in S_2, P(x, y)$

[•] $\forall y \in S_2, \forall x \in S_1, P(x, y)$

¹⁷ Tip: when the domains of the two variables are the same, we typically combine the quantifications, e.g., $\forall x \in S, \forall y \in S, P(x,y) \text{ into } \forall x,y \in S, P(x,y).$

The same is true of two consecutive existential quantifiers. Consider the statements "there exist an a in A and b in B such that a loves b" and "there exist a b in B and a in A such that a loves b." Again, they mean the same thing: in this case, we only care about one particular pair of people (one from A and one from B), so the order in which we pick the particular a and b doesn't matter. In general, the following two formulas are equivalent:

- $\exists x \in S_1, \exists y \in S_2, P(x, y)$
- $\exists y \in S_2, \exists x \in S_1, P(x, y)$

But even though consecutive quantifiers of the same type behave very nicely, this is not the case for a pair of alternating quantifiers. First, consider

$$\forall a \in A, \exists b \in B, Loves(a,b).$$

This can be translated as "For every person a in A, there exists a person b in B, such that a loves b." This is true: every person in A loves at least one person.

a (from A)	b (a person in B who a loves)
Breanna	Thelonious
Malena	Laura
Patrick	Stanley
Ella	Stanley

¹⁸ Or put a bit more naturally, "For every person a in A, a loves someone in B," which can be shortened even further to "Everyone in A loves someone in B."

Note that the choice of person who a loves depends on a: this is consistent with the latter part of the English translation, "a loves someone in B."

Let us contrast this with the similar-looking formula, where the order of the quantifiers has changed:

$$\exists b \in B, \forall a \in A, Loves(a,b).$$

This formula's meaning is quite different: "there exists a person b in B, where for every person a in A, a loves b." Put more naturally, "there is a person b in B that is loved by everyone in A" or "someone in B is loved by everyone in A".

b (from B)	Loved by everyone in A?
Sophia	No
Thelonious	No
Stanley	Yes
Laura	No

This is True because all people in A love Stanley. However, this would not be True if we removed the love connection between Malena and Stanley. In this case, Stanley would no longer be loved by everyone, and so no one in B is loved by everyone in A. But also notice that even if Malena no longer loves Stanley, the previous statement ("everyone in A loves someone") is still True!

So we would have a case where switching the order of quantifiers changes the meaning of a formula! In both cases, the existential quantifier $\exists b \in B$ involves making a *choice* of person from B. But in the first case, this quantifier occurs after a is quantified, so the choice of b is allowed to depend on the choice of a. In the second case, this quantifier occurs before a, and so the choice of b must be independent of the choice of a.

When reading a nested quantified expression, you should read it from left to right, and pay attention to the order of the quantifiers. In order to see if the statement is True, whenever you come across a universal quantifier, you must verify the statement for every single value that this variable can take on. Whenever you see an existential quantifier, you only need to exhibit *one* value for that variable such that the statement is True, and this value can depend on the variables to the left of it, but not on the variables to the right of it.

Writing sentences in predicate logic

Now that we have introduced the existential and universal quantifiers, we have a complete set of tools needed to represent all statements we'll see in this course. A general formula in predicate logic is built up using the existential and universal quantifiers, the propositional operators \neg , \land , \lor , \Rightarrow , and \Leftrightarrow , and arbitrary predicates. To ensure that the formula has a fixed truth value, we will require every variable in the formula to be quantified. We call a formula with no unquantified variables a sentence. So for example, the formula

$$\forall x \in \mathbb{N}, \ x^2 > y$$

is not a sentence: even though x is quantified, y is not, and so we cannot determine the truth value of this formula. If we quantify y as well, we get a sentence:

$$\forall x, y \in \mathbb{N}, \ x^2 > y.$$

However, don't confuse a formula being a sentence with a formula being True! As we'll see repeatedly throughout the course, it is quite possible to express both True and False sentences, and part of our job will be to determine whether a given sentence is True or False, and to prove it.

Manipulating negation

We have already seen some equivalences among logical formulas, such as the equivalence of $p \Rightarrow q$ and $\neg p \lor q$. While there are many such equivalences, the only other major type that is important for this course are the ones used to simplify negated formulas. Taking the negation of a statement is extremely common, because often when we are trying to decide if a statement is True, it is useful to know exactly what its negation means and decide whether the negation is more plausible than the original.

Given any formula, we can state its negation simply by preceding it by a ¬ symbol:

$$\neg (\forall x \in \mathbb{N}, \exists y \in \mathbb{N}, x \ge 5 \lor x^2 - y \ge 30).$$

However, such a statement is rather hard to understand if you try to transliterate each part separately: "Not for every natural number x, there exists a natural number y, such that x is greater than or equal to 5 or $x^2 - y$ is greater than or equal to 30."

¹⁹ Other texts will often refer to quantified variables as *bound variables*, and unquantified variables as *free variables*.

Instead, given a formula using negations, we apply some simplification rules to "push" the negation symbol to the right, closer the to individual predicates. Each simplification rule shows how to "move the negation inside" by one step, giving a pair of equivalent formulas, one with the negation applied to one of the logical operator or quantifiers, and one where the negation is applied to inner subexpressions.

- $\neg(\neg p)$ becomes p.
- $\neg (p \lor q)$ becomes $(\neg p) \land (\neg q)$.²⁰
- $\neg (p \land q)$ becomes $(\neg p) \lor (\neg q)$.
- $\neg(p \Rightarrow q)$ becomes $p \wedge (\neg q)$.²¹
- $\neg (p \Leftrightarrow q)$ becomes $(p \land (\neg q)) \lor ((\neg p) \land q))$.
- $\neg(\exists x \in S, P(x))$ becomes $\forall x \in S, \neg P(x)$.
- $\neg(\forall x \in S, P(x))$ becomes $\exists x \in S, \neg P(x)$.

It is usually easy to remember the simplification rules for \land , \lor , \forall , and \exists , since you simply "flip" them when moving the negation inside. The intuition for the negation of $p \Rightarrow q$ is that there is only one case where this is False: when p has occurred but q does not. The intuition for the negation of $p \Leftrightarrow q$ is to remember that \Leftrightarrow can be replaced with "have the same truth value," so the negation is "have different truth values."

Commas: avoid them!

Here is a common question from students who are first learning symbolic logic: "does the comma mean 'and' or 'then'?" As we discussed at the start of the course, we study to predicate logic to provide us with an unambiguous way of representing ideas. The English language is filled with ambiguities that can make it hard to express even relatively simple ideas, much less the complex definitions and concepts used in many fields of computer science. We have seen one example of this ambiguity in the English word "or," which can be inclusive or exlusive, and often requires additional words of clarification to make precise. In everyday communication, these ambiguous aspects of the English language contribute to its richness of expression. But in a technical context, ambiguity is undesirable: it is much more useful to limit the possible meanings to make them unambiguous and precise.

There is another, more insidious example of ambiguity with which you are probably more familiar: the comma, a tiny, easily-glazed-over symbol that people often infuse with different meanings. Consider the following statements:

- 1. If it rains tomorrow, I'll be sad.
- 2. David is cool, Toniann is cool.

Our intuitions tell us very different things about what the commas mean in each case. In the first, the comma means then, separating the hypothesis and conclusion of an implication. But in the second, the comma is used to mean and, the implicit joining of two separate sentences.²² The fact that we are all fluent in English means that our prior intuition hides the ambiguity in this symbol, but it is quite obvious when we put this into the more unfamiliar context of predicate logic, as

²⁰ The negation rules for AND and OR are known as deMorgan's laws.

²¹ Since $p \Rightarrow q$ is equivalent to $\neg p \lor q$.

²² Grammar-savvy folks will recognize this as a comma splice, which is often frowned upon but informs our reading nonetheless.

in the formula:

This, of course, is where the confusion lies, and is the origin of the question posed at the beginning of this section. Because of this ambiguity, never use the comma to connect propositions. We already have a rich enough set of symbols—including \land and \Rightarrow —that we do not need another one that is ambiguous and adds nothing new!

That said, keep in mind that commas do have two valid uses in predicate formulas:

- immediately after a variable quantification, or separating two variables with the same quantification
- separating arguments to a predicate

You can see both of these usages illustrated below, but please do remember that these are the *only* valid places for the comma within symbolic notation!

$$\forall x, y \in \mathbb{N}, \ \forall z \in \mathbb{R}, \ P(x, y) \Rightarrow Q(x, y, z)$$

Defining predicates

Throughout this course, we will study various mathematical objects that play key roles in computer science. As these objects become more complex, so too will our statements about them, to the point where if we try to write out everything using just basic set and arithmetic operations, our formulas won't fit on a single line! To avoid this problem, we create *definitions*, which we can use to express a long idea using a single term.²³

In this section, we'll look at one extended example of defining our own predicates and using them in our statements. Let's take some terminology that is already familiar to us, and make it precise using the language of predicate logic.

Definition 1.7. Let $n, d \in \mathbb{Z}$.²⁴ We say that d divides n, or n is divisible by d, when there exists a $k \in \mathbb{Z}$ such that n = dk. In this case, we use the notation $d \mid n$ to represent "d divides n."

Note that just like the equals sign = is a binary predicate, so too is |. For example, the statement 3 | 6 is True, while the statement 4 | 10 is False.²⁵

Example 1.9. Let's express the statement "For every integer x, if x divides 10, then it also divides 100" in two ways: with the divisibility predicate $d \mid n$, and without it.

• With the predicate: this is a universal quantification over all possible integers, and contains a logical implication. So we can write

$$\forall x \in \mathbb{Z}, \ x \mid 10 \Rightarrow x \mid 100.$$

• Without the predicate: the same structure is there, except we unpack the definition of divisibility, replacing every instance of $d \mid n$ with $\exists k \in \mathbb{Z}, n = dk$.

$$\forall x \in \mathbb{Z}, \ (\exists k \in \mathbb{Z}, \ 10 = kx) \Rightarrow (\exists k \in \mathbb{Z}, \ 100 = kx).$$

²³ This is completely analogous to using local variables or helper functions in programming to express *part* of an overall value or computation.

²⁴ You may be used to defining divisibility for just the natural numbers, but it will be helpful to allow for negative numbers in our work.

 25 Students often confuse the divisibility predicate with the horizontal fraction bar. The former is a *predicate* that returns a boolean; the latter is a function that returns a number. So $4 \mid 10$ is False, while $\frac{10}{4}$ is 2.5.

Note that each subformula in the parentheses has its own k variable, whose scope is limited by the parentheses.²⁶ However, even though this technically correct, it's often confusing for beginners. So instead, we'll tweak the variable names to emphasize their distinctness:

$$\forall x \in \mathbb{Z}, \ (\exists k_1 \in \mathbb{Z}, \ 10 = k_1 x) \Rightarrow (\exists k_2 \in \mathbb{Z}, \ 100 = k_2 x).$$

As you can see, using this new predicate makes our formula quite a bit more concise! But the usefulness of our definitions doesn't stop here: we can, of course, use our terms and predicates in further definitions.

Definition 1.8. Let $p \in \mathbb{N}$. We say p is prime when it is greater than 1 and the only natural numbers that divide it are 1 and itself.

Example 1.10. Let's define a predicate Prime(p) to express the statement that "p is a prime number," with and without using the divisibility predicate.

The first part of the definition, "greater than 1," is straightforward. The second part is a bit trickier, but a good insight is that we can enforce constraints on values through implication: if a number d divides p, then d = 1 or d = p. We can put these two ideas together to create a formula:

$$Prime(p): p > 1 \land (\forall d \in \mathbb{N}, \ d \mid p \Rightarrow d = 1 \lor d = p), \qquad \text{where } p \in \mathbb{N}.$$

To express this idea without using divisibility predicate, we substitute in the definition of divisibility. The underline shows the changed part.

$$Prime(p): p > 1 \land (\forall d \in \mathbb{N}, \ (\exists k \in \mathbb{Z}, \ p = kd) \Rightarrow d = 1 \lor d = p), \quad \text{where } p \in \mathbb{N}.$$

Example 1.11. Finally, let us express one of the more famous properties about prime numbers: "there are infinitely many primes." 28

We have just seen how to express the fact that a single number p is a prime number, but how do we capture "infinitely many"? The key idea is that because primes are natural numbers, if there are infinitely many of them, then they have to keep growing bigger and bigger.²⁹ So we can express the original statement as "every natural number has a prime number larger than it," or in the symbolic notation:

$$\forall n \in \mathbb{N}, \exists p \in \mathbb{N}, p > n \land Prime(p).$$

Of course, if we wanted to express this statement without either the Prime or divisibility predicates, we would end up with an extremely cumbersome statement:

$$orall n \in \mathbb{N}, \; \exists p \in \mathbb{N}, \; p > n \wedge p > 1 \wedge \Big(orall d \in \mathbb{N}, \; (\exists k \in \mathbb{Z}, \; p = kd) \Rightarrow d = 1 \lor d = p \Big).$$

This statement is terribly ugly, which is why we define our own predicates! Keep this in mind throughout the course: when you are given a statement to express, make sure you are aware of all of the relevant definitions, and make use of them to simplify your expression.

One last example: Fermat's Last Theorem

As payoff for the work that we have done so far, let us use predicate logic to express one of the most famous statements in mathematics: Fermat's Last Theorem. It

²⁶ That is, the k in the hypothesis of the implication is different from the k in the conclusion: they can take on different values, though they can also take on the same value.

²⁷ Unlike divisibility, we restrict primes to being positive.

28 Later on, we'll actually prove this statement!

²⁹ Another way to think about this is to consider the statement "every prime number is less than 9000. If this statement were True, then there could only be at most 8999 primes."

was first conjectured by the mathematician Pierre de Fermat in 1637 in the margin of a copy of the text *Arithmetica*, where he claimed that he had a proof that was too large to fit in the margin!³⁰ Despite this purported proof, for centuries this statement had no published proof. It wasn't until 1994 that Andrew Wiles finally proved this theorem.

Example 1.12. Fermat's Last Theorem states that there are no three positive integers a, b, and c that satisfy $a^n + b^n = c^n$ for any integer n > 2. To express this in predicate logic, we identify the relevant variables: a, b, c, and n. Are they universally or existentially quantified? The n certainly is universally quantified, since we say that the statement is "for any n > 2." The statement also makes a claim that no a, b, c satisfy the given equation, which we can rephrase as "there do not exist a, b, c satisfying..." Finally, we can express the condition n > 2 using an implication: if n > 2, then there is no solution to... Putting this together yields:

$$\forall n \in \mathbb{N}, \ n > 2 \Rightarrow \neg (\exists a, b, c \in \mathbb{Z}^+, \ a^n + b^n = c^n).$$

We can now simplify this statement by pushing the negation inwards, so that this statement becomes

$$\forall n \in \mathbb{N}, \ n > 2 \Rightarrow (\forall a, b, c \in \mathbb{Z}^+, \ a^n + b^n \neq c^n).$$

Exercise Break!

- 1.3 Let S be a set of people, C be the set of all countries, and let T be a predicate defined over $S \times C$ such that T(x,y) is True if and only if $x \in S$ has traveled to country $y \in C$. Express each of the following statements by a simple English sentence.
 - (a) $(\exists x \in S, T(x, France)) \land (\forall y \in S, T(y, Japan))$
 - (b) $\forall x \in S, \exists y \in C, T(x, y)$
 - (c) $\forall x, z \in S, \exists y \in C, T(x, y) \Leftrightarrow T(z, y)$
- 1.4 Write each of the statements below in predicate logic, and then write the contrapositive and converse of each statement.
 - (a) If all birds fly, and if Tweety is a bird, then Tweety flies.
 - (b) If it does not rain or it is not foggy, then the sailing race will be held and registration will go on.
 - (c) If rye bread is for sale at Ace Bakery, then rye bread was baked that day.

Our conventions for writing formulas

Mathematical expressions in predicate logic can become complicated very quickly. In order to avoid confusion and to make things as clear as possible we will follow some important conventions.

³⁰ "I have discovered a truly marvelous proof of this, which this margin is too narrow to contain."

Operator precedence

The longer and more complex our formulas, the harder they are to read and understand. For example, here is a rather more complicated formula:

$$\forall x, y \in \mathbb{N}, \ \exists z \in \mathbb{N}, \ x + y = z \land x \cdot y = z \Rightarrow x = y.$$

Whenever we mix different propositional operators together, or when we mix quantifiers with formulas containing predicates, we need to worry about which ones come first—i.e., which ones have higher precedence. Technically, we can just use parentheses around every operation, but this quickly becomes very tiring. Instead, we will use the following precedence levels, in decreasing order of precedence.³¹

- 1. ¬
- 2. V, A
- $3. \Rightarrow, \Leftrightarrow$
- 4. ∀, ∃

So for example the expression

$$(p \lor \neg q) \land r \Rightarrow ((s \lor t) \land u) \lor (\neg v \land w)$$

represents

$$\bigg(\big(p \vee (\neg q) \big) \wedge r \bigg) \Rightarrow \bigg(\big((s \vee t) \wedge u \big) \vee \big((\neg v) \wedge w \big) \bigg),$$

and the expression

$$\forall x, y \in \mathbb{N}, \ \exists z \in \mathbb{N}, \ x + y = z \land x \cdot y = z \Rightarrow x = y$$

represents

$$orall x,y\in \mathbb{N}, \ \Big(\exists z\in \mathbb{N}, \ \Big(ig(x+y=z\wedge x\cdot y=zig)\Rightarrow x=y\Big)\Big).$$

Associativity

There is one more notational simplification we will use to reduce the number of parentheses we need to write: the \wedge and \vee operators are each associative, meaning that

$$(p \wedge q) \wedge r$$
 is equivalent to $p \wedge (q \wedge r)$

and

$$(p \lor q) \lor r$$
 is equivalent to $p \lor (q \lor r)$.

This means that when we have a chain of ANDs, we do not need to write any parentheses to indicate the order in which they are evaluated, and can instead write

$$p_1 \wedge p_2 \wedge p_3 \wedge \ldots \wedge p_k$$

and similarly with a chain or ORs. It turns out that the biconditional operator is also associative, so the same convention applies.

However, keep in mind that the implication operator is not associative, and so you must always use parentheses to indicate the order they should be evaluated.

³¹ Combinations of operations at the same level must be disambiguated using parentheses.

Variable scope and naming

As we saw in the previous section, formulas involving multiple variables can be hard to understand: one has to keep careful track of each variable, what it represents, and where it can legitimately appear in the formula. To make this easier, we will always use distinct names for each variable to ensure there is no possibility of confusion about what a variable is referring to. Here is an example, where f is a unary function from $\mathbb N$ to $\mathbb N$:

$$(\forall x \in \mathbb{N}, \ f(x) \ge 5) \lor (\exists x \in \mathbb{N}, \ f(x) < 5).$$

In this statement, we have two different occurrences of quantified variables, but they have the same name. We will always prefer to write it in this equivalent form, where each occurrence has a distinct name:

$$(\forall x \in \mathbb{N}, f(x) \ge 5) \lor (\exists y \in \mathbb{N}, f(y) < 5).$$

We do this even when expanding the same definition multiple times, typically using subscripts to differentiate the occurrences:

$$x \mid 10 \Rightarrow x \mid 100$$

becomes

$$\left(\exists k_1 \in \mathbb{Z}, \ 10 = k_1 x\right) \Rightarrow \left(\exists k_2 \in \mathbb{Z}, \ 100 = k_2 x\right).$$

Each quantification of a variable will be followed by a formula, which will be the *scope* of this variable. For example $\forall x \in \mathbb{N}, \ f(x) \geq 5$ —the formula $f(x) \geq 5$ is the part of the statement that involves x.

Quantifiers are read left-to-right, which is why in $\forall a \in A, \exists b \in B$ the variable a is in scope when choosing b, but this is not true in $\exists b \in B, \forall a \in A$.

Finally, because we take quantifiers to have lowest precedence, the scope of a variable usually lasts until the end of the formula. The only time this is *not* the case is if the quantification is surrounded by parentheses, as in

$$(\forall x \in \mathbb{N}, \ \underline{f(x) \geq 5}) \lor (\exists y \in \mathbb{N}, \ \underline{f(y) < 5}).$$

Here, the scope of x is only the first underlined expressions, and the scope of y is only the second underlined expression.

2 Introduction to Proofs

In the previous chapter, we studied how to express statements precisely using the language of predicate logic. But just as English enables us to make both true and false claims, the language of predicate logic allows for the expression of both true and false sentences. In this chapter, we will turn our attention to analyzing and communicating the truth or falsehood of these statements. You will develop the skills required to answer the following questions:

- How can you figure out if a given statement is True or False?
- If you know a statement is True, how can you convince others that it is True? How can you do the same if you know the statement is False instead?
- If someone gives you an explanation of why a statement is True, how do you know whether to believe them or not?

These questions draw a distinction between the internal and external components of mathematical reasoning. When given a new statement, you'll first need to figure out for yourself whether it is true (internal), and then be able to express your thought process to others (external). But even though we make a separation, these two processes are certainly connected: it is only after convincing yourself that a statement is true that you should then try to convince others. And often in the process of formalizing your intuition for others, you notice an error or gap in your reasoning that causes you to revisit your intuition—or make you question whether the statement is actually true!

A mathematical proof is how we communicate ideas about the truth or falsehood of a statement to others. There are many different philosophical ideas about what constitutes a proof, but what they all have in common is that a proof is a mode of *communication*, from the person creating the proof to the person digesting it. In this course, we will focus on reading and creating our own written mathematical proofs, which is the standard proof medium in computer science.

As with all forms of communication, the style and content of a proof varies depending on the audience. In this course, the audience for all of our proofs will be an average CSC165 student (and not your TA or instructor). As we will discuss, your audience determines how formal a proof should be (here, quite formal), and what background knowledge you can assume is understood without explanation (here, not much).

Some basic examples

We're going to start out our exploration of proofs by studying a few simple statements. You may find our first few examples a bit on the easy side, which is fine. We are using them not so much for their ability to generate mathematical insight, but rather to model both the thinking and the writing that would go into approaching a problem.

Each example in this chapter is divided into three or four parts:

- 1. The statement that we want to prove or disprove. Sometimes, we'll specify whether to prove or disprove it, and other times deciding whether the statement is true or false is part of the exercise.
- 2. A translation of the statement into predicate logic. This step often provides insight into the logical structure of the statement that we are considering, which in turn informs the structure and techniques that we will use in our
- 3. A discussion to try to gain some intuition about why the statement is true. You'll tend to see that these are written very informally, as if we are talking to a friend on a whiteboard. The discussion usually will reveal the mathematical insight that forms the content of a proof. This is often the hardest part of developing a proof, so please don't skip these sections!
- 4. A formal proof. This is meant to be a standalone piece of writing, the "final product" of our earlier work. Depending on the depth of the discussion, the formal proof might end up being almost mechanical - a matter of formalizing our intuition.

With this in mind, let's dive right in!

Example 2.1. Prove that $15 \cdot 3^2 - 7 = 7 + (19 + 3)^2 / 4$.

Translation. Note that this statement has no logical operators, variables, or quantifiers. So the "translation" into predicate logic is simply itself:

$$15 \cdot 3^2 - 7 = 7 + (19 + 3)^2 / 4$$
.

Discussion. I can check whether this is true or not by putting both sides into my calculator.

Proof. This statement is true because both sides equal 128.1

That was perhaps an underwhelming proof, and rightfully so: statements that do not contain any variables are generally very straightforward to prove or disprove, because they usually amount to performing just some kind of calculation. However, almost all of the statements we care about involve quantified variables, and so we will next discuss how to deal with these quantifications so that the core of our proofs become "just a calculation."

Example 2.2. Prove that there exists a power of two bigger than 1000.

Translation. In order to translate this statement into predicate logic, I need to unpack two definitions in this statement. I know that "there exists" translates

¹ We are not going to evaluate you on your computational abilities. We expect that as a typical CSC165 student, you can check arithmetic expressions yourself. You can have the same expectation when writing your proofs.

into an existential quantifier, and all "powers of 2" have the form 2^n , where n is a natural number. So this statement becomes:

$$\exists n \in \mathbb{N}, \ 2^n > 1000.$$

Discussion. This must be true since I know that the powers of 2 grow to infinity (either from intuition, or a calculus class). I just need to do some calculations until I find a large enough value for n.

Proof. Let n = 10.

Then 2^n is a power of two, and $2^n = 1024$, which is greater than $1000.^2$

We can draw from this example a more general technique for structuring our existence proofs. A statement of the form $\exists x \in S, P(x)$ is True when at least one element of S satisfies P. The easiest way to convince someone that this is True is to actually find the concrete element that satisfies P, and then show that it does.³ This is so natural a strategy that it should not be surprising that there is a "standard proof format" when dealing with such statements.

A typical proof of an existential. Given statement to prove: $\exists x \in S, P(x)$. Proof. Let x =____. [Proof that P() is True.]

Note that the two blanks represent the same element of S, which you get to choose as a prover. Thus existence proofs usually come down to finding a correct element of the domain which satisfy the required properties.

Example 2.3. Prove that every real number n greater than 20 satisfies the inequality $1.5n - 4 \ge 3$.

Translation. Here the statement starts with an "every," which is a big hint about the formal structure of the statement: it is universally quantified.

What about the domain of n? The statement mentions real numbers, but there is the issue of the qualifying "greater than 20" as well. While we could define a set S to be the set of real numbers bigger than 20, instead we will express this condition as a hypothesis in an implication. The conclusion, 1.5n - 4 > 3, only needs to be true when n is greater than 20.

This gives us the full translation

$$\forall n \in \mathbb{R}, \ n > 20 \Rightarrow 1.5n - 4 > 3.$$

Discussion. I might first try to gain some intuition by substituting numbers for n. 25 is bigger than 20, and 1.5(25) - 4 = 33.5 > 3. But that idea is limited in

² Note again that we didn't add a sentence in our proof to "verify" that $2^{10} = 1024$, as this is easily checkable with a calculator.

³ Of course, this is not the only proof technique used for existence proofs. You'll study more sophisticated ways of doing such proofs in future courses.

scope to just one real number—appropriate for proving an existential, but not a universal. This statement is talking about an infinite number of real numbers, so I need to use an argument that will work on *any* real number bigger than 20.

This should be some straightforward algebraic manipulation. We start with the assumption that n > 20, and multiply by 1.5 then subtract 4; both of these operations will preserve the inequality.⁴

Proof. Let $n \in \mathbb{R}$ be an arbitrary real number. Assume that n > 20. We want to prove that $1.5n - 4 \ge 3$.

We can perform the following manipulations to our given inequality to result in the final inequality:

$$n>20$$
 $1.5n>30$ $1.5n-4>26$ $1.5n-4\geq 3$ (since $26>3$)

The above proof has a few interesting details. The first is that this was a proof of a universally-quantified statement. Unlike the previous example, where we proved a fact about just one number, here we proved a fact about an infinite set of numbers.

To do this, our proof introduced a variable n that could represent any real number. Unlike the previous existence proof, when we introduced this variable n we did not specify a concrete value like 10, but rather said that n was "an arbitrary real number," and then proceeded with the proof. As we get more comfortable, we will drop the English phrase part and just write "let $n \in S$ " to introduce n as an arbitrary element of S.⁵

A typical proof of a universal.

Given statement to prove: $\forall x \in S, P(x)$.

Proof. Let $x \in S$. (That is, let x be an arbitrary element of S.)

[Proof that P(x) is True].

However, this structure does not tell the full story. We also put a further restriction on n: "Assume that n > 20." Whenever we want to prove that an implication $p \Rightarrow q$ is true, we do so by assuming that p is true, and then proving that q must be true.

A typical proof of an implication (direct).

Given statement to prove: $p \Rightarrow q$.

Proof. Assume p.

⁴ Now is a good time to review the section on Inequalities.

⁵ You might notice that we use the same word "let" to introduce both existentially- and universallyquantified variables. However, you should always be able to tell how the variable is quantified based on whether it is given a concrete value or an "arbitrary" value in the proof. [Proof that q is True.]

Of course, these proof templates can be combined as the statements you prove grow more complex. In particular, statements of the form $\forall n \in S, P(n) \Rightarrow Q(n)$ are probably the most common type of statements you'll prove, and follow the standard setup of "Let $n \in S$ be an arbitrary element of S, and assume P(n) is True."6

⁶ Compare this with the first line of the previous proof.

Variables as representing arbitrary numbers

A good way of understanding what it means for n to be an arbitrary real number under the stated assumption is that we should be able to substitute any real number that satisfies the assumption (n > 20) into the body of the proof, and have the body still make sense. For example, if we substitute n=25 into the body of the previous proof, we can see that every line is valid:

We can perform the following manipulations to our given inequality to result in the final inequality:

$$25 > 20$$
 $1.5(25) > 30$
 $1.5(25) - 4 > 26$
 $1.5(25) - 4 > 3$ (since $26 > 3$)

However, the body does not necessarily make sense if we violate our assumption that n > 20! Below we show what our proof body looks like when we substitute n = 4. What is the problem with this body?

We can perform the following manipulations to our given inequality to result in the final inequality:

$$4 > 20$$
 $1.5(4) > 30$
 $1.5(4) - 4 > 26$
 $1.5(4) - 4 \ge 3$ (since $26 > 3$)

Unlike variables in programming, which refer to concrete values, but can change their values over time, variables in a mathematical proof never change their value. Even when we say n represents an arbitrary real number, this doesn't mean we can substitute different real numbers for n at different points in the proof! For example, the following proof snippet makes absolutely no sense:

We can perform the following manipulations to our given inequality to result in the final inequality:

$$25>20$$

$$1.5(16)>30$$

$$1.5(3000)-4>26$$

$$1.5(3.14159)-4\geq 3$$
 (since $26>3$)

At each line of the calculation, we substituted a different real number for n; as you might expect, the statements no longer logically flow. So we often say that a variable n represents an arbitrary and fixed element of the domain, to remind ourselves that the value of this variable will not change during the proof.

A note about inequalities, bounds, and approximation

You may have felt a little uneasy by the final step of our computation in the above proof, going from 1.5n-4>26 to $1.5n-4\geq 3$. In most calculations you would have done in high school (or perhaps even other university math classes), we never would have performed such a step. If we wanted to "solve" the inequality $1.5n-4\geq 3$, the "answer" we present would probably be $n\geq \frac{14}{3}$, not $n\geq 20$. What is different here?

We deliberately chose this example to bring up this point. There is a difference between *solving* an inequality to determine the exact range of values for a variable, and manipulating inequalities to produce more inequalities. Inequalities are fundamentally about *bounding* values, and are by definition inexact. In this course (and largely in computer science), we treat inequalities with a grain of salt, keeping in mind that they are just bounds. And when a bound is "as good as possible," we pay special attention to it: these bounds are not to be taken for granted, and must always be earned.⁷

⁷ We'll see what we mean by "as good as possible" later on.

What goes into a proof?

We have now seen our first few basic examples of formal mathematical proofs. In the next section, we will create more complex proofs by studying some definitions and properties based in number theory. But to ensure that we have a solid foundation before moving on, we will first take a step back and give names to two major components of every proof and guidelines for writing them, based on the examples we have already seen.

Proof header: setting up the proof

Every proof you write should start with a **proof header**. The main purpose of a proof header is to introduce all the variables and assumptions you'll use in your proof. The order of statements matters here: variables and assumptions should be introduced in the same order they appear in the translated statement, to avoid any potential problems with scope (this is particularly important when dealing with alternating quantifiers).

You must introduce every variable you use in your proof.⁸ Use the word let to introduce variables. Make sure that every variable you introduce has a different name.

f

[•] For a universally-quantified variable ($\forall x \in S$), introduce the variable in one of two ways:

⁸ This goes for variables that appear in the statement you're proving—they aren't "automatically" introduced.

"Let $x \in S$." or "Let x be an arbitrary element of S."

• For an existentially-quantified variable $(\exists x \in S)$, introduce the variable by setting it to a concrete element of S. For example, if $S = \mathbb{N}$, we might introduce x by saying:

```
"Let x = 5."
```

• For a local variable that does not appear in the original statement, introduce it like you would an existentially-quantified variable:

```
"Let \epsilon = x - |x|."
```

Such variables can be helpful in giving names to certain key expressions in your proof, much in the same way local variables are helpful in programming.

When trying to prove an implication in a universally-quantified statement, state that you are assuming the hypothesis of the implication. Always use the word assume to introduce your assumptions.

• For example, when proving the statement $\forall x \in \mathbb{N}, P(x) \Rightarrow Q(x)$, you would write:9

```
"Let x \in \mathbb{N}. Assume P(x)."
```

• If the hypothesis of the implication is multiple predicates connected by ANDs, you get to assume all of them. For example, when proving $\forall x \in \mathbb{N}, P_1(x) \land P_2(x) \land P_3(x) \land P_3($ $P_2(x) \wedge P_3(x) \Rightarrow Q(x)$, you would write:

```
Let x \in \mathbb{N}. Assume that P_1(x), P_2(x), and P_3(x) are all true.
```

If you assume a predicate, you may find it useful to restate your assumption with the expanded body of the predicate. While this is not required, it can be very helpful to make clearer to your reader what you're assuming, and possibly even introduce new variables that will play a role in your proof. For example, suppose we have the predicate P(x): " $x^3 < 10x + 300$ " (where $x \in \mathbb{N}$). If we are proving a statement of the form $\forall x \in \mathbb{N}, P(x) \Rightarrow Q(x)$, our proof header could be

Let
$$x \in \mathbb{N}$$
. Assume that $P(x)$ is true, i.e., that $x^3 < 10x + 300$.

As we start proving larger and more complicated statements, the construction of the proof header will prove to be extremely valuable in helping us figure out where to start. The two major components of the proof header—introducing variables and stating assumptions—can be done mechanically 10 simply from the structure of the statement alone. When we write a proof header, we "unwrap" the statement by peeling off quantifiers and assumptions, until we are left with the core of what we want to prove. Here is one example of this.

⁹ Warning: any variables involved in an assumption must be introduced (using let) before the assumption is made. Don't just write "Assume P(x)" if you haven't yet introduced x!

¹⁰ By "mechanically" here we mean "without much thought." The exception is figuring out what value to use for an existentially-quantified variable, so what we typically do is leave a blank in our proof header to come back to later.

Example 2.4. Let us write the proof header we would use to prove the following statement:

$$\forall x \in \mathbb{R}, \ \forall y \in \mathbb{N}, \ x > 10 \land y < x \Rightarrow (\exists z \in \mathbb{R}, \ P(x, y, z))$$

Proof. Let $x \in \mathbb{R}$ and let $y \in \mathbb{N}$. Assume that x > 10 and that y < x. Let z =____. We will prove that P(x, y, z) is true.

[Proof body goes here.]

In the above example, we took a fairly large and complex statement and used the proof header to get at the core of the proof: picking a value for z (indicated by the blank in the proof header) to prove the predicate P(x,y,z). We ended our proof header by explicitly stating our new goal: proving P(x,y,z). While this last part is not required, it is often very useful to remind the reader what the body of the proof is actually about, after having introduced all these variables and assumptions.

Proof body: the chain of reasoning

While the proof header sets up the proof, the *proof body* contains the actual reasoning that shows that a statement must be true. ¹¹ The proof body consists of a sequence of true statements called *deductions*, where each statement logically follows from a combination of the following sources of truth:

- Definitions
- Assumptions (made in the proof header)
- Previous deductions (made earlier in the proof body)
- External true statements

We use the metaphor of a *chain* to describe the body of a proof; proof bodies start with statements already known to be true, and then make logical deductions until reaching the statement that you're actually trying to prove. ¹²

Each sentence you write in the proof body should consist of two parts: the deduction you're making (i.e., what you're claiming to be true), and the reason for that deduction (what combination of definitions/assumptions/previous deductions/external true statements it follows from). Since this type of statement comprises about 90% of proof bodies, there are a few different common ways of saying this in English that you'll see (and use), including but not limited to:

[&]quot;Since [reason], [deduction]."

[&]quot;Because we know [reason], we can conclude [deduction]."

[&]quot;Then [deduction] (by the fact that [reason])."

[&]quot;It follows from [reason] that [deduction] is also true/holds."

¹¹ This is typically the part of a proof that people think of when they imagine what a proof is. However, the proof header is an essential component, both in terms of writing a coherent proof, and being a helpful step in actually figuring out how to prove something.

¹² Students sometimes ask: how do you know when a proof is over? Answer: when you've written a deduction that is the statement you wanted to prove.

Logical deductions

The most common form of logical deduction we use when writing proofs is modus ponens, which matches our intuition for what implication means. This rule says that if we already know p and $p \Rightarrow q$ are both true, then we can conclude that q is true. In a proof, we might write something like: "Because we know x > 10 and that x > 10 implies $x^2 - x > 90$, we can conclude that $x^2 - x > 90$.

The other very common form of logical deduction is called universal instantiation, which matches our intuition for what a universally-quantified statement means. This rule says that if we already know a universal like $\forall x \in S, P(x)$, and we have a variable y whose value is an element of the domain S, then we can conclude that P(y) must be true. In a proof, we might write something like: "Because we know that $y \in \mathbb{N}$ and that $\forall x \in \mathbb{N}, x^2 + 5x + 4$ is not prime, we can conclude that $y^2 + 5y + 4$ is not prime." In fact, we use this form of deduction every time we appeal to some "elementary" fact about numbers!

Writing reasons and deductions

Because writing proof bodies is the part that often requires a lot of thinking, you are given more flexibility; there aren't as strict guidelines as for the proof header. However, for every statement you make in the proof body, you should be able to answer the following two questions:

- 1. What deduction am I saying is true here?
- 2. What reason(s) am I giving for why this is true?

You must provide explicit reasons for all statements you make in your proof. Do not simply write (for example) "therefore [deduction]" without justification. Remember that your job in writing a proof is to convince another human being something is true; it is not your reader's job to search through your proof to figure out what reason you meant to give. A deduction that "obviously follows" for you might not be at all clear to another person, which is why providing justification is so important.

In later courses, and certainly as professionals, you'll be able to relax this and often leave justifications up to the reader to figure out, but this is not the case for this course. Remember that because we're all beginners here, we want to share exactly what our thinking is, to make sure our reasoning is actually correct. To put it another way: in the setting of this course, your goal is not to convince your reader that some sentence is True—we already know this—but reather to convince your reader that you are able to write a correct and complete proof!

To make your lives a little easier, there are two exceptions to this rule—that is, two types of deductions where you don't need to provide justification. They are:

- Any deduction whose truth can be verified using a calculator, and any comparison, divisibility and floor/ceiling operation on concrete numbers. For example, you can make deductions like "100 > 3 4" and "165 is not divisible by 6" without giving any justification.
- Any basic manipulation of an equality or inequality to get another valid equality or inequality described in the earlier section on inequalities. For example, you

can go from x > 4 to 2x > 8 without saying that you've multiplied both sides of the first inequality by 2 to get obtain the second.

For any other type of reasoning—including definitions, assumptions, prior deductions, and other external facts—you must reference them explicitly when making deductions. But this doesn't mean you need to repeat or write out the statements! Using some short phrases to at least indicate where the reasons are coming from is acceptable:

```
"By the previous deduction, ..."

"By the definition of divisibility, ..."

"By our first assumption, we can conclude ..."

"Using Claim 3, we know that ..."
```

The direction of a proof

Because we read proofs from top to bottom, the order in which we write statements matters tremendously. We have seen this already when discussing the proof header and the order in which we introduce variables. Even more is true: the proof header should always come before the proof body, so that the variables and assumptions have been clearly defined before we use them in our deductions.

Order also matters when writing deductions in a proof body, because one of the possible types of reasons supporting a deduction are *previous* deductions made. In a proof body, a series of calculations is read from top to bottom, where each line is a deduction whose reasons are the previous line and some basic manipulation. We should think of a block of calculation as a giant implication: *if* the first line is true, *then* the last line must also be true (it logically follows from the first). In a previous example where we wanted to prove that $\forall n \in \mathbb{N}, n > 20 \Rightarrow 1.5n - 4 \geq 3$, the calculation

$$n>20$$
 $1.5n>30$
 $1.5n-4>26$
 $1.5n-4\geq 3$ (since $26>3$)

really showed " $n > 20 \Rightarrow 1.5n - 4 \ge 3$."

This is fairly intuitive, but is often forgotten when we perform *calculations* (manipulation of equalities or inequalities) in a proof body. This is because we use calculations for a different purpose in a proof than how you often use calculations in math class. In a math class, you're used to manipulating equalities and inequalities to "solve" them, which really means performing an *algorithm* that gets you an answer. The reason this is different is that these algorithms always have you *start* with the thing you're trying to "solve" and arrive at an answer. Here's what you might have done in a math class with our inequality $1.5n-4 \ge 3$:

$$1.5n - 4 \ge 3$$
$$1.5n \ge 7$$
$$n \ge \frac{14}{3}$$

Then you would have arrived at your "answer" of $\frac{14}{3}$ and moved on to the next problem. However, in the top-down context of a proof, this calculation is not what we want! While each individual line does indeed follow from the previous one, because we read proofs top-down, this calculation really shows that $1.5n-4 \ge$ $3 \Rightarrow n \geq \frac{14}{3}$.

Note that these algorithms result in calculations that are backwards: they start with the equation/inequality we want to prove, and derive some simpler inequality from it. In a proof, however, we must start with simple inequalities (like assumptions from an implication in the original statement) and derive our target inequality from them. The moral of this section is that proceeding blindly with the algorithms for "solving" equations and inequalities in previous classes may be helpful for scratch work, but you should always be careful when transferring that work to your final proof, so that your calculations actual represent a true chain of reasoning that end with the statement you want to prove.

Much of the time, your scratch work calculations will be reversible, meaning that they can be written in the reverse order but still be logically correct. This is because many of the manipulations we do to equations/inequalities are "if and only ifs"; for example, adding the same quantity to both sides:

$$1.5n-4>3\Leftrightarrow 1.5n>7.$$

However, this isn't always true: for example, squaring both sides of an equation:

$$a = b \Rightarrow a^2 = b^2$$
 but $a^2 = b^2 \not\Rightarrow a = b$.

Rather than worry about which operations are reversible and which aren't, we always write our calculations in top-down order so that there is no confusion in our equations/inequalities about which implies which.

A new domain: number theory

One of the biggest questions that arises from the idea of "proof as communication" is determining how much detail to go into. For this course, we are assuming only basic knowledge of arithmetic, algebraic manipulations of equalities and inequalities, and standard elementary functions like powers, logarithms, and trigonometric functions, but no calculus. 13 However, there is even variation in the typical CSC165 student with experience in this area, so as much as possible in this course, we will introduce new mathematical domains to serve as the objects of study in our proofs.

This approach has three very nice benefits: first, by building domains from the ground up, we can specify absolutely the common definitions and properties that everyone may assume and use freely in proofs; second, these domains are the theoretical foundation of many areas of computer science, and learning about them here will serve you well in many future courses; and third, learning about new domains will help develop the skill of reading about a new mathematical context and understanding it.14 The definitions and axioms of a new domain communicate the foundation upon which we build new proofs - in order to prove things, we need to understand the objects that we're talking about first.

Our first foray into domain exploration will be into number theory, which you can think of as taking a type of entity with which we are quite familiar, and formalizing

¹³ So you may use, without justifications, various laws like $a^b \cdot a^c = a^{b+c}$ and $\sin^2 \theta + \cos^2 \theta = 1$.

¹⁴ In other words, you won't just learn about new domains; you'll learn how to learn about new domains!

definitions and pushing the boundaries of what we actually know about these numbers that we use every day. We'll start off by repeating and expanding on one definition from the previous chapter.

Definition 2.1. Let $n, d \in \mathbb{Z}$. We say that d divides n, or n is divisible by d, if and only if there exists a $k \in \mathbb{Z}$ such that n = dk.

In this case, we use the notation $d \mid n$ to represent "d divides n," and call d a divisor of n, and n a multiple of d.

Divisibility is a nice definition to work with because it contains an existential quantifier embedded in the definition. From this, we'll see some proofs with more complex structure, based on the greater complexity of the statement.

Example 2.5. Prove that 23 | 115.

Translation. We will expand the definition of divisibility to rewrite this statement in terms of simpler operations:

$$\exists k \in \mathbb{Z}, 115 = 23k.$$

Discussion. We just need to divide 115 by 23, right?

Proof. Let k = 5.

Then $115 = 23 \cdot 5 = 23 \cdot k$.

Example 2.6. Prove that there exists an integer that divides 104.

Translation. There is the key phrase "there exists" right in the problem statement, so we could write $\exists a \in \mathbb{Z}, \ a \mid 104$. We can once again expand the definition of divisibility to write: 15

$$\exists a, k \in \mathbb{Z}, 104 = ak.$$

Discussion. Basically, we need to pick a pair of divisors of 104. Since this is an existential proof and we get to pick both a and k, any pair of divisors will work.

Proof. Let a = -2 and let k = -52.

Then 104 = ak.

The previous example is the first one that had multiple quantifiers. In our proof, we had to give explicit values for both a and k to show that the statement held. Just as how a sentence in predicate logic must have all its variables quantified, a mathematical proof must introduce all variables contained in the sentence being proven.

Alternating quantifiers revisited

In the previous chapter, we saw how changing the order of an existential and universal quantifier changed the meaning of a statement. Now, we'll study how the order of quantifiers changes how we can introduce variables in a proof.

 15 We use the abbreviated form for two quantifications of the same type. **Example 2.7.** Prove that all integers are divisible by 1.

Translation. The statement contains a universal quantification: $\forall n \in \mathbb{Z}, 1 \mid n$. We can unpack the definition of divisibility to

$$\forall n \in \mathbb{Z}, \ \exists k \in \mathbb{Z}, \ n = 1 \cdot k.$$

Discussion. The final equation in the fully-expanded form of the statement is straightforward, and is valid when k equals n. But how should I introduce these variables? Answer: in the same order they are quantified in the statement.

Proof. Let $n \in \mathbb{Z}$. Let k = n.

Then $n = 1 \cdot n = 1 \cdot k$.

In this proof, we used an extremely important tool at our disposal when it comes to proofs with multiple quantifiers: any existentially-quantified variable can be assigned a value that depends on the variables defined before it.

In our proof, we first defined n to be an arbitrary integer. Immediately after this, we wanted to show that for this $n, \exists k \in \mathbb{N}, n = 1 \cdot k$. And to prove this, we needed a value for k—a "let" statement. Because we define k after having defined n, we can use n in the definition of k and say "Let k = n." It may be helpful to think about the analogous process in programming. We first initialize a variable n, and then define a new variable k that is assigned the value of n.

Even though this may seem obvious, one important thing to note is that the order of variables in the statement determines the order in which the variables must be introduced in the proof, and hence which variables can depend on which other variables. For example, consider the following erroneous "proof."

Example 2.8. (Wrong!) Prove that $\exists k \in \mathbb{Z}, \ \forall n \in \mathbb{Z}, \ n = 1 \cdot k$.

Proof. Let k = n. Let $n \in \mathbb{Z}$.

Then $n = 1 \cdot k$.

This proof may look very similar to the previous one, but it contains one crucial difference. The very first sentence, "Let k = n," is invalid: at that point, n has not yet been defined! This is the result of having switched around the order of the quantifiers, which forces k to be defined independently of whatever n is chosen.

Note: don't assume that just because one proof is invalid, that all proofs of this statement are invalid! We cannot conclude that this statement is false just because we found one proof that didn't work. 16 We'll next look at how to prove that this statement is indeed false.

¹⁶ A meta way of looking at this: a statement is true if there exists a correct proof of it.

False statements and disproofs

Suppose we have a friend who is trying to convince us that a certain statement X is false. If they tell you that statement X is false because they tried really hard to come up with a proof of it and failed, you might believe them, or you might wonder if maybe they just missed a crucial idea leading to a correct proof. An absence of proof is not enough to convince us that the statement is false.

Instead, we must see a disproof, which is simply a proof that the *negation* of the statement is true.¹⁸ For this section, we'll be using the simplification rules from the first chapter to make negations of statements easier to work with.

Here are two examples: the first one is quite simple, and is used to introduce the basic idea. The second is more subtle, and really requires good understanding of how we manipulate a statement to get a simple form for its negation.

Example 2.9. Disprove the following statement: every natural number divides 360.

Translation. This statement can be written as $\forall n \in \mathbb{N}, n \mid 360$. However, we want to prove that it is false, so we really need to study its negation.

$$\neg (\forall n \in \mathbb{N}, \ n \mid 360)$$
$$\exists n \in \mathbb{N}, \ n \nmid 360$$

Discussion. The original statement is obviously not true: the number 7 doesn't divide 360, for instance. Is that a proof? We wrote the negation of the statement in symbolic form above, and if we translate it back into English, we get "there exists a natural number which does not divide 360." So, yes. That's enough for a proof.

Proof. Let n = 7.

Then $n \nmid 360$, since $\frac{360}{7}$ is not an integer.

When we want disprove a universally-quantified statement ("every element of S satisfies predicate P"), the negation of that statement becomes an existentially-quantified one ("there exists an element of S that doesn't satisfy predicate P"). Since proofs of existential quantification involve just finding one value, the disproof of the original statement involves finding such a value which causes the predicate to be false (or alternatively, causes the negation of the predicate to be true). We call this value a **counterexample** for the original statement. In the previous example, we would say that 7 is a counterexample of the given statement.

A typical disproof of a universal (counterexample).

Given statement to disprove: $\forall x \in S, P(x)$.

Proof. We prove the negation, $\exists x \in S, \neg P(x)$. Let $x = ___$.

[Proof that $\neg P(___)$ is True.]

¹⁷ Maybe they skipped all their CSC165 classes.

¹⁸ In other words, if we can prove that $\neg X$ is true, then X must be false.

Now let's look at at a more complex disproof.

Example 2.10. Disprove the following claim: for all natural numbers a and b, there exists a natural number c which is less than a+b, and greater than both a and b, such that c is divisible by a or by b.

Translation. The original statement can be translated as follows. We've underlined the four different propositions which are joined with AND operators to make them stand out.

$$\forall a,b \in \mathbb{N}, \ \exists c \in \mathbb{N}, \ \underline{c < a + b} \land \underline{c > a} \land \underline{c > b} \land (a \mid c \lor b \mid c).$$

We'll derive the negation step by step, though once you get comfortable with the negation rules, you'll be able to handle even complex formulas like this one quite quickly.

$$\neg \left(\forall a,b \in \mathbb{N}, \ \exists c \in \mathbb{N}, \ \underline{c < a + b} \land \underline{c > a} \land \underline{c > b} \land (\underline{a \mid c \lor b \mid c}) \right)$$

$$\exists a,b \in \mathbb{N}, \ \neg \left(\exists c \in \mathbb{N}, \ \underline{c < a + b} \land \underline{c > a} \land \underline{c > b} \land (\underline{a \mid c \lor b \mid c}) \right)$$

$$\exists a,b \in \mathbb{N}, \ \forall c \in \mathbb{N}, \ \neg \left(\underline{c < a + b} \land \underline{c > a} \land \underline{c > b} \land (\underline{a \mid c \lor b \mid c}) \right)$$

$$\exists a,b \in \mathbb{N}, \ \forall c \in \mathbb{N}, \ \underline{c \ge a + b} \lor \underline{c \le a} \lor \underline{c \le b} \lor \left(\neg (\underline{a \mid c \lor b \mid c}) \right)$$

$$\exists a,b \in \mathbb{N}, \ \forall c \in \mathbb{N}, \ \underline{c \ge a + b} \lor \underline{c \le a} \lor \underline{c \le b} \lor \left(a \nmid c \land b \nmid c \right)$$

$$\exists a,b \in \mathbb{N}, \ \forall c \in \mathbb{N}, \ \underline{c \ge a + b} \lor \underline{c \le a} \lor \underline{c \le b} \lor \left(a \nmid c \land b \nmid c \right)$$

Discussion. That symbolic negation involved quite a bit of work. Let's make sure we can translate the final result back into English: there exist natural numbers a and b such that for all natural numbers $c, c \geq a + b$ or $c \leq a$ or $c \leq b$ or neither a nor b divide c. Hopefully this example illustrates the power of predicate logic: by first translating the original statement into symbolic logic, we were able to obtain a negation by applying some standard manipulation rules and then translating the resulting statement back into English. For a statement as complex as this one, it is usually easier to do this than to try to intuit what the English negation of the original is, at least when you're first starting out.

Okay, so how do we prove the negation? The existential quantifier tells us we get to pick a and b. Let's think simple: what if a and b are both 2? Then a + b = 4. If $c \geq 4$, the first clause in the OR is satisfied, and if $c \leq 2$, the second and third clauses are satisfied. So we only need to worry about when c is 3, because in this case the only clause that could possibly be satisfied is the last one, $a \nmid c \land b \nmid c$. Luckily, a and b are both 2, and 2 doesn't divide 3, so it seems like we're good in this case as well.

It was particularly helpful that we chose such small values for a and b, so that there weren't a lot of numbers in between them and their sum to care about. As you do your own proofs of existentially-quantified statements, remember that you have the power to pick values for these variables!

Proof. Let
$$a=2$$
 and $b=2$, and let $c \in \mathbb{N}$. We now need to prove that $c > a+b \lor c < a \lor c < b \lor (a \nmid c \land b \nmid c)$.

Substituting in the values for a and b, this gets simplified to:

$$c \ge 4 \lor c \le 2 \lor 2 \nmid c \tag{*}$$

To prove an OR, we only need one of the three parts to be true, and different ones can be true for different values of c.

However, precisely which part is true depends on the value of c. For example, we can't say that for an *arbitrary* value of c, that $c \ge 4$. So we'll split up the remainder of the proof into three cases for the values for c: numbers ≥ 4 , numbers < 2, and the single value 3.

Case 1. We will assume that $c \geq 4$, and prove the statement (*) is true.

In this case, the first part of the OR in (*) is true (this is exactly what we've assumed).

Case 2. We will assume that $c \leq 2$, and prove the statement (*) is true.

In this case, the second part of the OR in (*) is true (this is exactly what we've assumed).

Case 3. We will assume that c=3, and prove the statement (*) is true.

This case is the trickiest, because unlike the others, our assumption that c=3 is not verbatim one of the parts of (*). However, we note that $2 \nmid 3$, and so the third part of the OR is satisfied.

Since in all possible cases statement (*) is true, we conclude that this statement is always true.

Proof by cases

The previous proof illustrated a new proof technique known as **proof by cases**. Remember that for a universal proof, we typically let a variable be an arbitrary element of the domain, and then make an argument in the proof body to prove our goal statement. However, even when the goal statement is true for all elements of the domain, it isn't always easy to construct a single argument that works for all of those elements! Sometimes, different arguments are required for different elements. In this case, we divide the domain into different parts, and then write a separate argument for each part.

A bit more formally, we pick a set of unary predicates P_1, P_2, \ldots, P_k (for some positive integer k), such that for every element x in the domain, x satisfies at least one of the predicates (we say that these predicates are exhaustive). You should think of these predicates as describing how we divide up the domain; in the previous example, the predicates were:

$$P_1(c): c \le 2, \qquad P_2(c): c \ge 4, \qquad P_3(c): c = 3.$$

Then, we divide the proof body into cases, where in each case we assume that one of the predicates is True, and use that assumption to construct a proof that specifically works under that assumption.¹⁹

¹⁹ Recall that there's an equivalence between predicates and sets. Another way of looking at a proof by cases is that we divide the domain into subsets $S_1, S_2, \ldots S_k$, and then prove the desired statement separately for each of these subsets.

```
A typical proof by cases.
Given statement to prove: \forall x \in S, P(x). Pick a set of exhaustive predicates
P_1,\ldots,P_k of S.
Proof. Let x \in S. We will use a proof by cases.
Case 1. Assume P_1(x) is True.
[Proof that P(x) is True, assuming P_1(x).]
Case 2. Assume P_2(x) is True.
[Proof that P(x) is True, assuming P_2(x).]
Case k. Assume P_k(x) is True.
[Proof that P(x) is True, assuming P_k(x).]
```

Proof by cases is a very versatile proof technique, since it allows the combining of simpler proofs together to form a whole proof. Often it is easier to prove a property about some (or even most) elements of the domain than it is to prove that same property about all the elements. But do keep in mind that if you can find a simple proof which works for all elements of the domain, that's generally preferable than combining multiple proofs together in a proof by cases.

To see one natural use of proof by cases in number theory, we introduce the following theorem, which formalizes our intuitions about another familiar term: remainders.

Theorem 2.1. (Quotient-Remainder Theorem) For all $n \in \mathbb{Z}$ and $d \in \mathbb{Z}^+$, there exist $q, r \in \mathbb{Z}$ such that n = qd + r and 0 < r < d. Moreover, these q and r are unique (they are determined entirely by the values of n and d).

Definition 2.2. Let n, d, q, r be the variables in the previous theorem. We say that q and r are the quotient and remainder, respectively, when n is divided by d.

The reason this theorem is powerful is that it tells us that for any divisor $d \in \mathbb{Z}^+$, we can separate all possible integers into d different groups, corresponding to their possible remainders (between 0 and d-1) when divided by d. Let's see this how to use this fact to perform a proof by cases.

Example 2.11. Prove that for all integers x, $2 \mid x^2 + 3x$.

Translation. Using the divisibility predicate: $\forall x \in \mathbb{Z}, 2 \mid x^2 + 3x$. Or expanding the definition of divisibility: $\forall x \in \mathbb{Z}, \exists k \in \mathbb{Z}, x^2 + 3x = 2k$.

Discussion. We want to "factor out a 2" from the expression $x^2 + 3x$, but this only works if x is even. If x is odd, though, then both x^2 and 3x will be odd, and adding two odd numbers together produces an even number.

But how do we "know" that every number has to be either even or odd? And how

can we formalize the algebraic operations of "factoring out a 2" or "adding two odd numbers together"? This is where the Quotient-Remainder Theorem comes in.

Proof. Let $x \in \mathbb{Z}$. By the Quotient-Remainder Theorem, we know that when x is divided by 2, the two possible remainders are 0 and 1. We will divide up the proof into two cases based on these remainders.

Case 1: assume the remainder when x is divided by 2 is 0. That is, we assume there exists $q \in \mathbb{Z}$ such that x = 2q + 0. Let $k = 2q^2 + 3q$. We will show that $x^2 + 3x = 2k$.

We have:

$$x^{2} + 3x = (2q)^{2} + 3(2q)$$

$$= 4q^{2} + 6q$$

$$= 2(2q^{2} + 3q)$$

$$= 2k$$

Case 2: assume the remainder when x is divided by 2 is 1. That is, we assume there exists $q \in \mathbb{Z}$ such that x = 2q + 1. Let $k = 2q^2 + 5q + 2$. We will show that $x^2 + 3x = 2k$.

We have:

$$x^{2} + 3x = (2q + 1)^{2} + 3(2q + 1)$$
$$= 4q^{2} + 4q + 1 + 6q + 3$$
$$= 2(2q^{2} + 5q + 2)$$
$$= 2k$$

Generalizing statements

In this section, we will investigate another important skill for reading and writing proofs: the ability to *generalize* existing knowledge into more generic, and powerful, forms. As usual, we start with an example.

A first example

Example 2.12. Prove that for all integers x, if x divides (x + 5), then x also divides 5.

Translation. There is both a universal quantification and implication in this statement:²⁰

$$\forall x \in \mathbb{Z}, \ x \mid (x+5) \Rightarrow x \mid 5.$$

When we unpack the definition of divisibility, we need to be careful about how the quantifiers are grouped:

$$\forall x \in \mathbb{Z}, \ \left(\left(\exists k_1 \in \mathbb{Z}, \ x+5=k_1 x \right) \Rightarrow \left(\exists k_2 \in \mathbb{Z}, \ 5=k_2 x \right) \right).$$

²⁰ We weren't kidding that this is the most common form of statement.

Discussion. I need to prove that if x divides x + 5, then it also divides 5. So I can assume that x divides x + 5, and I need to prove that x divides 5. Since x is divisible by x, I should be able to subtract it from x + 5 and keep the result a multiple of x. Can I prove that using the definition of divisibility? I basically need to "turn" the equation $x + 5 = k_1 x$ into the equation $5 = k_2 x$.

Proof. Let x be an arbitrary integer. Assume that $x \mid (x+5)$, i.e., that there exists $k_1 \in \mathbb{Z}$ such that $x+5=k_1x$. We want to prove that there exists $k_2 \in \mathbb{Z}$ such that $5 = k_2 x$. Let $k_2 = k_1 - 1$.

Then we can calculate:

$$k_2x=(k_1-1)x$$

$$=k_1x-x$$

$$=(x+5)-x \qquad \qquad \text{(we assumed } x+5=k_1x\text{)}$$

$$=5$$

Whew, that was a bit longer than the proofs we've already done. There were a lot of new elements that we introduced here, so let's break them down:

• After introducing x, we wanted to prove the *implication* $x \mid (x+5) \Rightarrow x \mid 5$. To prove an implication, we needed to assume that the hypothesis was true, and then prove that the conclusion is also true. In our proof, we wrote "Assume $x \mid (x+5)$." This is not a claim that $x \mid (x+5)$ is True; rather, it is a way to consider what would happen if $x \mid (x+5)$ were True. The goal for the rest of the proof after that was to prove that $x \mid 5$.

Note that this proof did not prove that $\forall x \in \mathbb{Z}, x \mid x+5$: this is actually false! Instead, we proved that if x divides (x + 5), then it must also divide 5.

• When we assumed that $x \mid (x+5)$, what this really did was introduce a new variable $k_1 \in \mathbb{Z}$ from the definition of divisibility. This might seem a little odd, but take a moment to think about what this means in English. We assumed that x divides x + 5, which (by definition) is the same as assuming that there exists an integer k_1 such that $x+5=k_1x$. Given that such a number exists, we can give it a name and refer to it in the rest of our proof. 21

Generalizing our example

One of the most important meta-techniques in mathematical proof is that of generalization: taking a true statement (and a proof of the statement), and then replacing a concrete value in the statement with a universally quantified variable. For example, consider the statement from the previous example, $\forall x \in \mathbb{Z}, \ x \mid (x+5) \Rightarrow$ $x \mid 5$. It doesn't seem like the "5" serves any special purpose; it is highly likely that it could be replaced by another number like 165, and the statement would still hold.²²

But rather than replace the 5 with another concrete number and then re-proving the statement, we will instead replace it with a universally-quantified variable, and prove the corresponding statement. This way, we will know that in fact we could replace the 5 with any natural number, and the statement would still hold.

²¹ In other words, we introduced a variable into the proof through an assumption we made.

²² Concretely, consider the statement $\forall x \in \mathbb{Z}, \ x \mid (x+165) \Rightarrow x \mid 165, \text{ which}$ is at least as plausible as the original statement with 5's.

Example 2.13. Prove that for all $d \in \mathbb{Z}$, and for all $x \in \mathbb{Z}$, if x divides (x + d), then x also divides d.

Translation. This has basically the same translation as last time, except now we have an extra variable:

$$orall d,x\in \mathbb{Z},\; \Big(ig(\exists k_1\in \mathbb{Z},\;x+d=k_1xig)\Rightarrow ig(\exists k_2\in \mathbb{Z},\;d=k_2xig)\Big).$$

Discussion. I should be able to use the same set of calculations as last time.

Proof. Let d and x be arbitrary natural numbers. Assume that $x \mid (x+d)$, i.e., there exists $k_1 \in \mathbb{Z}$ such that $x+d=k_1x$.

We want to prove that there exists $k_2 \in \mathbb{Z}$ such that $d = k_2 x$. Let $k_2 = k_1 - 1$.

Then we can calculate:

$$k_2 x = (k_1 - 1)x$$

= $k_1 x - x$
= $(x + d) - x$
= d

This proof is basically the same as the previous one: we have simply swapped out all of the 5's with d's. We say that the proof did not depend on the value 5, meaning there was no place that we used some special property of 5, where we could have used a generic integer instead. We can also say that the original statement and proof generalize to this second version.

Why does generalization matter? By generalizing the previous statement from being about the number 5 to an arbitrary integer, we have essentially gone from one statement being true to an infinite number of statements being true. The more general the statement, the more useful it becomes. We care about exponent laws like $a^b \cdot a^c = a^{b+c}$ precisely because they apply to every possible number; regardless of what our concrete calculation is, we know we can use this law in our calculations.

Exercise Break!

2.1 Prove that for any three integers a, b, and c, if a divides both b and c, then a also divides b+c.

Hint: since the hypothesis is an AND of two statements, you get to assume both statements.

2.2 (Divisibility of linear combinations) Generalize the previous proof to prove the following statement:

$$orall a,b,c,p,q \in \mathbb{Z}, \ \Big(a \mid b \wedge a \mid c \Rightarrow a \mid (bp+cq) \Big).$$

This statement says that if you have two multiples of a, and then multiply them by any other two numbers and add the results, the final number must always be a multiple of a.

Proof by contrapositive

Let us now look at one example that is very similar to the previous one.

Example 2.14. Prove that for all integers x, if x does not divide x + 5, then x does not divide 5.

Translation. This is actually a little easier to translate than the examples we have just done. We'll keep the divisibility predicate in the statement for now.

$$\forall x \in \mathbb{Z}, x \nmid x + 5 \Rightarrow x \nmid 5.$$

Discussion. As a standard approach for an implication, we would first assume that x does not divide x + 5, and then prove that x does not divide 5. But assuming that x doesn't divide something seems less informative than knowing that it does divide something.

Luckily, we have a new proof technique to work with: an proof by contrapositive (also known as a form of indirect proof). Rather than try to prove the implication directly, we prove its contrapositive, which is logically equivalent to it.²³ Let's rewrite the statement using the contrapositive:

$$\forall x \in \mathbb{Z}, \ x \mid 5 \Rightarrow x \mid x + 5.$$

Now if we can assume $x \mid 5$, that gives us a lot to work with!

Proof. Let $x \in \mathbb{Z}$. We will prove the contrapositive statement: $x \mid 5 \Rightarrow x \mid x + 5$. So assume that $x \mid 5$.

[We leave it as an exercise to prove that $x \mid x+5$ under this assumption.]

When proving an implication, it is often the case that the assuming the hypothesis does not get you very far. Flipping the implication around to its contrapositive and assuming the negation of the conclusion might yield better results!

A typical proof of an implication (contrapositive/indirect proof).

Given statement to prove: $P \Rightarrow Q$.

Proof. Assume $\neg Q$.

[Proof that $\neg P$ is True.]

Characterizations

We will now look at a pair of related examples that both demonstrate how to prove a biconditional, and illustrate one of the common goals of mathematical study: finding alternative useful characterizations of definitions. In particular,

²³ Remember, the contrapositive of $p \Rightarrow q \text{ is } \neg q \Rightarrow \neg p.$

we'll show that prime numbers are exactly the numbers greater than 1 that satisfy the following predicate:

$$Atomic(n): \forall a, b \in \mathbb{N}, n \nmid a \land n \nmid b \Rightarrow n \nmid ab, \quad \text{where } n \in \mathbb{N}$$

Example 2.15. We'll first prove the following statement:²⁴

$$\forall n \in \mathbb{N}, \ \left(n > 1 \land \left(\forall a, b \in \mathbb{N}, \ n \nmid a \land n \nmid b \Rightarrow n \nmid ab\right)\right) \Rightarrow Prime(n) \tag{2.1}$$

After thinking for a while, it's not clear how to use the hypothesis to prove the conclusion. So, we'll try rewriting this statement using the contrapositive of the implication:

$$\forall n \in \mathbb{N}, \ \neg Prime(n) \Rightarrow \Big(n \leq 1 \lor \big(\exists a, b \in \mathbb{N}, \ n \nmid a \land n \nmid b \land n \mid ab\big)\Big) \tag{2.2}$$

Now, we can assume that n is not prime, and we only need to prove an existential (or that $n \leq 1$)! Not bad. We will prove statement 2.2; since it is logically equivalent to 2.1, this proof will also be a proof of 2.1.

Discussion. We're going to assume that n is not prime, and it's greater than 1 (this is the more interesting case). Let's look at the definition of Prime and negate it:

$$Prime(n): n > 1 \land (\forall d \in \mathbb{N}, d \mid n \Rightarrow d = 1 \lor d = n) \\ \neg Prime(n): n \leq 1 \lor (\exists d \in \mathbb{N}, d \mid n \land d \neq 1 \land d \neq n)$$

So then if we also assume that n > 1, then we can also assume that there exists a number d that divides n that is not 1 or n.

Let's look at an example to gain some intuition. If n=6, then we know $n=2\cdot 3$. From this, we need to pick an a and b such that $n\nmid a$, $n\nmid b$, and $n\mid ab$. In this case, we can just pick a=2 and b=3! Does this always work? Say now that n=12, so we could write $n=2\cdot 6$ or $n=3\cdot 4$. In all cases, as long as $n=n_1\cdot n_2$ where $1< n_1, n_2< n$, we can pick $a=n_1$ and $b=n_2$. Now onto the proof.

Proof. Let $n \in \mathbb{N}$. Assume that n is not prime. Then by negating the definition of prime, either $n \leq 1$ or there exists $d \in \mathbb{N}$, $d \mid n \wedge d \neq 1 \wedge d \neq n$. We divide our proof into two cases based on which part of the OR is true.

Case 1: Assume $n \leq 1$.

Then since the first part of the OR we want to prove is $n \leq 1$, this is true.

Case 2: Assume $\exists d \in \mathbb{N}, \ d \mid n \land d \neq 1 \land d \neq n$.

Expanding the definition of the divides predicate, this means that there also exists $k \in \mathbb{N}$ such that n = dk. We will prove the second part of the OR $(\exists a, b \in \mathbb{N} \dots)$. Let a = d and b = k. We want to prove that $n \nmid a$, $n \nmid b$, and $n \mid ab$.

We leave the proof body as an exercise; to complete this, we'll use a few external facts about divisibility.

What we have just proven is that if n is greater than 1 and satisfies the Atomic predicate, then it must be prime. This rules out the possibility that n = 6

²⁴ In English: "Every number that is greater than one and atomic must also be prime."

satisfies this property, for example. But what about n = 5? This statement doesn't actually tell us that 5 satisfies this property! So next, we'll prove the converse of the implication.

Example 2.16. Let's prove the following, which uses the converse of the implication from 2.1:25

²⁵ In English: "Every number that is prime must be greater than one and atomic."

$$\forall n \in \mathbb{N}, \ Prime(n) \Rightarrow \Big(n > 1 \land \big(\forall a, b \in \mathbb{N}, \ n \nmid a \land n \nmid b \Rightarrow n \nmid ab\big)\Big)$$
 (2.3)

It turns out that we can do a direct proof here, so we'll stick with this form and not write the contrapositive.

Discussion. Let's do an example to try to understand why it might be true. Consider the prime n = 7 and consider some arbitrary numbers a and b. The interesting case is when both a and b do not have 7 as a divisor, for example a=12 and b=10. We can check that $a \cdot b=120$ also doesn't have 7 as a divisor. But how do we prove this? The "obvious" way of showing this is to first write a and b as a product of their prime factors. Then $a \cdot b$ is just the product of all of the factors of a and b. In our example, for $a = 12, b = 10, a = 2 \cdot 2 \cdot 3$ and $b = 2 \cdot 5$. So $a \cdot b = 2 \cdot 2 \cdot 3 \cdot 2 \cdot 5$. Clearly this representation of $a \cdot b$ does not have 7 as a prime factor. Now because the prime factorization of any number is unique, it follows that $a \cdot b$ does not have 7 as a divisor.

But the problem with this proof is that we would have to prove that every number has a unique prime factorization. This is a bit hard, and isn't really necessary to prove the statement, so instead we'll use the following two facts that are easier to prove. They only rely on the properties of the greatest common divisor that we'll talk about in the next section.²⁶

$$\forall n, m \in \mathbb{N}, \ Prime(n) \land n \nmid m \Rightarrow (\exists r, s \in \mathbb{Z}, \ rn + sm = 1)$$
 (Claim 1)
 $\forall n, m \in \mathbb{N}, \ Prime(n) \land (\exists r, s \in \mathbb{Z}, \ rn + sm = 1) \Rightarrow n \nmid m$ (Claim 2)

How might we set up a proof using these claims? First, we note that we are assuming that n is prime. Say that we have two numbers a, b that are not divisible by n. Using Claim 1 twice, there exist r_1, s_1 (for a) and r_2, s_2 (for b) such that

$$r_1n + s_1a = 1$$
$$r_2n + s_2b = 1$$

Now what? We want to conclude that ab is also not divisible by n. To do this we will use Claim 2, which says that to conclude that ab is not divisible by n, it suffices to find r, s such that rn + s(ab) = 1. We can find r, s by multiplying the two equations together:

$$r_1r_2n^2 + r_2s_1an + r_1s_2bn + s_1s_2ab = 1$$

This can be rewritten as

$$(r_1r_2n + r_2s_1a + r_1s_2b)n + (s_1s_2)(ab) = 1$$

Proof. Let $n \in \mathbb{N}$. Assume that n is prime. We need to prove that n > 1 and that Atomic(n) are true.

For the first part, the definition of prime tells us immediately that n > 1.

For the second part, we want to prove that $(\forall a, b \in \mathbb{N}, n \nmid a \land n \nmid b \Rightarrow n \nmid ab)$. Let $a, b \in \mathbb{N}$, and assume that $n \nmid a$ and $n \nmid b$. We want to prove that $n \nmid ab$.

We'll first prove that there exist $r_3, s_3 \in \mathbb{Z}$, $r_3n + s_3ab = 1$. By Claim 1 and the assumption that n is prime, there exist $r_1, s_1, r_2, s_2 \in \mathbb{Z}$ such that $r_1n + s_1a = 1$ and $r_2n + s_2b = 1$. Let $r_3 = r_1r_2n + r_2s_1a + r_1s_2b$ and $s_3 = s_1s_2$.

Then we can multiply the first two equations to obtain:

$$(r_1n+s_1a)(r_2n+s_2b)=1$$
 $r_1r_2n^2+r_2s_1an+r_1s_2bn+s_1s_2ab=1$ $(r_1r_2n+r_2s_1a+r_1s_2b)n+(s_1s_2)ab=1$ $r_3n+s_3ab=1$

So then there exist $r_3, s_3 \in \mathbb{Z}$, $r_3n + s_3ab = 1$. Then using Claim 2 (and again the assumption that n is prime), we can conclude that $n \nmid ab$.

Putting everything together

To recap, we have now proved both of the following statements:

$$\forall n \in \mathbb{N}, \ n > 1 \land Atomic(n) \Rightarrow Prime(n) \tag{2.1}$$

$$\forall n \in \mathbb{N}, \ Prime(n) \Rightarrow n > 1 \land Atomic(n)$$
 (2.3)

These have the form $\forall n \in \mathbb{N}, \ P(n) \Rightarrow Q(n) \text{ and } \forall n \in \mathbb{N}, \ Q(n) \Rightarrow P(n)$; in other words, we know both directions of the implication are true, and so can express this using the biconditional operator, \Leftrightarrow . Thus we have proven:

$$\forall n \in \mathbb{N}, \ Prime(n) \Leftrightarrow n > 1 \land Atomic(n)$$

In other words, a natural number n is prime if and only if it is greater than one and atomic. The property "greater than one and atomic" is a *characterization* or *alternate definition* of the concept of prime numbers. Equivalent characterizations are very useful in mathematics and computer science as they often give a very different way to look at the same concept.

Greatest common divisor

Let us now introduce one more definition that you're probably familiar with, though again we will take some time to treat it more formally than what you may have seen before.

Definition 2.3. Let m, n be natural numbers which are not both 0. The greatest common divisor (gcd) of m and n, denoted gcd(m, n), is the maximum natural number d such that d divides both m and n.²⁷

We also define gcd(0,0) = 0 just to make the domain of the gcd operator all possible pairs of natural numbers.

To make it easier to translate this statement into symbolic form, we can restate the "maximum" part by saying that if e is any number which divides m and n, then e < d. Let $m, n, k \in \mathbb{N}$, not all of which are 0, and suppose $k = \gcd(m, n)$. Then k satisfies the following statement:

$$k \mid m \land k \mid n \land (\forall e \in \mathbb{N}, e \mid m \land e \mid n \Rightarrow e \leq k).$$

You might wonder whether this definition makes sense in all cases: is it possible for two numbers to have no divisors in common? But remember that one of the statements we proved in this chapter is that 1 divides every natural number. So at the very least, 1 is a common divisor between any two natural numbers.

Here is an example which makes use of both this definition, and the definition of prime from the previous chapter.

Example 2.17. Prove that for all natural numbers p and q, if p and q are distinct primes, then gcd(p,q) = 1.

Translation. Here is an initial translation which focuses on the structure of the above statement, but doesn't unpack any definitions:

$$\forall p, q \in \mathbb{N}, (Prime(p) \land Prime(q) \land p \neq q) \Rightarrow \gcd(p, q) = 1.$$

We could unpack the definitions of Prime and gcd, but doing so would not add any insight at this point. While we will almost certainly end up using these definitions in the discussion and proof sections, expanding it here actually obscures the meaning of the statement.

In general, use translation as a way of precisely specifying the structure of a statement; as we have seen repeatedly, the high-level structure of a statement is mimicked in the structure of its proof. And while you don't need to expand every definition in a statement, you should always keep in mind that definitions referred to in the statement will require unpacking in the proof itself.

Discussion. We know that primes don't have many divisors, and that 1 is a common divisor for any pair of numbers. So to show that gcd(p,q) = 1, we just need to make sure that neither p nor q divides the other (otherwise that would be a common divisor larger than 1).

Proof. Let $p, q \in \mathbb{N}$. Assume that p and q are both prime, and that $p \neq q$. We want to prove that gcd(p, q) = 1.

By the definition of primality, we know that $p \neq 1$. Also by the definition of primality, the only positive divisors of q are 1 and q itself. So then since $p \neq q$ (our assumption) and $p \neq 1$, we know that $p \nmid q$.

Then 1 is the only positive common divisor of p and q, so gcd(p,q) = 1.

²⁷ According to this definition, what is gcd(0, n) when n > 0?

Next, we will look at one of the strongest properties of the greatest common divisor: it is the smallest natural number that can be written as a sum of (positive or negative) multiples of the two numbers.

Theorem 2.2. Let a and b be arbitrary natural numbers, and assume at least one of them is non-zero. Then gcd(a,b) is the smallest positive integer such that there exist $p,q \in \mathbb{Z}$ with gcd(a,b) = ap + bq.

We will not prove this theorem here; instead, our main goal for stating it is to introduce a new proof technique: using an external statement as a step in a proof. This might sound kind of funny—after all, many of our proofs so far have relied on some algebraic manipulations which are valid but are really knowledge we learned prior to this course. The subtle difference is that those algebraic laws we take for granted as "obvious" because we learned them so long ago. But in fact our proofs can consist of steps which are statements that we know are true because of an external source, even one that we don't know how to prove ourselves.

This is a fundamental parallel between writing proofs and writing computer programs. In programming, we start with some basic building blocks of a language—data types, control flow constructs, etc.—but we often rely on libraries as well to simplify our tasks. We can use these libraries by reading their documentation and understanding how to use them, but don't need to understand how they are implemented. In the same way, we can use an external theorem in our proof by understanding what it means, but without knowing how to prove it.

Example 2.18. For all $a, b \in \mathbb{N}$, every integer that divides both a and b also divides gcd(a, b).

Translation. We can translate this statement as follows:

$$\forall a, b \in \mathbb{N}, \ \forall d \in \mathbb{Z}, \ (d \mid a \land d \mid b) \Rightarrow d \mid \gcd(a, b).$$

Discussion. This one is a bit tougher. All we know from the definition of gcd is that $d \leq \gcd(a,b)$, but that doesn't imply $d \mid \gcd(a,b)$ by any means. But given the context that we just discussed in the preceding paragraphs, I'd guess that we should also use the GCD Characterization Theorem to write $\gcd(a,b)$ as ap + bq. Oh, and one of the previous exercises showed that any number that divides a and b will divide ap + bq as well!

Proof. Let $a, b \in \mathbb{N}$ and $d \in \mathbb{Z}$. Assume that $d \mid a$ and $d \mid b$. We want to prove that $d \mid \gcd(a, b)$.

By the GCD Characterization Theorem, there exist integers $p, q \in \mathbb{Z}$ such that $gcd(a, b) = ap + bq.^{28}$

Then by the exercise on the divisibility of linear combinations, since $d \mid a$ and $d \mid b$ (by assumption), we know that $d \mid ap + bq$. Since gcd(a, b) = ap + bq, we conclude that $d \mid gcd(a, b)$.

²⁸ This line uses a known external fact that is an existential to *introduce* two variables p and q to use in our proof.

Modular arithmetic

The final definition in this chapter introduces some notation that is extremely commonplace in number theory, and by extension in many areas of computer sci-

ence. Often when we are dealing with relationships between numbers, divisibility is too coarse a relationship: as a predicate, it is constrained by the binary nature of its output. Instead, we often care about the remainder when we divide a number by another.

Definition 2.4. Let $a, b, n \in \mathbb{Z}$, with $n \neq 0$. We say that a is congruent to b modulo n if and only if $n \mid a - b$. In this case, we write $a \equiv b \pmod{n}$.

This definition captures the idea that a and b have the same remainder when divided by n. You should think of this congruence relation as being analogous to numeric equality, with a relaxation. When we write a = b, we mean that the numeric values of a and b are literally equal. When we write $a \equiv b \pmod{n}$, we we mean that if you look at the remainders of a and b when divided by n, those remainders are literally equal.

We will next look at how addition, subtraction, and multiplication all behave in an analogous fashion under modular arithmetic. The following proof is a little tedious because it is calculation-heavy; the main benefits here are practicing reading and using a new definition, and getting comfortable with this particular notation.

Example 2.19. Prove that for all $a, b, c, d, n \in \mathbb{Z}$, with $n \neq 0$, if $a \equiv c \pmod{n}$ and $b \equiv d \pmod{n}$, then:

- 1. $a+b \equiv c+d \pmod{n}$
- $2. \ a-b \equiv c-d \pmod{n}$
- 3. $ab \equiv cd \pmod{n}$

Translation. We will only show how to unpack the definitions in (2), as the other two are quite similar.

$$\forall a, b, c, d, n \in \mathbb{Z}, (n \neq 0 \land n \mid (a - c) \land n \mid (b - d)) \Rightarrow n \mid ((a - b) - (c - d)).$$

Proof. Let $a, b, c, d, n \in \mathbb{Z}$, and assume that $n \neq 0$, $n \mid (a - c)$, and $n \mid (b - d)$.

We will only prove (2), and leave (1) and (3) as exercises. This means we want to prove that $n \mid ((a-c)-(b-d))$.

By the previous exercise on the divisibility of linear combinations, since $n \mid (a-c)$ and $n \mid (b-d)$, it divides their difference:

$$n \mid (a-c)-(b-d)$$
 $n \mid (a-b)-(c-d)$ (rearranging terms)

You may be wondering why we left out division in the above theorem. Recall again the definition of divisibility: $a \mid b$ means that there exists $k \in \mathbb{N}$ such that b=ka. Not every pair of integers is related by divisibility, and this also transfers over to modular arithmetic as well.

However, we have all the tools necessary to prove the following quite remarkable fact.

²⁹ One warning: the notation $a \equiv b$ (mod n) is not exactly the same as mod or % operator you are familiar with from programming; here, both a and b could be much larger than n, or even negative.

Example 2.20. Let $a, b, p \in \mathbb{Z}$. If p is a prime number and a is not divisible by p, then there exists $k \in \mathbb{Z}$ such that $ak \equiv b \pmod{p}$.

Translation. This statement is quite complex! Remember that we focus on translation to examine the structure of the statement, so that we know how to set up a proof. We aren't going to expand every single definition for the sake of expanding definitions.

$$\forall a, b, p \in \mathbb{Z}, ((Prime(p) \land p \nmid a) \Rightarrow (\exists k \in \mathbb{Z}, ak \equiv b \pmod{p})).$$

Discussion. So this is saying that under the given assumptions, b is "divisible" by a modulo p. Somehow I'm supposed to use the fact that p is prime. The conclusion is "there exists a $k \in \mathbb{Z}$ such that..." so that I know that at some point I'll need to define a variable k in terms of a, b, and/or p, which satisfies the congruence.

Can I do k = b/a? That obviously would satisfy the congruence, but the example statement doesn't say that I can assume that a divides b... But if I could prove that $a \mid b$, then I would be able to write the proof. So is it true? The statement has to hold for *every* pair of numbers a and b where a isn't divisible by p, so I think I'm out of luck – after all, this includes cases where a > b.

Here's another idea: can I prove a less general statement? I could set b to always be 1, and try to show that there always exists a k such that $ak \equiv 1 \pmod{p}$. If I can show that, then multiplying both sides by b should do the trick.³⁰

[HINT: use the GCD Characterization Theorem.] Woah, I got a hint! Hmmm, that theorem talks about writing gcd as a sum of multiples. How does that help? Let me write down what I know and can assume:

- p is prime
- $p \nmid a$
- The gcd of two numbers can be written as the *sum of multiples* of the numbers.

And what I want to prove:

- $\exists k \in \mathbb{Z}, ak \equiv 1 \pmod{p}$. That's equivalent to:
- $\exists k \in \mathbb{Z}, p \mid (ak-1)$, using the definition of mod. That's equivalent to:
- $\exists k, d \in \mathbb{Z}, ak-1 = pd$. Hey, wait a second...
- $\exists k, d \in \mathbb{Z}, ak pd = 1$. That's writing 1 as a sum of multiples of a and p!

Now I just need to connect these two lines of reasoning.

Proof. Let $a,b,p\in\mathbb{N}$. Assume that p is prime and p does not divide a. We want to prove that there exists $k\in\mathbb{Z}$ such that $ak\equiv b\pmod{p}$. To do this, we are going to first prove two $subclaims.^{31}$

Claim 1.
$$gcd(a, p) = 1$$
.

Proof. By definition of **prime**, we know that the only two positive divisors of p are 1 and p. Since we have assumed that $p \nmid a$, this means that 1 is the only positive common divisor of p and a. So gcd(a, p) = 1.

³⁰ That's statement (3) from the previous example, by the way.

³¹ Think of these as helper functions in programming. They are smaller statements which we can use as steps in a larger proof.

Claim 2. There exists $k \in \mathbb{Z}$ such that $ak \equiv 1 \pmod{p}$.

Proof. By the previous claim, we now know that gcd(a, p) = 1. By Theorem 2.1, there exist $r, s \in \mathbb{Z}$ such that ar + ps = 1.

Let k = r. Then we can re-arrange this statement:

$$ak + ps = 1$$
 $ak - 1 = p(-s)$
 $p \mid (ak - 1)$
 $ak \equiv 1 \pmod{p}$

Finally, we can use these two claims to prove that there exists a $k' \in \mathbb{Z}$ such that $ak' \equiv b \pmod{p}$.

Let k' = kb. Then we have:

$$ak \equiv 1 \pmod{p}$$
 $akb \equiv b \pmod{p}$
 $ak' \equiv b \pmod{p}$

This theorem brings together elements from all of our study of proofs so far. We have both types of quantifiers, as well as some significant assumptions (as part of an implication). We even used the GCD Characterization Theorem for a key step in our proof. Finally, this proof introduced one more useful kind of structure: a subproof, or proof of a smaller claim that is used to prove the main result. Just as helper functions help organize a program, small claims and subproofs help organize a proof so that each part can be understood separately, before being combined into a whole.³² As your proofs grow longer and longer, make good use of this approach to keep your proofs readable and easy to understand. There is nothing worse than having to slog through pages and pages of a single proof without any sense of what claim is being proved, and how the claims fit together.

32 We can outline the previous proof in three steps: (1) Prove that gcd(a, p) = 1, (2) Prove that $\exists k \in \mathbb{Z}, \ ak \equiv 1 \pmod{p}, \text{ and (3)}$ Prove that $\exists k' \in \mathbb{Z}, \ ak' \equiv b \pmod{p}$.

Proof by contradiction

The final proof technique we will cover in this chapter is the proof by contradiction. Given a statement P to prove, rather than attempt to prove it directly we assume that its negation $\neg P$ is true, and then use this assumption to prove a statement Q and its negation $\neg Q$. We call Q and $\neg Q$ the contradiction that arises from the assumption that P is .

Why does this work? Essentially, we argue the if P is false, then statement Qmust be true, but its negation $\neg Q$ must also be true. But these two things can't be true at the same time, and so our original assumption must be wrong!

Proofs by contradiction are a more general form of the indirect proof-by-contrapositive we saw earlier in this chapter. They often take a bit more thought because it isn't

necessarily clear what the contradiction (statement Q) should be. We finish off this chapter by presenting one particularly famous proof by contradiction dating back to the Greek mathematician Euclid.³³

Theorem 2.3. There are infinitely many primes.

Proof. Assume that this statement is false, i.e., that there a finite number of primes. Let $k \in \mathbb{N}$ be the number of primes, and let p_1, p_2, \ldots, p_k be the prime numbers.

Our statement Q will be "for all $n \in \mathbb{N}$, n is prime if and only if n is one of $\{p_1, \ldots, p_k\}$." Q is True because of our assumption that there are a finite number of primes, and the definitions of k and p_1, \ldots, p_k .

Now we will show that Q is False. Define the number

$$P=1+\prod_{i=1}^k p_i=1+p_1 imes p_2 imes \cdots imes p_k.$$

There must be some prime p that divides P because P > 1. But $p \notin \{p_1, \ldots, p_k\}$, because otherwise p would divide $P - p_1 \times \cdots \times p_k = 1$, and no prime can divide 1. So then p is a prime that is not one of $\{p_1, \ldots, p_k\}$, and so Q is false. Contradiction!

³³ Although Euclid's original proof was written in an informal style, the idea was certainly there.

3 Induction

In the previous chapters we have studied how to express statements precisely using mathematical expressions, and how to analyze and prove the truth or falsehood of these statements using a variety of proof techniques. In this chapter, we will introduce a new and very important proof technique called **induction**, and use it to prove statements of the form, $\forall n \in \mathbb{N}, P(n)$.

You may wonder why we need this new technique when we were already proving universal statements in the last chapter just fine without induction. It turns out that many interesting statements in number theory and most other domains cannot be proved or disproved easily with just the techniques from the previous chapter. We will first motivate the principle of induction using an example from modular arithmetic. Then we will apply induction to other statements in number theory, and then to new domains, using induction to prove properties about sequences and to find expressions for various ways of counting combinatorial objects.

The principle of induction

Let us start with an example.

Example 3.1. Prove that for any $m, x, y, n \in \mathbb{N}$ such that $n \geq 1$, if $x \equiv y \pmod{m}$, then $x^n \equiv y^n \pmod{m}$.

It is not hard to show that this is true without using induction for n=2 as follows. By assumption, $x\equiv y\pmod m$, and therefore $x\cdot x\equiv y\cdot y\pmod m$, and thus $x^2\equiv y^2\pmod m$. In order to show that it is true for n=3, we can argue that since we already know that $x^2\equiv y^2\pmod m$, and $x\equiv y\pmod m$, then $x\cdot x^2\equiv y\cdot y^2\pmod m$ and thus $x^3\equiv y^3\pmod m$. Then we can prove that it is true for n=4 in exactly the same way, and so on. But in order to make the "and so on" mathematically rigorous, we need to use induction.

The first explicit formulation of the principle of induction was given by Pascal (as in Pascal's triangle) in 1665. However, its uses have been traced as far back as Plato (370 BC), and a variation of Euclid's proof of the existence of infinitely many primes (from around the same time period). We cannot stress enough the importance of the induction principle—it is *the* powerhorse behind nearly all proofs. The principle of induction applies to *universal* statements over the natural numbers—that is, statements of the form $\forall n \in \mathbb{N}, P(n)$. It cannot be used to prove statements of any other form! Note however that P(n) can be quite complicated and can involve other possibly nested quantifiers.

¹ This is Part 3 of Example 2.19 from the previous chapter.

In this course, we will study only the most basic form of induction, commonly called *simple* induction.² There are two steps to using this induction principle³:

- The base case is a proof that the statement holds for the first natural number, 0; that is, a proof that P(0) holds.
- The inductive step is a proof that for all $n \in \mathbb{N}$, if P(n) is true, then P(n+1) is also true. That is:

$$\forall n \in \mathbb{N}, \ P(n) \Rightarrow P(n+1).$$

Once the base case and inductive step are proven, by the principle of induction, one can conclude $\forall n \in \mathbb{N}, P(n)$.

Typical structure of a proof by induction.

Given statement to prove: $\forall n \in \mathbb{N}, P(n)$.

Proof. We prove this by induction on n.

Base Case: [Proof that P(0) is True.]

Inductive step: Let $n \in \mathbb{N}$, and assume that P(n) is true. (The assumption that P(n) is true is called the *induction hypothesis*.)

[Proof that P(n+1) is True.]

The point behind induction is that sometimes it isn't possible to give a direct proof for all n at once—sometimes we require knowing that the statement is true for smaller values in order to show that it is true for larger ones. Induction formalizes this idea—if you show it is true for the smallest element (the base case) and if you can show that as long as it is true for n then it is also true for the number right after n, then we can conclude that it is true for every n.

Why does the principle of induction work? This is essentially the domino effect. Assume you have shown the base case and the inductive step. In other words, you know P(0) is true, and you know that P(n) implies P(n+1) for every natural number k. Since you know P(0) from the base case and $P(0) \Rightarrow P(1)$ by the inductive step, we have P(1). Then since you now know P(1) and $P(1) \Rightarrow P(2)$ from the inductive step, we have P(2). Now since we know P(2) and $P(2) \Rightarrow P(3)$, we have P(3). And so on.

Examples from number theory

Let us see how to use induction to prove some statements from number theory.

Example 3.2. Prove that for every natural number n, $7 \mid 8^n - 1$.

Translation. We can write this as

$$\forall n \in \mathbb{N}, \ 7 \mid 8^n - 1.$$

² In CSC236, you'll learn about different forms of induction.

³ Notice that the two steps are a conjunction, so they may be presented in either order. Variable names (n, k, i, etc.) are up to you, provided you use each name to refer to a fixed value

Define the predicate P(n) as "7 | $8^n - 1$," where n is a natural number. This makes it clear how we will use induction: the statement becomes $\forall n \in \mathbb{N}, P(n)$.

Proof. Let P(n) be the statement that 7 divides $8^n - 1$; in other words, there exists an integer y such that $7 \cdot y = 8^n - 1$. Expressed formally, P(n) is:

$$\exists y \in \mathbb{Z}, \ 7 \cdot y = 8^n - 1.$$

We want to prove for all $n \in \mathbb{N}$ that P(n) holds.

Base Case: Let n = 0. We want to prove that P(0) is true.

We know that $8^0 - 1 = 0$, and that $7 \mid 0$. So P(0) holds.

Inductive Step: Let $k \in \mathbb{N}$, and assume that P(k) is true. That is, we assume that $7 \mid 8^k - 1$; unpacking the definition of divisibility, this means there exists y_k such that $8^k - 1 = 7y_k$.

Now we want to show that P(k+1) holds:

$$7 \mid 8^{k+1} - 1$$
, or in other words, $\exists y_{k+1} \in \mathbb{Z}, \ 8^{k+1} - 1 = 7y_{k+1}$.

How do we find this y_{k+1} ? In order to prove P(k+1) using P(k), we have to extract the expression $8^{k}-1$ out of the expression $8^{k+1}-1$. Thus we will rewrite $8^{k+1} - 1$ as follows:

$$8^{k+1} - 1 = 8^{k+1} - 8 + 7 = 8(8^k - 1) + 7.$$

Next, we use the *induction hypothesis*, which says that $7y_k = 8^k - 1$:

$$8^{k+1} - 1 = 8(8^k - 1) + 7$$

= $8(7y_k) + 7$
= $7(8y_k + 1)$

So let $y_{k+1} = 8y_k + 1$. Then $8^{k+1} - 1 = 7y_{k+1}$, and so $7 \mid 8^{k+1} - 1$. This completes the proof of the inductive step and thus the proof.

Let's do another example, which is quite similar to the previous one, but is useful for practicing this new technique.

Example 3.3. Prove that for every natural number n, $n(n^2 + 5)$ is divisible by 6.

Proof. Let P(n) be the statement that $n(n^2 + 5)$ is divisible by 6.

Base Case: Let n = 0.

When n=0, the expression $n(n^2+5)=0(0^2+5)=0$. So it is divisible by 6 and thus P(0) holds.

Inductive Step: Let $k \in \mathbb{N}$, and assume P(k) is true. That is, we assume $k(k^2 + 5)$ is divisible by 6. We want to prove that P(k+1) holds; i.e., that (k+1)((k+1)) $(1)^2 + 5$) is divisible by 6.

⁴ You'll see us start to merge or omit the "translation" and "discussion" sections into the proof in this and future chapters, as you become more experienced with reading and writing proofs.

As in the previous example, in order to prove P(k+1) holds using the assumption that P(k) holds, we somehow need to extract the expression $k(k^2+5)$ out of the expression $(k+1)((k+1)^2+5)$. Some algebraic manipulations follow:

$$(k+1)((k+1)^2+5) = (k+1)(k^2+2k+6)$$

$$= (k+1)((k^2+5)+(2k+1))$$

$$= k(k^2+5)+k(2k+1)+(k^2+5)+(2k+1)$$

$$= k(k^2+5)+3k^2+3k+6$$

$$= k(k^2+5)+3k(k+1)+6$$

By the induction hypothesis, the first term on the right-hand side, $k(k^2+5)$, is divisible by 6. For the second term, since k and k+1 are consecutive natural numbers, one of them is even and thus k(k+1) is a multiple of 2 and thus 3k(k+1) is divisible 6. Using the statement from Exercise ??, since each term on the right-hand side is a multiple of 6, their sum is also a multiple of 6, which completes the inductive step.

Now let us go back to our motivating example and prove it using induction.

Example 3.4. Prove that for any $m, x, y \in \mathbb{N}$ and for any $n \in \mathbb{N}$ that if $x \equiv y \pmod{m}$, we have $x^n \equiv y^n \pmod{m}$.

Translation. Expressed in predicate logic:

$$\forall m, x, y \in \mathbb{N}, \ \forall n \in \mathbb{N}, \ x \equiv y \pmod{m} \Rightarrow x^n \equiv y^n \pmod{m}.$$

We have deliberately separated the three variables m, x, y from n, for a reason we'll discuss in next section.

Discussion. In the informal argument given at the start of the chapter, we first fixed values for m, x, y and then proved the claim when n = 2. Then for these same values of m, x, y we proved it for n = 3 and so on. In order to formalize this, we will want to first fix $m, x, y \in \mathbb{N}$ once and for all, and then prove the statement by induction on n.

Proof. Let $m, x, y \in \mathbb{N}$. Let P(n) be the predicate $x \equiv y \pmod{m} \Rightarrow x^n \equiv y^n \pmod{m}$. We want to prove that $\forall n \in \mathbb{N}, P(n)$ by induction.⁵

Base Case: Let n = 0.

To prove this, we simply observe that when n=0, the conclusion of the implication says that $x^0 \equiv y^0 \pmod{m}$, which is trivially true because both sides equal 1.6

Inductive Step: Let $k \in \mathbb{N}$, and assume that P(k) is true. That is, we assume that

$$x \equiv y \pmod{m} \Rightarrow x^k \equiv y^k \pmod{m}$$
.

From this assumption we want to prove that P(k+1) is true, i.e., that

$$x \equiv y \pmod{m} \Rightarrow x^{k+1} \equiv y^{k+1} \pmod{m}$$
.

⁵ Note that this predicate only makes sense after we have introduced m, x, and y.

⁶ We didn't even need the assumption that $x \equiv y \pmod{m}$!

Note that P(k+1) has the form of an implication, so we know how we should proceed: assume the hypothesis, i.e., that $x \equiv y \pmod{m}$. Using our assumption that P(k) is true, and that $x \equiv y \pmod{m}$, we can conclude that $x^k \equiv y^k$ \pmod{m} .

We know from a previous example that

$$x^k \equiv y^k \pmod{m} \land x \equiv y \pmod{m} \Rightarrow x \cdot x^k \equiv y \cdot y^k \pmod{m}$$
.

Since the left-hand side of this implication is true, the right hand side must also be true. Therefore $x^{k+1} \equiv y^{k+1} \pmod{m}$, and this completes the proof.

One interesting subtlety in how we set up this proof is in how we chose the order of the variables m, x, y, n being quantified. You know already that changing the order of these variables doesn't change the meaning of the statement, because they are all universally-quantified. However, changing their order does change the proof that we would write!

A different way to proceed in this proof would be to write the statement as

$$\forall n \in \mathbb{N}, \ \forall m, x, y \in \mathbb{N}, \ x \equiv y \pmod{m} \Rightarrow x^n \equiv y^n \pmod{m}.$$

Doing it this way, we would define P(n) to be the (more complex) statement

$$\forall m, x, y \in \mathbb{N}, \ x \equiv y \pmod{m} \Rightarrow x^n \equiv y^n \pmod{m}.$$

If we had proceeded this way, then the base case, P(0) of the induction would be prove the implication for all values of m, x, y when n = 0. So in the base case we would first fix particular but arbitrary values of $m, x, y \in \mathbb{N}$ before proceeding with the proof. And again in the inductive step, we would need to prove P(n) implies P(n+1), which is a more complicated statement since the other variables m, x, yare not fixed but are universally quantified. When we have a universal statement such as this one that involves one universally quantified variable that we want to do induction on (in this case n), plus other universally quantified variables that we do not need to do induction on (in this case m, x, y), it is usually easier to first fix m, x, y and then do induction on n, as we did above, rather than the other way around.7

We will do one more example from number theory. This example is proving an inequality rather than an equality, and demonstrates how to use induction with a different starting number as the base case.

Example 3.5. Prove that for all natural numbers n greater than or equal to 3, $2n+1 \le 2^n$.

Translation. We do the usual thing and express the "greater than or equal to 3" as a hypothesis in an implication.

$$\forall n \in \mathbb{N}, \ n \geq 3 \Rightarrow 2n+1 \leq 2^n$$
.

This statement doesn't have exactly the right form for the induction technique we've learned, but if we define the predicate

$$P(n): 2n+1 \le 2^n$$
, where $n \in \mathbb{N}$

then the statement becomes $\forall n \in \mathbb{N}, n \geq 3 \Rightarrow P(n)$, which is close.

⁷ Remember that we can reorder consecutive variables with the same quantification in a statement without changing the meaning.

Discussion. The principle of induction relies on two things: a base case, which gives us a starting point, and the inductive step, which allows us to build on the base case to conclude the truth of the predicate for larger and larger natural numbers.

The particular number for the base case turns out not to be so important: if we prove that P(3) is true as our base, then the inductive step still allows us to conclude that $P(4), P(5), \ldots$ are all true!

Proof. Let P(n) be the predicate $2n+1 \le 2^n$. We'll prove that $\forall n \in \mathbb{N}, n \ge 3 \Rightarrow P(n)$ using induction.

Base Case: Let n = 3.

Plugging in n=3 into the left and right sides of the inequality, we get $7 \le 8$, which is true

Inductive Step: Let $k \in \mathbb{N}$ and assume $k \geq 3$. Assume P(k) is true: $2k + 1 \leq 2^k$. We want to prove P(k+1) is true: $2(k+1) + 1 \leq 2^{k+1}$.

As usual, to obtain this inequality we start with the one we get from the induction hypothesis:

$$2k+1 \le 2^k$$
 $2k+1+2 \le 2^k+2^k$ (since $2 \le 2^k$) $2(k+1)+1 \le 2^{k+1}$

Exercise Break!

Use induction to prove each of the following statements.

- 3.1 For all $n \in \mathbb{N}$, $9^n 1$ is divisible by 8.8
- 3.2 For all $n \in \mathbb{N}$, $5^{2n} 1$ is divisible by 6.
- 3.3 For all $n \in \mathbb{N}$, $x^n y^n$ is divisible by x y.
- 3.4 For all $n \in \mathbb{N}$, if $n \geq 6$ then $5n + 5 \leq n^2$.
- 3.5 For all $n \in \mathbb{N}$, if $n \ge 1$ then $2^{2^n} 1$ is divisible by at least n distinct primes.

⁸ Note: the first two statements follow immediately from a previous exercise, but we encourage you to prove them "from scratch" for the practice.

Combinatorics

Combinatorics is an area of mathematics concerned with counting objects, and more generally with analyzing patterns. A pattern is most typically a sequence of numbers and we will often want to derive a closed-form expression for a_k , the k^{th} number in the sequence, or for $\sum_{i=0}^k a_i$, the sum of the first k+1 numbers in the sequence.

⁹ Drawing inspiration from programming, sequence indexing starts at 0, not 1.

Example 3.6. We will start with a famous example. Consider the following sequence of numbers:

$$0, 1, 1, 2, 3, 5, 8, 13, 21, 34, \dots$$

Call the k^{th} element in the sequence a_k . For each k, what is a_k ? It isn't too hard to see that we obtain a_k by summing together the two previous numbers. That is, for all $k \geq 2$, $a_k = a_{k-1} + a_{k-2}$. This is a very famous sequence called the Fibonacci sequence.

Example 3.7. Another easier example is an arithmetic sequence. Suppose you start with \$10, and every month you earn \$200. How much money do you have after kmonths? At the start you have \$10; after one month you have \$210 dollars; after two months you have \$410 dollars, etc. In general this gives rise to the sequence:

$$a_0 = 10, \ a_1 = 210, \ a_2 = 410, \ a_3 = 610, \ a_4 = 810, \ldots$$

In general, $a_k = 10 + 200 \cdot k$.

Example 3.8. Another kind of sequence is obtained by multiplying the current amount by a fixed value each time. Suppose that now you start with \$10, but now you invest your money in a very lucrative place so that every month your money doubles. This gives rise to the sequence:

$$a_0 = 10$$
, $a_1 = 20$, $a_2 = 40$, $a_3 = 80$, $a_4 = 160$,...

It is not hard to see that in general, $a_k = 10 \times 2^k$. This is called a geometric sequence.

Example 3.9. Finally, one more example. Let $n \in \mathbb{N}$. Suppose that we want to sum all natural numbers starting at 0, up to and including n. That is, $a_k =$ $0+1+2+\cdots+k$. This gives rise to the infinite sequence:

$$a_0 = 0$$
, $a_1 = 1$, $a_2 = 3$, $a_3 = 6$, $a_4 = 10$, $a_5 = 15$,...

It turns out that we have the following closed-form expression for a_n : $a_n =$ $n \times (n+1)/2$.

Closed-form formulas, with proof!

In general, a sequence is an ordered list of numbers given by the outputs of a function $f: \mathbb{N} \to \mathbb{R}$, where $a_0 = f(0)$, $a_1 = f(1)$, etc. The sequences we will study are infinite: there is one term a_k for each natural number k. We call the function f an explicit or closed-form expression/formula for the sequence if f involves a fixed number of elementary operations 10. For example, the following is a closed-form expression for the Fibonacci sequence, known as Binet's formula:

$$a_n = \frac{(1+\sqrt{5})^n - (1-\sqrt{5})^n}{2^n\sqrt{5}}.$$

Nice sequences will have explicit formulas, but there are also examples of sequences that are complex and that do not have an explicit formula. We can often use induction in order to prove that a particular explicit formula computes the terms in a sequence. Let's see some examples of this.

¹⁰ Reasonable people may differ on whether a given operation is elementary. Ask when in doubt.

Translation. This statement can be translated as

$$\forall n \in \mathbb{N}, \ \sum_{j=1}^{n} j = n(n+1)/2.$$

Proof. Let P(n) be the statement $\sum_{j=1}^{n} j = n(n+1)/2$.

Base Case: Let n = 0.

In this case, the left side is the empty sum (which has value 0), and the right side is 0(0+1)/2=0.

Inductive Step: Let $k \in \mathbb{N}$ and assume that P(k) is true, i.e., that $\sum_{j=1}^{k} j = k(k+1)/2$. It is helpful to write down what we want to prove, which is P(k+1):

$$P(k+1): \sum_{j=1}^{k+1} j = \frac{(k+1)(k+2)}{2}.$$

Now we have:

$$\begin{split} \sum_{j=1}^{k+1} j &= \sum_{j=1}^{k} j + (k+1) \\ &= \frac{k(k+1)}{2} + (k+1) \\ &= \frac{k(k+1) + 2(k+1)}{2} \\ &= \frac{(k+1)(k+2)}{2} \end{split}$$
 (by induction hypothesis)

Strengthening the hypothesis

Example 3.11. Prove that the sum of the first n odd numbers is a perfect square.

Translation. This translates to the mathematical statement

$$orall n \in \mathbb{N}, \; \exists x \in \mathbb{N}, \; \sum_{i=0}^{n-1} (2i+1) = x^2.$$

Discussion. We will try to prove this by induction on n. Let P(n) be the statement that the sum of the first n odd numbers is a perfect square: $\exists x \in \mathbb{N} \sum_{i=0}^{n-1} (2i+1) = x^2$.

For the inductive step, we will assume P(k) and try to prove P(k+1):

$$\exists x_{k+1} \in \mathbb{N}, \ \sum_{i=0}^{(k+1)-1} (2i+1) = x_{k+1}^2.$$

From the inductive hypothesis we know that the sum of the first k terms in the above sum is a perfect square. But how can we use that to deduce that when we add the last term, 2k+1, to this perfect square that we will get yet another perfect square? We're stuck: our induction hypothesis is not enough to help us prove P(k+1).

Let's look at some examples and try to learn more. When n=1, the sum of just this one odd number is a perfect square, 1^2 . For n=2 we have $1+3=4=2^2$. For n=3 we have $1+3+5=9=3^2$. Now we start to see a pattern and we will conjecture that the sum of the first n odd numbers is equal to n^2 . We will try to prove this stronger statement instead!

Proof. Let P(n) be the predicate $\sum_{i=0}^{n-1} (2i+1) = n^2$. We will prove that $\forall n \in$ \mathbb{N} , P(n) by induction on n.

Base Case: Let n = 0.

In this case we have $\sum_{i=0}^{-1} (2i+1) = 0$ (since this is an empty sum), so P(0) is true.

Inductive Step: let $k \in \mathbb{N}$, and assume that P(k) holds. We want to prove P(k+1). From the induction hypothesis we now know that not only is the sum of the first k odd numbers a perfect square, but it is equal to k^2 . So then:

$$\sum_{i=0}^{k} (2i+1) = \sum_{i=0}^{k-1} (2i+1) + (2k+1)$$

$$= k^2 + (2k+1)$$
 (by induction hypothesis)
$$= (k+1)^2$$

Going beyond numbers

This next example is somewhat different in that we will want to prove something about objects that are not simply numbers.

Example 3.12. Prove that for every finite set S, $|\mathcal{P}(S)| = 2^{|S|}$, using induction. ¹¹

Translation. It may not be obvious how induction fits into this example, given that we are looking to prove something about sets, not natural numbers. There is, however, a nice approach we can take: perform induction using a variable representing the size of the set (note that the size of a finite set is always a natural number). 12

Our predicate is the following, defined for $n \in \mathbb{N}$:

$$P(n)$$
: every set S of size n satisfies $|\mathcal{P}(S)| = 2^n$

The original statement is then equivalent to $\forall n \in \mathbb{N}, P(n)$, and we can use induction!

Proof. Base case: let n = 0.

¹¹ Recall that $\mathcal{P}(S)$ is the power set of S, the set of all subsets of S. This statement is saying that if S has n elements, then it has exactly 2^n subsets.

¹² We say that we're performing induction on the size of the set.

In this case, there is only one set of size 0: S must be the empty set. The only subset of the empty set is the empty set itself, so $\mathcal{P}(S) = \{\emptyset\}$ (size 1), and $2^0 = 1$.

Inductive Step: Now let $k \in \mathbb{N}$ and assume that P(k) holds. We want to prove P(k+1). Note that the predicate P(k+1) is really a universally-quantified statement ("every set S") with a condition ("of size k+1"), so we can unwrap it a little more. Let S be a set, and assume S has size k+1. Let the elements of S be denoted by s_1,\ldots,s_{k+1} . We want to prove that the number of subsets of S is 2^{k+1} .

First, consider all subsets of S that do not contain the last element, s_{k+1} ; in other words, the subsets of $\{s_1, \ldots, s_k\}$. By the induction hypothesis, the number of such subsets is exactly 2^k .

Now consider all subsets of S that contain s_{k+1} . Again, the number of subsets of S that contain s_{k+1} is 2^k , since we can obtain these subsets by taking all 2^k subsets of $\{s_1, \ldots, s_k\}$, and adding s_{k+1} to each subset.

Thus in total there are $2^k + 2^k = 2^{k+1}$ subsets of S.

Here's another example: the size of a set obtained as the Cartesian product of two finite sets. Try to prove it as an exercise; note that while there are two natural number variables here (n and m), you only need to do induction on one of them (and you can pick).

Example 3.13. Prove that for all $n, m \in \mathbb{N}$, and for all sets A and B of size n and m, respectively, $|A \times B| = n \cdot m$.

Exercise Break!

- 3.6 Prove that for all natural numbers n, $\sum_{i=1}^{n} \frac{1}{i(i+1)} = \frac{n}{n+1}$.
- 3.7 Prove that for all natural numbers n, $\sum_{k=1}^{n} 4 \cdot 5^{k-1} = 5^n 1$.
- 3.8 (Handshake Theorem). Let $n \in \mathbb{N}$, and assume $n \geq 1$. Suppose you are at a party and n people (including yourself). At the end of the party, define a person's parity as Odd if they have shaken hands with an odd number of people, and Even if they have shaken hands with an even number of people. Prove that the number of people of odd parity must be even.

Incorrect proofs by induction

Just as it is important to be able to formulate a correct proof by induction, it is equally important to not be fooled by an incorrect proof! Consider this well-known example. Say we want to prove that all jellybeans have the same colour. Let P(n) be the statement that any set of n jellybeans all have the same colour. The base case is when there is only one jellybean, and it has one colour, so the statement P(1) is true.

Now let's assume that P(k) is true and try to prove that P(k+1) is true. Let $S = \{j_1, j_2, \dots, j_{k+1}\}$ be a set of (k+1) jellybeans. Consider the first k jellybeans in S: $S_1 = \{j_1, \dots, j_k\}$. By the induction hypothesis, they all must have the same colour. Now consider the last k jellybeans in S: $S_2 = \{j_2, \dots, j_{k+1}\}$. Again by the induction hypothesis, they must also have the same colour. Now since these two sets overlap, the two colours must be the same, thus the entire set j_1, \ldots, j_{k+1} of jellybeans has the same colour and we can conclude P(k+1).

We know that it is clearly wrong, so where exactly is the mistake? To find the error it is helpful to walk through the smallest possible counterexample—say for instance we have two jellybeans, where the first one is red and the second one is yellow. In this case we can see the mistake since the two sets S_1 and S_2 do not overlap.

Looking ahead: strong induction (optional)

The way that we expressed the induction principle above was to prove the base case P(0), and then give a general argument for P(n+1) assuming P(n). We said intuitively that this works by the domino effect: (1) Suppose we know that the first domino P(0) is down, and (2) we know that as long as P(n) is down, then so is P(n+1), then this implies (3) that all of the dominoes are down. However, we could have replaced (2) by (2') which states that as long as all of the first n dominoes are down, $P(0), \ldots, P(n)$, then so is P(n+1). As long as we know (1) and (2'), this still implies (3). Note that proving (2') rather than (2) may be easier since we can assume not only that P(n) is true, but that all of $P(0), P(1), \ldots, P(n)$ are true, in order to deduce that P(n+1) is true.

This is called the principle of strong induction. It turns out that strong induction and simple induction (the form we've been using in this chapter) are equivalent, but sometimes it can be easier to prove a statement using strong induction rather than simple induction. More formally, suppose that we want to prove $\forall n \in \mathbb{N}, n \geq n$ $k \Rightarrow P(n)$, where k is some natural number. The principle of strong induction can be used to prove this statement as follows.

- First, prove the base case P(k).
- Secondly, prove that for any fixed but arbitrary $n \geq k$, P(j) for all $j, k \leq j \leq n$ implies P(n+1).

Then we can conclude $\forall n \in \mathbb{N}, n \geq k \Rightarrow P(n)$. You will learn more about strong induction in CSC236/240.

Example 3.14. Prove that every integer n that is greater than or equal to 2 can be expressed as a product of one or more prime numbers.

Proof. Let P(n) be the statement that n can be expressed as a product of one or more prime numbers. The base case is when n=2. Since 2 is prime, 2 can be expressed as a product of one prime number (itself), and thus P(2) is true.

For the inductive step, let n be an integer, $n \geq 2$. And assume that for every integer j, $2 \le j \le n$, that j can be expressed as a product of one or more prime numbers. Now we want to prove P(n+1), that n+1 can also be expressed as a product of prime numbers. There are two cases. Either the integer n+1 is itself a prime number or it is not. If it is a prime number, then it is a product of one prime number (itself), and this case is complete. 13

The second case is when n+1 is not a prime number, and thus $n+1=a\cdot b$, where both a and b are positive integers that are both different from n+1 and 1. Since $2 \le a \le n$, and $2 \le b \le n$, by the induction hypothesis, both a and b can be written as the product of prime numbers, and thus $a \cdot b$ can also be written as the product of prime numbers and the proof is complete!

13 Note that we don't even need the induction hypothesis in this case!

Note that in this last example, it would have been futile to try to use simple induction since then we would only know that n is a product of prime numbers, which is useless in order to show that n+1 is the product of prime numbers.¹⁴

 14 After all, when $n \geq 2$, we know that n is not a factor of n+1.

4 Representations of Natural Numbers

An important issue in computing is our choice of representation for the objects that we wish to study. In particular, how to represent various types of numbers (natural numbers, rational numbers, real numbers) as well as other objects such as graphs. You are all familiar with the decimal (base 10) system for numbers. For example, to represent the positive integer three-hundred and twenty-four in its decimal form we would write "324". This is shorthand for $3 \times 10^2 + 2 \times 10^1 + 4 \times 10^0$. We know it is a decimal form because powers of 10 are used in the expression. You are probably so used to this representation that you don't even think about it anymore. But let's review the basic properties of decimal notation so that we set the standard for other representations that will be important.

Decimal representation of natural numbers

When you read a number such as "324" in decimal, you see a sequence of decimal digits, $d_{k-1}d_{k-2}\dots d_1d_0$, where each digit d_i is in $\{0,1,2,\dots,9\}$. The number that corresponds to this sequence of digits is $\sum_{i=0}^{k-1} d_i \times 10^i$. In words, the rightmost digit is multiplied by 10^0 , the next digit to the left is multiplied by 10^1 , and so on. Each digit to the left has a multiplier that is 10 times the multiplier of the previous digit. In our example "324", we have $d_2=3$, $d_1=2$, and $d_0=4$, and so the value is $3\times 10^2+2\times 10^1+4\times 10^0$.

Here are some useful properties of decimal representation:

- 1. To multiply a number by 10, you can just insert a 0 at the right end of its decimal form. That is, if a number n is represented by $d_{k-1}d_{k-2}\dots d_1d_0$, then the representation of $10\times n$ is $d_{k-1}d_{k-2}\dots d_1d_00$. For example, 10×324 is represented as 3240.
- 2. With the k decimal digit positions, exactly 10^k unique numbers (from 0 to $10^k 1$) can be represented. For example, using three decimal digits (k = 3), we can represent the numbers 0 through 999.

Binary representation of natural numbers

The binary (base 2) representation of a number uses the binary digits $\{0, 1\}$ instead of the ten decimal digits $\{0, 1, 2, \dots, 9\}$ We write numbers in binary in the same sort of way that we write numbers in our traditional base 10 system. Again we represent a number by a sequence of binary digits, $d_{k-1}d_{k-2}\dots d_1d_0$, but now

each digit d_i is 0 or 1. The value of the number corresponding to this sequence is: $\sum_{i=0}^{k-1} d_i \times 2^i$. Note that the *only* change in the expression is the change from powers of 10 to powers of 2. The number represented in its decimal form as 139 would represented in binary as: $1 \times 2^7 + 1 \times 2^3 + 1 \times 2^1 + 1 \times 2^0 = 10001011$. In the sum, the terms multiplied by the digit 0 were omitted. The rightmost digit is multiplied by $2^0 = 1$, the next to the left is multiplied by $2^1 = 2$, and so on. Each digit to the left has a multiplier that is 2 times the previous digit. The above properties about decimal representation continue to hold, but now the 10's are replaced by the new base, 2. Finally, we note that when discussing the binary representation of a number, the digits d_i are often called *bits*. To the right are some examples of numbers together in their decimal and binary representation.

Converting from binary to decimal

It is really easy to convert a number from its binary representation to its decimal representation. We express the number as a sum, expand out the powers in decimal, and add up using familiar decimal arithmetic. For example:

$$100101 = 1 \times 2^5 + 0 \times 2^4 + 0 \times 2^3 + 1 \times 2^2 + 0 \times 2^1 + 1 \times 2^0 = 32 + 0 + 0 + 4 + 0 + 1 = 37.$$

The binary expression 100101 and the decimal expression 37 are two ways for representing the same number.

Converting from decimal to binary

Here is a process for converting from the decimal representation of a number to its binary representation. Consider the decimal number 37. We start by finding the largest power of 2 that is less than or equal to 37. In this case it is 2^5 , since $2^5 = 32$ and $2^5 \le 37$, while $2^6 = 64$ and $2^6 \not \le 37$. We can then write $37 = 1 \times 2^5 + 5$. Now apply the same process with the unconverted remainder, the decimal number 5. The largest power of 2 that is less than or equal to 5 is 2^2 , so we get $5 = 2^2 + 1$. Continuing, the largest power of 2 that is less than or equal to 1 is 2^0 . We get $1 = 2^0 + 0$. With a remainder of 0, there is nothing left to convert. Now we collect everything together to get:

$$37 = (1 \times 2^5) + (0 \times 2^4) + (0 \times 2^3) + (1 \times 2^2) + (0 \times 2^1) + (1 \times 2^0) = 100101.$$

Properties of binary representation

Our first theorem shows that every natural number has a binary representation. We label the digits b_i since the base is 2, which makes the digits bits.

Theorem 4.1. For every natural number n, there exists $p \in \mathbb{N}$ and bits $b_p, \ldots, b_0 \in \{0, 1\}$ such that $n = \sum_{i=0}^{p} b_i 2^i$.

Proof. Rather than proving the statement as written, we will prove an equivalent statement that is more amenable to using our technique of induction from the previous chapter:¹

$$orall m \in \mathbb{N}, \ \left(orall n \in \mathbb{N}, \ n \leq m \Rightarrow \left(\exists p \in \mathbb{N}, \ \exists b_0, b_1, \ldots, b_p \in \{0,1\}, \ n = \sum_{i=0}^p b_i 2^i
ight)
ight)$$

Decimal	Binary
1	1
2	10
3	11
4	100
5	101
6	110
7	111
8	1000
9	1001
10	1010
11	1011
12	1100
13	1101
14	1110
15	1111
16	10000
17	10001
18	10010
19	10011
20	10100

¹ An English way of interpreting this statement is that "for all $m \in \mathbb{N}$, every number less than or equal to m has a binary representation.

We define the predicate P(m) to be the part after the $\forall m \in \mathbb{N}$, which can be translated as "every natural number less than or equal to m has a binary representation." We'll prove by induction on m that $\forall m \in \mathbb{N}, P(m)$.

Base case: Let m = 0.

Let $n \in \mathbb{N}$ and assume that $n \leq m$. There is only one possible number, namely n = 0, to consider. Let p = 0 and $b_0 = 0$. Then $0 = \sum_{i=0}^{p} b_i 2^i = 0 \times 2^0 = 0$.

Inductive step. Let $m \in \mathbb{N}$, and assume that P(m) is true, i.e., that every natural number less than or equal to m has a binary representation. We want to prove that P(m+1) is true.

Let $n \in \mathbb{N}$ and assume that n < m+1. If n < m, then by the induction hypothesis n has a binary representation. So we'll further assume that n = m + 1for the rest of this proof.²

We'll divide up the rest of the proof into two cases, depending on whether n is even or odd.

Case 1: Assume n is even, i.e., there exists $k \in \mathbb{N}$ such that n = 2k.

By one of our earlier properties of divisibility, we know that since $k \mid n, k < n$. Therefore by the induction hypothesis there exists $p \in \mathbb{N}$ and $b_p, \ldots, b_0 \in \{0, 1\}$ such that $k=\sum_{i=0}^p b_i 2^i$. Then $n=2\sum_{i=0}^p b_i 2^i=\sum_{i=0}^p b_i 2^{i+1}$.

Let p'=p+1, and let $b_0'=0$, and for all $i\in\{1,2,\ldots,p+1\}$, let $b_i'=b_{i-1}$. Then $n = \sum_{i=0}^{p'} b_i' 2^i.$

Case 2: Assume n is odd, i.e., there exists $k \in \mathbb{N}$ such that n = 2k + 1.

Similar to the previous case, by the induction hypothesis, there exists $p \in \mathbb{N}$ and $b_p,\ldots,b_0\in\{0,1\}$ such that $k=\sum_{i=0}^pb_i2^i$. Then $n=2\left(\sum_{i=0}^pb_i2^i\right)+1=$ $\left(\sum_{i=0}^p b_i 2^{i+1}\right) + 1.$

Let p'=p+1 and let $b_0'=1$, and for all $i\in\{1,2,\ldots,p+1\}$, let $b_i'=b_{i-1}$. Then $n = \sum_{i=0}^{p'} b'_i 2^i$.

One troubling issue with the representations that result from the statement of the previous theorem is that they are not unique.³ For example, the decimal number 14 can be represented in binary as 1110, but it can also be represented as 01110, 001110, 0001110 and so on. Computer scientists hate to have multiple ways to represent a particular entity, since each different representation can lead to a case to check. We want a rule that forces us to say which of those representations for 14 is the agreed upon unique representation. How can we choose? One way is to say that we want the one that does not have the uninformative leading 0's.

Theorem 4.2. For every number $n \in \mathbb{Z}^+$, there exist unique values $p \in \mathbb{N}$ and $b_p, \ldots, b_0 \in \{0, 1\}$ such that both of the following hold:

² Essentially, we're doing a proof by cases here, but one of the cases (n < m) is so simple that we're not writing full headers, because we'll use cases later on as well.

^{1.} $n = \sum_{i=0}^{p} b_i 2^i$ (i.e., this is a binary representation of n)

^{2.} $b_p = 1$ (this representation has no leading zeroes)

³ Remember that the existential quantifier says that at least one value of the domain satisfies a given property; not that exactly one does.

Dividing by two

Lemma 4.3. Let $n \in \mathbb{N}$, and assume $n \geq 2$. Let the binary representation of n be $b_p b_{p-1} \dots b_0$, where $b_p = 1$ (so no leading zeroes). Then the binary representation of $\lfloor n/2 \rfloor$ is $b_p b_{p-1} \dots b_1$ (i.e., the binary representation of n with the rightmost digit removed).

Proof. Let $n \in N$, and assume $n \geq 2$. Let $p \in \mathbb{N}$ and $b_0, b_1, \ldots, b_p \in \{0, 1\}$ be such that $n = \sum_{i=0}^p b_i 2^i$ and $b_p = 1$. We divide the proof into two cases, based on whether n is even or odd.

Case 1: Assume n is even. In this case, $b_0 = 0$, and thus

$$\left\lfloor \frac{n}{2} \right\rfloor = \frac{n}{2} \\
 = \frac{\sum_{i=0}^{p} b_i 2^i}{2} \\
 = \frac{\sum_{i=1}^{p} b_i 2^i}{2} \qquad \text{(since } b_0 = 0\text{)} \\
 = \sum_{i=1}^{p} b_i 2^{i-1} \\
 = \sum_{i=0}^{p-1} b_{i+1} 2^i$$

Case 2: Assume n is odd. In this case, $b_0 = 1$, and $\lfloor n/2 \rfloor = (n-1)/2$, and so:

$$\left\lfloor \frac{n}{2} \right\rfloor = \frac{n-1}{2} \\
 = \frac{\left(\sum_{i=0}^{p} b_{i} 2^{i}\right) - 1}{2} \\
 = \frac{\left(\sum_{i=1}^{p} b_{i} 2^{i}\right) + 1 \cdot 2^{0} - 1}{2} \\
 = \frac{\sum_{i=1}^{p} b_{i} 2^{i}}{2} \\
 = \sum_{i=1}^{p} b_{i} 2^{i-1} \\
 = \sum_{i=0}^{p-1} b_{i+1} 2^{i}$$
 (since $b_{0} = 1$)

Exercise Break!

- 4.1 In the proof of the Lemma on dividing by two, why did we need the restriction that n > 2? Where does the proof go wrong if n = 0 or n = 1?
- 4.2 Prove that for every n, the binary representation of n+1 contains exactly one bit that flips from 0 to 1. For example, n=7 in binary is 0111, and n=8 is

- 1000, and thus only one digit, d_3 flips from 0 to 1. Similarly going from 8 to 9, involves one bit flip, this time d_0 .
- 4.3 Our discussion in this chapter has been restricted to base 2 and base 10 representations. Which other integer bases are possible? Can you generalize (with proof) the previous theorems to other bases?

5 Analyzing Algorithm Running Time

When we first begin writing programs, we are mainly concerned with their correctness: do they work the way they're supposed to? As our programs get larger and more complex, we add in a second consideration: are they designed and documented clearly enough so that another person can read the code and make sense of what's going on? These two properties—correctness and design—are fundamental to writing good software. However, when designing software that is meant to be used on a large scale or that reacts instantaneously to a rapidly-changing environment, there is a third consideration which must be taken into account when evaluating programs: the amount of time the program takes to run.

In this chapter, you will learn how to formally analyze the running time of an algorithm, and explain what factors do and do not matter when performing this analysis. You will learn the notation used by computer scientists to represent running time, and distinguish between best-, worst-, and average-case algorithm running times.

A motivating example

Consider the following function, which prints out all the items in a list:

```
def print_items(lst: list) -> None:
    for item in lst:
        print(item)
```

What can we say about the running time of this function? An empirical approach would be to measure the time it takes for this function to run on a bunch of different inputs, and then take the average of these times to come up with some sort of estimate of the "average" running time.

But of course, given that this algorithm performs an action for every item in the input list, we expect it to take longer on longer lists, so taking an average of a bunch of running times loses important information about the inputs.¹

How about choosing one particular input, calling the function multiple times on that input, and averaging those running times? This seems better, but even here there are some problems. For one, the computer's hardware can affect running time; for another, computers all are running multiple programs at the same time, so what else is currently running on your computer also affects running time. So even running this experiment on one computer wouldn't necessarily be indicative of how long the function would take on a different computer, nor even how long it would take on the same computer running a different number of other programs.

¹ This is like doing a random poll of how many birthday cakes people have eaten without taking into account how old the respondents are.

While these sorts of timing experiments are actually done in practice for evaluating particular hardware or extremely low-level (close to hardware) programs, these details are often not helpful for the average software developer. After all, most software developers do not have control over the machine on which their software will be run.

So rather than use an empirical measurement of runtime, what we do instead is use an abstract representation of runtime: the number of "basic operations" an algorithm executes. However, there is a good reason "basic operation" is in quotation marks—this vague term raises a whole slew of questions:

- What counts as a "basic operation"?
- How do we tell which "basic operations" are used by an algorithm?
- Do all "basic operations" take the same amount of time?

The answers to these questions can depend on the hardware being used, as well as what programming language the algorithm is written in. Of course, these are precisely the details we wish to avoid thinking about.

For example, suppose we analyzed the running time of the print_items function, counting only the print calls as basic operations. Then for a list of length n, there are n print calls, so we would say that the running time of print_items on a list of length n is n basic operations.

But then a friend comes along, and says "No wait, the variable item must be assigned a new value of the list at every loop iteration, and that counts as a basic operation." Okay, so then we would say that there are n print calls and nassignments to item, for a total running time of 2n basic operations for an input list of length n.

But then another friend chimes in, saying "But print calls take longer than variable assignments, since they need to change pixels on your monitor, so you should count each print call as 10 basic operations." Okay, so then there are n print calls worth 10n basic operations, plus the assignments to item, for a total of 11n basic operations for an input list of length n.

And then another friend joins in: "But you need to factor in an overhead of calling the function as a first step before the body executes, which counts as 1.5 basic operations (slower than assignment, faster than print)." So then we now have a running time of 11n + 1.5 basic operations for an input list of length n.

And then another friend starts to speak, but you cut them off and say "That's it! This is getting way too complicated. I'm going back to timing experiments, which may be inaccurate but at least I won't have to listen to these increasing levels of fussiness."

The expressions n, 2n, 11n, and 11n + 1.5 may be different mathematically, but they share a common qualitative type of growth: they are all lines, i.e., grow linearly with respect to n. What we will study in the next section is how to make this observation precise, and thus avoid the tedium of trying to exactly quantify our "basic operations," and instead measure the overall rate of growth in the number of operations.

Asymptotic growth

Here is a quick reminder about function notation. When we write $f: A \to B$, we say that f is a function which maps elements of A to elements of B. In this chapter, we will mainly be concerned about functions mapping the natural numbers to the nonnegative real numbers, i.e., functions $f: \mathbb{N} \to \mathbb{R}^{\geq 0}$. Though there are many different properties of functions that mathematicians study, we are only going to look at one such property: describing the long-term (asymptotic) growth of a function. We will proceed by building up a few different definitions of comparing function growth, which will eventually lead into one which is robust enough to be used in practice.

Definition 5.1. Let $f,g:\mathbb{N}\to\mathbb{R}^{\geq 0}.$ We say that g is absolutely dominated by f if and only if for all $n \in \mathbb{N}$, $g(n) \leq f(n)$.

Example 5.1. Let $f(n) = n^2$ and g(n) = n. Prove that g is absolutely dominated by f.

Translation. This is a straightforward unpacking of a definition, which you should be very comfortable with by now: $\forall n \in \mathbb{N}, g(n) < f(n)$.

Proof. Let $n \in \mathbb{N}$. We want to show that $n \leq n^2$.

Case 1: Assume n = 0. In this case, $n^2 = n = 0$, so the inequality holds.

Case 2: Assume $n \geq 1$. In this case, we take the inequality $n \geq 1$ and multiply both sides by n to get $n^2 \ge n$, or equivalently $n \le n^2$.

Unfortunately, absolute dominance is too strict for our purposes: if $g(n) \leq f(n)$ for every natural number except 5, then we can't say that q is absolutely dominated by f. For example, the function g(n) = 2n is not absolutely dominated by $f(n) = n^2$, even though $g(n) \leq f(n)$ everywhere except n = 1. Here is another definition which is a bit more flexible than absolute dominance.

Definition 5.2. Let $f,g:\mathbb{N}\to\mathbb{R}^{\geq 0}$. We say that g is dominated by f up to a constant factor if and only if there exists a positive real number c such that for all $n \in \mathbb{N}$, $g(n) \leq c \cdot f(n)$.

Example 5.2. Let $f(n) = n^2$ and g(n) = 2n. Prove that g is dominated by f up to a constant factor.

Translation. Once again, the translation is a simple unpacking of the previous definition:4

$$\exists c \in \mathbb{R}^+, \ \forall n \in \mathbb{N}, \ q(n) < c \cdot f(n).$$

Discussion. The term "constant factor" is revealing. We already saw that n is absolutely dominated by n^2 , so if the n is multiplied by 2, then we should be able to multiply n^2 by 2 as well to get the calculation to work out.

Proof. Let c=2, and let $n\in\mathbb{N}$. We want to prove that $g(n)\leq c\cdot f(n)$, or in other words, $2n < 2n^2$.

² These are the domain and range which arise in algorithm analysis—an algorithm can't take "negative" time to run, after all.

³ Note that we aren't quantifying over f and g; the "let" in the example defines concrete functions that we want to prove something about.

⁴ Remember: the order of quantifiers matters! The choice of c is notallowed to depend on n.

Case 1: Assume n = 0. In this case, 2n = 0 and $2n^2 = 0$, so the inequality holds.

Case 2: Assume $n \ge 1$. Taking the assumed inequality $n \ge 1$ and multiplying both sides by 2n yields $2n^2 \ge 2n$, or equivalently $2n \le 2n^2$.

Intuitively, "dominated by up to a constant factor" allows us to ignore multiplicative constants in our functions. This will be very useful in our running time analysis because it frees us from worrying about the exact constants used to represent numbers of basic operations: n, 2n, and 11n are all equivalent in the sense that each one dominates the other two up to a constant factor.

However, this second definition is still a little too restrictive, as the inequality must hold for every value of n. Consider the functions $f(n) = n^2$ and g(n) = n + 90. No matter how much we scale up f by multiplying it by a constant, f(0) will always be less than g(0), so we cannot say that g is dominated by f up to a constant factor. And again this is silly: it is certainly possible to find a constant c such that $g(n) \le cf(n)$ for every value except n = 0. So we want some way of omitting the value n = 0 from consideration; this is precisely what our third definition gives us.

Definition 5.3. Let $f,g: \mathbb{N} \to \mathbb{R}^{\geq 0}$. We say that g is eventually dominated by f if and only if there exists $n_0 \in \mathbb{R}^+$ such that $\forall n \in \mathbb{N}$, if $n \geq n_0$ then $g(n) \leq f(n)$.

Example 5.3. Let $f(n) = n^2$ and g(n) = n + 90. Prove that g is eventually dominated by f.

Translation.

$$\exists n_0 \in \mathbb{R}^+, \ \forall n \in \mathbb{N}, \ n > n_0 \Rightarrow q(n) < f(n).$$

Discussion. Okay, so rather than finding a constant to scale up f, we need to argue that for "large enough" values of n, $n+90 \le n^2$. How do we know that value of n is "large enough?"

Since this is a quadratic inequality, it is actually possible to solve it directly using factoring or the quadratic formula. But that's not really the point of this example, so instead we'll take advantage of the fact that we get to choose the value of n_0 to pick one which is large enough.

Proof. Let $n_0 = 90$, let $n \in \mathbb{N}$, and assume $n \ge n_0$. We want to prove that $n + 90 \le n^2$.

We will start with the left-hand side and obtain a chain of inequalities that lead to the right-hand side.

$$n + 90 \le n + n$$
 (since $n \ge 90$)
 $= 2n$
 $\le n \cdot n$ (since $n \ge 2$)
 $= n^2$

Intuitively, this definition allows us to ignore "small" values of n and focus on the long term, or asymptotic, behaviour of the function. This is particularly important

for ignoring the influence of slow-growing terms in a function, which may affect the function values for "small" n, but eventually are overshadowed by the fastergrowing terms. In the above example, we knew that n^2 grows faster than n, but because an extra +90 was added to the latter function, it took a while for the faster growth rate of n^2 to "catch up" to n + 90.

Our final definition combines both of the previous ones, enabling us to ignore both constant factors and small values of n when comparing functions.

Definition 5.4. Let $f,g:\mathbb{N}\to\mathbb{R}^{\geq 0}$. We say that g is eventually dominated by f up to a constant factor if and only if there exist $c, n_0 \in \mathbb{R}^+$, such that for all $n \in \mathbb{N}$, if $n \geq n_0$ then $g(n) \leq c \cdot f(n)$.

In this case, we also say that g is Big-Oh of f, and write $g \in \mathcal{O}(f)$.

We use $\in \mathcal{O}(f)$ here because formally, we define $\mathcal{O}(f)$ to be the set of functions that are eventually dominated by f up to a constant factor:

$$\mathcal{O}(f) = \{g \mid g : \mathbb{N} \to \mathbb{R}^{\geq 0}, \ \exists c, n_0 \in \mathbb{R}^+, \ \forall n \in \mathbb{N}, \ n \geq n_0 \Rightarrow g(n) \leq c \cdot f(n) \}.$$

Example 5.4. Let $f(n) = n^3$ and $g(n) = n^3 + 100n + 5000$. Prove that $g \in \mathcal{O}(f)$.

Translation.

$$\exists c, n_0 \in \mathbb{R}^+, \ \forall n \in \mathbb{N}, \ n \geq n_0 \Rightarrow n^3 + 100n + 5000 \leq cn^3.$$

Discussion. It's worth pointing out that in this case, g is neither eventually dominated by f nor dominated by f up to a constant factor. So we'll really need to make use of both constants c and n_0 . They're both existentially-quantified, so we have a lot of freedom in how to choose them!

Here's an idea: let's split up the inequality $n^3 + 100n + 5000 < cn^3$ into three simpler ones:

$$n^3 \le c_1 n^3$$
 $100n \le c_2 n^3$
 $5000 < c_3 n^3$

If we can make these three inequalities true, adding them together will give us our desired result (setting $c = c_1 + c_2 + c_3$). Each of these inequalities is simple enough that we can "solve" them by inspection. Moreover, because we have freedom in how we choose n_0 and c, there are many different ways to satisfy these inequalities! To illustrate this, we'll look at two different approaches here.

Approach 1: focus on choosing n_0 .

It turns out we can satisfy the three inequalities even if $c_1 = c_2 = c_3 = 1$:

- $n^3 \le n^3$ is always true (so for all n > 0).
- $100n < n^3$ when n > 10.
- $5000 \le n^3$ when $n \ge \sqrt[3]{5000} \approx 17.1$

We can pick n_0 to be the largest of the lower bounds on n, $\sqrt[3]{5000}$, and then these three inequalities will be satisfied!

⁵ Or in other words, $n^3 + 100n +$ $5000 \in \mathcal{O}(n^3)$.

⁶ Exercise: prove this!

Approach 2: focus on choosing c.

Another approach is to pick c_1 , c_2 , and c_3 to make the right-hand sides large enough to satisfy the inequalities.

- $n^3 \le c_1 n^3$ when $c_1 = 1$.
- $100n \le c_2 n^3$ when $c_2 = 100$.
- $5000 \le c_3 n^3$ when $c_3 = 5000$, as long as $n \ge 1$.

Proof. (Using Approach 1) Let c=3 and $n_0=\sqrt[3]{5000}$. Let $n\in\mathbb{N}$, and assume that $n\geq n_0$. We want to show that $n^3+100n+5000\leq cn^3$.

First, we prove three simpler inequalities:

- $n^3 \le n^3$ (since the two quantities are equal).
- Since $n \ge n_0 \ge 10$, we know that $n^2 \ge 100$, and so $n^3 \ge 100n$.
- Since $n \ge n_0$, we know that $n^3 \ge n_0^3 = 5000$.

Adding these three inequalities gives us:

$$n^3 + 100n + 5000 \le n^3 + n^3 + n^3 = cn^3$$
.

Proof. (Using Approach 2) Let c = 5101 and $n_0 = 1$. Let $n \in \mathbb{N}$, and assume that $n \ge n_0$. We want to show that $n^3 + 100n + 5000 \le cn^3$.

First, we prove three simpler inequalities:

- $n^3 \le n^3$ (since the two quantities are equal).
- Since $n \in \mathbb{N}$, we know that $n \le n^3$, and so $100n \le 100n^3$.
- Since $1 \le n$, we know that $1 \le n^3$, and then multiplying both sides by 5000 gives us $5000 \le 5000n^3$.

Adding these three inequalities gives us:

$$n^3 + 100n + 5000 \le n^3 + 100n^3 + 5000n^3 = 5101n^3 = cn^3$$
.

One special case of Big-Oh: O(1)

So far, we have seen Big-Oh expressions like $\mathcal{O}(n)$ and $\mathcal{O}(n^2)$, where the function in parentheses has grown to infinity. However, not every function takes on larger and larger values as its input grows. Some functions are *bounded*, meaning they never take on a value larger than some fixed constant.

For example, consider the constant function f(n) = 1, which always outputs the value 1, regardless of the value of n. What would it mean to say that a function q is Big-Oh of this f? Let's unpack the definition of Big-Oh to find out.

$$g \in \mathcal{O}(f)$$

$$\exists c, n_0 \in \mathbb{R}^+, \ \forall n \in \mathbb{N}, \ n \geq n_0 \Rightarrow g(n) \leq c \cdot f(n)$$

$$\exists c, n_0 \in \mathbb{R}^+, \ \forall n \in \mathbb{N}, \ n \geq n_0 \Rightarrow g(n) \leq c \qquad \qquad \text{(since } f(n) = 1)$$

In other words, there exists a constant c such that q(n) is eventually always less than or equal to c. We say that such functions g are asymptotically bounded with respect to their input, and write $g = \mathcal{O}(1)$ to represent this.

Exercise Break!

5.1 Let $f: \mathbb{N} \to \mathbb{R}^{\geq 0}$, and let $y \in \mathbb{R}^+$ be an arbitrary positive real number. Prove that if $f \in \mathcal{O}(y)$, then $f \in \mathcal{O}(1)$ (this is why we write $\mathcal{O}(1)$ and usually never see $\mathcal{O}(2)$ or $\mathcal{O}(165)$).

Omega and Theta

Big-Oh is a useful way of describing the long-term growth behaviour of functions, but its definition is limited in that it is not required to be an exact description of growth. After all, the key inequality $g(n) \leq cf(n)$ can be satisfied even if f grows much, much faster than q. For example, we could say that $n+10 \in \mathcal{O}(n^{100})$ according to our definition, but this is not necessarily informative.

In other words, the definition of Big-Oh allows us to express upper bounds on the growth of a function, but does not allow us to distinguish between an upper bound that is tight and one that vastly overestimates the rate of growth.

In this section, we will introduce the final new pieces of notation for this chapter, which allow us to express tight bounds on the growth of a function.

Definition 5.5. Let $f, g: \mathbb{N} \to \mathbb{R}^{\geq 0}$. We say that g is Omega of f if and only if there exist constants $c, n_0 \in \mathbb{R}^+$ such that for all $n \in \mathbb{N}$, if $n \ge n_0$, then $g(n) \ge c \cdot f(n)$. In this case, we can also write $g \in \Omega(f)$.

You can think of Omega as the dual of Big-Oh: when $g \in \Omega(f)$, then f is a lower bound on the growth rate of q. For example, we can use the definition to prove that $n^2 - 5 \in \Omega(n)$.

We can now express a bound that is tight for a function's growth rate quite elegantly by combining Big-Oh and Omega: if f is asymptotically both a lower and upper bound for g, then g must grow at the same rate as f.

Definition 5.6. Let $f, g: \mathbb{N} \to \mathbb{R}^{\geq 0}$. We say that g is Theta of f if and only if g is both Big-Oh of f and Omega of f. In this case, we can write $g \in \Theta(f)$, and say that f is a **tight bound** on g.

Equivalently, g is Theta of f if and only if there exist constants $c_1, c_2, n_0 \in \mathbb{R}^+$ such that for all $n \in \mathbb{N}$, if $n \geq n_0$ then $c_1 f(n) \leq g(n) \leq c_2 f(n)$.

⁷ Most of the time, when people say "Big-Oh" they actually mean Theta, i.e., a Big-Oh upper bound is meant to be the tight one, because we rarely say upper bounds that overestimate the rate of growth. However, in this course we will always use Θ when we mean tight bounds, because we will

Example 5.5. Let $f(n) = n^2$ and g(n) = n + 10. Then $g \in \mathcal{O}(f)$, but $g \notin \Theta(f)$. That is, f is an upper bound for the growth rate of g, but it is not a tight upper bound.

Exercise Break!

5.2 Prove the statement in the previous example. Note that the correct translation uses an AND, so you'll actually need to prove two different statements here.

Properties of Big-Oh, Ometa, and Theta

If we had you always write chains of inequalities to prove that one function is Big-Oh/Omega/Theta of another, that would get quite tedious rather quickly. Instead, in this section we will prove some properties of this definition which are extremely useful for combining functions together under this definition. These properties can save you quite a lot of work in the long run. We'll illustrate the proof of one of these properties here; most of the others can be proved in a similar manner, while a few are most easily proved using some techniques from calculus.⁸

Elementary functions

The following theorem tells us how to compare four different types of "elementary" functions: constant functions, logarithms, powers of n, and exponential functions.

Theorem 5.1. For all $a, b \in \mathbb{R}^+$, the following statements are true:

- 1. If a > 1 and b > 1, then $\log_a n \in \Theta(\log_b n)$.
- 2. If a < b, then $n^a \in \mathcal{O}(n^b)$ and $n^a \notin \Omega(n^b)$.
- 3. If a < b, then $a^n \in \mathcal{O}(b^n)$ and $a^n \notin \Omega(b^n)$.
- 4. If a > 1, then $1 \in \mathcal{O}(\log_a n)$ and $1 \notin \Omega(\log_a n)$.
- 5. $\log_a n \in \mathcal{O}(n^b)$ and $\log_a n \notin \Omega(n^b)$.
- 6. If b > 1, then $n^a \in \mathcal{O}(b^n)$ and $n^a \notin \Omega(b^n)$.

Basic properties

Theorem 5.2. For all $f: \mathbb{N} \to \mathbb{R}^{\geq 0}$, $f \in \Theta(f)$.

Theorem 5.3. For all $f, g: \mathbb{N} \to \mathbb{R}^{\geq 0}$, $g \in \mathcal{O}(f)$ if and only if $f \in \Omega(g)$.

Theorem 5.4. For all $f, g, h : \mathbb{N} \to \mathbb{R}^{\geq 0}$:

- If $f \in \mathcal{O}(g)$ and $g \in \mathcal{O}(h)$, then $f \in \mathcal{O}(h)$.
- If $f \in \Omega(q)$ and $g \in \Omega(h)$, then $f \in \Omega(h)$.
- If $f \in \Theta(g)$ and $g \in \Theta(h)$, then $f \in \Theta(h)$.¹⁰

⁸ We discuss the connection between calculus and asymptotic notation in the following section, but this is *not* a required part of CSC165.

⁹ As a consequence of this, $g \in \Theta(f)$ if and only if $f \in \Theta(g)$.

¹⁰ Exercise: prove this using the first two.

Operations on functions

Definition 5.7. Let $f, g : \mathbb{N} \to \mathbb{R}^{\geq 0}$. We can define the sum of f and g as the function $f + g : \mathbb{N} \to \mathbb{R}^{\geq 0}$ such that

$$\forall n \in \mathbb{N}, \ (f+g)(n) = f(n) + g(n).$$

Theorem 5.5. For all $f, g, h : \mathbb{N} \to \mathbb{R}^{\geq 0}$, the following hold:

- 1. If $f \in \mathcal{O}(h)$ and $g \in \mathcal{O}(h)$, then $f + g \in \mathcal{O}(h)$.
- 2. If $f \in \Omega(h)$, then $f + g \in \Omega(h)$.
- 3. If $f \in \Theta(h)$ and $g \in \mathcal{O}(h)$, then $f + g \in \Theta(h)$.¹¹

¹¹ Exercise: prove this using the first

We'll prove the first of these statements.

Translation.

$$\forall f, g, h : \mathbb{N} \to \mathbb{R}^{\geq 0}, \ (f \in \mathcal{O}(h) \land g \in \mathcal{O}(h)) \Rightarrow f + g \in \mathcal{O}(h).$$

Discussion. This is similar in spirit to the divisibility proofs we did in the Introduction to Proofs chapter, which used a term (divisibility) that contained a quantifier. Here, we need to assume that f and g are both Big-Oh of h, and prove that f + q is also Big-Oh of h.

Assuming $f \in \mathcal{O}(h)$ tells us there exist positive real numbers c_1 and n_1 such that for all $n \in \mathbb{N}$, if $n \geq n_1$ then $f(n) \leq c_1 \cdot h(n)$. There similarly exist c_2 and n_2 such that $g(n) \leq c_2 \cdot h(n)$ whenever $n \geq n_2$. Warning: we can't assume that $c_1 = c_2$ or $n_1 = n_2$, or any other relationship between these two sets of variables.

We want to prove that there exist $c, n_0 \in \mathbb{R}^+$ such that for all $n \in \mathbb{N}$, if $n > n_0$ then $f(n) + g(n) \le c \cdot h(n)$.

The forms of the inequalities we can assume— $f(n) \le c_1 h(n), g(n) \le c_2 h(n)$ and the final inequality are identical, and in particular the left-hand side suggests that we just need to add the two given inequalities together to get the third. We just need to make sure that both given inequalities hold by choosing n_0 to be large enough, and let c be large enough to take into account both c_1 and c_2 .

Proof. Let $f, g, h : \mathbb{N} \to \mathbb{R}^{\geq 0}$, and assume $f \in \mathcal{O}(h)$ and $g \in \mathcal{O}(h)$. By these assumptions, there exist $c_1, c_2, n_1, n_2 \in \mathbb{R}^+$ such that for all $n \in \mathbb{N}$,

- if $n \geq n_1$, then $f(n) \leq c_1 \cdot h(n)$, and
- if $n \geq n_2$, then $g(n) \leq c_2 \cdot h(n)$.

We want to prove that $f + g \in \mathcal{O}(h)$, i.e., that there exist $c, n_0 \in \mathbb{R}^+$ such that for all $n \in \mathbb{N}$, if $n \ge n_0$ then $f(n) + g(n) \le c \cdot h(n)$.

Let $n_0 = \max\{n_1, n_2\}$ and $c = c_1 + c_2$. Let $n \in \mathbb{N}$, and assume that $n \geq n_0$. We now want to prove that $f(n) + g(n) \le c \cdot h(n)$.

Since $n_0 \geq n_1$ and $n_0 \geq n_2$, we know that n is greater than or equal to n_1 and n_2 as well. Then using the Big-Oh assumptions,

$$f(n) \leq c_1 \cdot h(n)$$

$$g(n) \leq c_2 \cdot h(n)$$

12 The definition of Big-Oh here has three quantifiers, but the idea is the same.

Adding these two inequalities together yields

$$f(n) + g(n) \le c_1 h(n) + c_2 h(n) = (c_1 + c_2)h(n) = c \cdot h(n).$$

Theorem 5.6. For all $f: \mathbb{N} \to \mathbb{R}^{\geq 0}$ and all $a \in \mathbb{R}^+$, $a \cdot f \in \Theta(f)$.

Theorem 5.7. For all $f_1, f_2, g_1, g_2 : \mathbb{N} \to \mathbb{R}^{\geq 0}$, if $g_1 \in \mathcal{O}(f_1)$ and $g_2 \in \mathcal{O}(f_2)$, then $g_1 \cdot g_2 \in \mathcal{O}(f_1 \cdot f_2)$. Moreover, the statement is still true if you replace Big-Oh with Omega, or if you replace Big-Oh with Theta.

Theorem 5.8. For all $f: \mathbb{N} \to \mathbb{R}^{\geq 0}$, if f(n) is eventually greater than or equal to 1, then $\lfloor f \rfloor \in \Theta(f)$ and $\lceil f \rceil \in \Theta(f)$.

Properties from calculus

[Note: this subsection is **not** part of the require course material for CSC165. It is presented mainly for the nice connection between Big-Oh notation and calculus.]

Our asymptotic notation of \mathcal{O} , Ω , and Θ are concerned with the comparing the long-term behaviour of two functions. It turns out that the concept of "long-term behaviour" is captured in another object of mathematical study, familiar to us from calculus: the *limit* of the function as its input approaches infinity.

Formally, we have the following two definitions: 13

$$\begin{split} \lim_{n \to \infty} f(n) &= L: \ \forall \epsilon \in \mathbb{R}^+, \ \exists n_0 \in \mathbb{N}, \ \forall n \in \mathbb{N}, \ n \geq n_0 \Rightarrow |f(n) - L| < \epsilon, \\ & \text{(where } f: \mathbb{N} \to \mathbb{R} \text{ and } L \in \mathbb{R}) \\ \lim_{n \to \infty} f(n) &= \infty: \ \forall M \in \mathbb{R}^+, \ \exists n_0 \in \mathbb{N}, \ \forall n \in \mathbb{N}, \ n \geq n_0 \Rightarrow f(n) > M \end{split}$$
 (where $f: \mathbb{N} \to \mathbb{R}$)

Using just these definitions and the definitions of our asymptotic symbols \mathcal{O} , Ω , and Θ , we can prove the following pretty remarkable results:

Theorem 5.9. For all $f, g : \mathbb{N} \to \mathbb{R}^{\geq 0}$, if $g(n) \neq 0$ for all $n \in \mathbb{N}$, then the following statements hold:

- (i) If there exists $L \in \mathbb{R}^+$ such that $\lim_{n \to \infty} f(n)/g(n) = L$, then $g \in \Omega(f)$ and $g \in \mathcal{O}(f)$. (In other words, $g \in \Theta(f)$.)
- (ii) If $\lim_{n\to\infty} f(n)/g(n) = 0$, then $f \in \mathcal{O}(g)$ and $g \notin \mathcal{O}(f)$.
- (iii) If $\lim_{n\to\infty} f(n)/g(n) = \infty$, then $g \in \mathcal{O}(f)$ and $f \notin \mathcal{O}(g)$.

Proving this theorem is actually a very good (lengthy) exercise for a CSC165 student; they involve keeping track of variables and manipulating inequalities, two key skills you're developing in this course! And they do tend to be useful in practice (although again, not for this course) to proving asymptotic bounds like $n^2 \in \mathcal{O}(1.01^n)$. But note that the converse of these statements is not true; for example, it is possible (and another nice exercise) to find functions f and g such that $g \in \Theta(f)$, but $\lim_{n \to \infty} f(n)/g(n)$ is undefined.

¹³ We're restricting our attention here to functions with domain N because that's our focus in computer science.

Back to algorithms

Let us return to our example at the beginning of the chapter:

```
def print_items(lst: list) -> None:
       for item in lst:
           print(item)
3
```

How can we use our asymptotic notation to help us analyze the running time of this algorithm? Remember that we have proposed expressions like n, 2n, 11n, 11n + 1.5, where n is the length of the input list.

By using asymptotic notation, we no longer need to worry about the constants involved, and so don't need to worry about whether a single call to print counts as one or ten "basic operations." Moreover, by focusing on the long-term growth, we can also ignore lower-order terms like the 1.5 in 11n + 1.5. ¹⁴

Just as switching from measuring real time to counting "basic operations" allows us to ignore the computing environment in which the program runs, switching from an exact step count to asymptotic notation allows us to ignore machine- and programming language-dependent constants involved in the execution of the code.

Having ignored all these external factors, our analysis will concentrate on how the size of the input influences the running time of a program, where we measure running time just using asymptotic notation, and not exact expressions.

Warning: the "size" of the input to a program can mean different things depending on the type of input, or even depending on the program itself. Whenever you perform a running time analysis, be sure to clearly state how you are measuring and representing input size.

Because constants don't matter, we will use a very coarse measure of "basic operation" to make our analysis as simple as possible. For our purposes, a basic operation (or step) is any block of code whose running time does not depend on the size of the input. 15

This includes all primitive language operations like most assignment statements, arithmetic calculations, and list and string indexing. The one major statement type which does not fit in this category is a function call—the running time of such statements depends on how long that particular function takes to run. We'll revisit this in more detail later.

The runtime function

print_items is an example of a special type of program: one whose runtime depends only on the size of the input list, and not the contents of the list. That is, we expect that print_items takes the same amount of time on every list of length 100. We can make this a little more clear by introducing one piece of notation that will come in handy for the rest of the chapter.

Definition 5.8. Let func be an algorithm. For every $n \in \mathbb{N}$, we define the set $\mathcal{I}_{func,n}$ to be the set of allowed inputs to func of size n.

Example 5.6. For example, $\mathcal{I}_{print\ items,100}$ is simply the set of all lists of length 100. $\mathcal{I}_{print\ items,0}$ is the set containing just one input: the empty list.

¹⁴ The formal grounding for this is in the section of properties of Theta.

¹⁵ To belabour the point a little, this depends on how we define input size. For integers, we usually will assume they have a fixed size in memory (e.g., 32 bits), which is why arithmetic operations take constant time. But of course if we allow numbers to grow infinitely, this is no longer true, and performing arithmetic operations will no longer take constant time.

We can restate our observation about print_items in terms of these sets: for all $n \in \mathbb{N}$, every element of $\mathcal{I}_{print_items,n}$ has the *same* runtime when passed to print_items.

Definition 5.9. Let func be an algorithm whose runtime depends only on its input size. We define the running time function of func as $RT_{func}: \mathbb{N} \to \mathbb{R}^{\geq 0}$, where $RT_{func}(n)$ is equal to the running time of func when given an input of size n.¹⁶

The goal of a *runtime analysis* for func is to find a function f (consisting of just elementary functions) such that $RT_{func} \in \Theta(f)$.

Our first technique for performing this runtime analysis follows four steps:

- 1. Identify the blocks of code which can be counted as a single basic operation, because they don't depend on the input size.
- 2. Identify any loops in the code, which cause basic operations to repeat. You'll need to figure out how many times those loops run, based on the size of the input. Be *exact* when counting loop iterations.
- 3. Use your observations from the previous two steps to come up with an expression for the number of basic operations used in this algorithm—i.e., find an exact expression for $RT_{func}(n)$.
- 4. Use the properties of asymptotic notation to find an elementary function f such that $RT_{func} \in \Theta(f(n))$.

Because Theta expressions depend only on the fastest-growing term in a sum, and ignores constants, we don't even need an exact, "correct" expression for the number of basic operations. This allows us to be rough with our analysis, but still get the correct Theta expression.

Example 5.7. Consider the function print_items. We define input size to be the number of items of the input list. Perform a runtime analysis of print_items.

Proof. For this algorithm, each iteration of the loop can be counted as a single operation, because nothing in it (including the call to print) depends on the size of the input list. 17

So the running time depends on the number of loop iterations. Since this is a for loop over the lst argument, we know that the loop runs n times, where n is the length of lst.

Thus the total number of basic operations performed is n, and so the running time is $RT_{print\ items}(n) = n$, which is $\Theta(n)$.

It is quite possible to have nested loops in a function body, and analyze the running time in the same fashion. The simplest method of tackling such functions is to count the number of repeated basic operations in a loop starting with the *innermost* loop and working your way out.

Example 5.8. Consider the following function.

¹⁶ We will often abbreviate "running time" to "runtime".

¹⁷ This is actually a little subtle. If we consider the size of individual list elements, it could be the case that some take a much longer time to print than others (imagine printing a string of one-thousand characters vs. the number 5). But by defining input size purely as the number of items, we are implicitly ignoring the size of the individual items. The running time of a call to print does *not* depend on the length of the input list.

```
def print_sums(lst: list) -> None:
    for item1 in lst:
        for item2 in lst:
            print(item1 + item2)
```

Perform a runtime analysis of print_sums. (For the remainder of this course, we will assume input size for a list is always its length, unless something else is specified.)

Proof. Let n be the length of lst.

The inner loop (for item2 in lst) runs n times (once per item in lst), and each iteration is just a single basic operation.

But the entire inner loop is itself repeated, since it is inside another loop. The outer loop runs n times as well, and each of its iterations takes n operations.

So then the total number of basic operations is

```
RT_{print sums}(n) = \text{steps for the inner loop} \times \text{number of times inner loop is repeated}
                      = n^2
```

So the running time of this algorithm is $\Theta(n^2)$.

Students often make the mistake, however, that the number of nested loops should always be the exponent of n in the Big-Oh expression. However, things are not that simple, and in particular, not every loop takes n iterations.

Example 5.9. Consider the following function:

```
def f(lst: List[int]) -> None:
       for item in lst:
           for i in range(10):
3
               print(item + i)
```

Perform a runtime analysis of this function.

Proof. Let n be the length of the input list lst. The inner loop repeats 10 times, and each iteration is again a single basic operation, for a total of 10 basic operations. The outer loop repeats n times, and each iteration takes 10 steps, for a total of 10n steps. So the running time of this function is $\Theta(n)$. (Even though it has a nested loop!)

Alternative, more concise analysis. The inner loop's running time doesn't depend on the number of items in the input list, so we can count it as a single basic operation.

The outer loop runs n times, and each iteration takes 1 step, for a total of n steps, which is $\Theta(n)$.

¹⁸ E.g., two levels of nested loops always becomes $\Theta(n^2)$.

When we are analyzing the running time of two blocks of code executed in sequence (one after the other), we add together their individual running times. The sum theorems are particularly helpful here, as it tells us that we can simply compute Theta expressions for the blocks individually, and then combine them just by taking the fastest-growing one. Because Theta expressions are a simplification of exact mathematical function expressions, taking this approach is often easier and faster than trying to count an exact number steps for the entire function.¹⁹

Example 5.10. Analyze the running time of the following function, which is a combination of two previous functions.

```
^{19} E.g., \Theta(n^2) is simpler than 10n^2+0.001n+165.
```

```
def combined(lst: list) -> None:
    # Loop 1
for item in lst:
    for i in range(10):
        print(item + i)

# Loop 2
for item1 in lst:
    for item2 in lst:
        print(item1 + item2)
```

Proof. Let n be the length of 1st. We have already seen that the first loop runs in time $\Theta(n)$, while the second loop runs in time $\Theta(n^2)$.²⁰

By Theorem 5.5, we can conclude that combined runs in time $\Theta(n^2)$. (Since $n \in \mathcal{O}(n^2)$.)

²⁰ By "runs in time $\Theta(n)$," we mean that the number of basic operations of the second loop is a function $f(n) \in \Theta(n)$.

Loop iterations with changing costs

Consider the following function:

```
def all_pairs(lst: list) -> None:
    i = 0
    while i < len(lst):
        j = 0
        while j < i:
            print(i + j)
            j = j + 1
        i = i + 1</pre>
```

Like previous examples, this function has a nested loop. However, unlike those examples, here the inner loop's running time depends on the current value of i, i.e., which iteration of the outer loop we're on.

This means we cannot take the previous approach of calculating the cost of the inner loop, and multiplying it by the number of iterations of the outer loop; this only works if the cost of each outer loop iteration is the same.

So instead, we need to manually add up the cost of each iteration of the outer loop, which depends on the number of iterations of the inner loop. More specifically, since j goes from 0 to i-1, the number of iterations of the inner loop is i, and each iteration of the inner loop counts as one basic operation. So the cost of the

i-th iteration of the outer loop is i+1, where the 1 comes from counting the assignment statements in the outer loop.

So then to compute the total cost, we must add up the cost of each iteration. Let n be the length of the input list, and RT_{all} pairs (n) be the running time of all_pairs on a list of length n.

$$RT_{all_pairs}(n) = \sum_{i=0}^{n-1} (i+1) = \sum_{i'=1}^{n} i' = \frac{n(n+1)}{2} + n \in \Theta(n^2).$$

Helper functions

Finally, let us return to how we deal with helper functions in our analysis. Suppose we are asked to analyze the running time of the following function under the assumption that the helper functions do not change the size of lst:

```
def uses_helpers(lst: list) -> None:
    x = helper1(lst)
    y = helper2(lst)
    return x + y
```

As with analyzing any other sequential program, we simply take the sum of each individual code block's running time. That is, we take the running time of helper1 when given input lst, the running time of helper2 when given input lst, and the single basic operation for return x + y, and add these together. We do not need to add any "extra overhead" for calling functions: while this overhead often exists, it does not depend on the size of the input, and so we treat this as a single basic operation that can be ignored.²¹

Example 5.11. Prove that if helper1 runs in time $\Theta(n^2)$ and helper2 runs in time $\Theta(n^3)$, where the n in both cases is the size of their input list, then uses_helper runs in time $\Theta(n^3)$.

Proof. Let n be the size of the input to uses_helpers. Then because helper1 is called on the same input, it takes time $\Theta(n^2)$. Similarly, helper2 takes time $\Theta(n^3)$. Finally, the cost of the return statement is $\Theta(1)$.

Taking the sum of these yields a total running time of $\Theta(n^3)$.

Note that unlike previous examples, this analysis was an implication: the running time of uses_helpers depends on the running times of helper1 and helper2. It is important to keep this in mind when both writing and analyzing your code: it is easy to skim over a helper function call because it takes up so little visual space, but that one call might make the difference between a $\Theta(n)$ and $\Theta(2^n)$ running time.

Some trickier examples

Students often get the impression that runtime analysis is all about counting the level of nested loops. Our goal here is to convince you that runtime analysis

²¹ Any constant number of basic operations is dominated by terms that grow with the size of the input.

isn't always straight-forward, and in fact can lead to surprising results, even for simple-looking algorithms!

Example 5.12. Let us analyze the runtime of the following function, which determines whether a number is prime.

```
def is_prime(n: int) -> bool:
    if n < 2:
       return False
    d = 2
5
    while d < n:
6
       if n % d == 0:
                        # Since d divides n, n cannot be prime.
         return False
       d = d + 1
q
                   # If the loop doesn't find a divisor, n is prime.
    return True
```

While this code is structurally very simple, consisting of a just a single loop with a standard increment, its runtime function is unlike any other we have seen before. This loop can return early, but in a way which is quite unpredictable, as it depends on when a divisor of n is found. It is possible to be more precise, and say that "the number of loop iterations is equal to one less than the smallest divisor of ngreater than 1," but this isn't expressible in terms of elementary mathematical functions!

To the right, we show a graph of the running times (measured as number of loop iterations) of this function for the first 100 values of n. This nicely illustrates the difficulty with trying to summarize the runtime of is_prime in a single Theta expression. There is an upper bound of n-2 iterations (this is what occurs when no divisor between 1 and n is found), and a lower bound of a single iteration (when the first number, d=2, is a divisor of n), and some other dots in between. So we could say that the runtime of is_prime is $\mathcal{O}(n)$ and $\Omega(1)$, but in fact it is neither $\Theta(n)$ nor $\Theta(1)!^{22}$

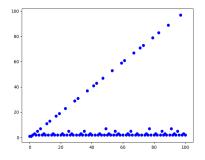
Example 5.13. Let's go one step further with the previous example, and study a function that uses is_prime as a helper.

```
def print_primes(n: int) -> None:
    for k in range(2, n + 1):
        if is_prime(k):
            print(k)
```

What is the asymptotic running time of print_primes as a function of n? It seems at first glance this should be straightforward to analyze, as the code in this function's body is structurally simple.

The problem, of course, lies in the is_prime helper. Because it stops as soon as it finds a factor of n between 2 and n-1, the number of iterations that occur can vary between 1 and n-2. Note that is_prime only goes through all n-2iterations if n is prime.

So if we want to analyze the running time of print_primes, we need to add up the cost of running is_prime for each number between 2 and $n-1.^{23}$ Let RT_{print} primes(n) represent the running time of print_primes(n), and RT_{is} prime(n)time operations in print_primes and



²² So our goal of finding an elementary Theta expression for an algorithm's runtime isn't always possible.

²³ We can ignore the other constantis_prime.

represent the running time of is_prime(n).

$$RT_{print_primes}(n) = \sum_{k=2}^{n} RT_{is_prime}(k)$$

How do we evaluate this sum? We could say that the running time of $is_prime(k)$ is at most k-2, but this forces us to change the equality into an inequality:

$$egin{split} RT_{print_primes}(n) & \leq \sum_{k=2}^{n} (k-2) \ & = \sum_{k=2}^{n} k - 2(n-1) \ & = \sum_{k=1}^{n} k - 2(n-1) - 1 \ & = rac{n(n+1)}{2} - 2n + 1 \end{split}$$

In other words, we get a quadratic (n^2) running time here. But because our analysis over-estimated the running time of $is_prime(k)$, this is only an *upper bound* on the running time: RT_{print} $primes(n) \in \mathcal{O}(n^2)$.

In fact, this analysis did not take into account is_prime stopping early at all! However, it is not at all obvious how to take this into account in our analysis, since we lack the mathematical tools required to think about when and how is_prime stops early for the different values of k.

However, here is one simple argument that we could use to get a *lower bound* on the running time of this function. We observed that when is_prime's input k is prime, its runtime is k-2. So what do we get if we take the original expression for $RT_{print \ primes}(k)$ and throw out all the terms except when k is prime?

$$egin{aligned} RT_{print_primes}(n) &= \sum_{k=2}^{n} RT_{is_prime}(k) \ &\geq \sum_{\substack{k \leq n \ k ext{ is prime}}} T_2(k) \ &= \sum_{\substack{k \leq n \ k ext{ is prime}}} (k-2) \ &= (\sum_{\substack{k \leq n \ k ext{ is prime}}} k) - 2 imes (\# ext{ of primes} \leq n) \ &= k ext{ is prime} \end{aligned}$$

We know from number theory that the sum of the primes $\leq n$ is roughly $\frac{n^2}{\log n}$, and the number of primes $\leq n$ is roughly $\frac{n}{\log n}$. This means that $RT_{print_primes}(n) \in \Omega\left(\frac{n^2}{\log n}\right)$.

Notice that this doesn't match our upper bound! Does that mean that one of these is wrong? Not quite—it means that the true running time is somewhere between $\frac{n^2}{\log n}$ and n^2 , but we would need to perform a better analysis to determine what it is.²⁴

²⁴ And of course, there's no guarantee that the runtime is Theta of any elementary function!

Our next example considers a standard loop, with a twist in how the loop variable changes at each iteration.

```
def twisty(n: int) -> None:
    x = n
    while x > 1:
    if x % 2 == 0:
        x = x / 2
    else:
        x = 2*x - 2
```

Even though the individual lines of code in this example are simple, they combine to form a pretty complex situation. The challenge with analyzing the runtime of this function is that, unlike previous examples, here the loop counter x does not always get closer to the loop stopping condition; sometimes it does (when divided by two), and sometimes it increases!

The key insight into analyzing the runtime of this function is that we don't just need to look at what happens after a single loop iteration, but instead perform a more sophisticated analysis based on *multiple* iterations.²⁵ More concretely, we'll prove the following claim.

Claim 3. For any value of x greater than 2, after two iterations of the loop the value of x decreases by at least one.

Proof. Let x_0 be the value of variable x at some iteration of the loop, and assume $x_0 > 2$. Let x_1 be the value of x after one loop iteration, and x_2 the value of x after two loop iterations. We want to prove that $x_2 \le x_0 - 1$.

We divide up this proof into four cases, based on the remainder of x_0 when dividing by four.²⁶ We'll only do two cases here to illustrate the main idea, and leave the last two cases as an exercise.

Case 1: Assume $4 \mid x_0$, i.e., $\exists k \in \mathbb{Z}, x_0 = 4k$.

In this case, x_0 is even, so the if branch executes in the first loop iteration, and so $x_1 = \frac{x_0}{2} = 2k$. And so then x_1 is also even, and so the if branch executes again: $x_2 = \frac{x_1}{2} = k$.

So then $x_2 = \frac{1}{4}x_0 \le x_0 - 1$ (since $x_0 \ge 4$), as required.

Case 2: Assume $4 \mid x_0 - 1$, i.e., $\exists k \in \mathbb{Z}, x_0 = 4k + 1$.

In this case, x_0 is odd, so the else branch executes in the first loop iteration, and so $x_2 = 2x_0 - 2 = 8k$. Then x_1 is even, and so $x_2 = \frac{x_1}{2} = 4k$.

So then $x_2 = 4k = x_0 - 1$, as required.

Cases 3 and 4: left as exercises.

So this claim tells us that after every two iterations, the value of x decreases by at least 1. Since x starts at n and the loop terminates when x reaches 1 (or less), there are at most 2(n-1) loop iterations.²⁷ So then since each loop iteration takes constant time, the total running time of this algorithm is $\mathcal{O}(n)$.

 $^{^{25}}$ As preparation, try tracing twisty on inputs 7, 9, and 11.

²⁶ The intuition here is that this determines whether x_0 is even/odd, and whether x_1 is even/odd.

²⁷ Contrast this with earlier examples that had the loop counter increase/decrease by 1 at *every* iteration.

Exercise Break!

- 5.3 The analysis we performed in the previous example is incomplete for a few reasons; our goal with this set of exercises is to complete it here.
 - (a) Complete the last two cases in the proof of the claim.
 - (b) State and prove an analogous statement for how much x must decrease by after three loop iterations.
 - (c) Find an exact upper bound on the number of loop iterations taken by this algorithm. Your upper bound should be smaller (and therefore more accurate) than the one given in the example.
 - (d) Finally, find, with proof, a good lower bound on the number of loop iterations taken by this algorithm.

Worst-case and best-case running times

In the previous section, we saw how to use asymptotic notation to characterize the rate of growth of the number of "basic operations" as a way of analyzing the running time of an algorithm. This approach allows us to ignore details of the computing environment in which the algorithm is run, and machine- and languagedependent implementations of primitive operations, and instead characterize the relationship between the input size and number of basic operations performed.

However, this focus on just the input size is a little too restrictive. Even though we can define input size differently for each algorithm we analyze, we tend not to stray too far from the "natural" definitions (e.g., length of list). In practice, though, algorithms often depend on the actual value of the input, not just its size. For example, consider the following function, which searches for an even number in a list of integers.

```
def has_even(numbers: List[int]) -> bool:
    for number in numbers:
        if number % 2 == 0:
        return True
    return False
```

Because this function returns as soon as it finds an even number in the list, its running time is not necessarily proportional to the length of the input list.

The running time of a function can vary even when the input size is fixed. Or using the notation of the previous section, the inputs in $\mathcal{I}_{has_even,10}$ do not all have the same runtime. The question "what is the running time of has_even on an input of length n?" does not make sense, as for a given input the runtime depends not just on its length but on which of its elements are even.

And because our asymptotic notation is used to describe the growth rate of *functions*, we cannot use it to describe the growth of a whole range of values with respect to increasing input sizes. A natural approach to fix this problem is to focus on the *maximum* of this range, which corresponds to the *slowest* the algorithm could run for a given input size.

Definition 5.10. Let func be a program. We define the following function, called the worst-case running time function of func:²⁸

```
WC_{func}(n) = \max \{ \text{running time of executing } f(x) \mid x \in \mathcal{I}_{func,n} \}
```

Note that WC_{func} is a function, not a (constant) number: it returns the maximum possible running time for an input of size n, for every natural number n. And because it is a function, we can use asymptotic notation to describe it, saying things like "the worst-case running time of this function is $\Theta(n^2)$."

The goal of worst-case runtime analysis for func is to find an elementary function f such that $WC_{func} \in \Theta(f)$.

However, it takes a bit more work to obtain tight bounds on a worst-case running time than on the runtime functions of the previous section. Let's think about just the worst-case running time for now. It is difficult to compute the *exact maximum* number of basic operations performed by this algorithm for every input size, which requires that we identify an input for each input size, count its maximum number of basic operations, and then prove that every input of this size takes at most this number of operations. Instead, we will generally take a two-pronged approach: proving matching *upper* and *lower bounds* on the worst-case running time of our algorithm.

Upper bounds on the worst-case runtime

Definition 5.11. Let func be a program, and WC_{func} its worst-case runtime function. We say that a function $f: \mathbb{N} \to \mathbb{R}^{\geq 0}$ is an upper bound on the worst-case runtime if and only if WC_{func} is absolutely dominated by f.

We use absolute dominance rather than the more refined Big-Oh because there's a very intuitive way to unpack this definition.

²⁸ Here, "running time" is measured in exact number of basic operations. We are taking the maximum/minimum of a set of numbers, *not* a set of asymptotic expressions.

```
\forall n \in \mathbb{N}, \ WC_{func}(n) \leq f(n)
\iff \forall n \in \mathbb{N}, \; \max \left\{ \text{running time of executing func(x)} \; | \; x \in \mathcal{I}_{func,n} \right\} \leq f(n)
\iff \forall n \in \mathbb{N}, \ \forall x \in \mathcal{I}_{func,n}, \ \text{running time of executing func(x)} \leq f(n)
```

The last line comes from the fact that if we know the maximum of a set of numbers is less than some value K, then all numbers in that set must be less than K. Thus an upper bound on the worst-case runtime is equivalent to an upper bound on the runtimes of all inputs.

But how do we find such an upper bound? And what does it mean to upper bound all runtimes of a given input size? We'll illustrate the technique in our next example.

Example 5.14. Prove that f(n) = n + 1 is an upper bound for the worst-case runtime of has_even.

Translation. To translate this statement, we can use the equivalent form we just discussed, keeping in mind that all lists are valid inputs to has_even:

"For every $n \in \mathbb{N}$ and every list numbers of length n, the runtime of has_even(numbers) is $\le n + 1$."

Discussion. Before starting our proof, there is only one point we want to highlight: even though we're in a completely different context, all the techniques of proof we learned earlier still apply! In particular, the translated statement begins with two universal quantifiers, and just knowing this alone should anticipate how we'll start our proof.

Proof. We will let $n \in \mathbb{N}$, and let numbers be an arbitrary list of length n. We want to show that has_even(numbers) takes at most n+1 basic operations.

Note that we can't assume anything about the values inside numbers. However, we can still make some observations about the code:

- The loop (for number in numbers) iterates at most n times. Each loop iteration counts as a single basic operation, so the loop takes at most n basic operations.
- The return False statement (if it is executed) counts as 1 basic operation.

The total number of basic operations possible is simply their sum: n+1.

Note that we did not prove that has_even(numbers) takes exactly n+1 basic operations for an arbitrary input numbers (this is false); we only proved an upper bound on the number of operations. And in fact, we don't even care that much about the exact number: what we ultimately care about is the asymptotic growth rate, which is linear for n+1. This allows us to conclude that the worst-case running time of has_even is $\mathcal{O}(n)$, where n is the length of the input list. Note that we must use Big-Oh here, not Theta: we don't yet know that this upper bound is tight.²⁹

²⁹ If this is surprising, note that we could have done the above proof but replaced n+1 by 5000n+165 and it would still have been valid.

Lower bounds on the worst-case runtime

So how do we prove our upper bound is tight? Since we've just shown that $WC(n) \in \mathcal{O}(n)$, we need to prove the corresponding lower bound $WC(n) \in \Omega(n)$. But what does it mean to prove a lower bound on the maximum of a set of numbers? Suppose we have a set of numbers S, and say that "the maximum of S is at least 50." This doesn't tell us what the maximum of S actually is, but it does give us one piece of information: there has to be a number in S which is at least 50.

The key insight is that the converse is also true—if I tell you that S contains the number 50, then you can conclude that the maximum of S is at least 50.

$$\max(S) \ge 50 \Leftrightarrow (\exists x \in S, x \ge 50).$$

Using this idea, we'll give a formal definition for a lower bound on the worst-case runtime of an algorithm.

Definition 5.12. Let func be a program, and WC_{func} is worst-case runtime function. We say that a function $f: \mathbb{N} \to \mathbb{R}^{\geq 0}$ is a lower bound on the worst-case runtime if and only if f is absolutely dominated by WC_{func} .

In an analogous fashion to the upper bound, we unpack this definition:

```
\forall n \in \mathbb{N}, \ WC_{func}(n) \geq f(n)
\Longleftrightarrow \forall n \in \mathbb{N}, \text{ max } \{\text{running time of executing } \mathsf{f}(\mathsf{x}) \mid x \in \mathcal{I}_{func,n}\} \geq f(n)
\iff \forall n \in \mathbb{N}, \ \exists x \in \mathcal{I}_{func,n}, \ \text{running time of executing } f(x) \geq f(n)
```

Remarkably, the crucial difference between this definition and the one for upper bounds is a change of quantifier: now the input x is existentially quantified, meaning we get to pick it. Or really, our goal is to find a whole set of inputs, one per input size, whose runtime is larger than a lower bound. So to find a lower bound on the worst-case running time, we need a set of inputs, one per input size, whose running time is "large" (i.e., close to the upper bound of n+1). Technically, we need an input family whose runtime is $\Omega(n+1)$, but in this case, it's actually possible to obtain exactly this number of steps.

Prove that the function f(n) = n + 1 is a lower bound on the worst-case runtime of has_even.

Translation. We'll state the equivalent form in English, mainly to remind you about the intuition here.

"For every $n \in \mathbb{N}$, there exists an input list numbers such that has_even(numbers) takes at least n+1 basic operations.

Proof. Let $n \in \mathbb{N}$. Let numbers be the list of length n consisting of all 1's. We'll prove that has_even(numbers) takes at least n+1 basic operations.

In this case, the if condition in the loop is always false, so the loop never stops early. Therefore it iterates exactly n times (once per item in the list), with each iteration taking one basic operation.

Finally, the return False statement executes, which is one basic operation. So the total number of basic operations for this input is n+1, which is $\Omega(n)$.

Putting it all together

Finally, we can combine our upper and lower bounds on $WC_{has\ even}$ to obtain a tight asymptotic bound.

Example 5.15. The worst-case running time of has_even is $\Theta(n)$, where n is the length of the input list.

Proof. Since we've proved that $WC_{has\ even}$ is in $\mathcal{O}(n)$ and in $\Omega(n)$, it is in $\Theta(n)$.

To summarize, to obtain a tight bound on the worst-case running time of a function, we need to do two things:

- Use the properties of the code to obtain an asymptotic upper bound on the worst-case running time. We would say something like $WC_f(n) \in \mathcal{O}(g(n))$.
- Find a family of inputs whose running time is $\Omega(q(n))$ (with proof, of course). This will prove that $WC_f(n) \in \Omega(g(n))$, and so we can conclude that $WC_f(n) \in$ $\Theta(g(n))$.

A note about best-case runtime

In this section, we focused on worst-case runtime, the result of taking the maximum runtime for every input size. It is also possible to define a best-case runtime function by taking the minimum possible runtimes, and obtain tight bounds on the best case through an analysis that is completely analogous to the one we just performed. In practice, however, the best-case runtime of an algorithm is usually not as useful to know—we care far more about knowing just how slow an algorithm is than how fast it can be.

Don't assume bounds are tight!

It is likely unsatisfying to hear that upper and lower bounds really are distinct things that must be computed separately. Our intuition here pulls us towards the bounds being "obviously" the same, but this is really a side effect of the examples we have studied so far in this course being rather straightforward. But this won't always be the case: the study of more complex algorithms and data structures exhibits quite a few cases where obtaining an upper bound involves a completely different argument from a lower bound.

Let's look at one such example that deals with manipulating strings.

Example 5.16. We say that a string is a *palindrome* when it can be read the same forwards and backwards; example of palindromes are "abba", "racecar", and "z". 30 We say that a string s_1 is a prefix of another string s_2 when s_1 is a substring of s_2 that starts at index 0 of s_2 . For example, the string "abc" is a prefix of "abcdef".

The algorithm below takes a non-empty string as input, and returns the length of the longest prefix of that string that is a palindrome. For example, the string

³⁰ Every string of length 1 is considered a palindrome.

"attack" has two non-empty prefixes that are palindromes, "a" and "atta", and so our algorithm will return 4.

```
def palindrome_prefix(s: str) -> int:
     n = len(s)
     for prefix_length in range(n, 0, -1): # goes from n down to 1
       # Check whether s[0:prefix_length] is a palindrome
       is_palindrome = True
       for i in range(prefix_length):
         if s[i] != s[prefix_length - 1 - i]:
           is_palindrome = False
           break
       # If a palindrome prefix is found, return the current length.
11
       if is_palindrome:
12
         return prefix_length
13
```

Note that even though the only return statement is inside the for loop, this algorithm is guaranteed to find a palindrome prefix, since the first letter of s by itself is a palindrome.

The code presented here is structurally simple, with a nested for loop. Indeed, it is not too hard to prove that the worst-case runtime of this function is $\mathcal{O}(n^2)$, where n is the length of the input string. What is harder, however, is showing that the worst-case runtime is $\Omega(n^2)$. To do so, we must find an input family whose runtime is $\Omega(n^2)$. There are two points in the code that can lead to fewer than the maximum loop iterations occurring, and we want to find an input family that avoids both of these. The difficulty is that these two points are caused by different types of inputs! The inner break statement occurs as soon as the algorithm detects that a prefix is not a palindrome, while the return statement occurs when the algorithm has determined that a prefix is a palindrome! To make this tension more explicit, let's consider two extreme input families that seem plausible at first glance, but which do not have a runtime that is $\Omega(n^2)$.

- \bullet The entire string s is a palindrome. In this case, in the first iteration of the outer loop, the entire string is checked. The inner loop indeed does not break, but unfortunately this means that the is_palindrome variable remains true after the inner loop occurs, and the outer loop returns during its very first iteration. Since the inner loop runs for n iterations and all of the individual operations are constant time, this input family takes $\Theta(n)$ time to run.
- The entire string s consists of different letters. In this case, the only palindrome prefix is just the first letter of s itself. This means that the outer loop will run for all n iterations, only returning in its last iteration (when prefix_length is 1). However, the inner loop will always stop after its first iteration, since it starts by comparing the first letter of s with another letter, which is guaranteed to be different by our choice of input family. This again leads to a $\Theta(n)$ running time.

The key idea is that we want to choose an input family that doesn't contain a long palindrome (so the outer loop runs for many iterations), but whose prefixes "look" like palindromes (so the inner loop runs for many iterations). Let $n \in \mathbb{Z}^+$. We define the input s_n as follows:

- $s_n[\lceil n/2 \rceil] = b$
- Every other character in s_n is equal to a.

Note that s_n is very close to being a palindrome: if that single character b were changed to an a, then s_n would be the all-a's string, which is certainly a palindrome. But by making the centre character a b, we not only ensure that the longest palindrome of s_n has length roughly n/2 (so the outer loop iterates roughly n/2times), but also that the "outer" characters of each prefix of s_n containing more than n/2 characters are all the same (so the inner loop iterates many times to find the mismatch between a and b). It turns out that this input family does indeed have an $\Omega(n^2)$ runtime! We'll leave the details as an exercise.

Average-case analysis

So far, we have only been concerned with the extremes of algorithm analysis. However, in practice this type of analysis sometimes ends up being misleading, with a variety of algorithms and data structures having a poor worst-case performance still yet performing well on the vast majority of inputs.

Some reflection makes this not too surprising; focusing on the maximum of a set of numbers says very little about the "typical" number in that set, or, more precisely, nothing about the *distribution* of numbers in that set.

A bit more concretely, suppose we have an algorithm func, and we look at the set of running times

```
Times_{func,n} = \{ \text{running time of executing func}(x) \mid x \in \mathcal{I}_{func,n} \}.
```

We have seen that we define the worst-case running time with the maximum running time in this set.³¹ Our final topic of this chapter will be to look at another measure of the running time: taking the average of the numbers in this set.

A first example

Consider the following algorithm, which searches for a particular item in a list.

```
def search(lst: List[int], x: int) -> bool:
       for item in lst:
           if item == x:
3
               return True
       return False
```

Let n represent the length of 1st. The loop body counts as one basic operation, and so the running time of this algorithm is proportional on the number of loop iterations. The loop can iterate between 1 and n times, leading to an upper bound on the worst-case of $\mathcal{O}(n)$ and a lower bound on the best-case of $\Omega(1)$. We'll leave it as an exercise to show that these bounds are tight (this is basically the same analysis we did in the previous section). But what can we say about the average of all possible inputs of length n?

Well, for one thing, we need to precisely define what we mean by "all possible inputs of length n." Because we don't have any restrictions on the elements stored 31 Don't forget that the worst-case running time is a function that uses not just one but all of the $Times_{func,n}$ sets.

in the input list, it seems like there could be an infinite number of lists of length n to choose from, and we cannot take an average of an infinite set of numbers.

So let us focus on one particular set of allowable inputs. We define the set \mathcal{I}_n of inputs to be pairs (lst, 1) where lst is any permutation of the numbers $\{1, 2, \ldots, n\}$, and we are always searching for the number 1 in the list.³²

Example 5.17. Given this set of inputs \mathcal{I}_n , prove that the average-case running time of search is $\Theta(n)$.

32 Since 1 is always in 1st, we might hope that the average running time is faster because of early returns.

Proof. We first want to calculate an exact expression for

$$Avg_{search}(n) = rac{1}{|\mathcal{I}_n|} \sum_{(lst,1) \in \mathcal{I}_n} ext{ running time of search(lst, 1)}.$$

Note that $|\mathcal{I}_n| = n!$, since this is the number of permutations of $\{1, \ldots, n\}$.

$$Avg_{search}(n) = rac{1}{n!} \sum_{(lst,1) \in \mathcal{I}_n} ext{running time of search(lst, 1)}.$$

Also, we want to make explicit that the summation ranges over values for lst, so we define S_n to be the set of all permutations of $\{1, \ldots, n\}$, and write

$$Avg_{search}(n) = rac{1}{n!} \sum_{lst \in S_n} ext{ running time of search(lst, 1)}.$$

Now, the running time of search(lst, 1) is the number of loop iterations performed, and this is exactly equal to one plus the index that 1 appears in lst.33

So we can rewrite the sum as follows:

$$Avg_{search}(n) = \frac{1}{n!} \sum_{lst \in S_n} (1 + ext{index of 1 in lst})$$

Now, it might be challenging to compute this sum, since 1 could appear in any position in 1st. However, we can split up S_n based on the index that 1 appears:

$$\begin{split} Avg_{search}(n) &= \frac{1}{n!} \sum_{i=0}^{n-1} \sum_{\substack{lst \in S_n\\1 \text{ is at lst[i]}}} (1 + \text{index of 1 in lst}) \\ &= \frac{1}{n!} \sum_{i=0}^{n-1} \sum_{\substack{lst \in S_n\\1 \text{ is at lst[i]}}} (1 + i) \end{split}$$

For the inner summation, we are not using 1st in the summation, so it just adds up i a bunch of times. To figure out the number of times i is added together, we need to count the number of lists 1st which have 1 at index i. There are (n-1)!such lists: once we have fixed index i to be 1 in the list, the remaining spots can be any of the (n-1)! permutations of $\{2,\ldots,n\}$. Using this allows us to obtain

³³ The "one plus" is because list indexing starts at 0, not 1.

a final expression for $Avg_{search}(n)$:

$$\begin{split} Avg_{search}(n) &= \frac{1}{n!} \sum_{i=0}^{n-1} \sum_{\substack{1 \text{ is at lst[i]} \\ 1 \text{ is at lst[i]}}} (1+i) \\ &= \frac{1}{n!} \sum_{i=0}^{n-1} (1+i)(n-1)! \\ &= \frac{1}{n} \sum_{i=0}^{n-1} (1+i) \\ &= \frac{1}{n} \sum_{i'=1}^{n} i' \qquad \text{(setting } i' = i+1) \\ &= \frac{1}{n} \cdot \frac{n(n+1)}{2} \\ &= \frac{n+1}{2} \end{split}$$

In other words, the average running time of search on this set of inputs is $\frac{n+1}{2}$ $\Theta(n)$.

Example 5.18. Now consider the set of inputs \mathcal{I}_n^l , which contains all pairs (lst, x) where lst is a permutation of $\{1, \ldots, n\}$ and x is any number between 1 and $n.^{34}$

34 Note that x is still guaranteed to be

Proof. While we want to perform the basically same calculation:

$$Avg_{search}(n) = rac{1}{|\mathcal{I}_n'|} \sum_{(lst,x) \in \mathcal{I}_n'} ext{running time of search(lst, x)}.$$

Note that this seems like a generalization of the previous set of inputs: we now have $|\mathcal{I}'_n| = n \cdot n!$, since now for each permutation we have n choices for x. However, we can do some manipulation of the sum to obtain the exact expression we computed in the previous example:

$$egin{align*} Avg_{search}(n) &= rac{1}{|\mathcal{I}_n'|} \sum_{(lst,x) \in \mathcal{I}_n'} ext{running time of search(lst, x)} \ &= rac{1}{n \cdot n!} \sum_{(lst,x) \in \mathcal{I}_n'} ext{running time of search(lst, x)} \ &= rac{1}{n \cdot n!} \sum_{x=1}^n \sum_{lst \in S_n} ext{running time of search(lst, x)} \ &= rac{1}{n} \sum_{x=1}^n \left(rac{1}{n!} \sum_{lst \in S_n} ext{running time of search(lst, x)}
ight) \end{aligned}$$

We have done two main things: explicitly pulled out the summation over x, so now the part in parentheses has a fixed x value; we pulled in the constant 1/n!, which makes the term in parentheses look exactly like our previous calculation, except with 1 replaced by x.

Why is this useful? Well, we already know that

$$rac{1}{n!}\sum_{lst\in S_n}$$
 running time of search(lst, 1) $=rac{n+1}{2}$.

But in our above proof, we didn't really use any special properties of 1 at all, other than the fact it was one of the numbers guaranteed to be in the list. So in fact, for any value of x between 1 and n, the same equality holds:

$$rac{1}{n!}\sum_{lst\in S_n}$$
 running time of search(lst, x) $=rac{n+1}{2}$.

This results in an absolutely massive simplification of our original expression:

$$egin{aligned} Avg_{search}(n) &= rac{1}{n} \sum_{x=1}^n \left(rac{1}{n!} \sum_{lst \in S_n} & ext{running time of search(lst, x)}
ight) \ &= rac{1}{n} \sum_{x=1}^n rac{n+1}{2} \ &= rac{n+1}{2} \end{aligned}$$

This leads to an average-case running time of $\frac{n+1}{2}$ steps, which is $\Theta(n)$.³⁵

Notice that we do not need to compute an upper and lower bound separately, since in this case we have computed an exact average. (Much like if we had the exact set of inputs, we can compute the exact max and exact min, and don't need to compute upper and lower bounds separately.)

Like worst-case and best-case running times, the average-case running time is a function which relates input size to some measure of program efficiency. In this particular example, we found that for the given set of inputs \mathcal{I}_n for each n, the average-case running time is asymptotically equal to that of the worst-case.

This might sound a little disappointing, but keep in mind the positive information this tells us: the worst-case input family here is not so different from the average case, i.e., it is fairly representative of the algorithm's running time as a whole.

It is not always the case that the average-case running time is asymptotically the same as the worst-case running time. It is certainly possible for the averagecase to be asymptotically the same as the best-case, or lie somewhere in between best- and worst-cases. It is also very sensitive to the set of inputs you choose to analyze, as you'll explore in the exercise. In CSC263/CSC265, you will return to this idea of average-case input with more sophisticated examples, looking not just at more complex functions, but also introducing the notions of probability into the analysis, allowing different inputs to be chosen more frequently than others.

Exercise Break!

5.4 Consider this alternate set of inputs for search: \mathcal{J}_n , where for each input $(lst,x) \in \mathcal{J}_n$, lst has length n, and x and the elements of lst are all between the numbers 1 and 10 (of course, lst can now contain duplicates).

35 Given the symmetry for different possible x values, it is perhaps not too surprising that the exact step count is the same for the two examples. You would expect this to change, however, if we expanded the possible values of x to, say, $1, \ldots, 2n$.

Show that the average-case running time of search on this set of inputs is $\Theta(1)$, i.e., is constant with respect to the length of the input list.

You'll find the following formula helpful:

$$\sum_{i=0}^{n-1} ir^i = \frac{nr^n}{r-1} + \frac{r-r^{n+1}}{(r-1)^2}.$$

6 Graphs and Trees

Our final mathematical domain of study is a powerful and ubiquitous way of representing entities and the relationships between them. If this sounds generic, that's because it is: this type of representation is abstract enough that we can use it to model concepts as varied as geographic locations and routes, animals and plants in an ecosystem, or people in a social network.

In this chapter, you will begin your study of *graph theory*, learning how to precisely define different types of these models, called *graphs*, and (of course) state and prove properties of these entities. While we are only scratching the surface in this chapter, the material you learn here will serve as a useful foundation in many future courses in computer science.

Initial definitions

Let us start with some basic definitions.

Definition 6.1. A graph is a pair of sets (V, E), which are defined as follows:

- V is a set of objects; each element of V is called a vertex of the graph.
- a set E of pairs of objects from V, where each pair (v_1, v_2) consists of two distinct vertices—i.e., $v_1, v_2 \in V$ and $v_1 \neq v_2$ —and is called an edge of the graph.

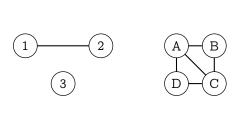
Order does not matter in the pairs, and so (v_1, v_2) and (v_2, v_1) represent the same edge.¹

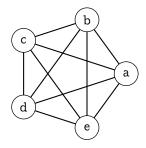
The conventional notation to introduce a graph is to write G = (V, E), where G is the graph itself, V is its vertex set, and E is its edge set.

Intuitively, the set of vertices of a graph represents a collection of objects, and the set of edges of a graph represent the relationships between those objects. For example, if we wanted to use the terminology of graphs to describe Facebook, we could say that each Facebook user is a *vertex*, while each friendship between two Facebook users is an *edge* between the corresponding vertices.

We often draw graphs using dots to represent vertices, and line segments to represent edges. We have drawn some examples of graphs below.

¹ In future courses, you'll study a variants of graphs called *directed graphs*, where vertex order in an edge does matter.





Example 6.1. Consider the graph on the right. How many vertices and how many edges does it have?

Discussion. This isn't a proof question, but just an exercise in terminology. To answer this, I have to be comfortable with the terminology *vertices* and *edges*, as well as pictorial representations of graphs. I just need to remember that dots correspond to vertices, and lines correspond to edges. (There are seven vertices and eleven edges.)

Now that we have these definitions in hand, let us prove our first general graph property. Unlike the previous example, here we will not have a concrete graph to work with, but instead have to work with an arbitrary graph.²

Example 6.2. Prove that for all graphs
$$G = (V, E)$$
, $|E| \leq \frac{|V|(|V|-1)}{2}$.

Translation. The statement we're proving universially quantifies G. Since how we declare a graph variable looks syntactically different ("G = (V, E)") than declaring a numeric variable, we'll adopt an assumed domain of "set of all graphs" for the rest of this chapter rather than introducing a "set of all graphs" explicitly.

$$orall G=(V,E)\in \mathcal{G},\,\,|E|\leq rac{|V|(|V|-1)}{2}.$$

Note that the *structure* of the statement is pretty straightforward, with the only tricky bit being that G is not an arbitrary *number*, but an arbitrary *graph*.

Discussion. So I'm trying to prove a relationship between the number of edges and vertices in any possible graph. I can't assume anything about the structure of the graph: it could have any number of vertices and edges, and this property should still hold.

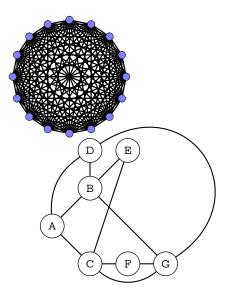
Because the inequality says that |E| is less than or equal to some expression, we can try to figure out what the maximum possible number of edges in G is. So the question is: Given n vertices, how many different edges could there be?

The answer is a straightforward application of the counting work we did earlier: each edge is formed by *choosing* two vertices, where order does not matter, and duplicate edges are not allowed.

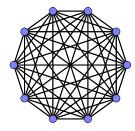
Proof. Let
$$G=(V,E)$$
 be an arbitrary graph. We want to prove that $|E|\leq \frac{|V|(|V|-1)}{2}$.

Each edge in G consists of a pair of vertices from V, where order does not matter. There are exactly $\frac{|V|(|V|-1)}{2}$ possible pairs of vertices, and so there are a maximum of this many possible edges.

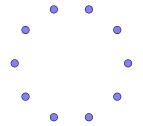
So
$$|E| \leq \frac{|V|(|V|-1)}{2}$$
.



² Reading this, you should immediately expect to see a universal quantification over the set of all possible graphs.



A graph with all possible edges.



A graph with no edges.

Exercise Break!

- 6.1 What is the fewest number of edges a graph could have, in terms of its number of vertices?
- 6.2 Let $n \in \mathbb{Z}^+$. Find, with proof, the number of distinct graphs with the vertex set $V = \{1, 2, \dots, n\}.$

We say two such graphs are distinct when one of them has an edge (u, v) and the other one does not have this edge with the same vertices.

Paths and connectedness

Often when we use graphs in modelling the real world, it is not sufficient to capture just a single relationship between entities. Our goal now is to use individual edges, which represent some sort of relationship between vertices, to build up extended, indirect connections between vertices. In a social network, for example, we want to be able to go from friends to "friends of friends," and even "friends of friends of friends of friends." In a graph representing roads between cities, we want to be able to go from "a route between cities using one road" to "a route between cities using k roads." We use the following definitions to make precise these notions of "indirect" relationships.

Definition 6.2. Let G = (V, E), and let $v_1, v_2 \in V$. We say that v_1 and v_2 are adjacent if and only if there exists an edge between them, i.e., $(v_1, v_2) \in E$. Equivalently, we can also say that v_1 and v_2 are neighbours.³

Definition 6.3. Let G = (V, E) and let $u, u' \in V$. A path between u and u' is a sequence of distinct vertices $v_0, v_1, v_2, \ldots, v_k \in V$ which satisfy the following properties:

- $v_0 = u$ and $v_k = u'$. (The endpoints of the path are u and u'.)
- Each consecutive pair of vertices are adjacent. (So v_0 and v_1 are adjacent, and so are v_1 and v_2 , v_2 and v_3 , etc.)

We allow k to be zero; this path would be just a single vertex v_0 .

The length of a path is one less than the number of vertices in the sequence (so the above sequence would have length k); more intuitively, the length of the path is the number of *edges* which are used by this sequence.

We say that u and u' are connected if and only if there exists a path between u and u'. 5 Because we allow zero-length paths, a vertex is always connected to itself.

We say that graph G is connected if and only if for all pairs of vertices $u, v \in V$, uand v are connected.

Being connected is a fundamental property of graphs. Imagine, for example, a geographical representation where each graph vertex is a city, and each edge a road between two cities. If this graph is not connected, then there is at least one pair of cities for which it is not possible to get from one to the other by road.

³ Remember that order doesn't matter in the edge pairs, so this is a symmetric relationship.

⁴ Like edges, paths are directionless; a path from u to u' is also a path from u' to u.

⁵ This definition is existentiallyquantified; there could be more than one path between u and u'.

Example 6.3. Consider the graph on the right.

- 1. Are the vertices A and B adjacent?
- 2. Are the vertices A and B connected?
- 3. What is the length of the shortest path between vertices B and F?
- 4. Prove that this graph is not connected.

Discussion. Parts (1) through (3) are exercises in understanding the definitions we've just read.

- 1. A and B are not adjacent: there is no edge between them.
- 2. A and B are connected: there is a path A, F, G, B between them.
- 3. There is a path of length two between B and F: B, G, F. How do we know this is the shortest one? The only path of length one that could be between B and F is simply the sequence B, F; but this is not a path because B and F are not adjacent.

Part 4 is a bit more complicated, and warrants a formal proof.

Translation. Let us first translate the statement "this graph is not connected." We'll let G=(V,E) refer to this graph (and corresponding vertex and edge sets). So we can write this statement as "G is not connected," but that's not very illuminating. Let us unpack the definition of connected for graphs, which requires every pair of vertices in the graph to be connected:

G is not connected

 $\iff \neg (G \text{ is connected})$

 $\iff \neg (\forall u, v \in V, u \text{ and } v \text{ are connected})$

 $\iff \exists u, v \in V, u \text{ and } v \text{ are *not* connected}$

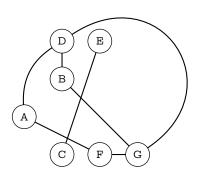
 $\iff \exists u, v \in V$, there is no path between u and v

We actually went a step further and unpacked the definition of connected for vertex pairs as well. Hopefully this makes it clear what it is we need to show: that there exist two vertices in the graph which do not have a path between them.

Proof. Let u=B and v=E be vertices in the above graph. We will show that B and E are not connected.

Suppose for a contradiction that there exists a path v_0, v_1, \ldots, v_k between B and E, where $v_0 = E$. Since v_0 and v_1 must be adjacent, and C is the only vertex adjacent to E, we know that $v_1 = C$. Since we know $v_k = B$, the path cannot be over yet; i.e., $k \geq 2$.

So what about v_2 ? By the definition of path, we know that v_2 must be adjacent to C, and must be distinct from E and C. But the only vertex that's adjacent to C is E, and so v_2 cannot exist, which gives us our contradiction.



⁶ This is both a review of logical manipulation rules and of practicing unpacking definitions!

Exercise Break!

6.3 Let $n \in \mathbb{Z}^+$. Find, with proof, the maximum length of a path in a graph with n vertices. (For extra practice, first express the problem in predicate logic.)

Now let us look at one extremely useful property of connectedness: the fact that if two vertices in a graph are both connected to a third vertex, then they are also connected to each other.

Example 6.4. Let G = (V, E) be a graph, and let $u, v, w \in V$. If v is connected to both u and w, then u and w are connected.⁷

Translation. Once again, after we get over the fact that we are quantifying over the set of all possible graphs, the translation is pretty straightforward, as the statement's structure is not that complex. To make the formula even more concise, we'll use the predicate Conn(G, u, v) to mean that "u and v are connected vertices in G."

$$\forall G = (V, E), \ \forall u, v, w \in V, \ (Conn(G, u, v) \land Conn(G, v, w)) \Rightarrow Conn(G, u, w).$$

Discussion. Let's examine the structure of the statement first. We have an arbitrary graph and three vertices in that graph. Because we're proving an implication, we assume its hypothesis: that u and v are connected, and that v and ware connected. We need to prove that u and w are also connected.

Let's rephrase that by unpacking the definition of "connected." We can assume that there is a path between u and v, and between v and w. We need to prove that there is a path between u and w. Phrased that way, it may seem obvious what to do: create a path between u and w by joining the path between u and vand the one between v and w.

There's only one problem with this: the paths between u and v and v and w might contain some vertices in common, and paths are not allowed to have duplicate vertices. We can fix this, however, by using a simple idea: find the first point of intersection between the paths, and join them at that vertex instead.

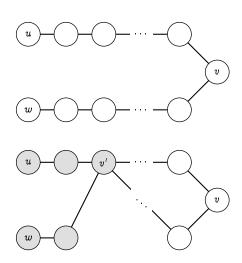
Proof. Let G = (V, E) be a graph, and $u, v, w \in V$. Assume that u and v are connected, and v and w are connected. We want to prove that u and w are connected.

Let P_1 be a path between u and v, and P_2 be a path between v and w. (By the definition of connectedness, both of these paths must exist.)

Handling multiple shared vertices: Let $S \subseteq V$ be the set of all vertices which appear on both P_1 and P_2 . Note that this set is not empty, because $v \in S$. Let v'be the vertex in S which is closest to u in P_1 . This means that no vertex in P_1 between u and v' is in S, or in other words, is also on P_2 .

Finally, let P_3 be the path formed by taking the vertices in P_1 from u to v', and then the vertices in P_2 from v' to w. Then P_3 has no duplicate vertices, and is indeed a path between u and w. By the definition of connectedness, this means that u and w are connected.

⁷ In other words, vertex-connectedness is a transitive property.



Exercise Break!

6.4 Prove or disprove the following statement: For all graphs G = (V, E) and vertices $v_1, v_2, v_3 \in V$, if v_1 and v_2 are not connected and v_1 and v_3 are not connected, then v_2 and v_3 are not connected.

A limit for connectedness

Intuitively, since connectivity is based on paths between vertices, which in turn are built from edges, it is natural to think that we can "force" a graph to be connected by simply adding more edges to it. In this section, we will investigate this by trying to answer the question: "how many edges does it take to ensure that a graph is connected?"

Example 6.5. For all $n \in \mathbb{Z}^+$, there exists an $M \in \mathbb{Z}^+$ such that for all graphs G = (V, E), if |V| = n and $|E| \ge M$, then G is connected.

Translation. The structure of this statement is a little more complex, but you should be able to handle this with all the work you've previously done. Keep in mind that we have three alternating quantifications—n, M, and G = (V, E)—as well as a couple of hypotheses in an implication.

$$\forall n \in \mathbb{Z}^+, \exists M \in \mathbb{Z}^+, \forall G = (V, E), (|V| = n \land |E| > M) \Rightarrow G \text{ is connected.}$$

Since this is already a little long, we won't unpack the definition of connected here, but be ready to do so in the discussion/proof to follow.

Discussion. There are two important things to note in the statement structure. The first is that because M is existentially-quantified, we get to pick its value. The second is that because this quantification happens after n, the value of M is allowed to depend on n. This turns out to be a great power indeed.

For example, if we set $M = n^2$, then because we know that no graph exists with n vertices and n^2 or more edges, 8 the implication becomes vacuously true. This is a valid proof, but not that interesting.

Instead, let's set $M = \frac{n(n-1)}{2}$, i.e., force the graph G to have all possible edges. The proof will still be straight-forward, but at least such a graph exists.

Proof. Let $n \in \mathbb{Z}^+$, let $M = \frac{n(n-1)}{2}$, and let G = (V, E) be a graph. Assume that |V| = n and $|E| \ge M$. We need to prove that G is connected.

Because the maximum number of edges in a graph with n vertices is exactly $\frac{n(n-1)}{2}$, this means that G must have all possible edges. Then any two vertices $u, v \in V$ are adjacent, and hence connected. So then G is connected.⁹

The previous example shows the danger of making statements using existential quantifiers: often it is easy to prove that a particular value exists, but what we really care about is the "best" possible value. We don't want just any M, but

⁸ By our example on the maximum number of edges a graph can have.

⁹ Review the definitions of "connected" if you aren't sure about the last two sentences here.

the smallest possible one which forces a graph to be connected. For instance, it would be much more interesting if we could prove the following statement, with M=2n:

$$\forall n \in \mathbb{Z}^+, \ \forall G = (V, E), \ (|V| = n \land |E| \ge 2n) \Rightarrow G \text{ is connected.}$$

Unfortunately, this statement is false, and in fact the value M=2n is not even close, as we'll prove next.

Example 6.6. Let $n \in \mathbb{Z}^+$, and assume n > 1. Then there exists a graph G =(V,E), such that |V|=n and $|E|=\frac{(n-1)(n-2)}{2}$, and G is not connected.

Translation.

$$\forall n \in \mathbb{Z}^+, \ n > 1 \Rightarrow \left(\exists G = (V, E), \ |V| = n \land |E| = \frac{(n-1)(n-2)}{2} \land G \text{ is not connected}\right).$$

Discussion. This statement looks a little different than the one from the previous example, but in fact is essentially its negation. ¹⁰ Here, we are asked to show that for any n, there is a graph with n vertices and $\frac{(n-1)(n-2)}{2}$ edges, but which is still not connected.

So how do we prove this? This time we can choose the graph, though we are constrained by the number of vertices and edges the graph must have. The expression $\frac{(n-1)(n-2)}{2}$ is a big hint, as it looks suspiciously like the maximum number of edges on n-1 vertices. . .

Proof. Let $n \in \mathbb{Z}^+$, and assume n > 1. Let G = (V, E) be the graph defined as follows:11

- $V = \{v_1, v_2, \dots, v_n\}.$
- $E = \{(v_i, v_j) \mid i, j \in \{1, \dots, n-1\} \text{ and } i < j\}$. That is, E consists of all edges between the first n-1 vertices, and has no edges connected to v_n .

We need to show three things:

- (i) |V| = n. (ii) $|E| = \frac{(n-1)(n-2)}{2}$.
- (iii) G is not connected.

For (i), we have explicitly labelled the n vertices in V, and so it is clear that |V|=n.

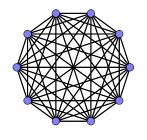
For (ii), we have chosen all possible pairs of vertices from $\{v_1, v_2, \dots, v_{n-1}\}$ for the edges. There are exactly $\frac{(n-1)(n-2)}{2}$ such edges.

For (iii), because v_n is not adjacent to any other vertex, it cannot be connected to any other vertex. So G is not connected.

We have now proved that a graph with a fairly large number of edges can still not be connected. It is worth noting that $\frac{(n-1)(n-2)}{2} = \frac{n(n-1)}{2} - (n-1)$. That

¹⁰ More precisely, the parts starting with the quantification of G are negations of each other.

¹¹ This is the first time we're defining a concrete graph in a proof, rather than introducing an arbitrary graph.



is, there is a graph that is missing only n-1 edges from the set of all possible of edges, but is still not connected. The question becomes: can we go higher still? Is it possible for a graph on n vertices to have more than $\frac{(n-1)(n-2)}{2}$ edges and yet still be not connected? Or is the best possible M from our original question indeed $\frac{(n-1)(n-2)}{2} + 1$?

It turns out that the latter is true, and this will be the last, and most challenging, proof we do in this section.

Example 6.7. Let $n \in \mathbb{Z}^+$. For all graphs G = (V, E), if |V| = n and $|E| \geq n$ $\frac{(n-1)(n-2)}{2} + 1$, then G is connected.

Translation.

$$\forall n \in \mathbb{Z}^+, \ \forall G = (V, E), \ \left(|V| = n \land |E| \ge \frac{(n-1)(n-2)}{2} + 1 \right) \Rightarrow G \text{ is connected.}$$

Discussion. So we are back to our original example, except now the M has been picked for us, and we are using an edge number of $\frac{(n-1)(n-2)}{2} + 1$. It is tempting for us to base our proof on the previous example: after all, if we start with a graph that has n-1 of its vertices all adjacent to each other, and then add one more edge to the remaining vertex, the new graph is certainly connected. However, this line of thinking relies on a particular starting point for the structure of G, which we cannot assume anything about (other than the number of vertices and edges, of course).

The problem is that even with these restrictions on the number of edges and vertices, it is hard to conceptualize enough common structure among such graphs to use in a proof. 12

What is more promising, though, is trying to take a graph which satisfies the constraints on its number of edges and vertices, and then remove a vertex to make the graph smaller, and argue two things:

- the smaller graph is connected
- the vertex we removed is adjacent to at least one vertex in the smaller graph

This idea of "removing a vertex" from a graph to make the problem smaller and simpler can be formalized using induction, and is in fact one of the most common proof strategies when dealing with graphs. 13 The one thing to keep in mind here is that we're doing induction on n, but the predicate we need to prove—contains quantifiers, making it more complex.

You'll notice that the inductive step in this proof is more complicated, and is split up into cases, and involves a sub-proof inside. As you read through this proof, look for both the structure as well as content of the proof: both are vital to understand.

Proof. We will proceed by induction on n. More precisely, define the following predicate over the positive integers:

$$P(n): \forall G=(V,E), \ \, \left(|V|=n \wedge |E| \geq \frac{(n-1)(n-2)}{2} + 1\right) \Rightarrow G \text{ is connected}.$$

In words, P(n) says that for every graph G with n vertices and at least $\frac{(n-1)(n-2)}{2}$ + 1 edges, G must be connected. We want to prove that $\forall n \in \mathbb{Z}^+, P(n)$ using induction.

¹² If that's too abstract, just imagine trying to complete the statement "Every graph with n vertices and at least $\frac{(n-1)(n-2)}{2} + 1$ edges is/has..."

¹³ We weren't kidding about the usefulness of induction.

Base Case: Let n = 1. This is a good exercise in substitution:

$$P(1): \forall G = (V, E), (|V| = 1 \land |E| > 1) \Rightarrow G$$
 is connected

This statement is vacuously true: no graph exists that has only one vertex and at least one edge, since an edge requires two vertices.

Inductive Step: Let $k \in \mathbb{Z}^+$, and assume that P(k) holds. We need to prove that P(k+1) also holds, i.e.:

$$P(k+1): orall G=(V,E), \;\; \left(|V|=k+1 \wedge |E| \geq rac{k(k-1)}{2}+1
ight) \Rightarrow G ext{ is connected.}$$

Let G=(V,E), and assume that |V|=k+1 and $|E|\geq \frac{k(k-1)}{2}+1$. We now need to prove that G is connected. We will split up this proof into two cases.

<u>Case 1</u>: Assume $|E| = \frac{(k+1)k}{2}$, i.e., G has all possible edges. In this case, G is certainly connected.

<u>Case 2</u>: Assume $|E| < \frac{(k+1)k}{2}$. We now need to prove the following claim. Claim 4. G has a vertex in G with between one and k-1 neighbours, inclusive. ¹⁴

Proof. Since G has fewer than the maximum number of possible edges, there exists a vertex pair (u, v) which is not an edge. Both u and v have at most k-1neighbours, since there are k-1 vertices in G other than these two.

We leave showing that both u and v have at least one neighbour as an exercise.

Using this claim, we let v be a vertex which has at most k-1 neighbours. Let G' = (V', E') be the graph which is formed by taking G and removing v from V, and all edges in E which use v. Then |V'| = |V| - 1 = k, i.e., we've decreased the number of vertices by one. This is good because we're trying to do induction on the number of vertices.

However, in order to use P(k), we need not just that the number of vertices to be k, but that the number of edges is at least $\frac{(k-1)(k-2)}{2} + 1.15$ This is what we'll show next.

$$\begin{split} |E'| &= |E| - \text{number of removed edges} \\ &\geq |E| - (k-1) & \text{(at most } k-1 \text{ edges removed)} \\ &\geq \frac{k(k-1)}{2} + 1 - (k-1) & \text{(assumption on } |E|) \\ &= \frac{(k-2)(k-1)}{2} + 1 \end{split}$$

Now that we have this, we can finally use the induction hypothesis: since |V'| = kand $|E'| \geq \frac{(k-2)(k-1)}{2} + 1$, we conclude that G' is connected.

Finally, let us use the fact that G' is connected to show that G is also connected. First, any two vertices not equal to v are connected in G because they are connected in G'. What about v, the vertex we removed from G to get G'? Recall our claim: v has at least one neighbour, so call it w. Then v is connected to w, but



¹⁴ Since there are k+1 vertices total, this claim is saying that there exists a vertex that has at least one neighbour, but not the maximum number of neighbours.

¹⁵ Remember that P(k) is an implication: if the graph has the appropriate number of vertices and edges, then it is connected.

because G' is connected, w is connected to every other vertex in G. By a previous example, we know that v must be connected to all of these other vertices.

Exercise Break!

These questions concern the proof that we just saw.

- 6.5 Let $n \in \mathbb{Z}^+$, and let G = (V, E) be a graph. Prove that if |V| = n and $|E| \ge \frac{(n-1)(n-2)}{2} + 1$, then every vertex in G has at least one neighbour.
- 6.6 It may have struck you as a little strange that we used cases in our proof of the inductive step.

What goes wrong with the argument in the second case if we try to include the case when G has all $\frac{(k+1)k}{2}$ possible edges? (Hint: this is actually quite subtle, and took us a while to pinpoint ourselves!)

Cycles and trees

We spent the last section investigating how many edges a graph would need to force it to be connected. We will now turn to the dual question: how many edges is a graph *forced* to have if it is connected? Rather than taking a graph and adding edges to it to see how far we can go without it becoming connected, we now ask how many edges can we *remove* from a connected graph without disconnecting it.

We might consider some simple examples to gain some intuition here. For example, suppose we have a graph with n vertices which is just a path.

This has n-1 edges, and if you remove any edge from it, the resulting graph will be disconnected (we leave a proof of this as an exercise).

But this isn't the only possible configuration for such a graph. The one on the right certainly isn't a path; you may recognize it as a "tree," though we won't define this term formally until later in this chapter.

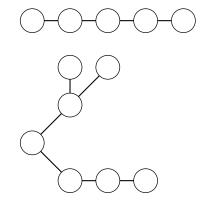
Indeed, removing any edge from this graph disconnects it, and you might notice by counting that the number of edges is again one fewer than the number of vertices.

It turns out that these examples do give us the right intuition: any connected graph G=(V,E) must have $|E|\geq |V|-1.^{18}$ The tricky part is proving this. Once again, we must struggle with the fact that even though the previous examples gave us some intuition, it is a challenge to generalize these examples to obtain an argument that works on all graphs satisfying these vertex and edge counts.

To get a formal proof, we'll need some way of characterizing exactly when we can remove an edge from a graph without disconnecting it. The following definition is an excellent start.

Definition 6.4. Let G = (V, E) be a graph. A cycle in G is a sequence of vertices v_0, \ldots, v_k satisfying the following conditions:

- ¹⁶ Or, how many edges are *sufficient* for graph connectedness.
- ¹⁷ Or, how many edges are *necessary* for graph connectedness.



¹⁸ The contrapositive is also an interesting statement: if a graph has fewer than |V|-1 edges, it cannot be connected.

- k ≥ 3
- $v_0 = v_k$, and all other vertices are distinct from each other and v_0
- · each consecutive pair of vertices is adjacent

In other words, a cycle is like a path, except it starts and ends at the same vertex. The length of a cycle is the number of edges used by the sequence, which is also the number of distinct vertices in the sequence (the above notation describes a cycle of length k). Cycles must have length at least three; two adjacent vertices are not considered to form a cycle.

To use our example of cities and roads, if there is a cycle in the graph, it is possible to make a trip which starts and ends at the same city, and travels no road or city more than once.

Getting back to our motivation, cycles are a form of "connectedness redundancy" in a graph. Vertices in a cycle are all obviously connected to each other, but even if one edge is removed, the result is a path. In this case, the cycle's vertices are still connected to each other—albeit with possibly a much longer path to travel. Even though the diagrams on the right illustrate this property for a cycle itself, we will now show that this property holds even when this cycle is part of a larger graph.

Example 6.8. Let G = (V, E) be a graph and $e \in E$. If G is connected and e is in a cycle of G, then the graph obtained by removing e from G is still connected.

Translation. There are a lot of quantified variables here, and some assumptions which are perhaps not obvious from the English. It is certainly a worthwhile exercise to translate this statement explicitly. The trickiest part is the condition on e (that it is part of a cycle of G); remember that we generally represent such conditions as assumptions in a logical implication.

For brevity, we will use the notation G - e to represent the graph obtained by removing edge e from G.

 $\forall G = (V, E), \ \forall e \in E, \ (G \text{ is connected} \land e \text{ is in a cycle of } G) \Rightarrow G - e \text{ is connected}.$

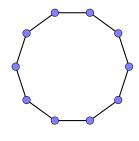
Discussion. This is a statement about a particular transformation: if we start with a connected graph and remove an edge in a cycle, then the resulting graph is still connected.

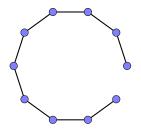
We get to assume that the original graph is connected and has a cycle, but that's it. We don't know anything else about the graph's structure, nor even which edge in the cycle e is.

That said, it seems like we should be able to simply make an argument based on the transitivity of connectedness: if we remove the edge (u, v) from the cycle, then we already know that u and v are still connected, so all the other vertices should still be connected too).

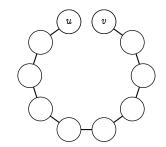
Proof. Let G = (V, E) be a graph, and $e \in E$ be an edge in the graph. Assume that G is connected and that e is in a cycle. Let $G' = (V, E \setminus \{e\})$ be the graph formed from G by removing edge e. We want to prove that G' is also connected, i.e., that any two vertices in V are connected in G'.

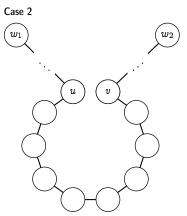
Let $w_1, w_2 \in V$. By our assumption, we know that w_1 and w_2 are connected in











G. We want to show that they are also connected in G', i.e., there is a path in G' between w_1 and w_2 .

Let P be a path between w_1 and w_2 in G (such a path exists by the definition of connectedness). We divide our proof into two cases: one where P uses the edge e, and another where it does not.

<u>Case 1</u>: P does not contain the edge e. Then P is a path in G' as well (since the only edge that was removed is e).

<u>Case 2</u>: P does contain the edge e. Let u be the endpoint of e which is closer to w_1 on the path P, and let v be the other endpoint.

This means that we can divide the path P into three parts: P_1 , the part from w_1 to u, the edge (u, v), and then P_2 , the part from v to w_2 . Since P_1 and P_2 cannot use the edge (u, v)—no duplicates—they must be paths in G' as well. So then w_1 is connected to u in G', and w_2 is connected to v in G'. But we know that u and v are also connected in G' (since they were part of the cycle), and so by the transitivity of connectedness, w_1 and w_2 are connected in G'.

This example tells us that if we have a connected graph with a cycle, it is always possible to remove an edge from the cycle and still keep the graph connected. Since we are interested in talking about the minimum number of edges necessary for connecting a graph, we'll now think about graphs which don't have any cycles.

Definition 6.5. A tree is a graph that is connected and has no cycles.

We would like to say that trees are the "minimally-connected" graphs: that is, the graphs which have the fewest number of edges possible but are still connected. It may be tempting to simply assert this based on the definition and what we have already proven, but let G be a connected graph, and consider the following statements carefully:

- 1. If G has a cycle, then there exists an edge e in G such that G e is connected.
- 2. If G is a tree, then it does not have a cycle.
- 3. If G does not have a cycle, then there does not exist an edge e in G such that G e is connected.

We know that (1) is true by the previous example. (2) is true simply by the definition of "tree." How do we know (3) is true?

In fact, we don't. The statements (1) and (3) may look very similar, but they are *not* logically equivalent. In fact, (3) is logically equivalent to the *converse* of (1): if we let P be the statement "G has a cycle" and Q be the statement "there exists an edge e in G such that G - e is connected," then (1) is simply $P \Rightarrow Q$, while (3) is $\neg P \Rightarrow \neg Q$.

So we actually need to prove (3) directly, which is what we'll do next.

Example 6.9. Let G be a graph. Prove that if G does not have a cycle, then there does not exist an edge e in G such that G - e is connected.

Translation.

 $\forall G = (V, E), G \text{ does not have a cycle} \Rightarrow \neg (\exists e \in E, G - e \text{ is connected}).$

In general, having to prove that there does not exist some object satisfying some given conditions is challenging; it is often easier to assume such an object exists, and then prove that its existence violates one or more of the given assumptions. This can be formalized by writing the contrapositive form of our original statement.

$$\forall G = (V, E), \ (\exists e \in E, \ G - e \text{ is connected}) \Rightarrow G \text{ has a cycle.}$$

Discussion. So we can assume that there exists an edge e with this nice property that removing it keeps the graph connected. From this, we need to prove that G has a cycle. Note that we only need to show that a cycle exists—it may or may not have anything to do with e, but it is probably a good bet that it does.

The key insight is that if we remove e, we remove one possible path between its endpoints. But since the graph must still be connected after removing e, there must be another path between its endpoints.

Proof. Let G = (V, E) be a graph. Assume that there exists an edge $e \in E$ such that G - e is still connected.

Let $G' = (V, E \setminus \{e\})$ be the graph obtained by removing e from G. Our assumption is that G' is connected.

Let u and v be the endpoints of e. By the definition of connectedness, there exists a path P in G' between u and v; this path does not use e, since e isn't in G'. Then taking the path P and adding the edge e to it is a cycle in G.

Thus we now can state and prove the following fact about trees.

Example 6.10. Let G be a tree. Prove that removing any edge from G disconnects the graph.

Proof. This follows directly from the previous claim. By definition, G does not have any cycles, and so there does not exist an edge that can be removed from Gwithout disconnecting it.

We can say that a tree is the "backbone" of a connected graph. While a connected graph may have many edges and many cycles, it is possible to identify an underlying tree structure in the graph that, if it remains unchanged, ensures the graph remains connected, regardless of any other edges removed. 19

Now, let us return to our original motivation of counting edges to prove the following remarkable result, which says that the number of edges in a tree depends only on the number of vertices.

Theorem 6.1. Let G = (V, E) be a tree. Then |E| = |V| - 1.

Translation.

$$\forall G = (V, E), G \text{ is a tree} \Rightarrow |E| = |V| - 1.$$

¹⁹ In fact, many such trees may exist. This insight is the basis of minimum spanning trees, a well-studied problem in computer science that you will learn about in future courses.

Discussion. We have previously observed that this property seems to hold on trees that we drew ourselves. But of course this is not a formal proof, since we cannot assume anything about the particular structure of a tree.

A natural alternate strategy is to take a tree, remove a vertex from it, and use induction to show that the resulting tree satisfies this relationship between its numbers of vertices and edges.

This only works, though, if we can pick a vertex whose removal from G results in a tree—and in particular, results in a connected graph. To do this, we need to pick a vertex that is at the "end" of the tree.

Rather than proceeding with the proof directly, we recognize that a likely claim we'll need to use in our proof is that picking such an "end" vertex is always possible. Rather than embedding a subproof within the main proof, we will do it separately first.

Lemma 6.2. Let G = (V, E) be a tree. If $|V| \geq 2$, then G has a vertex that has exactly one neighbour.

Translation.

 $\forall G = (V, E), (G \text{ is a tree} \land |V| \ge 2) \Rightarrow (\exists v \in V, v \text{ has exactly one neighbour}).$

Discussion. What does it mean for a vertex to have exactly one neighbour? Intuitively, it means that we're at the "end" of the tree, and can't go any further. This makes sense visually on a diagram, but how can we formalize this? Suppose we start at an arbitrary vertex, and traverse edges to try to get as far away from it as possible. Because there are no cycles, we cannot revisit a vertex. But the path has to end somewhere, so it seems like its endpoint must have just one neighbour.

Proof. Let G = (V, E) be a tree. Assume that $|V| \geq 2$. We want to prove that there exists a vertex $v \in V$ which has exactly one neighbour.

Let u be an arbitrary vertex in V. Let v be a vertex in G that is at the maximum possible distance from u, i.e., the path between v and u has maximum possible length (compared to paths between u and any other vertex). We will prove that v has exactly one neighbour.

Let P be the path between v between u. We know that v has at least one neighbour: the vertex immediately before it on P. v cannot be adjacent to any other vertex on P, as otherwise G would have a cycle. Also, v cannot be adjacent to any other vertex w not on P, as otherwise we could extend P to include w, and this would create a longer path.

And so v has exactly one neighbour (the one on P immediately before v).

With this lemma in hand, we can now give a complete proof of the number of edges in a tree. The key will be to use induction, removing from the original graph a vertex with just one neighbour, so that the number of edges also only changes by one. But how can we use induction on a statement that starts with $\forall G = (V, E)$? We are used to seeing induction used with a statement of the form $\forall n \in \mathbb{N}$ or $\forall n \in \mathbb{Z}^+$. To this end, we introduce a variable n to stand for the number of vertices in a graph, and then apply induction using the number of vertices. The statement that we will prove becomes

$$\forall n \in \mathbb{Z}^+, \ \forall G = (V, E), \ (G \text{ is a tree} \land |V| = n) \Rightarrow |E| = n - 1.$$

Proof. We will proceed by induction on n, the number of vertices in the tree. Let P(n) be the following statement (over positive integers):

$$P(n): \forall G = (V, E), (G \text{ is a tree} \land |V| = n) \Rightarrow |E| = n - 1.$$

We want to prove that $\forall n \in \mathbb{Z}^+, P(n)$.

<u>Case 1</u>: Let n=1. Let G=(V,E) be an arbitrary graph, and assume that G is a tree with one vertex.

In this case, G cannot have any edges. Then |E| = 0 = n - 1.

Case 2: Let $k \in \mathbb{Z}^+$, and assume that P(k) is true, i.e., for all graphs G = (V, E), if G is a tree and |V|=k, then |E|=k-1. We want to prove that P(k+1) is also true. Unpacking P(k+1), we get:

$$\forall G = (V, E), (G \text{ is a tree} \land |V| = k+1) \Rightarrow |E| = k.$$

So let G = (V, E) be a tree, and assume |V| = k + 1. We want to prove that |E|=k.

By the previous tree Lemma, since k+1 > 2, there exists a vertex $v \in V$ that has exactly one neighbour. Let G'=(V',E') be the graph obtained by removing vand the one edge on v from G. Then |V'| = |V| - 1 = k and |E'| = |E| - 1.

We know that G' is also a tree. Then the induction hypothesis applies, and we can conclude that |E'| = |V'| - 1 = k - 1.

This means that |E| = |E'| + 1 = k, as required.

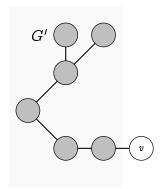
Combining everything together, we can conclude the following required number of edges for any connected graph.

Since every connected graph contains at least one tree (just keep removing edges in cycles until you cannot remove any more), this constraint on the numbers of edges in a tree translates immediately into a lower bound on the number of edges in any connected graph (in terms of the number of vertices of that graph).

Theorem 6.3. Let G = (V, E) be a graph. If G is connected, then $|E| \ge |V| - 1$.

Exercise Break!

- 6.7 Adapt the proof of the tree Lemma to prove that for any tree G = (V, E), if $|V| \geq 2$ then G has at least two vertices with exactly one neighbour.
- 6.8 Prove the following claim. Let G = (V, E) be a tree, and let v be a vertex in G that has exactly one neighbour. Prove that the graph obtained by removing v from G is also a tree.



- 6.9 (Longer) Let G = (V, E) be a graph. We say that a graph is approximately connected when it is connected, or when there exists a pair of distinct vertices $u, v \in V$ such that $G' = (V, E \cup \{(u, v)\})$ is connected.
 - a) Find, with proof, the maximum number M (in terms of |V|) such that if G has at least M edges, it must be approximately connected.
 - b) Find, with proof, the minimum number m (in terms of |V|) such that if G has fewer than m edges, it cannot be approximately connected.

Rooted trees

The definition of "tree" that we have used so far—a connected graph with no cycles—is actually more general than what you may be familiar with from typical computer science applications. This is because trees themselves do not enforce an orientation or ordering amongst vertices, while in practice almost all of their uses involve a notion of hierarchy that elevates some vertices above others.

For this type of application, we specialize our more general definition to add this notion of hierarchy. Note that this definition is a "cosmetic" one in the sense that it does not actually say anything different about the *structure* of a graph, but merely how we interpret the vertices of the graph.

Definition 6.6. A **rooted tree** is either an empty tree, or a tree that has exactly one vertex labelled as its **root**.²⁰

Simply by designating one vertex in a tree as special, we immediately obtain a sense of direction in the tree; we can now use distance from the root as a partial ordering of the vertices, and talk about moving "away from the root" or "towards the root" when traversing edges. We typically represent this sense of direction visually by drawing rooted trees with the root vertex at the top, although of course this is merely a convention.

We will now introduce some new terminology that emerge naturally from this orientation. Note that much of the terminology matches our intuition for relationships among relatives in a family tree.

Definition 6.7. Let G=(V,E) be a non-empty rooted tree, and $r\in V$ be the root of the tree. Let $v\in V$ be an arbitrary vertex (including, but not limited to, r itself).

The parent of v is its neighbour which is closer to r than v is. A **child** of v is any of its other neighbours (which are further from r than v is). 21

An ancestor of v is any vertex on the path between r and v, not including v itself. (Equivalently, an ancestor of v is its parent, its parent's parent, its parent's parent, etc.)

A descendant of v is any vertex w such that v is on the path between r and w. (Equivalently, a descendant of v is its child, its child's child, its child's child, etc.)

A leaf of a rooted tree is any vertex which has no children.²²

Example 6.11. Consider the rooted tree on the right.

²⁰ So when you hear the typical computer scientist talking about trees, they're really talking about rooted trees.

²¹ Equivalently, the parent is the vertex immediately before v on the path from r to v.

²² Note that all leaves of a rooted tree have at most one neighbour. The previous tree lemma can be used to show that each rooted tree has at least one leaf.



- 1. What is the parent of A?
- 2. What are the children of C?
- 3. What are the ancestors of B?
- 4. What are the ancestors of D?
- 5. What are the descendants of C?
- 6. What are the descendants of B?

Discussion. This is another simple check on the terminology.

The only ones of note are (4) and (6). Since vertex D is the root of the tree (remember the convention of drawing the root of the tree at the top of the diagram), it has no ancestors, and similarly, because B is a leaf, it has no descendants.

Definition 6.8. The height of a non-empty rooted tree is one plus the length of the longest path between the root and a leaf.²³ The "one plus" is to ensure that we are counting vertices instead of edges-e.g., a tree which consists of just the root vertex has height 1, not height 0.

The height of the *empty* rooted tree (i.e., a rooted tree with no vertices) is defined to be zero.

We have already studied the relationship between the numbers of vertices and edges in connected graphs. This question is far less interesting when it comes to trees, because there is an exact relationship between the number of vertices and edges in a tree (|E| = |V| - 1).

But for rooted trees, we get another fundamental relationship to study: how the number of vertices influences the height of the tree. This is a question which is fundamental to many computer science applications of rooted trees, which typically traverse a tree by starting at its root and going down. Such algorithms take a longer amount of time depending on how tall the tree is.

Theorem 6.4. Let $n \in \mathbb{N}$, and assume $n \geq 2$. Then the following statements hold.

- 1. Every rooted tree with n vertices has height ≥ 2 .
- 2. There exists a rooted tree with n vertices with height equal to 2.
- 3. Every rooted tree with n vertices has height $\leq n$.
- 4. There exists a rooted tree G with n vertices with height equal to n.

Discussion. Note that there are four different things to prove here. Two of them are universally-quantified statements, establishing universal bounds on the height of any rooted tree. Two of them are existentially-quantified statements, saying that the proposed bounds are tight, i.e., they can be met exactly.

These proofs are not very challenging, and we'll leave them as an exercise.²⁴

What is more interesting, and what is often done in practice, is to try to restrict the structure of a rooted tree by restricting the number of children each vertex can have. The following definition is one of the most common such restrictions.

Definition 6.9. A binary rooted tree is a rooted tree where every vertex has at most two children.²⁵

Our last proof in this course is captures one such relationship between height and number of vertices in binary rooted trees.

²³ Many texts define height as just the length of the longest path, which counts edges rather than vertices. It doesn't make a big difference, but counting vertices makes some of our future calculations look a little cleaner.

 $^{^{24}}$ Hint: think about the "extreme" of possible tree structures.

 $^{^{25}}$ This means each vertex has at most three neighbours in total: one parent, two children.

Example 6.12. Let $h \in \mathbb{N}$. Let G = (V, E) be a binary rooted tree, and assume that the height of G is $\leq h$. Then $|V| \leq 2^h - 1$.

Translation.

 $\forall h \in \mathbb{N}, \ \forall G = (V, E), \ (G \text{ is a binary rooted tree} \land G \text{ has height } \leq h) \Rightarrow |V| \leq 2^h - 1.$

Discussion. The key insight here is that binary rooted trees are themselves composed of smaller binary rooted trees. If we take G and remove its root, then we get obtain two binary rooted trees, both of which have height $\leq h-1$. We should then be able to use induction to prove the inequality.

Proof. We will prove this statement by induction on h. More precisely, let P(h) be the statement that for every binary rooted tree G=(V,E) of height $\leq h$, $|V| < 2^h - 1$.

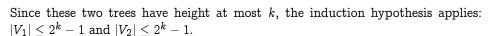
<u>Base case</u>: Let h = 0. In this case, the only binary rooted tree of height 0 is empty, i.e., has no vertices. Then |V| = 0 and $2^h - 1 = 0$, so the inequality holds.

Inductive Step: Let $k \in \mathbb{N}$, and assume that P(k) holds. We want to prove that P(k+1) is also true. More precisely, we can write:

 $P(k+1): \forall G=(V,E), (G \text{ is a binary rooted tree} \land G \text{ has height } \leq k+1) \Rightarrow |V| \leq 2^{k+1}-1.$

So let G = (V, E) be a binary rooted tree which has height $\leq k + 1$. We will show that $|V| \leq 2^{k+1} - 1$.

Let $r \in V$ be the root of G. Consider what happens when we remove r from G. We are left with two smaller binary rooted trees, $T_1 = (V_1, E_1)$ and $T_2 = (V_2, E_2)$. Note that one or both of these trees could be empty (i.e., have no vertices or edges), and this is perfectly acceptable.



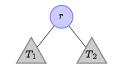
Then $|V| = |V_1| + |V_2| + 1$ (the number of vertices in each of the two smaller trees, plus the root):

$$|V| = |V_1| + |V_2| + 1$$

$$\leq (2^k - 1) + (2^k - 1) + 1$$

$$= 2 \cdot 2^k - 1$$

$$= 2^{k+1} - 1$$



7 Looking Ahead

There are many beautiful ideas in Computer Science that make fundamental use of mathematical expression and reasoning. While we cannot do justice to these topics in these notes (many of them are deep), we would like to give you a glimpse of the power of mathematical reasoning in Computer Science. You will learn these and other topics in depth in other Computer Science courses at University of Toronto, including CSC236/CSC240, CSC263/CSC265, CSC373, CSC438, CSC448, CSC463, and CSC473.

Turing's legacy: the limitations of computation

What are the limits of computation? Are there functions that we want to get a computer to calculate but that are beyond the capability of computers? This abstract and fuzzy question was formalized precisely by Alan Turing even before computers were invented! Namely, he defined a **Turing machine**, which is a purely mathematical model of computation. It is simple enough to reason about, yet powerful enough to capture any conceivable computational device!

After defining Turing machines, Turing proved that there are important problems that cannot be computed by any Turing machine. Because of the universality of the Turing machine, this then implies that these problems cannot be solved on any computer!

Before we try to explain the main ideas behind the proof, we would like to point out that mathematical expression is fundamental to even formulate the question. The abstraction of computation via the mathematical Turing machine model is essential to express a statement that talks about whether a given function can be computed.

The most famous problem that cannot be solved by any Turing machine (and thus by any computer) is called the *Halting Problem*. Informally, the input to the Halting Problem is a program, P, written in some programming language, together with an input to the program, x. The Halting Problem should output True for the pair (P, x) if and only if program P halts on input x. The obvious way to try to solve the Halting Problem on input (P, x) is to simply run or simulate P on the input x and see what happens. If P does halt on x, then our simulation will also halt and we will eventually discover that P halts on x. But what happens when P does not halt on x? In this case we are in trouble! What Turing proved is that it is basically impossible for a computer program to figure out with certainty whether an arbitrary program P will halt on a particular input x. That is, there is no clairvoyant way to examine a program to determine whether not it will halt

¹ By halt we mean that if we had an infinite amount of memory, then running P on x would eventually stop—that is, it would not get into any infinite loops.

² This is a worst-case result: there is no procedure that can decide for all programs P and for all inputs x whether or not P halts on x. But in special cases, it may be easy to determine what will happen.

on an input. Essentially the only thing that one can do is to run the program and see what happens.

We will focus on decision problems; that is, on problems that compute functions f from the natural numbers to $\{0,1\}$. Since we want to prove a negative result, we can pick any problem that we'd like, so we aren't cheating by focusing on decision problems.³ Furthermore, we will assume that the input to our decision problem is encoded in binary, so the input is just some finite-length string of zeroes and ones, and the output is either zero (False) or one (True). We are going to try to explain the main ideas behind the halting problem without getting into too much notation.

First, we have to define our formal model of computation, the Turing machine (TM). We won't go into any details of Turing machines. They are a beautiful abstraction of computation, but these details aren't really necessary to understand the main thing that we want to prove in this chapter—that certain natural and important functions are beyond the power of computation. The only thing that you will need to know about Turing machines is that they are just programs in a simple programming language where we will assume an unbounded amount of computational memory. If M is a TM for computing a decision problem, it takes as input an arbitrary natural number, encoded by a binary string, s. For each s, the TM may or may not halt on s. If it does halt, then it outputs either zero (reject) or one (accept). Turing machines satisfy the following important properties:

- 1. Turing machines are a universal model of computation—any program written in any standard programming language can be converted to an equivalent Turing machine (TM) program.
- 2. Turing machines can be enumerated.⁴

Both of these properties are not unreasonable—if you think of your favorite programming language, such as Python, it should be clear that both of these properties hold.

The first main idea is to come up with one explicit decision problem that cannot be computed by a TM. This first problem will not be the Halting Problem but will instead be a problem that we will construct to make the proof easier for us.⁵ By property (2) above, TM programs can be enumerated, so let us write them as M_1, M_2, \ldots , where M_i is the i^{th} TM in the enumeration. Now consider the following decision problem, called \mathcal{D} (for the diagonal language): The input to \mathcal{D} is, as usual, a natural number i (encoded in binary). The output is 1 if either M_i does not halt on input i, or if M_i halts and outputs 0 on input i. Otherwise, if M_i halts and outputs 1 on i, then D on i outputs 0. In other words, \mathcal{D} does the opposite of what M_i does on input i—if M_i rejects i (either by not halting or by halting and not accepting), then \mathcal{D} accepts i, and if M_i accepts input i, then \mathcal{D} rejects i. The very cool thing is that we can prove that the decision problem \mathcal{D} is not computed by any TM! Why is this? We want to prove that for every $j \in \mathbb{N}$, that M_j does not compute \mathcal{D} . So fix some arbitrary $j \in \mathbb{N}$, and consider M_j on input j—by construction it does the opposite thing that \mathcal{D} does on input j, and therefore M_j does not compute \mathcal{D} . Since we have proven this for every j, it follows that there is no Turing machine that computes $\mathcal{D}!^{6}$

Okay, so thus far we have found one explicit decision problem, \mathcal{D} , that cannot be computed by any TM. Now we want to prove that some specific decision problem

³ Indeed, decision problems turn out to be powerful enough anyway! That is, for any $f: \mathbb{N} \to \mathbb{N}$, there is a corresponding decision problem such that this problem can be computed if and only if the original function f can be computed.

⁴ By enumerated we mean that there is an algorithm that on input i can output the first i TM's, M_1 , M_2 , ...,

⁵ The proof method is called diagonalization, and was first used by Cantor in order to argue there is no bijective mapping from the natural numbers to the real numbers.

⁶ The main point here is that the set of all functions from the natural numbers to $\{0,1\}$ is huge—much, much larger than the set of all Turing machines since we have assumed that they can be enumerated Thus, at a high level the idea is the same as Cantor's, but here we are showing

(the Halting Problem) also cannot be computed by any TM. At this point, we need to be more precise about what we mean by the Halting Problem. We define the Halting Problem \mathcal{H} , as follows. The input is a pair (i,j) where both i and jare natural numbers. The output should be 1 (accept) if M_i halts on input j, and should be 0 (reject) otherwise.

To show that \mathcal{H} is not computable by any TM, we will introduce a second idea called a reduction that is extremely powerful and used extensively in Computer Science. In fact, you've seen this idea already although it didn't have this fancy name—it is none other than a proof by contradiction. Say that we want to prove $\neg A$, and we already know $\neg B$. Suppose that we can prove $A \Rightarrow B$. Then assume for sake of contradiction that A is true, thus by modus ponens it follows that Bis true, which contradicts $\neg B$. To instantiate this in our setting, we let B be the statement that \mathcal{D} is computable by some TM, and let A be the statement that \mathcal{H} is computable by a TM. Since we have already proven $\neg B$, it is just left to prove $A \Rightarrow B$; that is, we want to prove that if \mathcal{H} is computable by a TM, then \mathcal{B} is also computable by a TM, in order to get a contradiction and therefore conclude that \mathcal{H} is not computable. For this choice of A and B, proving $A \Rightarrow B$ is called a reduction (from B to A) because we are showing that computing B essentially reduces to the task of computing A.

So our remaining task is therefore to show that if we can compute \mathcal{H} , then we can compute \mathcal{D} by a TM. Here we will have to wave our hands a little bit, since we haven't even formally defined Turing machines! But we did say that they satisfy property (1), and thus we will argue informally that if we have an algorithm for \mathcal{H} , then we can also construct an algorithm for \mathcal{D} . How would we compute \mathcal{D} in the first place? Remember that the input is a number i, and we want to determine of M_i halts and accepts i. The first step on input i is to actually find the TM program M_i . This can be carried out by enumerating all TMs until we get to the i^{th} one.⁸

Now that we have M_i , how can we tell if M_i accepts i? If we just simulate M_i on input i, we may run into a problem if M_i doesn't halt on i since in that case our simulation will run forever and we will never know when to stop the simulation and output 1. But we are saved by the fact that we are assuming that we have an algorithm for \mathcal{H} ! Thus we can first run the algorithm for \mathcal{H} on the input pair (i,i). If it accepts, then we know that M_i halts on i, so in this case we can go ahead and simulate M_i on i, and return the opposite answer. If on the other hand the algorithm for \mathcal{H} on (i, i) rejects, then we know that M_i does not halt on i, so we should just return 1 (and not bother to do the simulation). Thus informally we have argued that if \mathcal{H} is computed by some TM, then \mathcal{D} is also computed by some TM, so we can conclude that \mathcal{H} is not computable!

Other undecidable problems

Using this idea of a reduction, we can now prove that many other problems of interest are also not computable by any Turing machine. One of the most famous of these problems is called Hilbert's Tenth Problem. In 1900, the Second International Congress of Mathematicians was held in Paris, France, where David Hilbert, one of the greatest mathematicians in the world, was invited to deliver one of the main lectures. His lecture has become very famous because in his lecture, entitled "Mathematical Problems," he formulated 23 major mathematical problems that he

⁷ But we said that inputs should be single numbers and not pairs of numbers! To handle this, we can encode a pair of numbers (i, j) by the single number $2^i \times 3^j$. Check that i and j can be uniquely extracted from 2×3^{j} .

⁸ This is very inefficient by it will suffice for our purposes here. There are much more efficient ways to do this.

felt were the most important open problems in all of mathematics to be studied in the coming century. Several of them have turned out to be very influential for mathematics of the 20th century. Some famous examples are: determining the truth or falsity of the continuum hypothesis, the Reimann hypothesis, formulating the axioms of physics, and proving that the axioms of arithmetic are consistent.

One of the most important is his tenth problem, called "Determining the solvability of a Diophantine equation" and asks, given a polynomial equation with any number of variables and integer coefficients, to devise an algorithm to determine whether the equation has an integer solution. This was open for a very long time until in 1970 Yuri Matiyasevich finally resolved Hilbert's tenth problem by proving that it has no solution since it is undecidable! The proof is a complicated reduction using insights from Julia Robinson, and a connection to Fibonacci numbers.

Gödel's legacy: the limitations of proofs

Another very famous problem that is not computable is called the Entscheidungsproblem. Informally, this is the problem of determining whether or not a mathematical statement is valid. We start with a fixed set of axioms (such as the axioms of Peano arithmetic, the most standard set of axioms for reasoning in number theory). The input is a mathematical sentence s, and the output should be 0 (reject) if s is not a logical consequence of the axioms, and 1 (accept) if s is a logical consequence of the axioms. This problem is undecidable by Matiyasevich's theorem, since the existence of solutions for Diophantine equations are a special type of mathematical statement. However, it is also possible give a simpler reduction showing that the Entscheidung problem is undecidable. Philosophically this is quite interesting as it proves that mathematics cannot be fully automated.

Closely connected to the Entscheidung problem is Hilbert's second problem, to prove that the axioms of arithmetic are consistent. In 1931 Kurt Gödel proved his famous incompleteness theorems, essentially showing that there is no reasonable set of axioms that can capture 10 all sentences that are true about the natural numbers. While his proof did not mention anything about computers or computability, we now know that his theorems are in fact very closely connected to undecidability, and can be proven using the ideas of reductions.

P versus NP

In the 60's and 70's, the complexity class \mathcal{P} emerged. It captures those decision problems that can be computed efficiently—where the number of basic computation steps in order to arrive at the answer is at most polynomial in the input length. That is, the runtime is $n^{O(1)}$. There are many examples of important problems in \mathcal{P} and you will study them in many of your courses. For example all of these problems have polynomial-time algorithms: detecting whether a graph contains a cycle, determining whether a graph contains a perfect matching, and computing the greatest common divisor of two numbers. A larger class of decision problems is known as \mathcal{NP}^{11} and contains important problems such as whether a graph contains a clique of size n/2, and whether there is a boolean assignment to the variables of a propositional formula forcing it to true. \mathcal{NP} -complete problems are the hardest problems in the class \mathcal{NP} and the best algorithms for these prob-

⁹ Entscheidung is the German word for "decision."

¹⁰ By "capture" we mean that the set of sentences that are logically consequences of the axioms should be exactly those sentences that are true over the natural numbers.

 $^{^{11} \}mathcal{NP}$ stands for nondeterministic polynomial time

lems run in time that is exponential in n—that is, in time $2^{O(n)}$. The class \mathcal{NP} is very important because it contains many many important problems that range across all disciplines, including fundamental problems in computational biology, physics, machine learning, and of course computer science. For all of these problems, all known algorithms run in exponential time, which makes them completely infeasible to solve. On the other hand, it is not known if it is possible to solve these problems much more efficiently, say in polynomial time. The \mathcal{P} versus \mathcal{NP} problem is the open problem of whether or not any of the \mathcal{NP} -complete problems can be solved in polynomial time, and is one of the most important open problems in mathematics and computer science today. 12

Other cool applications: Cryptography

As we mentioned in the introduction to these notes, cryptography is the study of algorithms and protocols for doing cool things across the Internet in the presence of adversaries. The techniques and tools that have been developed in cryptography are often very surprising and incredibly creative. Cryptography is in some sense the flip side of complexity theory. Whereas lower bounds in complexity theory prove that certain problems are inherently hard in that they require an infeasible amount of time in order to solve, cryptography uses this hardness in order to develop protocols! That is, who are these adversaries anyway? They are people or other computers, and thus they are limited to performing polynomialtime computation. In cryptography, the computational hardness of problems is used to an advantage—to build protocols for various tasks, where the security of the protocols can be proven under the assumptions that the adversaries are polynomially-bounded, and that certain problems in complexity theory are infeasible.

¹² It turns out that if one can get a polynomial-time algorithm for any \mathcal{NP} -complete problem, then all problems in \mathcal{NP} also have efficient algorithms. This was proving by Cook and independently by Levin in the early 70's.