CSC 311: Introduction to Machine Learning Lecture 3 - Bagging, Linear Models I

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Outline

1 Introduction

- **2** Bias-Variance Decomposition
- 3 Bagging
- 4 Linear Regression
- **5** Vectorization
- 6 Optimization
- **7** Feature Mappings
- 8 Regularization

- HW1 is due on June 05 (10% late penalty for each late day, no credit after 3 days).
- I have arranged TA office hours (on website) for the assignment.
- Go to the earliest possible ones you can attend.
- Manage your time well! If you wait till the last TA session, you may a long wait to ask your question.

Today

- Today we will introduce ensembling methods that combine multiple models and can perform better than the individual members.
 - ▶ We've seen many individual models (KNN, decision trees)
- We will see bagging:
 - ▶ Train models independently on random "resamples" of the training data.
- We will introduce linear regression, our first parametric learning algorithm.
 - ▶ This will exemplify how we'll think about learning algorithms for the rest of the course.





3 Bagging

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- prediction y at a query **x** is a random variable (where the randomness comes from the choice of dataset),
- y_{\star} is the optimal deterministic prediction, and
- t is a random target sampled from the true conditional $p(t|\mathbf{x})$.

$$\mathbb{E}[(y-t)^2] = \underbrace{(y_{\star} - \mathbb{E}[y])^2}_{\text{bias}} + \underbrace{\operatorname{Var}(y)}_{\text{variance}} + \underbrace{\operatorname{Var}(t)}_{\text{Bayes error}}$$

Bias/Variance Decomposition



Bias/variance decomposes the expected loss into three terms:

- bias: how wrong the expected prediction is (corresponds to under-fitting)
- variance: the amount of variability in the predictions (corresponds to over-fitting)

• Bayes error: the inherent unpredictability of the targets Often loosely use "bias" for "under-fitting" and "variance" for "over-fitting".

Visualizing Bias/Variance Decomposition

An overly **simple** model (e.g. KNN with large k) might have

• high bias

(cannot capture the structure in the data)

• low variance

(enough data to get stable estimates)



Visualizing Bias/Variance Decomposition

An overly **complex** model (e.g. KNN with k = 1) might have

• low bias

(learns all the relevant structure)

• high variance

(fits the quirks of the data you happened to sample)



Bias/Variance Decomposition: Another Visualization

• The following graphic summarizes the previous two slides:



A: Bayes error



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Bagging Motivation

- Sample m independent training sets from p_{sample} .
- Compute the prediction y_i using each training set.
- Compute the average prediction $y = \frac{1}{m} \sum_{i=1}^{m} y_i$.
- How does this affect the three terms of the expected loss?
 - Bias: unchanged, since the averaged prediction has the same expectation

$$\mathbb{E}[y] = \mathbb{E}\left[\frac{1}{m}\sum_{i=1}^{m} y_i\right] = \mathbb{E}[y_i]$$

Variance: reduced,

since we are averaging over independent predictions

$$\operatorname{Var}[y] = \operatorname{Var}\left[\frac{1}{m}\sum_{i=1}^{m} y_i\right] = \frac{1}{m^2}\sum_{i=1}^{m}\operatorname{Var}[y_i] = \frac{1}{m}\operatorname{Var}[y_i].$$

 Bayes error: unchanged, since we have no control over it

Intro ML (UofT)

- In practice, p_{sample} is often expensive to sample from. So training separate models on independently sampled datasets is very wasteful of data!
- Given training set \mathcal{D} , use the empirical distribution $p_{\mathcal{D}}$ as a proxy for p_{sample} . This is called bootstrap aggregation or bagging.
 - Take a dataset \mathcal{D} with n examples.
 - ▶ Generate *m* new datasets ("resamples" or "bootstrap samples")
 - Each dataset has n examples sampled from \mathcal{D} with replacement.
 - \blacktriangleright Average the predictions of models trained on the m datasets.
- One of the most important ideas in statistics!
 - Intuition: As $|\mathcal{D}| \to \infty$, we have $p_{\mathcal{D}} \to p_{\text{sample}}$.

Bagging Example 1/2

Create m = 3 datasets by sampling from D with replacement. Each dataset contains n = 7 examples.



Bagging Example 2/2

Generate prediction y_i using dataset D_i . Average the predictions.



- Classifier i outputs a prediction y_i
- y_i can be real-valued $y_i \in [0,1]$ or a binary value $y_i \in \{0,1\}$
- Average the predictions and apply a threshold.

$$y_{\text{bagged}} = \mathbb{I}\left(\frac{1}{m}\sum_{i=1}^{m}y_i > 0.5\right)$$

• Same as majority vote.

Bagging Properties

- A bagged classifier can be stronger than the average model.
 - ▶ E.g. on "Who Wants to be a Millionaire", "Ask the Audience" is much more effective than "Phone a Friend".
- But, if m datasets are NOT independent, don't get the $\frac{1}{m}$ variance reduction.
- Reduce correlation between datasets by introducing *additional* variability
 - Invest in a diversified portfolio, not just one stock.
 - Average over multiple algorithms, or multiple configurations of the same algorithm.

- A trick to reduce correlation between bagged decision trees: For each node, choose a random subset of features and consider splits on these features only.
- Probably the best black-box machine learning algorithm.
 - works well with no tuning.
 - widely used in Kaggle competitions.

Reduces over-fitting by averaging predictions.

In most competition winners.

A small ensemble often better than a single great model.

Limitations:

- Does not reduce bias in case of squared error.
- Correlation between classifiers means less variance reduction. Add more randomness in Random Forests.
- Weighting members equally may not be the best. Weighted ensembling often leads to better results if members are very different.



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Overview

- Third learning algorithm of the course: linear regression.
 - ► Task: predict scalar-valued targets (e.g. stock prices)
 - ► Architecture: linear function of the inputs
- While KNN was a complete algorithm, linear regression exemplifies a modular approach that will be used throughout this course:
 - choose a model describing the relationships between variables of interest
 - define a loss function quantifying how bad the fit to the data is
 - choose a regularizer saying how much we prefer different candidate models (or explanations of data)
 - ▶ fit a model that minimizes the loss function and satisfies the constraint/penalty imposed by the regularizer, possibly using an optimization algorithm
- Mixing and matching these modular components give us a lot of new ML methods.

Supervised Learning Setup



In supervised learning:

- There is input $\mathbf{x} \in \mathcal{X}$, typically a vector of features (or covariates)
- There is target $t \in \mathcal{T}$ (also called response, outcome, output, class)
- Objective is to learn a function $f : \mathcal{X} \to \mathcal{T}$ such that $t \approx y = f(\mathbf{x})$ based on some data $\mathcal{D} = \{(\mathbf{x}^{(i)}, t^{(i)}) \text{ for } i = 1, 2, ..., N\}.$

• Model: In linear regression, we use a *linear* function of the features $\mathbf{x} = (x_1, \ldots, x_D) \in \mathbb{R}^D$ to make predictions y of the target value $t \in \mathbb{R}$:

$$y = f(\mathbf{x}) = \sum_{j} w_j x_j + b$$

- y is the prediction
- w is the weights
- ► b is the bias (or intercept)
- w and b together are the parameters
- We hope that our prediction is close to the target: $y \approx t$.

What is Linear? 1 feature vs D features



- If we have only 1 feature: y = wx + b where $w, x, b \in \mathbb{R}$.
- y is linear in x.

- If we have D features: $y = \mathbf{w}^{\top} \mathbf{x} + b$ where $\mathbf{w}, \mathbf{x} \in \mathbb{R}^{D}$, $b \in \mathbb{R}$
- y is linear in **x**.

Relation between the prediction y and inputs \mathbf{x} is linear in both cases.

Linear Regression - Loss Function

- A loss function $\mathcal{L}(y,t)$ defines how bad it is if, for some example **x**, the algorithm predicts y, but the target is actually t.
- Squared error loss function:

$$\mathcal{L}(y,t) = \frac{1}{2}(y-t)^2$$

- y t is the residual, and we want to make this small in magnitude
- The $\frac{1}{2}$ factor is just to make the calculations convenient.
- Cost function: loss function averaged over all training examples

$$\begin{aligned} \mathcal{J}(\mathbf{w}, b) &= \frac{1}{2N} \sum_{i=1}^{N} \left(y^{(i)} - t^{(i)} \right)^2 \\ &= \frac{1}{2N} \sum_{i=1}^{N} \left(\mathbf{w}^\top \mathbf{x}^{(i)} + b - t^{(i)} \right)^2 \end{aligned}$$

• Terminology varies. Some call "cost" *empirical* or *average loss*.

Intro ML (UofT)

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Vectorization

• The prediction for one data point can be computed using a for loop:

```
y = b
for j in range(M):
    y += w[j] * x[j]
```

• Excessive super/sub scripts are hard to work with, and Python loops are slow, so we vectorize algorithms by expressing them in terms of vectors and matrices.

$$\mathbf{w} = (w_1, \dots, w_D)^\top$$
 $\mathbf{x} = (x_1, \dots, x_D)^\top$
 $y = \mathbf{w}^\top \mathbf{x} + b$

• This is simpler and executes much faster:

y = np.dot(w, x) + b

Why vectorize?

- The equations, and the code, will be simpler and more readable. Gets rid of dummy variables/indices!
- Vectorized code is much faster
 - Cut down on Python interpreter overhead
 - ▶ Use highly optimized linear algebra libraries (hardware support)
 - ▶ Matrix multiplication very fast on GPU (Graphics Processing Unit)

Switching in and out of vectorized form is a skill you gain with practice

- Some derivations are easier to do element-wise
- Some algorithms are easier to write/understand using for-loops and vectorize later for performance

Vectorization

• We can organize all the training examples into a design matrix **X** with one row per training example, and all the targets into the target vector **t**.



• Computing the predictions for the whole dataset:

$$\mathbf{X}\mathbf{w} + b\mathbf{1} = \begin{pmatrix} \mathbf{w}^T \mathbf{x}^{(1)} + b \\ \vdots \\ \mathbf{w}^T \mathbf{x}^{(N)} + b \end{pmatrix} = \begin{pmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{pmatrix} = \mathbf{y}$$

Vectorization

• Computing the squared error cost across the whole dataset:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + b\mathbf{1}$$
$$\mathcal{J} = \frac{1}{2N} \|\mathbf{y} - \mathbf{t}\|^2$$

- Sometimes we may use $\mathcal{J} = \frac{1}{2} ||\mathbf{y} \mathbf{t}||^2$, without a normalizer. This would correspond to the sum of losses, and not the averaged loss. The minimizer does not depend on N (but optimization might!).
- We can also add a column of 1's to design matrix, combine the bias and the weights, and conveniently write

$$\mathbf{X} = \begin{bmatrix} 1 & [\mathbf{x}^{(1)}]^{\top} \\ 1 & [\mathbf{x}^{(2)}]^{\top} \\ 1 & \vdots \end{bmatrix} \in \mathbb{R}^{N \times (D+1)} \text{ and } \mathbf{w} = \begin{bmatrix} b \\ w_1 \\ w_2 \\ \vdots \end{bmatrix} \in \mathbb{R}^{D+1}$$

Then, our predictions reduce to $\mathbf{y} = \mathbf{X}\mathbf{w}$.

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Solving the Minimization Problem

Our goal is to minimize the cost function $\mathcal{J}(\mathbf{w})$.

Recall from calculus: the minimum of a smooth function (if it exists) occurs at a critical point, i.e. point where the derivative is zero.

$$\nabla_{\mathbf{w}} \mathcal{J} = \frac{\partial \mathcal{J}}{\partial \mathbf{w}} = \begin{pmatrix} \frac{\partial \mathcal{J}}{\partial w_1} \\ \vdots \\ \frac{\partial \mathcal{J}}{\partial w_D} \end{pmatrix}$$

Solutions may be direct or iterative.

- Direct solution: set the gradient to zero and solve in closed form directly find provably optimal parameters.
- Iterative solution: repeatedly apply an update rule that gradually takes us closer to the solution.

Direct Solution: Calculus

- Lets consider a cartoon visualization of $\mathcal{J}(w)$ where w is single dimensional
- Left We seek $w = w^*$ that minimizes $\mathcal{J}(w)$
- **Right** The gradients of a function can tell us where the maxima and minima of functions lie
- Strategy: Write down an algebraic expression for $\nabla_w \mathcal{J}(w)$. Set equation to 0. Solve for w



Direct Solution: Calculus

- We seek w to minimize $\mathcal{J}(\mathbf{w}) = \frac{1}{2} \|\mathbf{X}\mathbf{w} \mathbf{t}\|^2$
- Taking the gradient with respect to \mathbf{w} and setting it to $\mathbf{0}$, we get:

$$abla_{\mathbf{w}} \mathcal{J}(\mathbf{w}) = \mathbf{X}^{\top} \mathbf{X} \mathbf{w} - \mathbf{X}^{\top} \mathbf{t} = \mathbf{0}$$

See course notes for additional details.

• Optimal weights:

$$\mathbf{w}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{t}$$

• Linear regression is one of only a handful of models in this course that permit direct solution.

- Many optimization problems don't have a direct solution.
- A more broadly applicable way to minimize the cost function: gradient descent.
- Gradient descent is an iterative algorithm, which means we apply an update repeatedly until some criterion is met.
- We initialize the weights to something reasonable (e.g. all zeros) and repeatedly adjust them in the direction of steepest descent.

Gradient Descent

- Observe:
 - if $\partial \mathcal{J}/\partial w_j > 0$, then decreasing \mathcal{J} requires decreasing w_j .
 - if $\partial \mathcal{J}/\partial w_j < 0$, then decreasing \mathcal{J} requires increasing w_j .



• The following update always decreases the cost function for small enough α (unless $\partial \mathcal{J} / \partial w_j = 0$):

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{J}}{\partial w_j}$$
Gradient Descent

• The following update always decreases the cost function for small enough α (unless $\partial \mathcal{J} / \partial w_j = 0$):

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{J}}{\partial w_j}$$

- $\alpha > 0$ is a learning rate (or step size).
 - The larger α is, the faster **w** changes.
 - ▶ Values are typically small, e.g. 0.01 or 0.0001.
 - We'll see later how to tune the learning rate.
 - If cost is the total loss rather than average loss, a smaller learning rate will be needed (α' = α/N).

Gradient Descent

• Gradient descent gets its name from the gradient. Recall the definition of the gradient:

$$\nabla_{\mathbf{w}} \mathcal{J} = \frac{\partial \mathcal{J}}{\partial \mathbf{w}} = \begin{pmatrix} \frac{\partial \mathcal{J}}{\partial w_1} \\ \vdots \\ \frac{\partial \mathcal{J}}{\partial w_D} \end{pmatrix}$$

The gradient is the direction of fastest *increase* in \mathcal{J} .

• Update rule in vector form:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}$$

• Update rule for linear regression:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) \, \mathbf{x}^{(i)}$$

Gradient descent updates w in the direction of fastest *decrease*.
Once it converges, we get a critical point, i.e. ∂J/∂w = 0.

Intro ML (UofT)

- GD is applicable to a much broader set of models
- GD is easier to implement than direct solutions
- For regression in high-dimensional space, GD is more efficient than direct solution
 - ► For example, the linear regression direction solution $(\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{t}$ requires matrix inversion, which is $\mathcal{O}(D^3)$.
 - ▶ Each GD update costs $\mathcal{O}(ND)$ or less with stochastic gradient descent.
 - Huge difference if $D \gg 1$

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Feature Mapping (Basis Expansion)

Can we use linear regression to model a non-linear relationship?



- Map the input features to another space using $\psi(\mathbf{x}) : \mathbb{R}^D \to \mathbb{R}^d$.
- Treat the mapped feature (in \mathbb{R}^d) as the input of a linear regression procedure.

Polynomial Feature Mapping

Fit the data using a degree-M polynomial function of the form:

$$y = w_0 + w_1 x + w_2 x^2 + \dots + w_M x^M = \sum_{i=0}^M w_i x^i$$

- The feature mapping is $\boldsymbol{\psi}(x) = [1, x, x^2, ..., x^M]^{\top}$.
- $y = \psi(x)^{\top} \mathbf{w}$ is linear in w_0, w_1, \dots
- Use linear regression to find **w**.
- In general, ψ can be any function. Another example: $\psi(x) = [1, \sin(2\pi x), \cos(2\pi x), \sin(4\pi x), ...]^{\top}$.



 $y = w_0$



-Pattern Recognition and Machine Learning, Christopher Bishop.

$$y = w_0 + w_1 x$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Model Complexity and Generalization



Under-fitting (M=0): Model is too simple, does not fit the data. Good model (M=3): Achieves small test error, generalizes well. Over-fitting (M=9): Model is too complex, fits perfectly.



Model Complexity and Generalization



- As *M* increases, the magnitude of coefficients gets larger.
- For M = 9, the coefficients have become finely tuned to the data.
- Between data points, the function exhibits large oscillations.

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- The degree M of the polynomial controls the model's complexity.
- The value of M is a hyperparameter for polynomial expansion, just like k in KNN. We can tune it using a validation set.
- Restricting the number of parameters / basis functions (M) is a crude approach to controlling the model complexity.
- Another approach: keep the model large, but regularize it
 - ▶ Regularizer: a function that quantifies how much we prefer one hypothesis vs. another

L^2 (or ℓ_2) Regularization

• Encourage the weights to be small by choosing the L^2 penalty as our regularizer.

$$\mathcal{R}(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|_2^2 = \frac{1}{2} \sum_j w_j^2.$$

• The regularized cost function makes a tradeoff between the fit to the data and the norm of the weights.

$$\mathcal{J}_{\text{reg}}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \lambda \mathcal{R}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \frac{\lambda}{2} \sum_{j} w_{j}^{2}$$

- If you fit training data poorly, \mathcal{J} is large. If the weights are large in magnitude, \mathcal{R} is large.
- Large λ penalizes weight values more.
- λ is a hyperparameter we can tune with a validation set.

Intro ML (UofT)

L^2 (or ℓ_2) Regularization

• The geometric picture:



L^2 Regularized Least Squares: Ridge regression

For the least squares problem, we have $\mathcal{J}(\mathbf{w}) = \frac{1}{2N} \|\mathbf{X}\mathbf{w} - \mathbf{t}\|^2$.

• When $\lambda > 0$ (with regularization), regularized cost gives

$$\begin{split} \mathbf{w}_{\lambda}^{\text{Ridge}} &= \operatorname*{argmin}_{\mathbf{w}} \mathcal{J}_{\text{reg}}(\mathbf{w}) = \operatorname*{argmin}_{\mathbf{w}} \frac{1}{2N} \|\mathbf{X}\mathbf{w} - \mathbf{t}\|_{2}^{2} + \frac{\lambda}{2} \|\mathbf{w}\|_{2}^{2} \\ &= (\mathbf{X}^{\top}\mathbf{X} + \lambda N\mathbf{I})^{-1} \mathbf{X}^{\top} \mathbf{t} \end{split}$$

- The case $\lambda = 0$ (no regularization) reduces to least squares solution!
- Can also formulate the problem as

$$\underset{\mathbf{w}}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{t}\|_{2}^{2} + \frac{\lambda}{2} \|\mathbf{w}\|_{2}^{2}$$

with solution

$$\mathbf{w}_{\lambda}^{\text{Ridge}} = (\mathbf{X}^{\top}\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^{\top}\mathbf{t}.$$

Gradient Descent under the L^2 Regularization

.

• Gradient descent update to minimize \mathcal{J} :

$$\mathbf{w} \leftarrow \mathbf{w} - lpha rac{\partial}{\partial \mathbf{w}} \mathcal{J}$$

 The gradient descent update to minimize the L² regularized cost *J* + λ*R* results in weight decay:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial}{\partial \mathbf{w}} \left(\mathcal{J} + \lambda \mathcal{R} \right)$$
$$= \mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \frac{\partial \mathcal{R}}{\partial \mathbf{w}} \right)$$
$$= \mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \mathbf{w} \right)$$
$$= (1 - \alpha \lambda) \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}$$

Linear regression exemplifies recurring themes of this course:

- choose a model and a loss function
- formulate an optimization problem
- solve the minimization problem using one of two strategies
 - direct solution (set derivatives to zero)
 - gradient descent
- vectorize the algorithm, i.e. represent in terms of linear algebra
- make a linear model more powerful using features
- improve the generalization by adding a regularizer