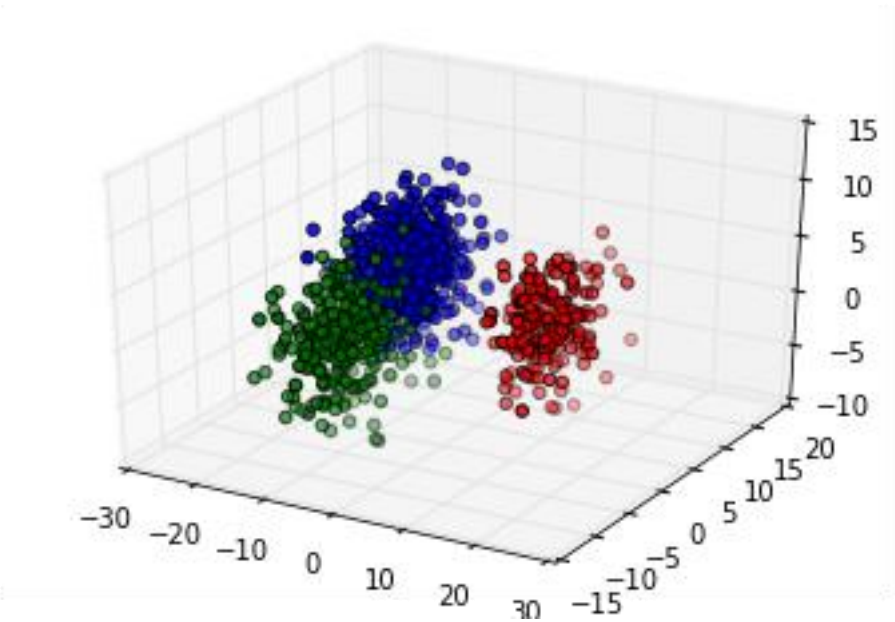
Mixtures of Gaussians and EM



CSC411/2515: Machine Learning and Data Mining, Winter 2018

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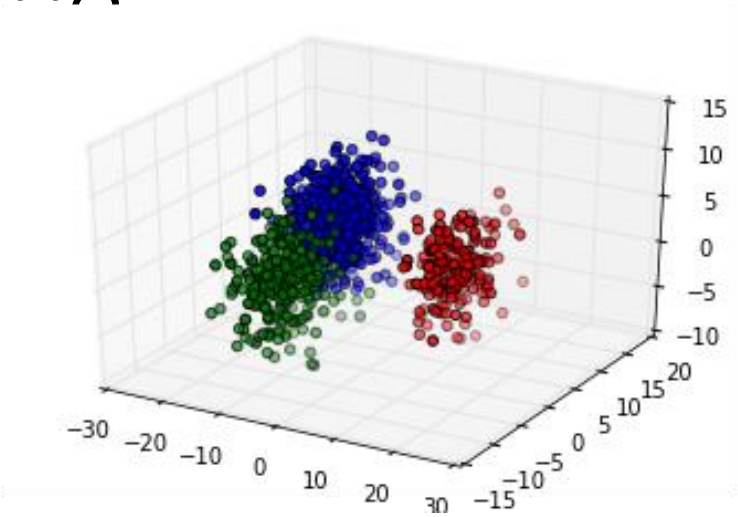
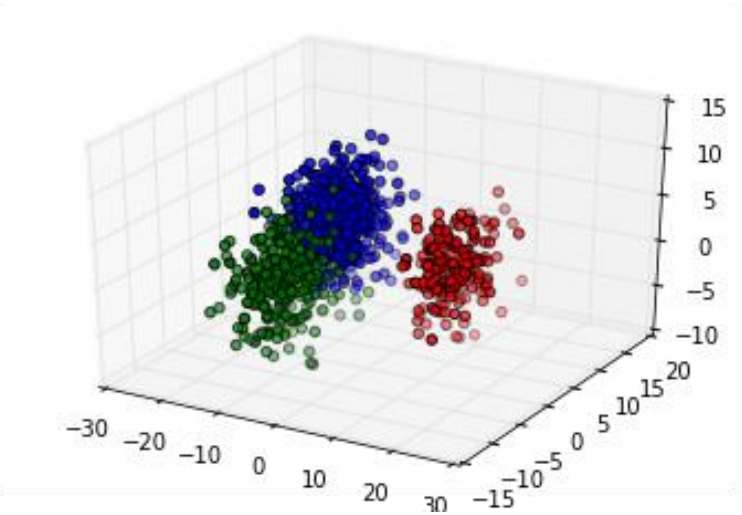
Unsupervised Learning



- Suppose the data (i.e., x's) belongs to different classes, but we don't have the labels (i.e., we don't have the y's)
- Won't to characterize the different x's somehow (e.g., "$x^{(i)}$ belongs to cluster B," there are 3 different clusters of data)
- Or to compute features that could be useful for classification (e.g., (1, 0, 0) if the x belongs to Cluster A, (0, 1, 0) if the x belongs to Cluster B, (0, 0, 1) if the x belongs to Cluster C)
  - If we can figure out how to compute those features using a large unlabelled dataset, we could then use them to perform supervised learning on a small labelled dataset
  - Like using the AlexNet features to classify faces

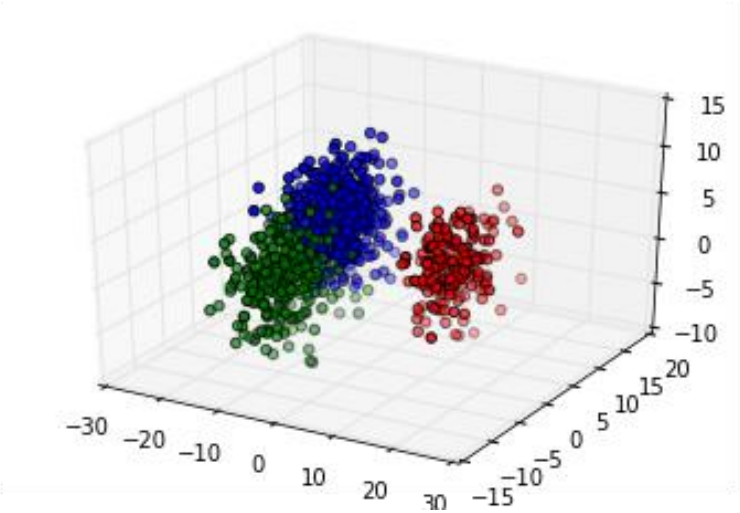
A Generative View



To generate a datapoint:

- Pick Cluster A with probability P_A, Cluster B with probability P_B, …
- If we picked Cluster cl, sample random coordinates from $N(\mu_{cl}, \Sigma_{cl})$

A Generative View



- If the data is well-described as several “clouds” of points, we can generate a datapoint that looks like it was sampled from the training set by picking a cloud and then picking a coordinate from the cloud.
- “Clouds” can be conveniently described as multivariate Gaussians

Mixture of Gaussians

- $P(x|\pi, \mu, \Sigma) = \sum_{cl} P(x|\mu, \Sigma, cl)P(cl|\pi)$ by the law of total probability
  - Weighted sum of the likelihoods for all the clusters, weighted by the probabilities of the clusters
- $P(x|\pi, \mu, \Sigma) = \sum_{cl} P(x|\mu, \Sigma, cl)P(cl|\pi) =$

$$= \sum_{cl} P(x|\mu_{cl}, \Sigma_{cl})\pi_{cl}$$

Learning a Mixture of Gaussians

- Let $z^{(i)}$ by the cluster to which point *i* is assigned
- If we knew all the $z^{(i)}$, we could learn the Gaussians one-by-one. But we don't. Instead, we can try to estimate

$$w_{cl}^{(i)} = p\left(z^{(i)} = cl \middle| x^{(i)}, \pi, \mu, \Sigma\right) = \frac{\mathrm{P}\left(\mathrm{x}^{(i)} \middle| \mu_{cl}, \Sigma_{cl}\right)\pi_{cl}}{P\left(x^{(i)} | \pi, \mu, \Sigma\right)} \propto \mathrm{P}\left(\mathrm{x}^{(i)} \middle| \mu_{cl}, \Sigma_{cl}\right)\pi_{cl}$$

- But we don't know μ, Σ, π either! But if we estimate the z's, it's easy to estimate μ, Σ, π.

Learning a Mixture of Gaussians

- E-step:
- Want to estimate the cluster assignments $z^{(i)}$.

$$\phi_{cl}^{(i)} = \mathrm{P}\left(\mathrm{x}^{(i)} \middle| \mu_{cl}, \Sigma_{cl}\right)\pi_{cl}$$

$$w_{cl}^{(i)} = p\left(z^{(i)} = cl \middle| x^{(i)}, \pi, \mu, \Sigma\right) = \frac{\mathrm{P}\left(\mathrm{x}^{(i)} \middle| \mu_{cl}, \Sigma_{cl}\right)\pi_{cl}}{P(x^{(i)}|\pi, \mu, \Sigma)} \propto \phi_{cl}^{(i)}$$

$$w_{cl}^{(i)} = \frac{\phi_{cl}^{(i)}}{\sum_{cl'} \phi_{cl'}^{(i)}}$$

Learning a Mixture of Gaussians

- M-step: Assume probabilistic cluster assignments were done

$$\pi_{cl} = \frac{1}{m}\sum_i w_{cl}^{(i)}$$

$$\mu_{cl} = \frac{\sum_i w_{cl}^{(i)} x^{(i)}}{\sum_i w_{cl}^{(i)}}$$

$$\Sigma_{cl} = \frac{\sum_i w_{cl}^{(i)} \left(x^{(i)} - \mu_{cl}\right)\left(x^{(i)} - \mu_{cl}\right)^T}{\sum_i w_{cl}^{(i)}}$$

Learning a Mixture of Gaussians

- Start with an initial guess of π, μ, Σ
- Repeat:
  - Perform E-step to estimate the (probabilistic) cluster assignments of each point

$$w_{cl}^{(i)} = p\left(z^{(i)} = cl \middle| x^{(i)}, \pi, \mu, \Sigma\right)$$

  - Assume cluster assignments, and re-estimate π, μ, Σ based on them

Learning a Mixture of Gaussians

- Very easy to get stuck in local optima
- Example:
  - A Gaussian whose variance is very small, and whose mean is very close to one point x
  - The E-step will only assign x to that Gaussian since the variance of the Gaussian is very small so the likelihood for any other point is small
  - The M-step will make the mean exactly equal to x, and make the variance even smaller
- Solution: start with Gaussians with large variances

Learning a Mixture of Gaussians

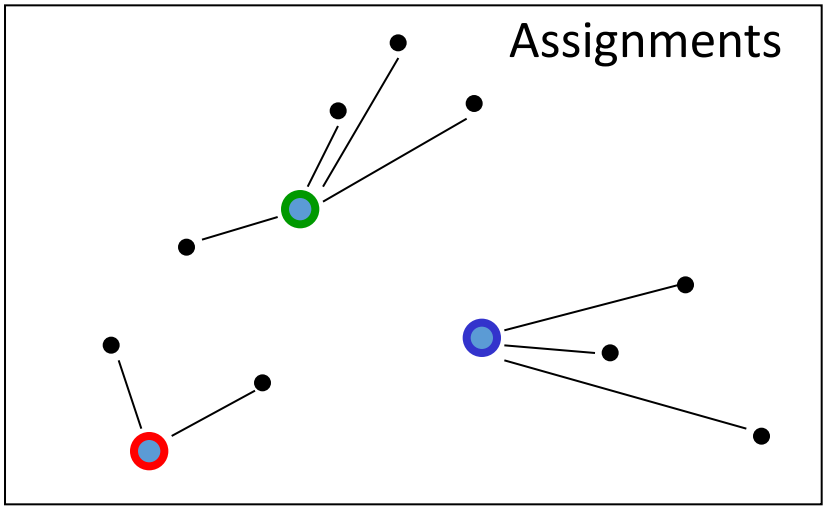
- How do we select the number of clusters?
- Try different numbers of clusters, select the number of clusters that maximizes the probability density of the validation set
  - Imagine fitting a very small-variance Gaussian to every point in the training set: this would give a very small probability density to the validation set

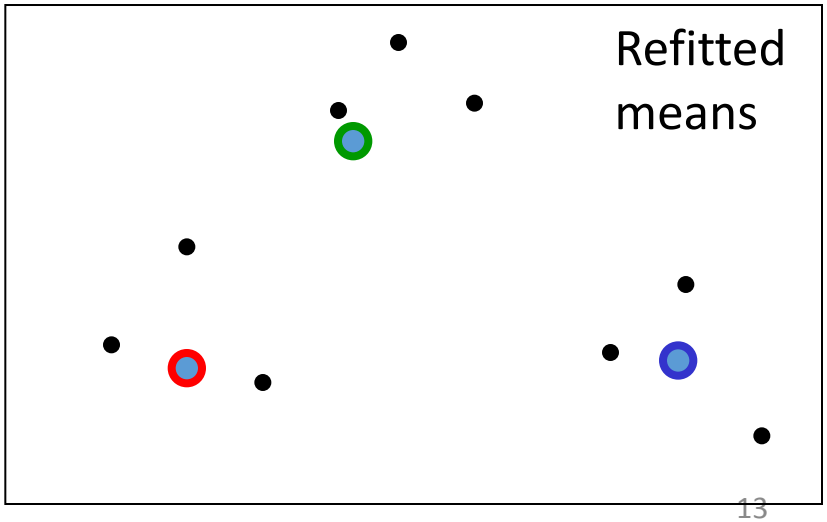
K-means

- K-means is an algorithm for finding centres of clusters
- Simpler than Mixture of Gaussians, but the same idea

K-means

- Assignment step: assign each datapoint to the closest cluster
- Refitting step: Move each cluster center to the average of the points assigned to the cluster





Slide from Geoff Hinton

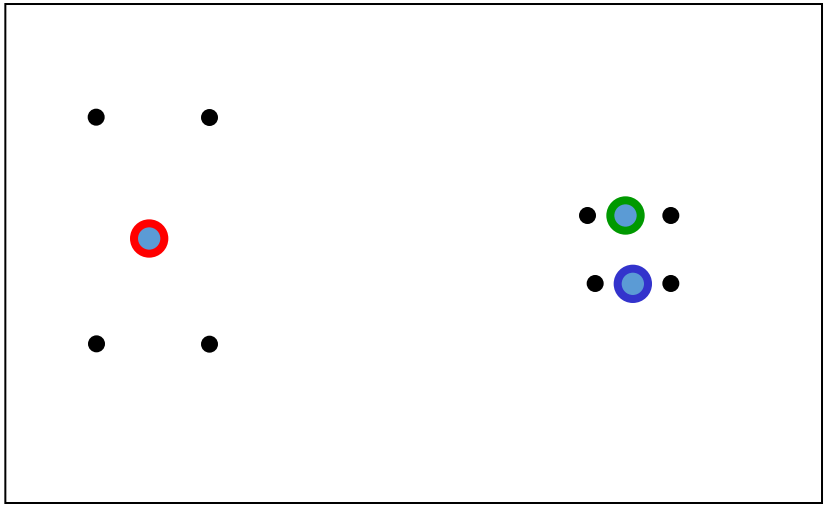
Why K-means converges

- Whenever an assignment is changed, the sum squared distances of datapoints from their assigned cluster centers is reduced
- Whenever a cluster center is moved the sum squared distances of the datapoints from their currently assigned cluster centers is reduced.
- If the assignments do not change in the assignment step, we have converged.

Slide from Geoff Hinton

K-means: local optima

- You could get back local optima with k-means
- Try multiple starting points
  - How to evaluate how good the result is?



Slide from Geoff Hinton

Speeding up Learning: MoG

- Run k-means first, initialize the means of the Gaussians to be the means obtained using k-means