CPSC 540: Machine Learning

More Mixtures

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Last Time: Mixture of Gaussians

- We discussed density estimation with a mixture of Gaussians,

$$p(x \mid \mu, \Sigma, \pi) = \sum_{c=1}^{k} \pi_c \underbrace{p(x \mid \mu_c, \Sigma_c)}_{\text{PDF of Gaussian } c},$$

  where PDF is written as convex combination of Gaussian PDFs.
  - Convex combination is needed so that probability integrates to 1.

- More flexible than a single Gaussian.
- With enough Gaussians, can approximate any continuous PDF.

- More generally, we can have mixtures of any distributions.
  - Today we'll discuss mixture of Bernoullis.
  - You can also do mixture of student t, mixture of Poisson, and so on.

Digression: Supervised Learning with Density Estimation

- Density estimation can be used for supervised learning:
  - 340 discussed generative models that model joint probability of x^i and y^i,
$$\begin{aligned} p(y^i|x^i) &\propto p(x^i, y^i) \\ &= p(x^i \mid y^i)p(y^i). \end{aligned}$$
  - Estimating $p(x^i, y^i)$ is a density estimation problem.
    - Naive Bayes models $p(x^i \mid y^i)$ as product of independent distributions.
    - Linear discriminant analysis (LDA) assumes $p(x^i \mid y^i)$ is Gaussian (shared Σ).
    - Gaussian discriminant analysis (GDA) allows each class to have its own covariance.
  - Generative models were unpopular for a while, but are now back:
    - Naive Bayes regression is being used for CRISPR gene editing.
    - Generative adversarial networks (GANs) and variational autoencoders (deep learning).
    - We believe that most human learning is unsupervised.

Previously: Independent vs. General Discrete Distributions

- We previously considered density estimation with discrete variables,

$$X = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},$$

  and considered two extreme approaches:
  - Product of independent Bernoullis:

$$p(x^i \mid \theta) = \prod_{j=1}^{d} p(x_j^i \mid \theta_j).$$

    Easy to fit but strong independence assumption:
    - Knowing x_j^i tells you nothing about x_k^i.
  - General discrete distribution:

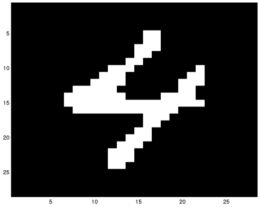
$$p(x^i \mid \theta) = \theta_{x^i}.$$

    No assumptions but hard to fit:
    - Parameter vector θ_{x^i} for each possible x^i.

Independent vs. General Discrete Distributions on Digits

- Consider handwritten images of digits:

$$x^i = \text{vec}\left(\quad \right),$$



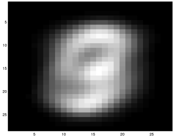
so each row of X contains all pixels from one image of a 0, 1, 2, …, or a 9.

- Previously we had labels and wanted to recognize that this is a 4.
- In density estimation we want probability distribution over images of digits.

- Given an image, what is the probability that it's a digit?
- Sampling from the density estimator it should generate images of digits.

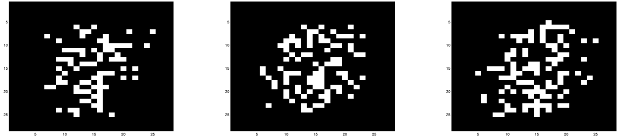
Independent vs. General Discrete Distributions on Digits

- We can visualize probabilities in independent Bernoulli model as an image:



  - We have a parameter θ_j for each pixel j, set to ("number of heads at pixel j")$/n$

- Samples generated from independent Bernoulli model:

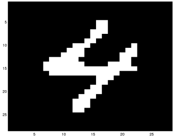


  - Flip a coin that lands hands with probability θ_j for each pixel j.

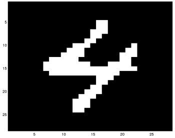
- This is clearly a terrible model: misses dependencies between pixels.

Independent vs. General Discrete Distributions on Digits

- Here is a sample from the MLE with the general discrete distribution:



- Here is an image with a probability of 0:



- This model memorized training images and doesn't generalize.
  - MLE puts probability at least $1/n$ on training images, and 0 on non-training images.

- A model lying between these extremes is the mixture of Bernoullis.

Mixture of Bernoullis

- Consider a coin flipping scenario where we have two coins:
  - Coin 1 has $\theta_1 = 0.5$ (fair) and coin 2 has $\theta_2 = 1$ (biased).

- Half the time we flip coin 1, and otherwise we flip coin 2:

$$
\begin{aligned}
p(x^i = 1 | \theta_1, \theta_2) &= \pi_1 p(x^i = 1|\theta_1) + \pi_2 p(x^i = 1|\theta_2) \\
&= \frac{1}{2}\theta_1 + \frac{1}{2}\theta_2.
\end{aligned}
$$

- With one variable this mixture model is not very interesting:
  - It's equivalent to flipping one coin with $\theta = 0.75$.

- But with multiple variables mixture of Bernoullis can model dependencies...

Mixture of Independent Bernoullis

- Consider a mixture of independent Bernoullis:

$$p(x \mid \theta_1, \theta_2) = \frac{1}{2} \underbrace{\prod_{j=1}^{d} p(x_j|\theta_{1j})}_{\text{first set of Bernoullis}} + \frac{1}{2} \underbrace{\prod_{j=1}^{d} p(x_j|\theta_{2j})}_{\text{second set of Bernoulli}} .$$

- Conceptually, we now have two sets of coins:
  - Half the time we throw the first set, half the time we throw the second set.

- With $d = 4$ we could have $\theta_1 = \begin{bmatrix} 0 & 0.7 & 1 & 1 \end{bmatrix}$ and $\theta_2 = \begin{bmatrix} 1 & 0.7 & 0.8 & 0 \end{bmatrix}$.
  - Half the time we have $p(x_3^i = 1) = 1$ and half the time it's 0.8.

- Have we gained anything?
  - In this example knowing $x_1 = 1$ tells you that $x_4 = 0$.
  - So this can model dependencies: $\underbrace{p(x_4 = 1 \mid x_1 = 1)}_{0} \neq \underbrace{p(x_4 = 1)}_{0.5}$.

Mixture of Independent Bernoullis

- General mixture of independent Bernoullis:

$$p(x^i \mid \Theta) = \sum_{c=1}^{k} \pi_c p(x^i \mid \theta_c),$$

  where Θ contains all the model parameters.

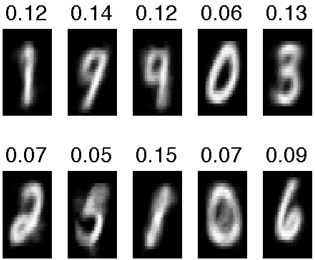
- Mixture of Bernoullis can model dependencies between variables
  - Individual mixtures act like clusters of the binary data.
  - Knowing cluster of one variable gives information about other variables.

- With k large enough, mixture of Bernollis can model any discrete distribution.
  - Hopefully with $k << 2^d$.

Mixture of Independent Bernoullis

- Plotting parameters θ_c with 10 mixtures trained on MNIST:digits.

(hand-written images of the the numbers 0 through 9)



http://pmtk3.googlecode.com/svn/trunk/docs/demoOutput/bookDemos/%2811%29-Mixture_models_and_the_EM_algorithm/mixBerMnistEM.html

- Remember this is unsupervised: it hasn't been told there are ten digits.
  - Density estimation tries to figure out how the world works.

Mixture of Independent Bernoullis

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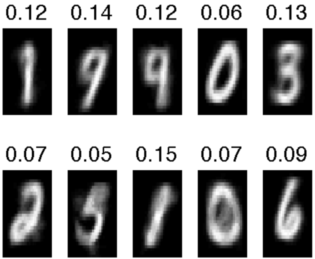


http://pmtk3.googlecode.com/svn/trunk/docs/demoOutput/bookDemos/%2811%29-Mixture_models_and_the_EM_algorithm/mixBerMnistEM.html

- You could use this model to "fill in" missing parts of an image:
  - By finding likely cluster/mixture, you find likely values for the missing parts.

Outline

Learning with Hidden Values

- We often want to learn with unobserved/missing/hidden/latent values.
- For example, we could have a dataset like this:

$$X = \begin{bmatrix} N & 33 & 5 \\ L & 10 & 1 \\ F & ? & 2 \\ M & 22 & 0 \end{bmatrix}, y = \begin{bmatrix} -1 \\ +1 \\ -1 \\ ? \end{bmatrix}.$$

- Missing values are very common in real datasets.
- An important issue to consider: why is data missing?

Missing at Random (MAR)

- We'll focus on data that is missing at random (MAR):
    - Assume that the reason ? is missing does not depend on the missing value.
    - This definition doesn't agree with intuitive notion of "random":
        - A variable that is *always* missing would be "missing at random".
        - The intuitive/stronger version is missing completely at random (MCAR).
- Examples of MCAR and MAR for digit data:
    - Missing random pixels/labels: MCAR.
    - Hide the the top half of every digit: MAR.
    - Hide the labels of all the "2" examples: not MAR.
- We'll consider MAR, because otherwise you need to model why data is missing.

Imputation Approach to MAR Variables

- Consider a dataset with MAR values:

$$X = \begin{bmatrix} N & 33 & 5 \\ F & 10 & 1 \\ F & ? & 2 \\ M & 22 & 0 \end{bmatrix}, y = \begin{bmatrix} -1 \\ +1 \\ -1 \\ ? \end{bmatrix}.$$

- Imputation method is one of the first things we might try:
  0. Initialization: find parameters of a density model (often using "complete" examples).
  1. Imputation: replace each ? with the most likely value.
  2. Estimation: fit model with these imputed values.

- You could also alternate between imputation and estimation.
  - Block coordinate optimization, treating ? values as more parameters.

Semi-Supervised Learning

- Important special case of MAR is semi-supervised learning.

$$X = \begin{bmatrix} \quad \end{bmatrix}, \quad y = \begin{bmatrix} \, \end{bmatrix},$$

$$\bar{X} = \begin{bmatrix} \quad \end{bmatrix}, \quad \bar{y} = \begin{bmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{bmatrix}.$$

- Motivation for training on labeled data (X, y) and unlabeled data $\bar{X}$:
  - Getting labeled data is usually expensive, but unlabeled data is usually cheap.

Semi-Supervised Learning

- Important special case of MAR is semi-supervised learning.

$$X = \begin{bmatrix} & & & \\ & & & \end{bmatrix}, \quad y = \begin{bmatrix} \\ \end{bmatrix},$$

$$\bar{X} = \begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \\ & & & \end{bmatrix}, \quad \bar{y} = \begin{bmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{bmatrix},$$

- Imputation approach is called self-taught learning:
  - Alternate between guessing $\bar{y}$ and fitting the model with these values.

Back to Mixture Models

- To fit mixture models we often introduce n MAR variables z^i.
- Why???
- Consider mixture of Gaussians, and let z^i be the cluster number of example i:
  - So $z^i \in \{1, 2, \cdots, k\}$ tells you which Gaussian generated example i.
  - Given the z^i it's easy to optimize the means and variances (μ_c, Σ_c):
    - Fit a Gaussian to examples in cluster i.
  - Given the (μ_c, Σ_c) it's easy to optimize the clusters z^i:
    - Find the cluster with highest $p(x^i | \mu_c, \Sigma_c)$.

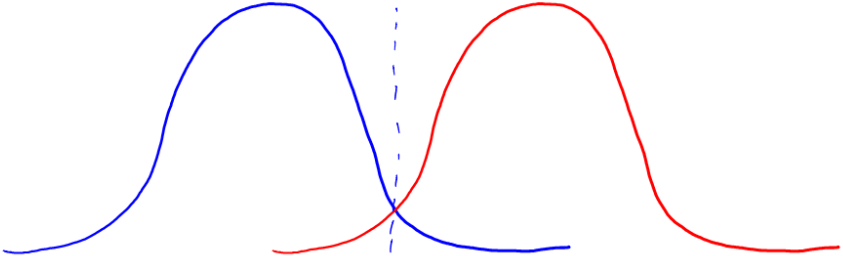
Imputation Approach for Mixtures of Gaussians

- Consider mixture of Gaussians with the choice $\Sigma_c = I$ for all c.
- Here is the imputation approach for fitting a mixtures of Gaussian:
  - Randomly pick some initial means μ_c.
  - Assigns x^i to the closest mean..
    - Given μ_c, for each x^i set z^i to the c maximizing $p(x^i \mid \mu_c)$
  - Set μ_c to the mean of the points assigned to cluster c.
    - Given the clusters/mixtures z^i, find the MLE of each mean.
- This is exactly k-means clustering.
  - With variable Σ_c, distance to mean will be measured in $\|\cdot\|_{\Sigma_c}$-norms.

K-Means vs. Mixture of Gaussians

- K-means can be viewed as fitting mixture of Gaussians (common Σ_c).
  - But variable Σ_c in mixture of Gaussians allow non-convex clusters.

With same covariance, clusters are convex.



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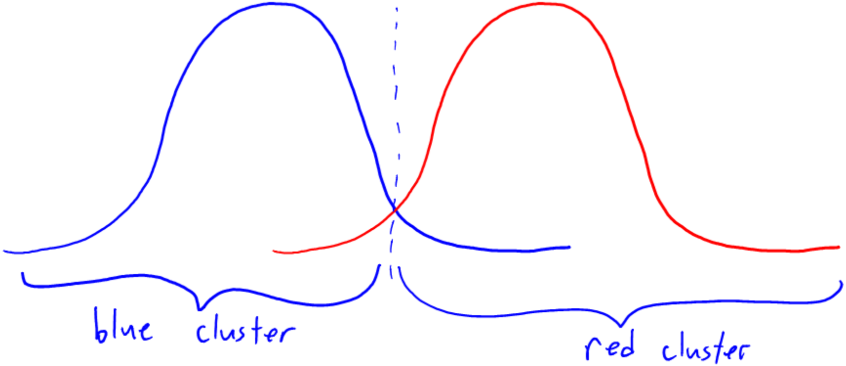

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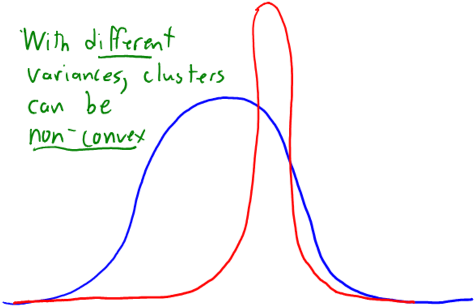

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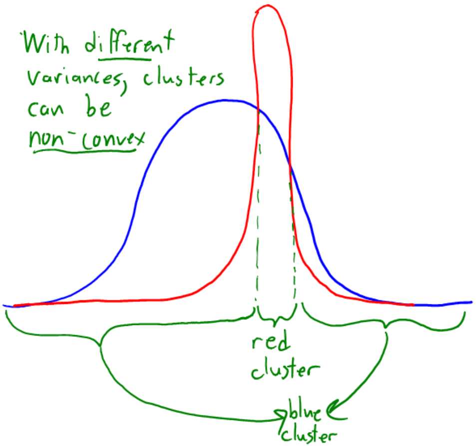

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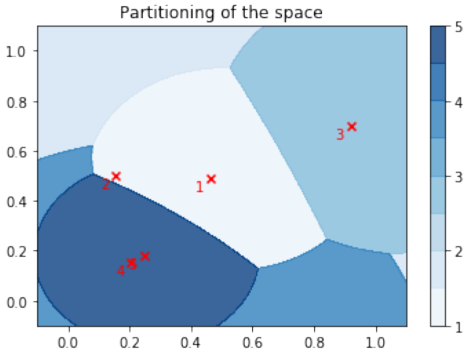

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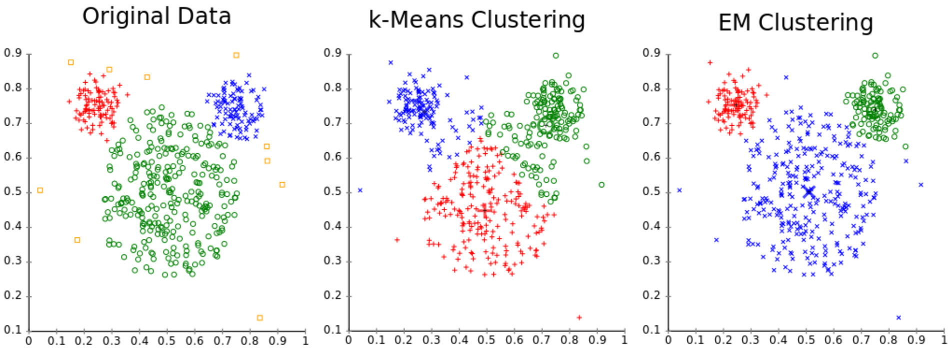

https://en.wikipedia.org/wiki/K-means_clustering

Drawbacks of Imputation Approach

- The imputation approach to MAR variables is simple:
  - Use density estimator to "fill in" the missing values.
  - Now fit the "complete data" using a standard method.
- But "hard" assignments of missing values lead to propagation of errors.
  - What if cluster is ambiguous in k-means clustering?
  - What if label is ambiguous in "self-taught" learning?
- Ideally, we should use probabilities of different assignments ("soft" assignments):
  - If the MAR values are obvious, this will act like the imputation approach.
  - For ambiguous examples, takes into account probability of different assignments.
- Expectation maximization (EM) considers probability of all imputations of ?.

Summary

- Mixture of Bernoullis can model dependencies between discrete variables.
    - Probability of belonging to mixtures is a soft-clustering of examples.
- Missing at random: fact that variable is missing does not depend on its value.
- Imputation approach to handling missing data.
    - Guess values of hidden variables, then fit the model (and usually repeat).
    - K-means is a special case, if we introduce "cluster number" as MAR variables.
- Next time: one of the most cited papers in statistics.