# CPSC 540: Machine Learning

## Mixture Models, Expectation Maximization

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# Admin

- Assignment 2:
  - Due tonight.
  - 1 late day to hand it in Wednesday.
  - 2 late days to hand it in next Wednesday.
- Class cancelled Wednesday:
  - So you can go to the TensorFlow lecture at the same time (check website for location).
- Assignment 3:
  - Out later this week.

# Last Time: Density Estimation

- Last time we started discussing unsupervised task of density estimation.
  - Given data $X$, estimate probability density $p(\hat{x}^i)$.

$$X = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \quad \hat{X} = \begin{bmatrix} ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \end{bmatrix}$$

- What is the probability of having $\hat{x}^i = \begin{bmatrix} 1 & 1 & 0 & 0 \end{bmatrix}$ in test data?

- A "master" ML problem that lets you solve many other problems...

# 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 $y^i$,

$$\begin{aligned} p(y^i|x^i) &\propto p(x^i, y^i) \\ &= p(x^i|y^i)p(y^i). \end{aligned}$$

  - Estimating $p(x^i, y^i)$ is a density estimation problem.
    - Naive Bayes models $p(x^i|y^i)$ as product of independent distributions.
    - Linear discriminant analysis (LDA) models $p(x^i|y^i)$ as a multivariate Gaussian.
  - Generative models have been unpopular for a while, but are coming back:
    - Naive Bayes regression is being used for CRISPR gene editing.
    - Generative adversarial networks and variational autoencoders (deep learning).
    - We believe that most human learning is unsupervised.

# Last Time: Multivariate Gaussian

- The multivariate normal distribution models PDF of vector $x$ as

$$p(x|\mu,\Sigma) = \frac{1}{(2\pi)^{\frac{d}{2}}|\Sigma|^{\frac{1}{2}}}\exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

  where $\mu \in \mathbb{R}^d$ and $\Sigma \in \mathbb{R}^{d\times d}$ and $\Sigma \succ 0$.

- Closed-form MLE:

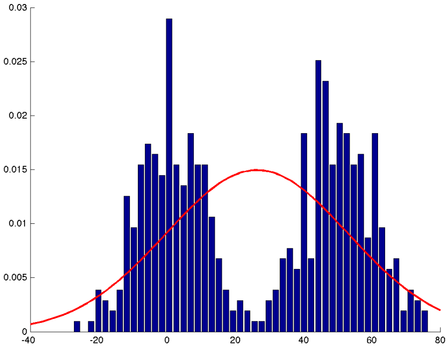
$$\mu = \frac{1}{n}\sum_{i=1}^{n} x^i, \quad \Sigma = \frac{1}{n}\sum_{i=1}^{N}\underbrace{(x^i-\mu)(x^i-\mu)^T}_{d\times d}.$$

- Closed under several operations: products of PDFs, marginalization, conditioning.
- Light-tailed: assumes all data is close to mean.
  - Not robust to outliers or data far away from mean.

# Outline

# 1 Gaussian for Multi-Modal Data

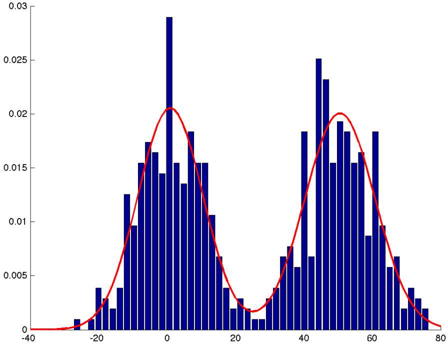
- Major drawback of Gaussian is that it's uni-modal.
  - It gives a terrible fit to data like this:




- If Gaussians are all we know, how can we fit this data?

# 2 Gaussians for Multi-Modal Data

- We can fit this data by using two Gaussians




- Instead of assuming data comes from one Gaussian, we assume:
  - Half the time it comes from Gaussian 1.
  - Half the time it comes from Gaussian 2.

# Mixture of Gaussians

- Our probability density in the previous example is given by

$$p(x \mid \mu_1, \mu_2, \Sigma_1, \Sigma_2) = \frac{1}{2}\underbrace{p(x \mid \mu_1, \Sigma_1)}_{\text{Gaussian 1}} + \frac{1}{2}\underbrace{p(x \mid \mu_2, \Sigma_2)}_{\text{Gaussian 2}},$$

  where $p(x|\mu_c, \Sigma_c)$ is the PDF of a Gaussian.

- If data comes from one Gaussian more often than the other, we could use

$$p(x \mid \mu_1, \mu_2, \Sigma_1, \Sigma_2, \pi_1, \pi_2) = \pi_1\underbrace{p(x \mid \mu_1, \Sigma_1)}_{\text{Gaussian 1}} + \pi_2\underbrace{p(x \mid \mu_2, \Sigma_2)}_{\text{Gaussian 2}},$$

  where $\pi_1 + \pi_2 = 1$ and both are non-negative.

# Mixture of Gaussians

- If instead of 2 Gaussians we need $k$ Gaussians, our PDF would be

$$p(x \mid \mu, \Sigma, \pi) = \sum_{c=1}^{k} \pi_c p(x \mid \mu_c, \Sigma_c),$$

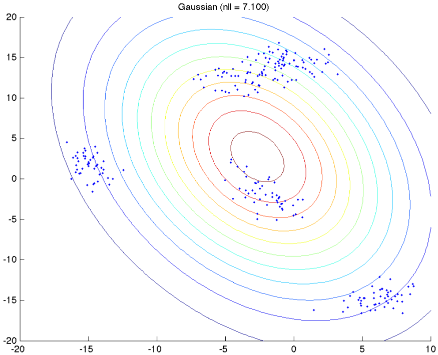
where $(\mu_c, \Sigma_c)$ are the parameters mixture/cluster $c$.

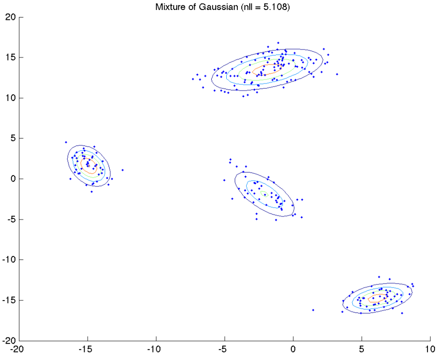
  - To make the $\pi_c$ probabilities we need that $\pi_c \geq 0$ and $\sum_{c=1}^{k} \pi_c = 1$.

- This is called a mixture of Gaussians model.
  - We can use it to model complicated densities with Gaussians (like RBFs).

# Mixture of Gaussians

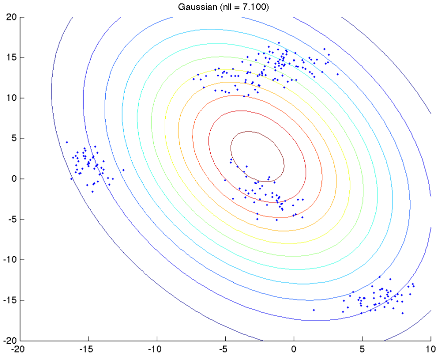
- Gaussian vs. Mixture of 4 Gaussians for 2D multi-modal data:

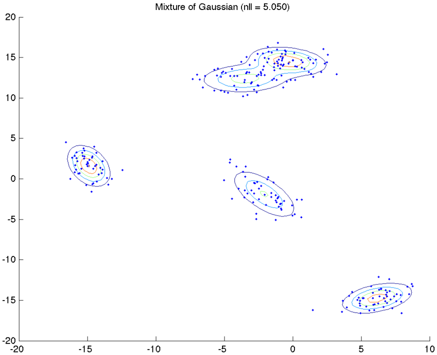


# Mixture of Gaussians

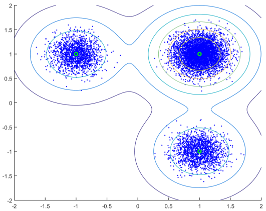
- Gaussian vs. Mixture of 5 Gaussians for 2D multi-modal data:



# Mixture of Gaussians

- How a mixture of Gaussian "generates" data:
  1. Sample cluster $c$ based on prior probabilities $\pi_c$ (categorical distribution).
  2. Sample example $x$ based on mean $\mu_c$ and covariance $\Sigma_c$.




- We usually fit these models with expectation maximization (EM):
  - EM is a general method for fitting models with hidden variables.
  - For mixture of Gaussians: we treat cluster $c$ as a hidden variable.

# Last Time: Independent vs. General Discrete Distributions

- We also 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:

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

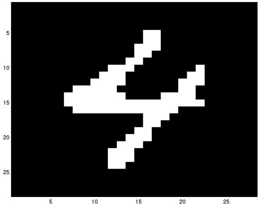
    Easy to fit but strong independence assumption:
    - Knowing $x_j$ tells you nothing about $x_k$.
  - General discrete distribution:

    $$p(x|\theta) = \theta_x.$$

    No assumptions but hard to fit:
    - Parameter vector $\theta_x$ for each possible $x$.

# Independent vs. General Discrete Distributions on Digits

- Consider handwritten images of digits:

$x^i = \text{vec}\Bigg($   $\Bigg)$,

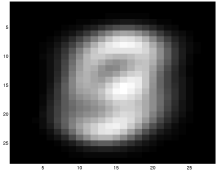
  so each row of $X$ contains all pixels from one image of a 0, 1, 2, . . . , 9.
- Previously we had labels and wanted to recognize that this is a 4.

- In density estimation we want probability distribution over images of digits.

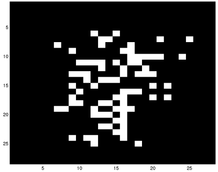
- Given an image, what is the probability that it's a digit?
- Sampling from the density should generate images of digits.

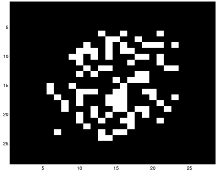
# Independent vs. General Discrete Distributions on Digits

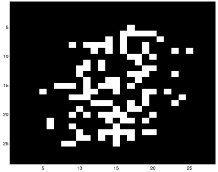
- We can visualize probabilities in independent Bernoulli model as an image:




- Samples generated from independent Bernoulli model:



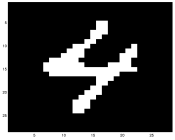



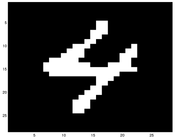

- This is clearly a terrible model: misses dependencies between pixels.

# Independent vs. General Discrete Distributions on Digits

- Here is a sample from the MLE with a 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:

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

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

- But this gets more interesting with multiple variables...

# 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 $\theta_2 = \begin{bmatrix} 1 & 0.7 & 0.8 & 0 \end{bmatrix}$.

- Have we gained anything?
  - In the mixture of Bernoullis the variables are not independent:
    - In this example knowing $x_1 = 1$ gives you the cluster, which gives you $x_4 = 0$.
    - So we have dependencies: $\underbrace{p(x_4 = 1|x_1 = 1)}_{0} \neq \underbrace{p(x_4 = 1)}_{0.5}$.

# Mixture of Independent Bernoullis

- General mixture of independent Bernoullis:

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

  where $\Theta$ contains all the model parameters.

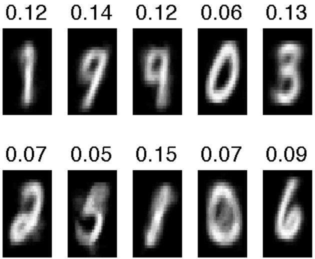
- Mixture of Bernoullis can model dependencies between variables
  - Individual Bernoullis act like clusters of the binary data.
  - Knowing cluster of one variable gives information about other variables.

- With $k$ large enough, mixtures are sufficient to model any discrete distribution.
  - Possibly with $k << 2^d$.

# Mixture of Independent Bernoullis

- Plotting parameters $\theta_c$ with 10 mixtures trained on MNIST:digits.

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



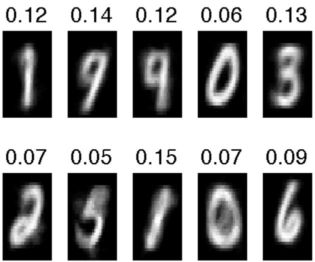

http://pmtk3.googlecode.com/svn/trunk/docs/demoOutput/bookDemos/%2811%29-Mixture_models_and_the_EM_algorithm/mixBerMnistEM.html

- 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

- Plotting parameters $\theta_c$ 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

- 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:

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

- 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):
  - The assumption that ? 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.

# Semi-Supervised Learning

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

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

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

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

# Semi-Supervised Learning

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

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

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

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

# 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 $i$:
  - Given the $z^i$ it's easy to optimize the means and variances $(\mu_c, \Sigma_c)$:
    - Fit a Gaussian to examples in cluster $i$.
  - Given the $(\mu_c, \Sigma_c)$ it's easy to optimize the clusters $z^i$:
    - Find the cluster with highest $p(x^i|\mu_c, \Sigma_c)$.
- If all clusters have the same covariance $\Sigma_c = \Sigma$, this is k-means clustering.
  - $\mu_c$ is the mean of cluster $c$ and $z^i$ is the nearest mean.

# Outline

# Drawbacks of Imputationa 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 Notation

- Expectation maximization (EM) is an optimization algorithm for MAR values:
  - Applies to problems that are easy to solve with "complete" data (i.e., you knew $H$).
  - Allows probabilistic or "soft" assignments to MAR values.
- EM is the most cited paper in statistics?
- EM notation: we use $O$ as observed variables and $H$ as hidden variables.
  - Mixture models: observe data $O = \{X\}$ but don't observe clusters $H = \{z^i\}_{i=1}^n$.
  - Semi-supervised learning: observe $O = \{X, y, \hat{X}\}$ but don't observe $H = \{\hat{y}\}$.
- When we choose one $H$ by imputation it's called "hard" EM.
- We use $\Theta$ as parameters we want to optimize.

# Complete Data and Marginal Likelihoods

- Assume observing $H$ makes "complete" likelihood $p(O, H|\Theta)$ "nice".
  - It has a closed-form MLE for Bernoulli or Gaussians, NLL convex for logistic, etc.

- From marginalization rule, likelihood of $O$ in terms of "complete" likelihood is

$$p(O|\Theta) = \sum_{H_1}\sum_{H_2}\cdots\sum_{H_m} p(O, H|\Theta) = \sum_{H} p(O, H|\Theta).$$

  where we sum (or integrate) over all $H$ (the "marginal likelihood" of $O$).

- The marginal log-likelihood thus has the form

$$-\log p(O|\Theta) = -\log\left(\sum_{H} p(O, H|\Theta)\right),$$

- which has a sum inside the log.
  - This does not preserve convexity: minimizing it is usually NP-hard.

# Expectation Maximization Bound

- To compute $\Theta^{t+1}$, the approximation used by EM and hard-EM is

$$-\log p(O|\Theta) = -\log\left(\sum_H p(O,H|\Theta)\right) \approx -\sum_H \alpha_H^t \log p(O,H|\Theta),$$

where $\alpha_H^t$ is a weight for the assignment $H$ to the hidden variables.

- In hard-EM we set $\alpha_H^t = 1$ for the most likely $H$ given $\Theta^t$ (all other $\alpha_H^t = 0$).

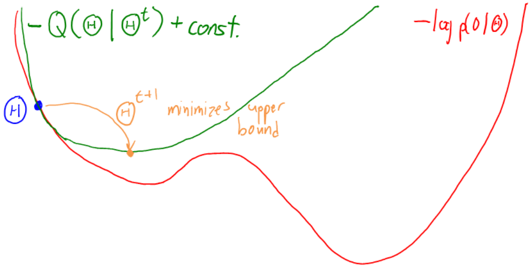
- In soft-EM we set $\alpha_H^t = p(H|O,\Theta^t)$, weighting $H$ by probability given $\Theta^t$.

- We'll show the EM approximation minimizes an upper bound,

$$-\log p(O|\Theta) \leq \underbrace{-\sum_H p(H|O,\Theta^t)\log p(O,H|\Theta)}_{Q(\Theta|\Theta^t)} + \text{const.},$$

# Expectation Maximization as Bound Optimization

- Expectation maximization is a bound-optimization method:
  - At each iteration we optimize a bound on the function.




- In gradient descent, our bound came from Lipschitz-continuity of the gradient.
- In EM, our bound comes from expectation over hidden variables (non-quadratic).

# Expectation Maximization (EM)

- So EM starts with $\Theta^0$ and sets $\Theta^{t+1}$ to maximize $Q(\Theta|\Theta^t)$.
- This is typically written as two steps:
  1. E-step: Define expectation of complete log-likelihood given $\Theta^t$,

$$Q(\Theta|\Theta^t) = \sum_H \underbrace{p(H|O,\Theta^t)}_{\text{fixed weight}} \underbrace{\log p(O,H|\Theta)}_{\text{nice term}}$$
$$= \mathbb{E}_{H|O,\Theta^t}[\log p(O,H|\Theta)],$$

     which is a weighted version of the "nice" $\log p(O,H)$ values.
  2. M-step: Maximize this expectation,

$$\Theta^{t+1} = \underset{\Theta}{\operatorname{argmax}}\, Q(\Theta|\Theta^t).$$

# Convergence Properties of Expectation Maximization

- We'll show that

$$\log p(O|\Theta^{t+1}) - \log p(O|\Theta^t) \geq Q(\Theta^{t+1}|\Theta^t) - Q(\Theta^t|\Theta^t),$$

  that guaranteed progress is at least as large as difference in $Q$.

- Does this imply convergence?
  - Yes, if likelihood is bounded above.
- Does this imply convergence to a stationary point?
  - No, although many papers say that it does.
    - Could have maximum of $3$ and objective values of $1, 1 + 1/2, 1 + 1/2 + 1/4, \ldots$

- Almost nothing is known about rate of convergence.

# Summary

- Mixture models write probability as convex combination of probabilities.
    - Model dependencies between variables even if components are independent.
    - 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.
- Semi-supervised learning: learning with labeled and unlabeled data.
- Expectation maximization:
    - Optimization with MAR variables, when knowing MAR variables make problem easy.

- Next time: what "parts" make up your personality? (Beyond PCA)