CPSC 540: Machine Learning

Mixture Models, Expectation Maximization

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Winter 2017

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,

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

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  - 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.

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    - 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 $\Sigma \succ 0$.

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- Closed-form MLE:

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

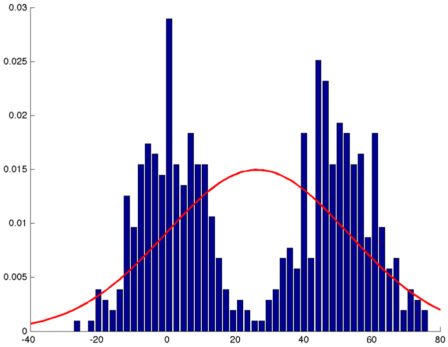
- Closed under several operations: products of PDFs, marginalization, conditioning.
- Light-tailed: assumes all data is close to mean.
  - Not robust to outliers or data far away from mean.

Outline

1. Mixture Models
2. Learning with Hidden Values
3. Expectation Maximization

1 Gaussian for Multi-Modal Data

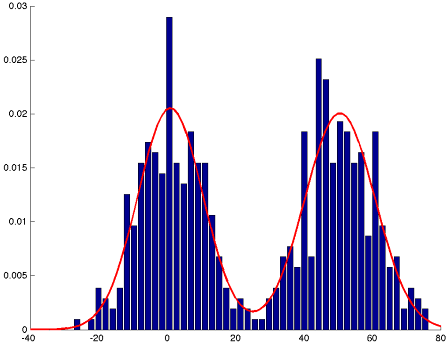
- Major drawback of Gaussian is that it's uni-modal.
  - It gives a terrible fit to data like this:



- 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.

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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 (μ_c, Σ_c) are the parameters mixture/cluster c.

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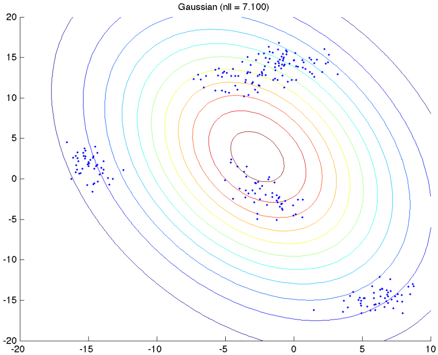
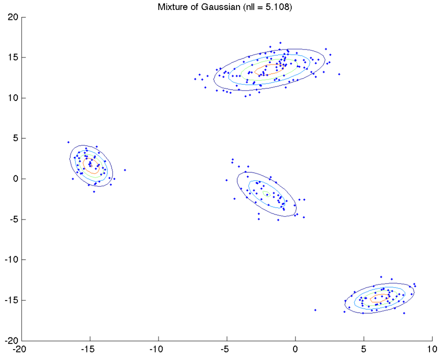
  where (μ_c, Σ_c) are the parameters mixture/cluster c.
  - To make the π_c probabilities we need that $\pi_c \geq 0$ and $\sum_{c=1}^{k} \pi_c = 1$.

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

Mixture of Gaussians

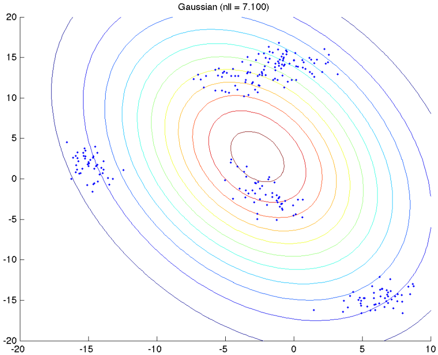
- Gaussian vs. Mixture of 4 Gaussians for 2D multi-modal data:

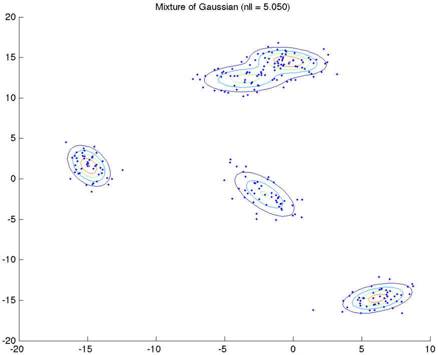




Mixture of Gaussians

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





Mixture of Gaussians

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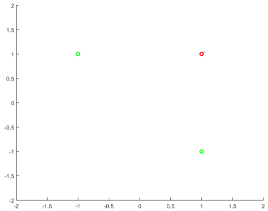
  1. Sample cluster c based on prior probabilities π_c (categorical distribution).
  2. Sample example x based on mean μ_c and covariance Σ_c.



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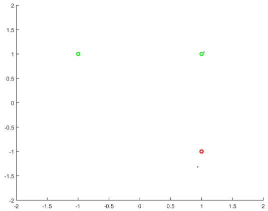

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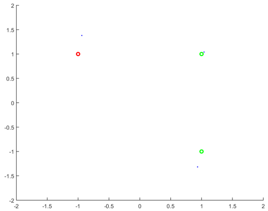

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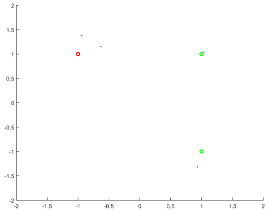

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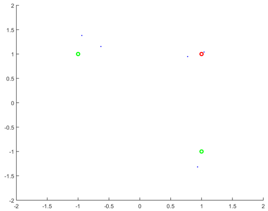

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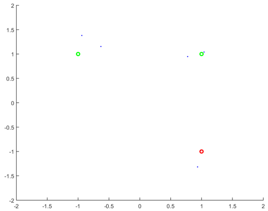

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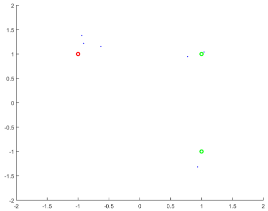

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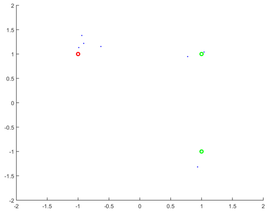

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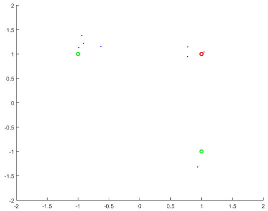

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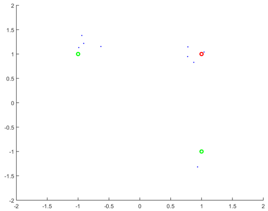

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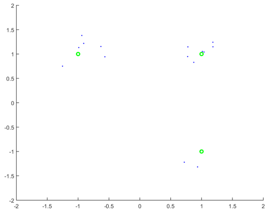

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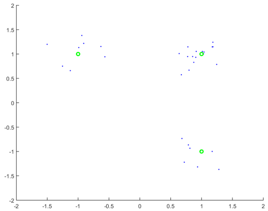

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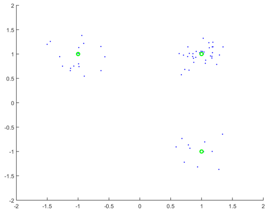

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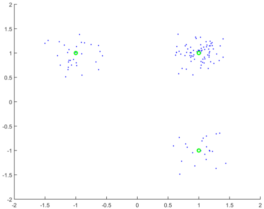

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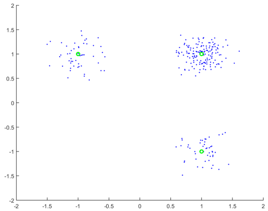

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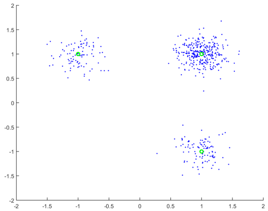

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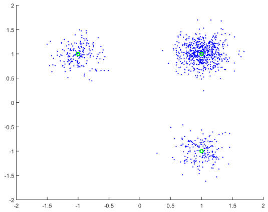

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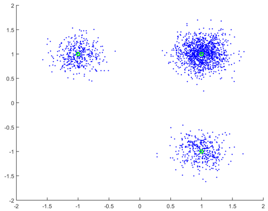

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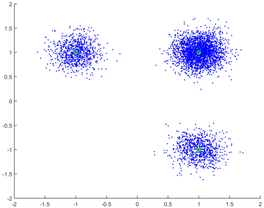

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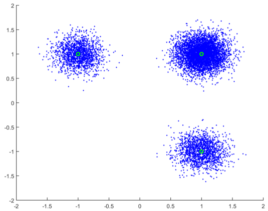

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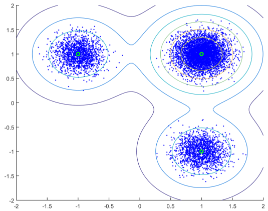

- We usually fit these models with expectation maximization (EM):
  - EM is a general method for fitting models with hidden variables.
  - For mixture of Gaussians: we treat cluster c as a hidden variable.

Last Time: Independent vs. General Discrete Distributions

- We also considered density estimation with discrete variables,

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

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  - 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.

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

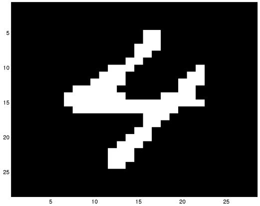
$$p(x|\theta) = \theta_x.$$

    No assumptions but hard to fit:
    - Parameter vector θ_x for each possible x.

Independent vs. General Discrete Distributions on Digits

- Consider handwritten images of digits:

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



so each row of X contains all pixels from one image of a 0, 1, 2, $\dots$, 9.

- Previously we had labels and wanted to recognize that this is a 4.

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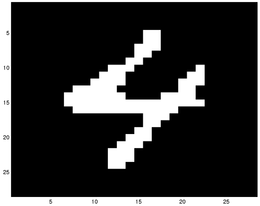
$$x^i = \text{vec}\left(\right.$$  $$\left.\right),$$

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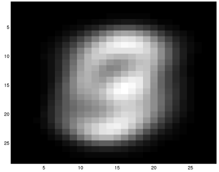
- In density estimation we want probability distribution over images of digits.

- 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:



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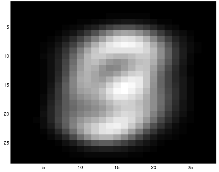
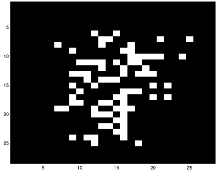
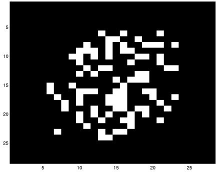
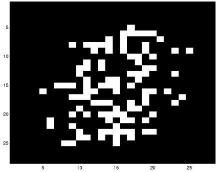


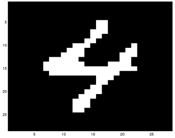
- Samples generated from independent Bernoulli model:

- 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:



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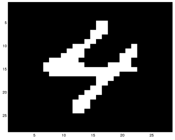
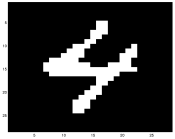


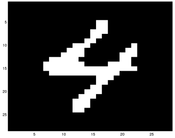
- Here is an image with a probability of 0:



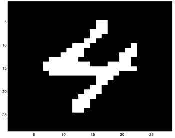
- This model memorized training images and doesn't generalize.
  - MLE puts probability at least $1/n$ on training images, and 0 on non-training images.

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).

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- 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.
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- 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:
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- 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?

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- 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 Θ contains all the model parameters.

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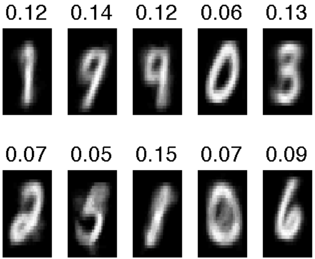
- Mixture of Bernoullis can model dependencies between variables
  - Individual Bernoullis act like clusters of the binary data.
  - Knowing cluster of one variable gives information about other variables.

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

Mixture of Independent Bernoullis

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

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



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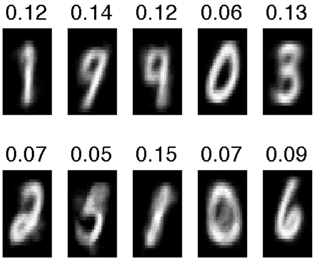

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- Remember this is unsupervised: it hasn't been told there are ten digits.
  - Density estimation tries to figure out how the world works.

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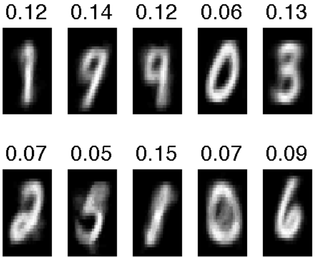

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- You could use this model to "fill in" missing parts of an image:
  - By finding likely cluster/mixture, you find likely values for the missing parts.

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:

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

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

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  - 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:

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- You could also alternate between imputation and estimation.

Semi-Supervised Learning

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

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

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- 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

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

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    - 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.
  - μ_c is the mean of cluster c and z^i is the nearest mean.

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- 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.

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- EM notation: we use O as observed variables and H as hidden variables.
    - Mixture models: observe data $O = \{X\}$ but don't observe clusters $H = \{z^i\}_{i=1}^n$.
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- When we choose one H by imputation it's called "hard" EM.

- We use Θ as parameters we want to optimize.

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

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

Expectation Maximization Bound

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

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

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

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

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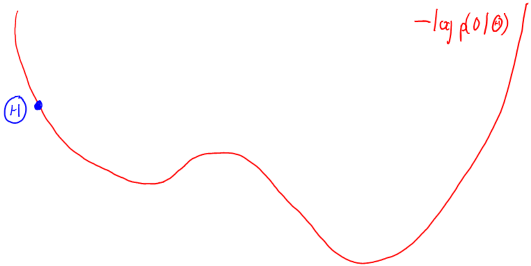
  - At each iteration we optimize a bound on the function.



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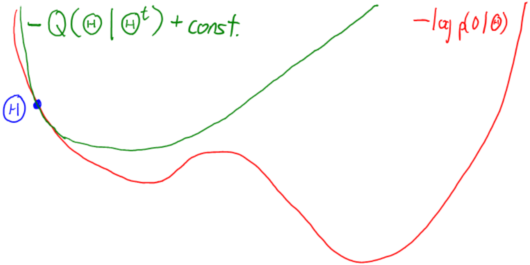

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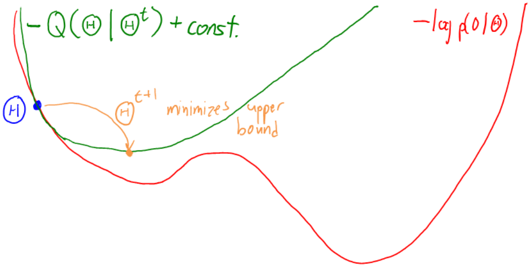

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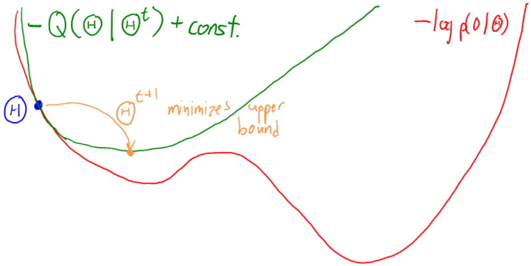

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which is a weighted version of the “nice” $\log p(O,H)$ values.

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     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

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

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- 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

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- 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)