# Clustering

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Slide Credit: Professor Fei Sha

11/20/15

# Outline

1. Administration
2. Brief review of last lecture
3. Clustering

# Grading

- Grades for midterm and project proposal will be available by next Tuesday
- HW5 grades available next Tuesday or Thursday
- For midterm, we will not be giving physical exams back, but you can see them during Nikos' office hours

# HW6

- Last Homework assignment
- I will post by next Tuesday
- Due on the last day of class

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# Neural Networks – Basic Idea

## Learning nonlinear basis functions and classifiers

- Hidden layers are nonlinear mappings from input features to new representation
- Output layers use the new representations for classification and regression

## Learning parameters

- Backpropogation = Stochastic gradient descent

# Summary of the course so far

**Supervised learning** has been our focus

- Setup: given a training dataset $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$, we learn a function $h(\boldsymbol{x})$ to predict $\boldsymbol{x}$'s true value $y$ (i.e., regression or classification)
- Linear vs. nonlinear features
  1. Linear: $h(\boldsymbol{x})$ depends on $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$
  2. Nonlinear: $h(\boldsymbol{x})$ depends on $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$, which in terms depends on a kernel function $k(\boldsymbol{x}_m, \boldsymbol{x}_n) = \boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)$,
- Loss function
  1. Squared loss: least square for regression (minimizing residual sum of errors)
  2. Logistic loss: logistic regression
  3. Exponential loss: AdaBoost
  4. Margin-based loss: support vector machines
- Principles of estimation
  1. Point estimate: maximum likelihood, regularized likelihood

# cont'd

- Optimization
  1. Methods: gradient descent, Newton method
  2. Convex optimization: global optimum vs. local optimum
  3. Lagrange duality: primal and dual formulation
- Learning theory
  1. Difference between training error and generalization error
  2. Overfitting, bias and variance tradeoff
  3. Regularization: various regularized models

# Supervised versus Unsupervised Learning

**Supervised** Learning from labeled observations

- Labels 'teach' algorithm to learn mapping from observations to labels
- Classification, Regression

# Supervised versus Unsupervised Learning

**Supervised** Learning from labeled observations

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**Unsupervised** Learning from unlabeled observations

- Learning algorithm must find latent structure from features alone
- Can be goal in itself (discover hidden patterns, exploratory analysis)
- Can be means to an end (preprocessing for supervised task)
- Clustering (Today)
- Dimensionality Reduction: Transform an initial feature representation into a more concise representation (Next)

# Outline

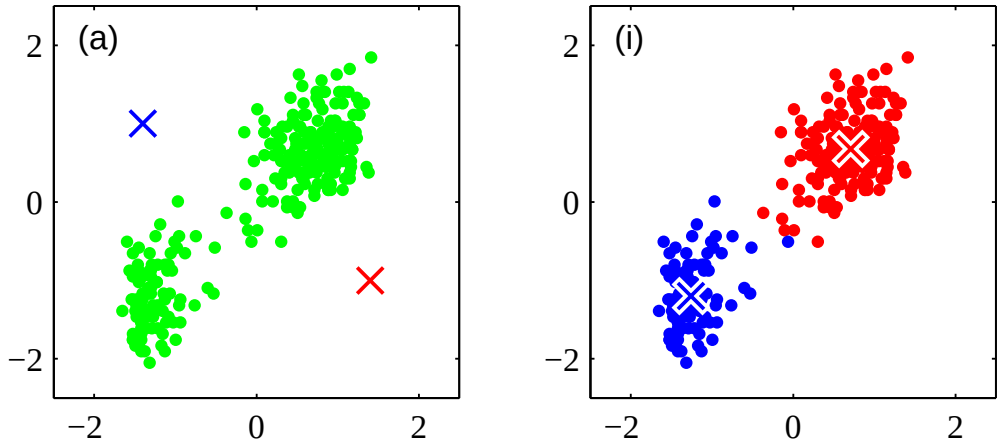
1. Administration
2. Brief review of last lecture
3. Clustering
   - K-means
   - Gaussian mixture models

# Clustering

**Setup** Given $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^N$ and $K$, we want to output

- $\{\boldsymbol{\mu}_k\}_{k=1}^K$: prototypes of clusters
- $A(\boldsymbol{x}_n) \in \{1, 2, \ldots, K\}$: the cluster membership, i.e., the cluster ID assigned to $\boldsymbol{x}_n$

**Toy Example** Cluster data into two clusters.




**Applications**

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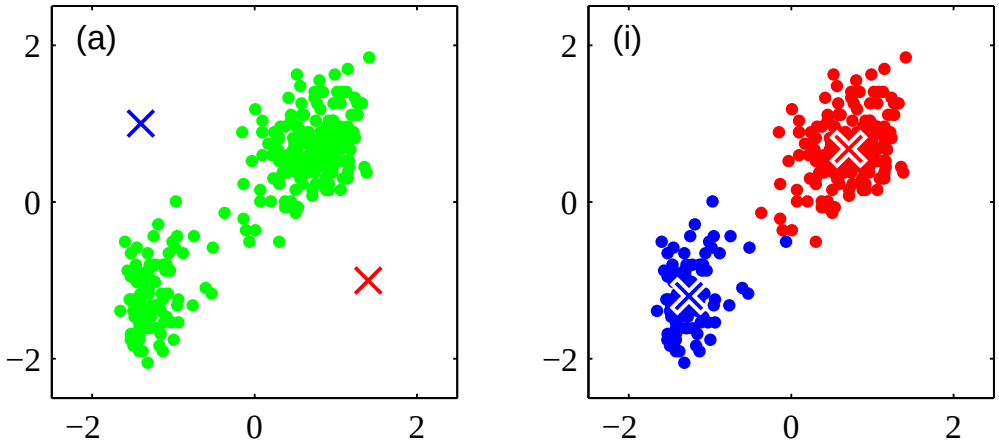
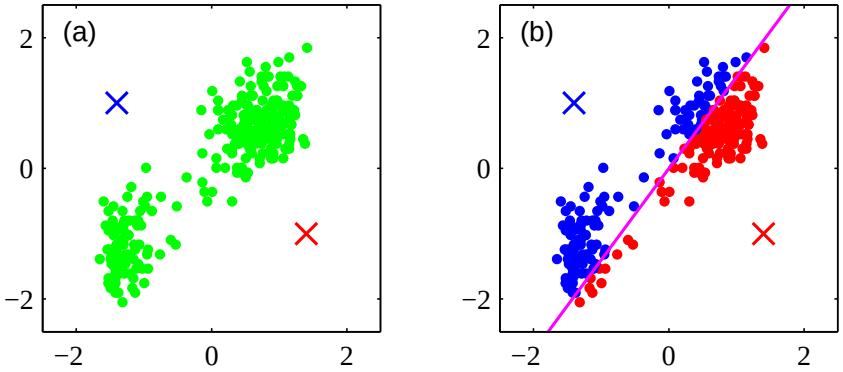



## Applications

- Identify communities within social networks
- Find topics in news stories
- Group similiar sequences into gene families

# K-means example



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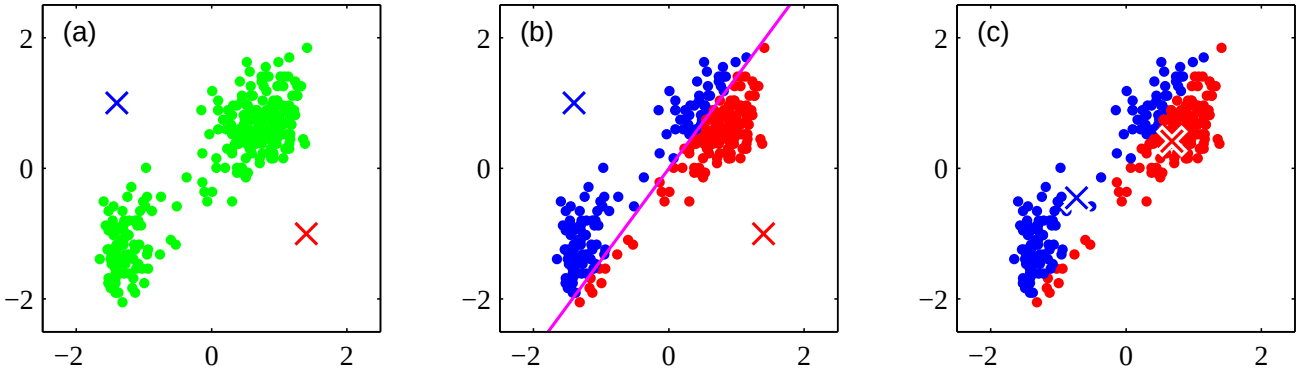

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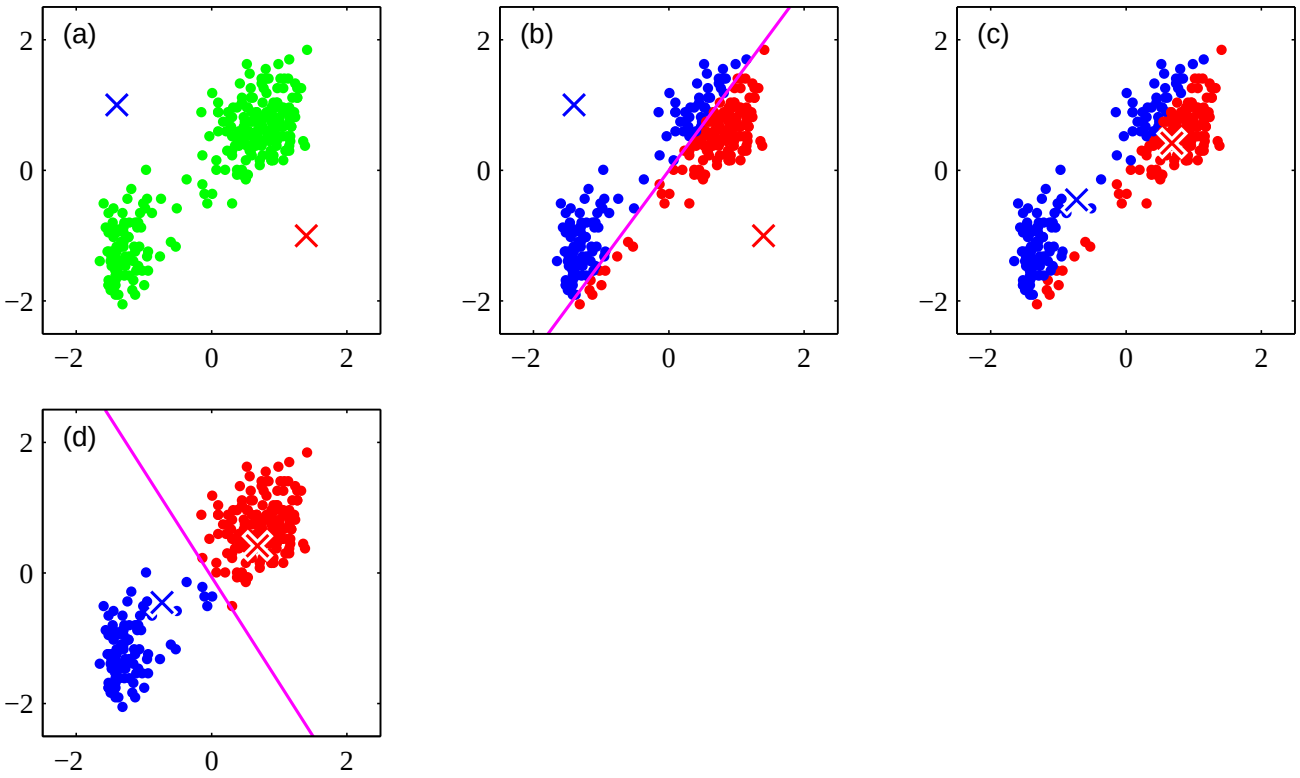

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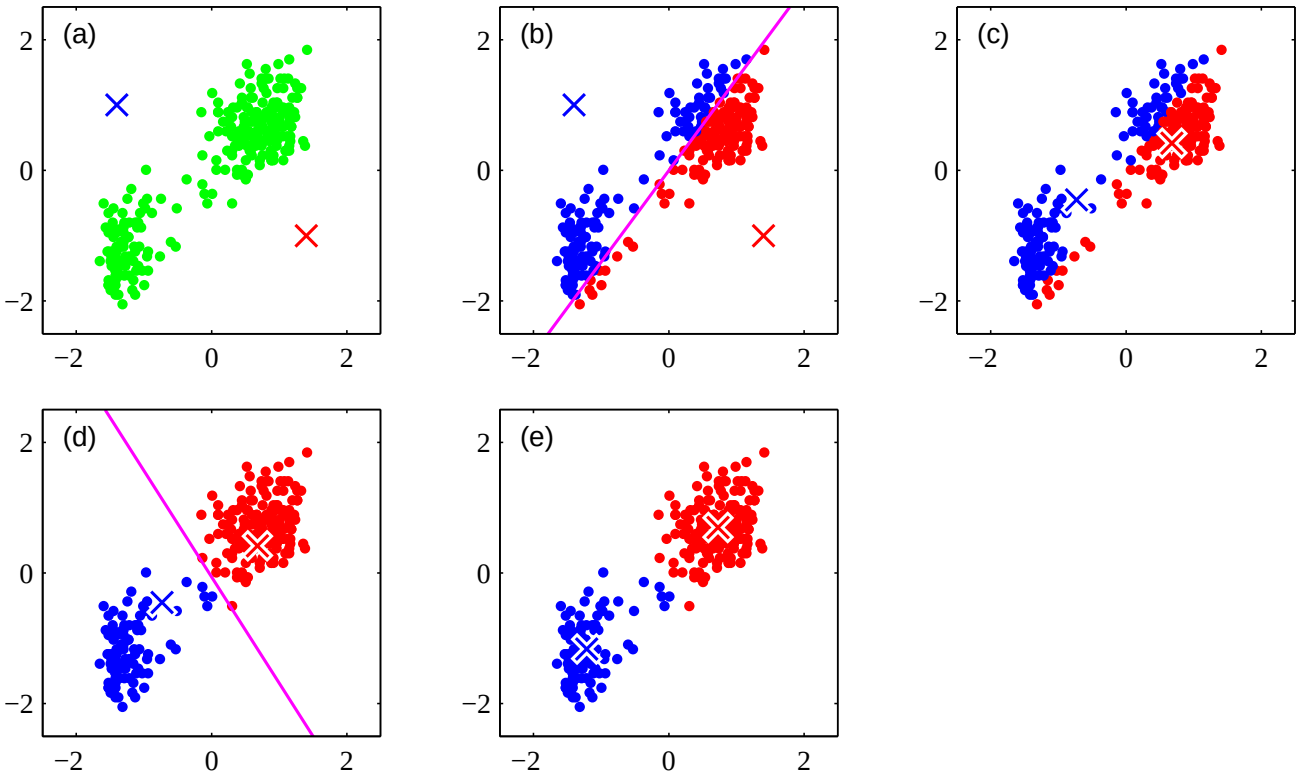

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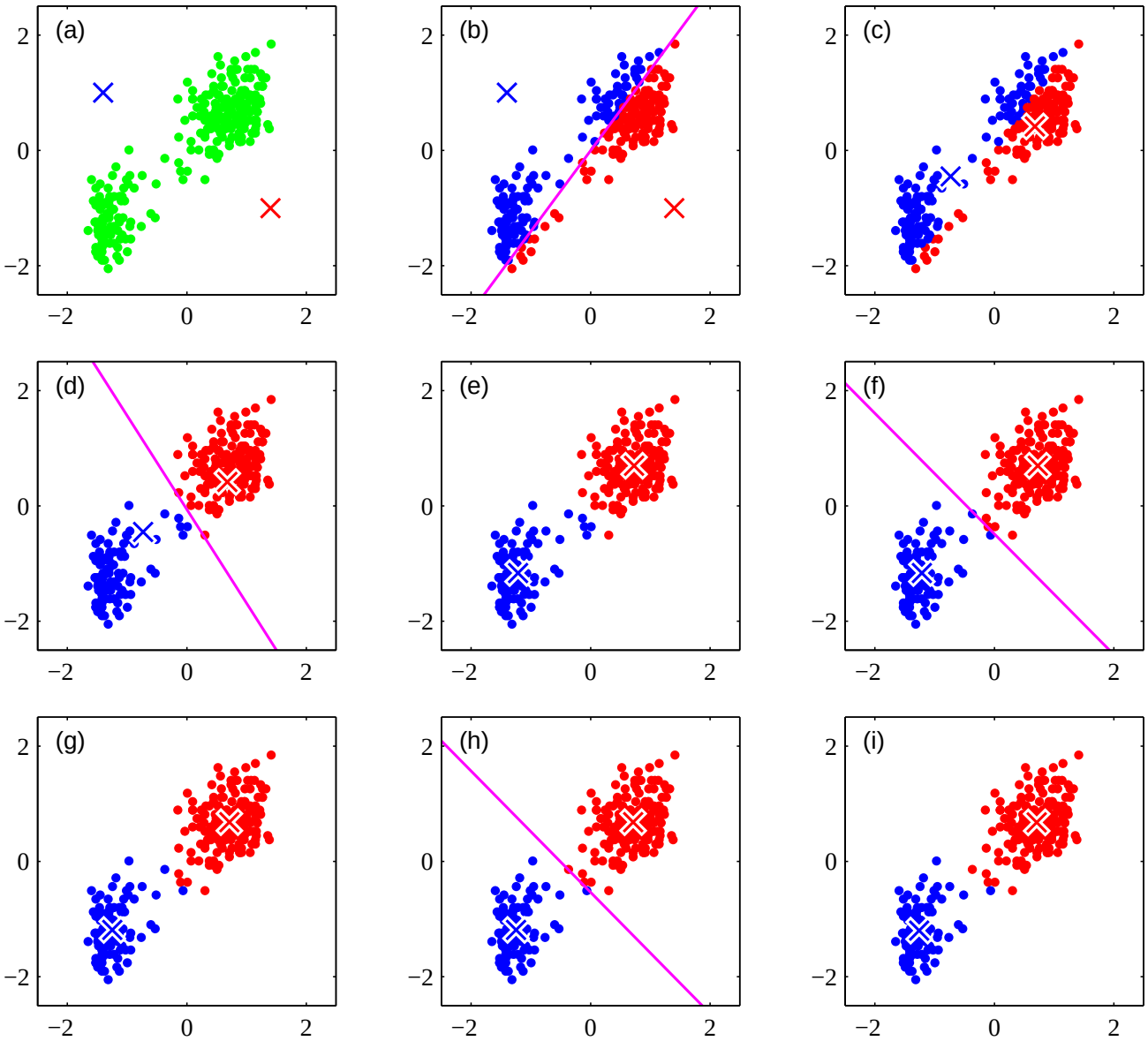

# K-means clustering

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**Distortion measure** (clustering objective function, cost function)

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$

where $r_{nk} \in \{0, 1\}$ is an indicator variable

$$r_{nk} = 1 \quad \text{if and only if} \quad A(\boldsymbol{x}_n) = k$$

# Algorithm

**Minimize distortion measure** alternative optimization between $\{r_{nk}\}$ and $\{\boldsymbol{\mu}_k\}$

- **Step 0** Initialize $\{\boldsymbol{\mu}_k\}$ to some values

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- **Step 1** Assume the current value of $\{\boldsymbol{\mu}_k\}$ fixed, minimize $J$ over $\{r_{nk}\}$, which leads to the following cluster assignment rule

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

# Algorithm

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- **Step 0** Initialize $\{\boldsymbol{\mu}_k\}$ to some values
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$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

- **Step 2** Assume the current value of $\{r_{nk}\}$ fixed, minimize $J$ over $\{\boldsymbol{\mu}_k\}$, which leads to the following rule to update the prototypes of the clusters

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk}\boldsymbol{x}_n}{\sum_n r_{nk}}$$

- **Step 3** Determine whether to stop or return to Step 1

# Remarks

- Prototype $\boldsymbol{\mu}_k$ is the mean of data points assigned to the cluster $k$, hence 'K-means'
- The procedure reduces $J$ in both Step 1 and Step 2 and thus makes improvements on each iteration
- No guarantee we find the global solution; quality of local optimum depends on initial values at Step 0 ($k$-means++ is a neat approximation algorithm)

# Application: vector quantization

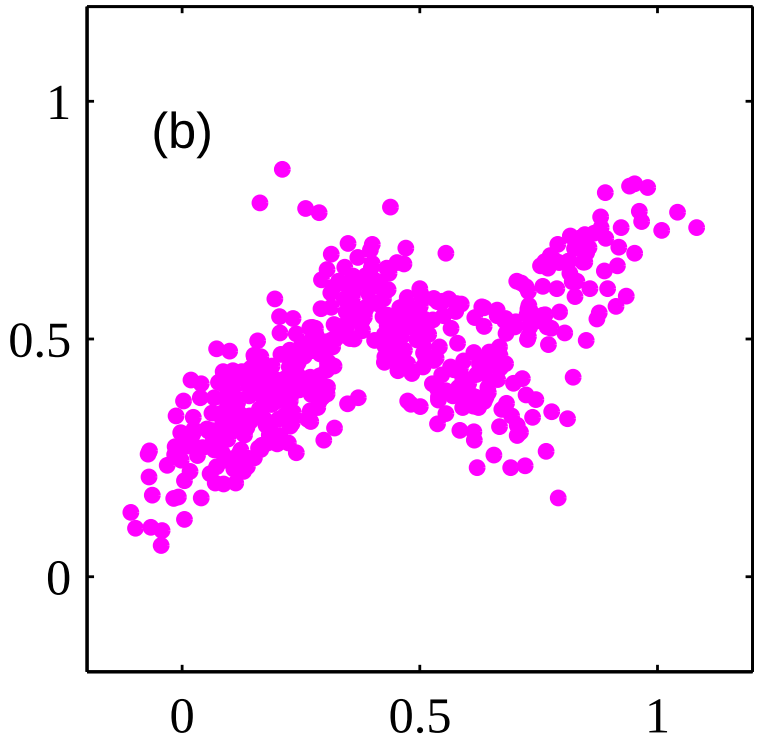
- Replace data point with associated prototype $\boldsymbol{\mu}_k$
- In other words, compress the data points into i) a codebook of all the prototypes; ii) a list of indices to the codebook for the data points
- Lossy compression, especially for small $K$

Clustering pixels and vector quantizing them. From left to right: Original image, quantized with large $K$, medium $K$, and a small $K$. Details are missing due to the higher compression (smaller $K$).

# Probabilistic interpretation of clustering?

We can impose a probabilistic interpretation of our intuition that points stay close to their cluster centers

- How can we model $p(\boldsymbol{x})$ to reflect this?

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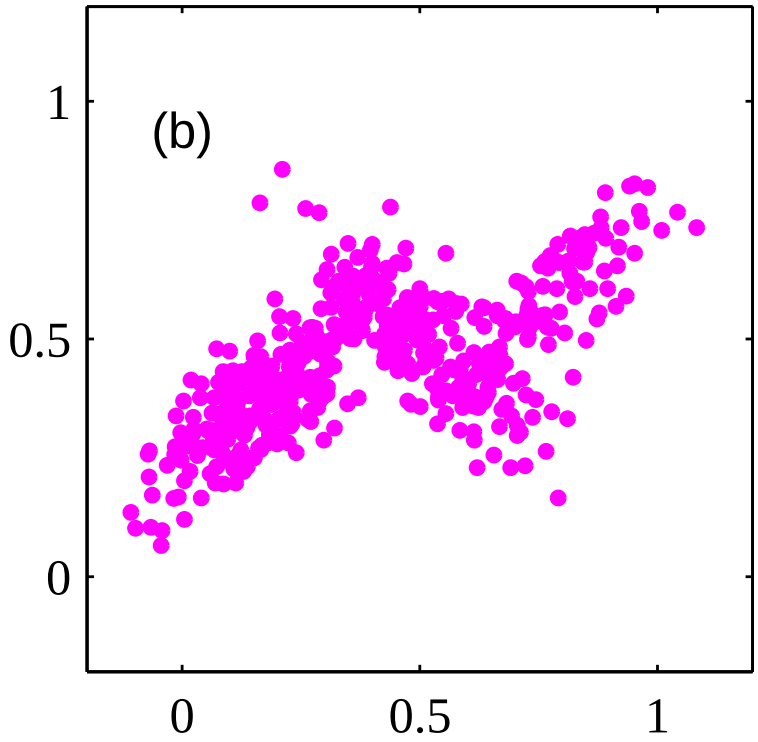
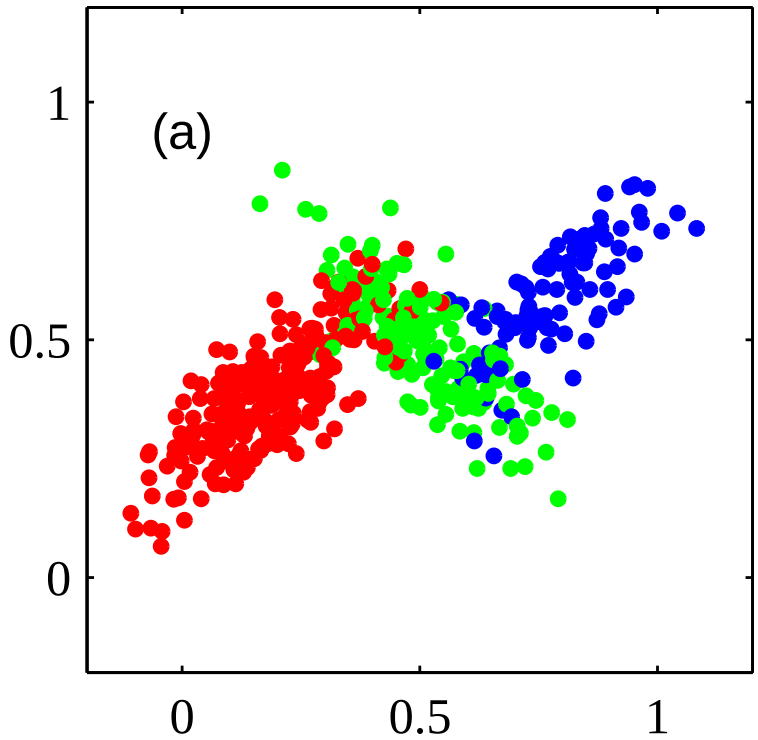



- Data points seem to form 3 clusters
- We cannot model $p(\boldsymbol{x})$ with simple and known distributions
- E.g., the data is not a Guassian b/c we have 3 distinct concentrated regions

# Gaussian mixture models: intuition

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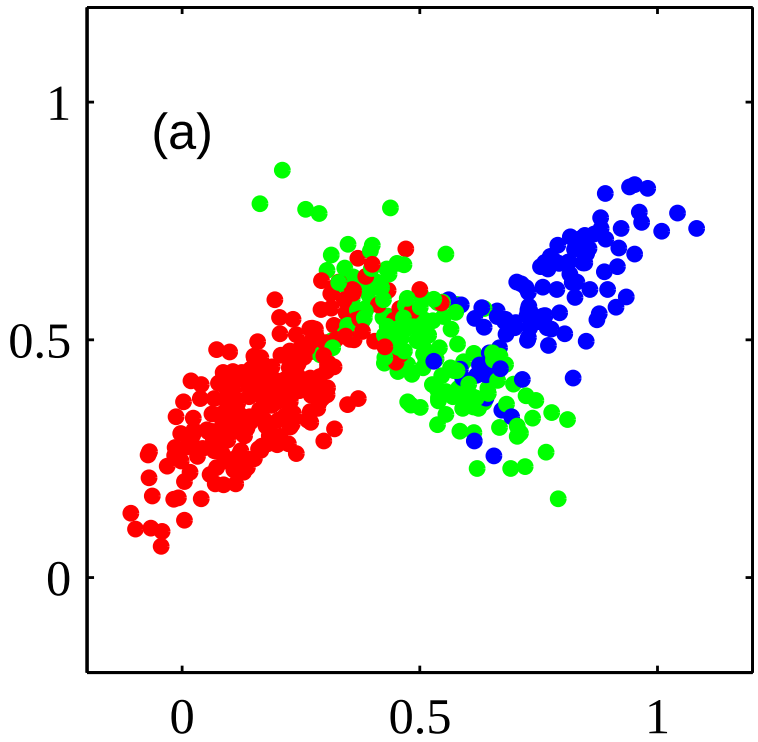


- We can model *each* region with a distinct distribution
- Common to use Gaussians, i.e., Gaussian mixture models (GMMs) or mixture of Gaussians (MoGs).
- We don't know *cluster assignments* (label) or *parameters* of Gaussians or *mixture components*!
- We need to learn them all from our *unlabeled* data $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^N$

# Gaussian mixture models: formal definition

A Gaussian mixture model has the following density function for $\boldsymbol{x}$

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- $K$: the number of Gaussians — they are called (mixture) components
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$$\forall\ k,\ \omega_k > 0, \quad \text{and} \quad \sum_k \omega_k = 1$$

The properties ensure $p(\boldsymbol{x})$ is a properly normalized probability density function.

# GMM as the marginal distribution of a joint distribution

Consider the following joint distribution

$$p(\boldsymbol{x}, z) = p(z)p(\boldsymbol{x}|z)$$

where $z$ is a discrete random variable taking values between $1$ and $K$.

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Then, the marginal distribution of $\boldsymbol{x}$ is

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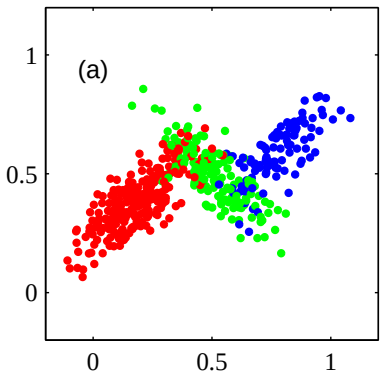
Namely, the Gaussian mixture model

# GMMs: example




The conditional distribution between $\boldsymbol{x}$ and $z$ (representing color) are

$$p(\boldsymbol{x}|z = red) = N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$$
$$p(\boldsymbol{x}|z = blue) = N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$$
$$p(\boldsymbol{x}|z = green) = N(\boldsymbol{x}|\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3)$$

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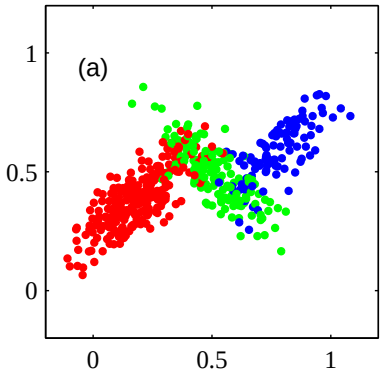


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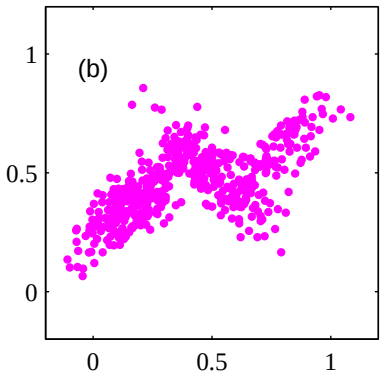


The marginal distribution is thus

$$p(\boldsymbol{x}) = p(red)N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + p(blue)N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) + p(green)N(\boldsymbol{x}|\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3)$$

# Parameter estimation for Gaussian mixture models

The parameters in GMMs are $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$. To estimate, consider the simple (and unrealistic) case first.

**We have labels $z$** If we assume $z$ is observed for every $\boldsymbol{x}$, then our estimation problem is easier to solve. Our training data is augmented:

$$\mathcal{D}' = \{\boldsymbol{x}_n, z_n\}_{n=1}^N$$

$z_n$ denotes the region where $\boldsymbol{x}_n$ comes from. $\mathcal{D}'$ is the *complete* data and $\mathcal{D}$ the *incomplete* data. How can we learn our parameters?

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Given $\mathcal{D}'$, the maximum likelihood estimation of the $\boldsymbol{\theta}$ is given by

$$\boldsymbol{\theta} = \arg\max \log \mathcal{D}' = \sum_n \log p(\boldsymbol{x}_n, z_n)$$

# Parameter estimation for GMMs: complete data

The *complete* likelihood is decomposable

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_n \log p(z_n)p(\boldsymbol{x}_n|z_n) = \sum_k \sum_{n:z_n=k} \log p(z_n)p(\boldsymbol{x}_n|z_n)$$

where we have grouped data by its values $z_n$. Let us introduce a binary variable $\gamma_{nk} \in \{0, 1\}$ to indicate whether $z_n = k$. We then have

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$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_k \sum_n \gamma_{nk} \log p(z = k)p(\boldsymbol{x}_n|z = k)$$

We use a "dummy" variable $z$ to denote all the possible values cluster assignment values for $\boldsymbol{x}_n$

$\mathcal{D}'$ specifies this value in the complete data setting

# Parameter estimation for GMMs: complete data

From our previous discussion, we have

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_k \sum_n \gamma_{nk} \left[\log \omega_k + \log N(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right]$$

Regrouping, we have

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_k \sum_n \gamma_{nk} \log \omega_k + \sum_k \left\{ \sum_n \gamma_{nk} \log N(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

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The term inside the braces depends on $k$-th component's parameters. It is now easy to show that (left as an exercise) the MLE is:

$$\omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

What's the intuition?

# Intuition

Since $\gamma_{nk}$ is binary, the previous solution is nothing but

- For $\omega_k$: count the number of data points whose $z_n$ is $k$ and divide by the total number of data points (note that $\sum_k \sum_n \gamma_{nk} = N$)
- For $\boldsymbol{\mu}_k$: get all the data points whose $z_n$ is $k$, compute their mean
- For $\boldsymbol{\Sigma}_k$: get all the data points whose $z_n$ is $k$, compute their covariance matrix

This intuition is going to help us to develop an algorithm for estimating $\boldsymbol{\theta}$ when we do not know $z_n$ (incomplete data).

# Parameter estimation for GMMs: incomplete data

When $z_n$ is not given, we can guess it via the posterior probability

$$p(z_n = k|\boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{p(\boldsymbol{x}_n)} = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n|z_n = k')p(z_n = k')}$$

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To compute the posterior probability, we need to know the parameters $\boldsymbol{\theta}$!

Let's pretend we know the value of the parameters so we can compute the posterior probability.

How is that going to help us?

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We define $\gamma_{nk} = p(z_n = k|\boldsymbol{x}_n)$

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- Each $\boldsymbol{x}_n$ is assigned to a component fractionally according to $p(z_n = k|\boldsymbol{x}_n)$

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- Each $\boldsymbol{x}_n$ is assigned to a component fractionally according to $p(z_n = k|\boldsymbol{x}_n)$

We now get the same expression for the MLE as before!

$$\omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

But remember, we're 'cheating' by using $\boldsymbol{\theta}$ to compute $\gamma_{nk}$!

# Iterative procedure

We can alternate between estimating $\gamma_{nk}$ and using the estimated $\gamma_{nk}$ to compute the parameters (same idea as with $K$-means!)

- Step 0: initialize $\boldsymbol{\theta}$ with some values (random or otherwise)
- Step 1: compute $\gamma_{nk}$ using the current $\boldsymbol{\theta}$
- Step 2: update $\boldsymbol{\theta}$ using the just computed $\gamma_{nk}$
- Step 3: go back to Step 1

Questions:

- Is this procedure reasonable, i.e., are we optimizing a sensible criteria?
- Will this procedure converge?

The answers lie in the *EM algorithm* — a powerful procedure for model estimation with unknown data (next lecture).