Machine Learning

CSCI 5622 Fall 2020

Prof. Claire Monteleoni

Today

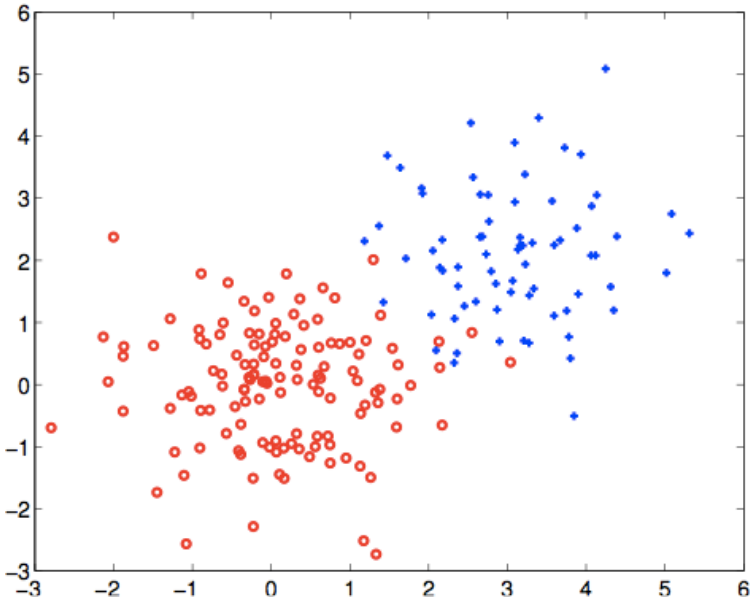
- Intro. to Generative Learning / probabilistic models
  - Maximum likelihood parameter estimation
  - Mixture models
  - Expectation maximization (EM)

with much credit to S. Dasgupta and T. Jaakkola

Training/test data generation

- We assume that the training (and test) examples are drawn as samples (generated) from some unknown distribution

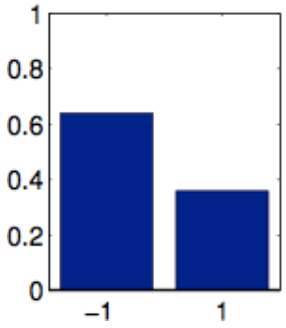
$$(\underline{x}, y) \sim P(\underline{x}, y) = P(\underline{x})P(y|\underline{x}) = P(\underline{x}|y)P(y)$$



- We can always think of these samples $(\underline{x}, y)$ as having been generated in two steps: first y, then $\underline{x}$ given y

$$y \sim P(y), \quad \underline{x} \sim P(\underline{x}|y)$$

Generative modeling: estimation



$P(y;\hat{\theta})$

$P(\underline{x}|y=-1;\hat{\theta})$

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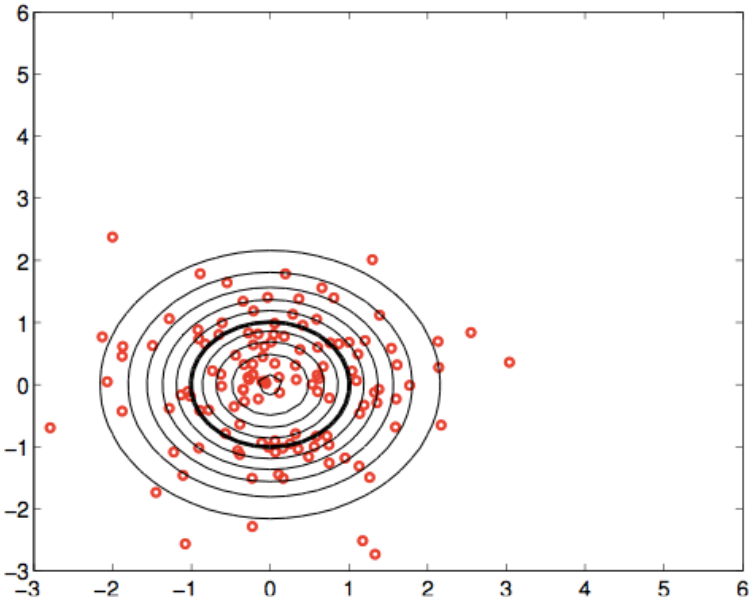
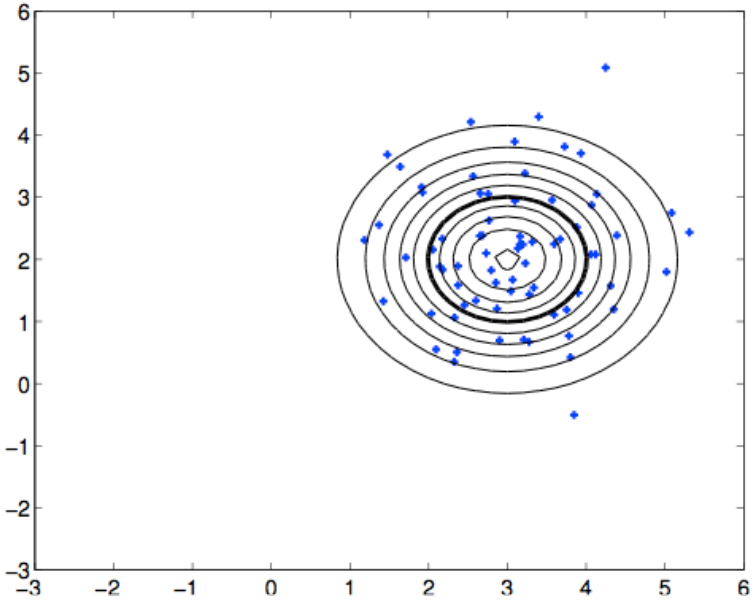




Maximum likelihood estimation

- Our parameterized Gaussian model is

$$P(\underline{x}, y; \theta) = P(\underline{x}|y; \theta)P(y; \theta) = N(\underline{x};\, \mu_y, \sigma_y^2 I)\, P(y; \theta)$$

- We find parameters $\theta = (\underline{\mu}_+, \underline{\mu}_-, \sigma_+^2, \sigma_-^2, q)$ that maximize the log-likelihood of the training data (examples and labels)

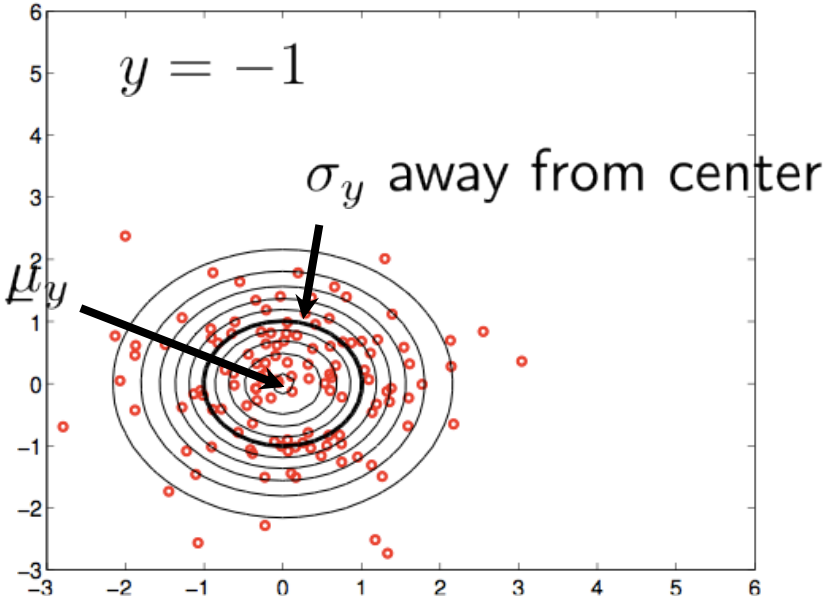
$$l(D; \theta) = \sum_{i=1}^{n} \log P(\underline{x}_i, y_i; \theta) = \sum_{i=1}^{n} \left[\log P(\underline{x}_i|y_i; \theta) + \log P(y_i; \theta) \right]$$

Generative modeling

- We can use simple spherical Gaussian models for the class-conditional distributions

$$P(\underline{x}|y;\theta) = N(\underline{x};\, \underline{\mu}_y, \sigma_y^2 I)$$

$$= \frac{1}{(2\pi\sigma_y^2)^{d/2}} \exp\left\{ -\frac{1}{2\sigma_y^2}\|\underline{x} - \underline{\mu}_y\|^2 \right\}$$



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$$+ \sum_{i=1}^{n} \left[\delta(y_i, 1) \log q + \delta(y_i, -1) \log(1 - q) \right]$$

indicator function

Maximum likelihood estimation

$$l(D;\theta) = \sum_{i=1}^{n} \left[-\frac{d}{2}\log(2\pi\sigma_{y_i}^2) - \frac{1}{2\sigma_{y_i}^2}\|\underline{x}_i - \mu_{y_i}\|^2 \right]$$

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$$\frac{\partial}{\partial q} l(D;\theta) = \frac{\sum_{i=1}^{n} \delta(y_i, 1)}{q} - \frac{\sum_{i=1}^{n} \delta(y_i, -1)}{1-q} = 0$$

Maximum likelihood estimation

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$$\Rightarrow \hat{q} = \frac{1}{n}\sum_{i=1}^{n} \delta(y_i, 1)$$

fraction of points labeled +1

Maximum likelihood estimation

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$$\Rightarrow \hat{\mu}_y = \frac{1}{\sum_{i=1}^{n} \delta(y, y_i)} \sum_{i=1}^{n} \delta(y, y_i)\, \underline{x}_i$$

average of points in class y

Maximum likelihood estimation

$$l(D;\theta) = \sum_{i=1}^{n} \left[-\frac{d}{2}\log(2\pi\sigma_{y_i}^2) - \frac{1}{2\sigma_{y_i}^2}\|\underline{x}_i - \mu_{y_i}\|^2 \right]$$

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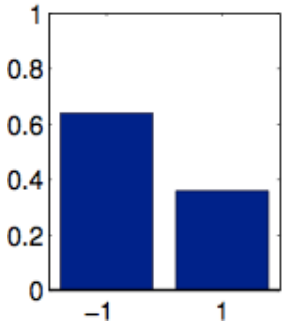
$$\Rightarrow \hat{\sigma}_y^2 = \frac{1}{d\sum_{i=1}^{n}\delta(y, y_i)} \sum_{i=1}^{n} \delta(y, y_i)\,\|\underline{x}_i - \hat{\mu}_y\|^2$$

average per dimension squared error in class y

Generative modeling: classification



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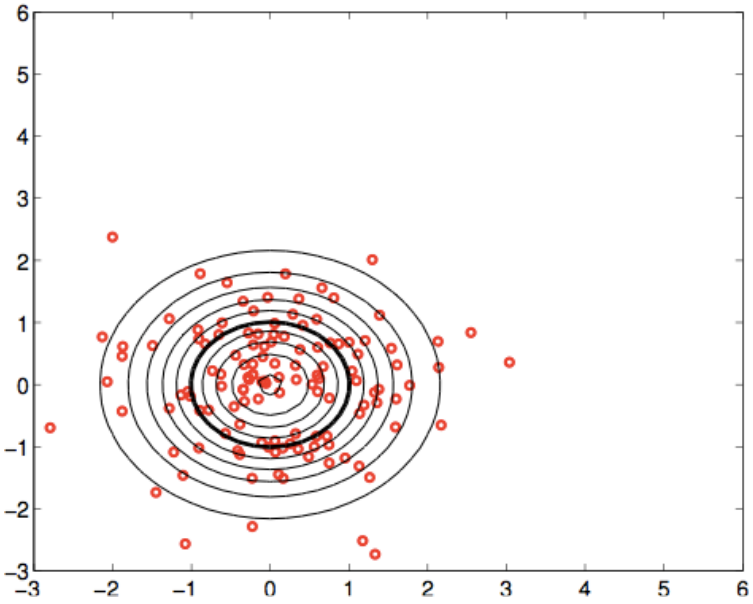

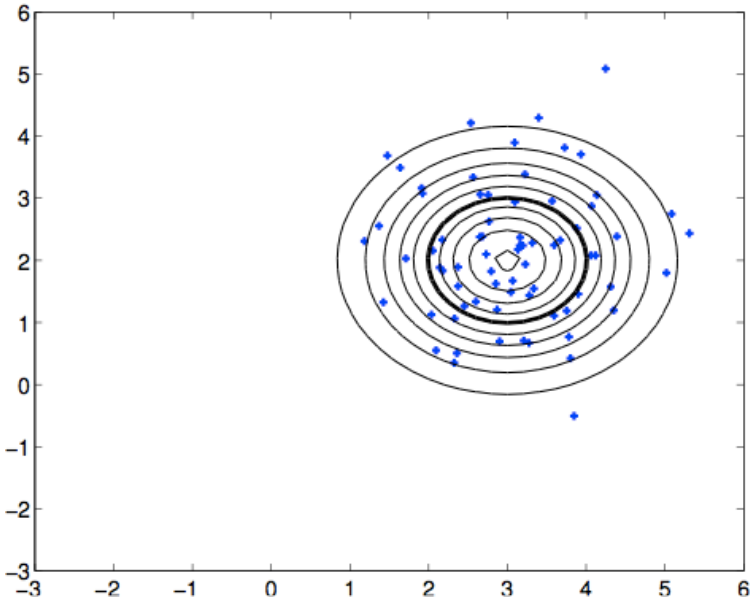

Decision boundary

- We predict the most likely label for $\underline{x}$ (cf. minimum probability of error classifier)

$$\hat{y} = \arg\max_{y} P(\underline{x}, y; \hat{\theta})$$

- The resulting decision boundary corresponds to all $\underline{x}$ such that

$$\log \frac{P(\underline{x}, y=1; \hat{\theta})}{P(\underline{x}, y=-1; \hat{\theta})} = \log \frac{P(y=1; \hat{\theta})}{P(y=-1; \hat{\theta})} + \log \frac{P(\underline{x}|y=1; \hat{\theta})}{P(\underline{x}|y=-1; \hat{\theta})} = 0$$

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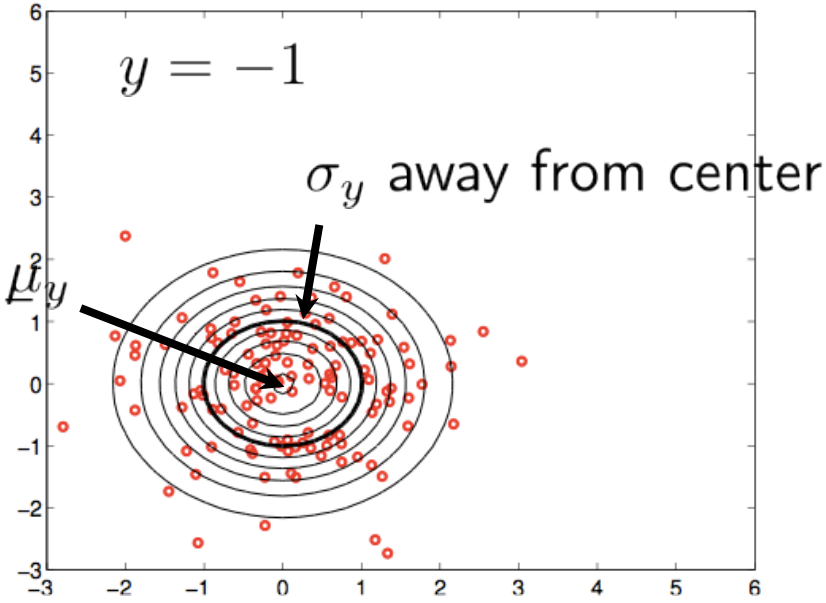

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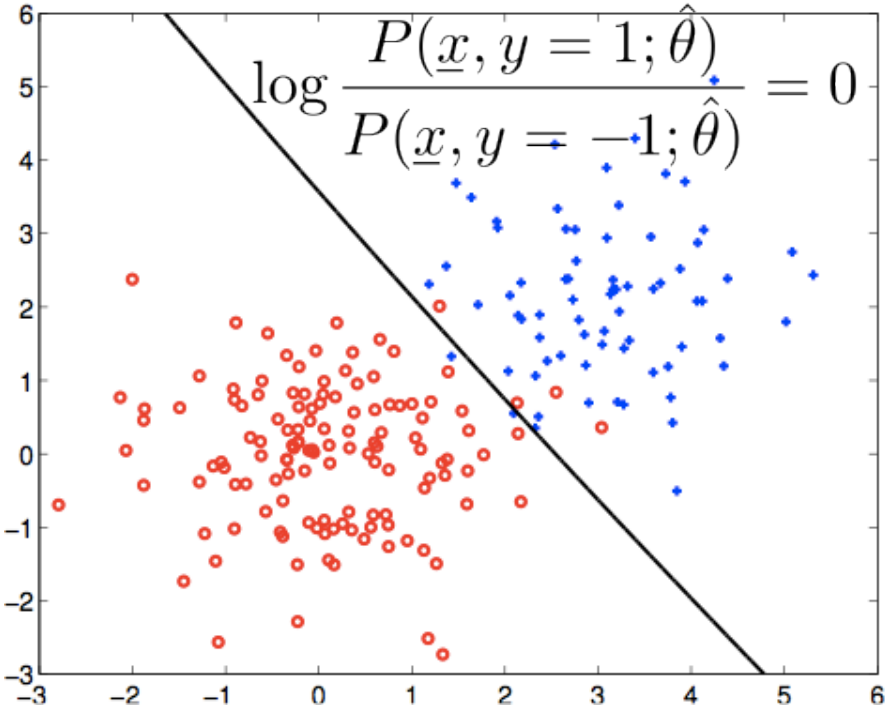
$$\begin{aligned}
\log \frac{P(\underline{x}, y=1; \hat{\theta})}{P(\underline{x}, y=-1; \hat{\theta})} &= \log \frac{P(y=1; \hat{\theta})}{P(y=-1; \hat{\theta})} + \log \frac{P(\underline{x}|y=1; \hat{\theta})}{P(\underline{x}|y=-1; \hat{\theta})} \\
&= \log \frac{\hat{q}}{1-\hat{q}} - \frac{d}{2} \log(\frac{\hat{\sigma}_{+1}^2}{\hat{\sigma}_{-1}^2}) \\
&\quad - \frac{1}{2\sigma_{+1}^2} \|\underline{x} - \underline{\mu}_{+1}\|^2 + \frac{1}{2\sigma_{-1}^2} \|\underline{x} - \underline{\mu}_{-1}\|^2 \\
&= 0
\end{aligned}$$

- This is linear in $\underline{x}$ if $\sigma_{+1}^2 = \sigma_{-1}^2$ (otherwise quadratic)

Decision boundary

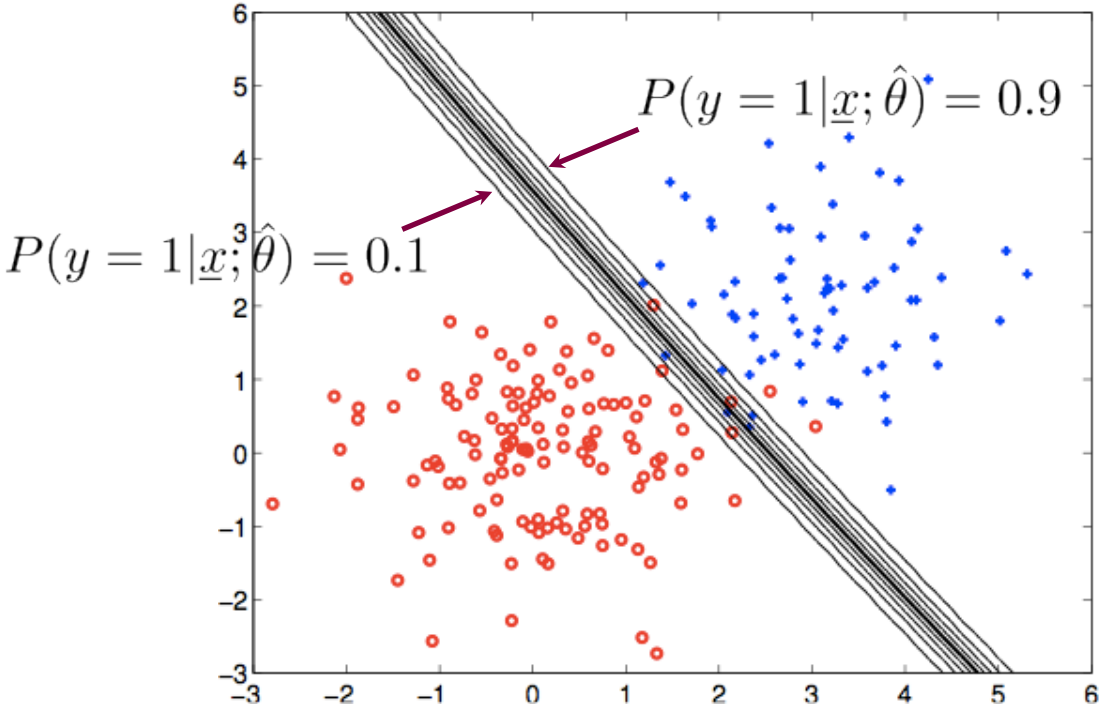


- This is very close to the optimal since the data were generated from two Gaussians with the same variance

Probabilistic predictions

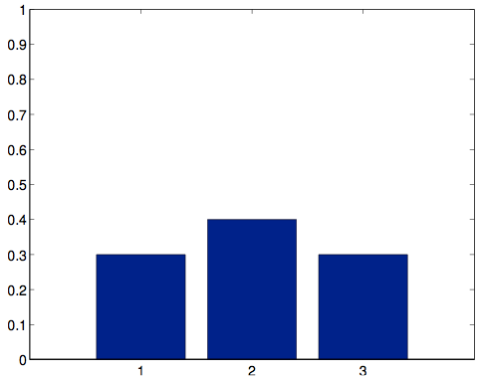
- The model also permits us to evaluate probabilities over the possible class labels such as

$$P(y = 1|\underline{x}; \hat{\theta}) = \frac{P(\underline{x}, y = 1; \hat{\theta})}{\sum_{y' \in \{-1,1\}} P(\underline{x}, y'; \hat{\theta})}$$



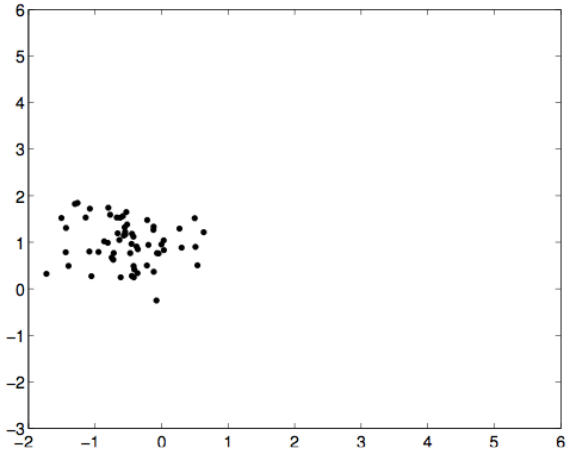
A mixture model

three types $z = 1, 2, 3$

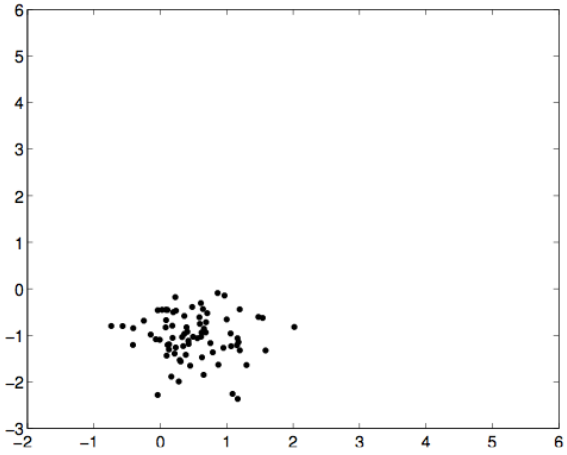


$P(z; \hat{\theta})$

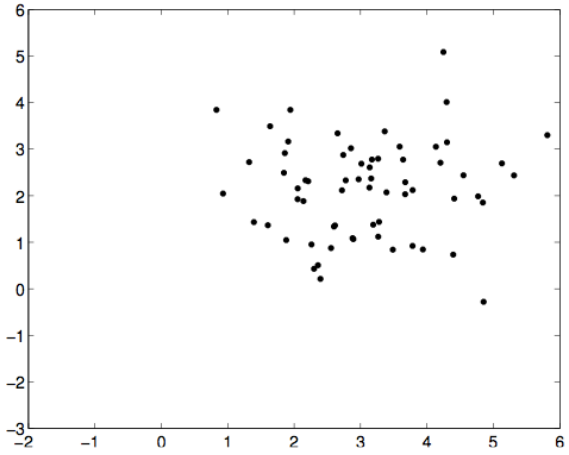
$P(\underline{x}|z = 1; \hat{\theta})$



$P(\underline{x}|z = 2; \hat{\theta})$

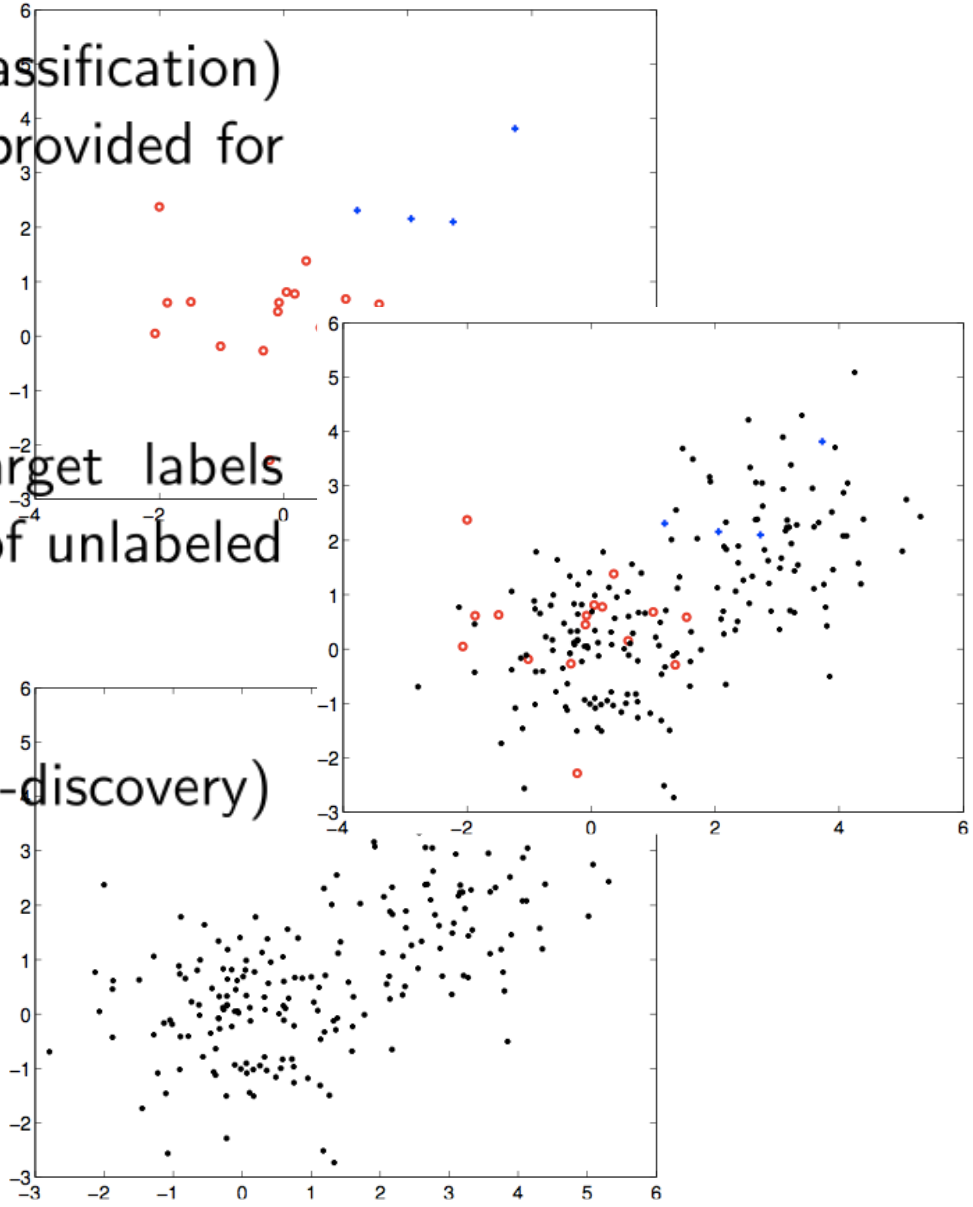


$P(\underline{x}|z = 3; \hat{\theta})$



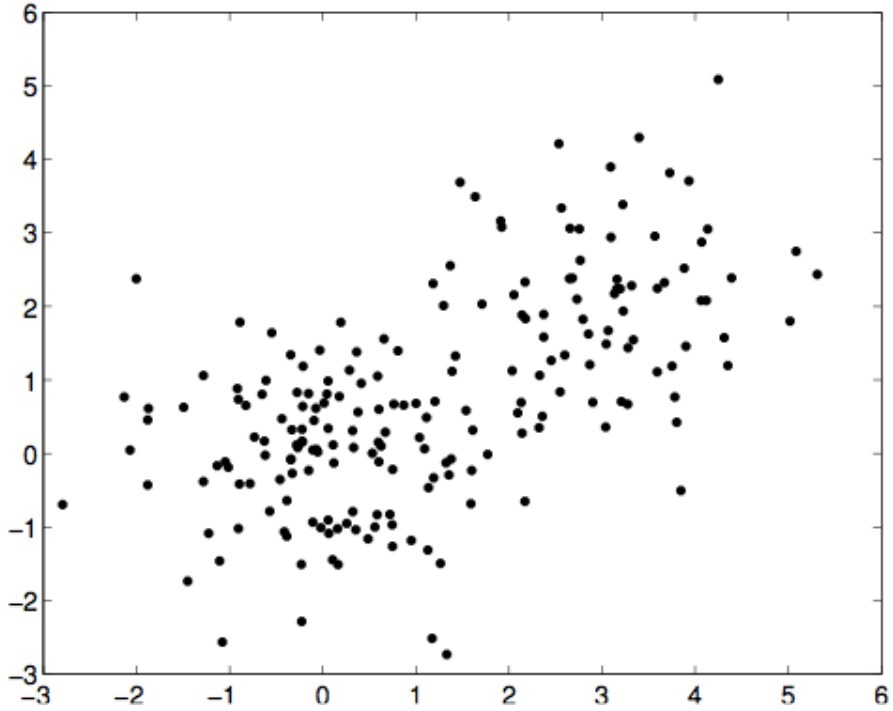
Classification - class discovery

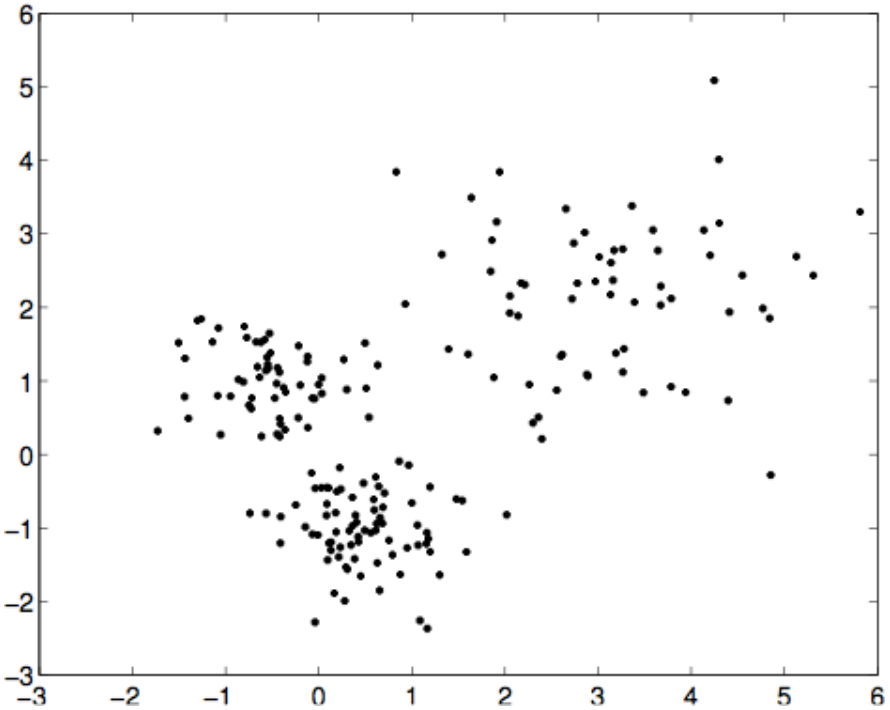
- Supervised learning (e.g., classification)
  - target labels (responses) provided for each example
- Semi-supervised learning
  - in addition to a few target labels we have a large number of unlabeled examples
- Unsupervised learning (class-discovery)
  - all examples are unlabeled



Class or type discovery

- There may be many underlying classes or "types" of examples
- Each class may itself consist of different sub-types
- Our goal is to discover how the data may have been generated from a "mixture" of underlying types





Mixtures and latent variables

- A k-component mixture model with parameters θ

$$P(\underline{x}, z; \theta) = P(\underline{x}|z; \theta)P(z; \theta)$$

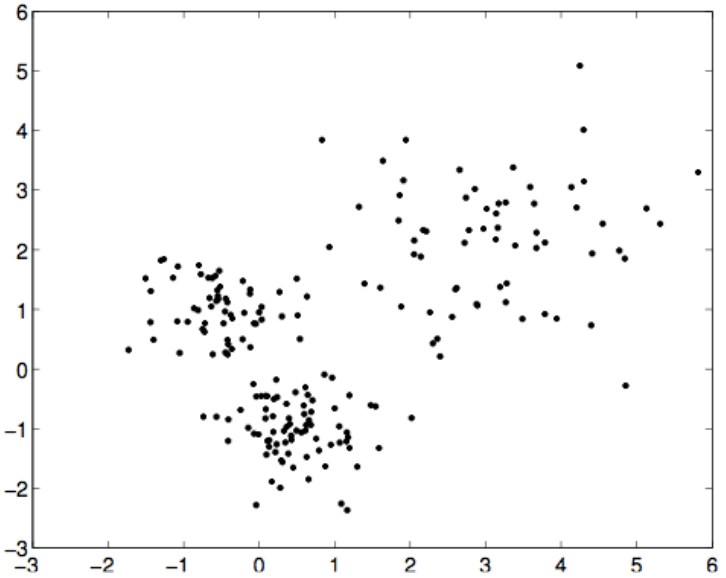
$$z \sim P(z; \theta) \text{ sample type } z = 1, \ldots, k$$

$$\underline{x} \sim P(\underline{x}|z; \theta) \text{ sample } \underline{x} \text{ given type } z$$

- The type z is latent (unobserved). The marginal distribution over $\underline{x}$ is given by the mixture

$$P(\underline{x}; \theta) = \sum_{z=1}^{k} P(\underline{x}|z; \theta)P(z; \theta)$$

$$\underline{x} \sim P(\underline{x}; \theta) \text{ sample } \underline{x}$$



Mixture estimation

- Consider a $k-$component mixture of spherical Gaussians

$$P(z;\theta) = \theta_z, \quad \sum_{z=1}^{k} \theta_z = 1$$

$$P(\underline{x}|z;\theta) = N(\underline{x};\, \underline{\mu}_z, \sigma_z^2 I)$$

where $\theta = \{\underline{\mu}_1, \ldots, \underline{\mu}_k, \sigma_1^2, \ldots, \sigma_k^2, \theta_1, \ldots, \theta_k\}$.

- We estimate the mixture parameters by maximizing the log-likelihood of the observed data $D = \{\underline{x}_1, \ldots, \underline{x}_n\}$

$$l(D;\theta) = \sum_{i=1}^{n} \log P(\underline{x}_i;\theta) = \sum_{i=1}^{n} \log \sum_{z=1}^{k} P(\underline{x}_i|z;\theta) P(z;\theta)$$

- This would be much easier if we knew the value of z corresponding to each $\underline{x}_i$ (complete data).

Mixture estimation: complete data

- If we knew the type z_i corresponding to each $\underline{x}_i$ then we would maximize the *complete log-likelihood*

$$\sum_{i=1}^{n} \log P(\underline{x}_i, z_i; \theta) = \sum_{i=1}^{n} \sum_{z=1}^{k} \delta(z, z_i) \log P(\underline{x}_i, z; \theta)$$

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- Just as in the classification context, finding the maximizing parameters is simple (based on separately estimating the Gaussians from the points assigned to them)

$$\hat{\theta}_z = \frac{\sum_{i=1}^{n} \delta(z, z_i)}{n}$$

$$\hat{\mu}_z = \frac{1}{\sum_{i=1}^{n} \delta(z, z_i)} \sum_{i=1}^{n} \delta(z, z_i)\, \underline{x}_i$$

$$\hat{\sigma}_z^2 = \frac{1}{d \sum_{i=1}^{n} \delta(z, z_i)} \sum_{i=1}^{n} \delta(z, z_i) \left\| \underline{x}_i - \hat{\mu}_z \right\|^2$$

The EM-algorithm

Initialize: select the initial parameters $\theta^{(0)}$

E-step: fix the current parameters $\theta^{(m)}$, evaluate posterior assignments (divide each point softly across the mixture components)

$$p(z|i) = P(z|\underline{x}_i; \theta^{(m)}), \quad z = 1, \ldots, k, \quad i = 1, \ldots, n$$

M-step: fix the posterior assignments $p(z|i)$, find new parameters $\theta^{(m+1)}$ by maximizing the expected complete log-likelihood

$$\sum_{i=1}^{n} \sum_{z=1}^{k} p(z|i) \log P(\underline{x}_i, z; \theta)$$

with respect to θ

Mixture estimation: E-step

- The difficulty now is that we have to *complete* the data by inferring values for the missing types z_i

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- Given the mixture parameters θ our best guess about the value of z_i corresponding to $\underline{x}_i$ is given by the posterior

$$p(z|i) = P(z|\underline{x}_i;\theta) = \frac{P(\underline{x}_i|z;\theta)P(z;\theta)}{\sum_{z'=1}^{k} P(\underline{x}_i|z';\theta)P(z';\theta)}$$

  Note that these "soft" posterior assignments $p(z|i)$ depend on the current setting of the parameters θ

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  Note that these "soft" posterior assignments $p(z|i)$ depend on the current setting of the parameters θ

- The soft assignments help us stochastically fill-in the missing type values. We therefore maximize the *expected log-likelihood* with respect to θ for fixed soft assignments

$$\sum_{i=1}^{n}\sum_{z=1}^{k} p(z|i)\log P(\underline{x}_i, z;\theta)$$

Mixture estimation: M-step

- As we have filled in the missing values, the estimation step is again easy. We simply use the "soft" posterior assignments $p(z|i)$ in place of the indicators $\delta(z, z_i)$

$$\hat{\theta}_z = \frac{\sum_{i=1}^{n} p(z|i)}{n}$$

$$\hat{\mu}_z = \frac{1}{\sum_{i=1}^{n} p(z|i)} \sum_{i=1}^{n} p(z|i)\, \underline{x}_i$$

$$\hat{\sigma}_z^2 = \frac{1}{d \sum_{i=1}^{n} p(z|i)} \sum_{i=1}^{n} p(z|i)\, \|\underline{x}_i - \hat{\underline{\mu}}_z\|^2$$

- These new parameters $\hat{\theta}$ can in turn be used to derive better soft assignments and so on.

[E-step]

The EM-algorithm

Initialize: select the initial parameters $\theta^{(0)}$

E-step: fix the current parameters $\theta^{(m)}$, evaluate posterior assignments (divide each point softly across the mixture components)

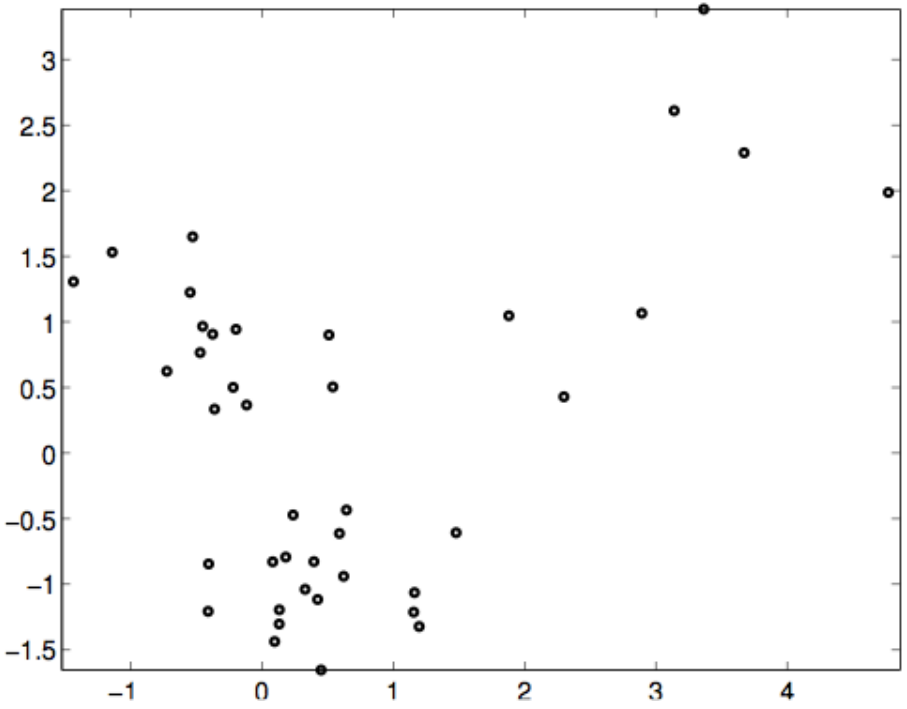
$$p(z|i) = P(z|\underline{x}_i; \theta^{(m)}), \quad z = 1, \ldots, k, \quad i = 1, \ldots, n$$

M-step: fix the posterior assignments $p(z|i)$, find new parameters $\theta^{(m+1)}$ by maximizing the expected complete log-likelihood

$$\sum_{i=1}^{n} \sum_{z=1}^{k} p(z|i) \log P(\underline{x}_i, z; \theta)$$

with respect to θ

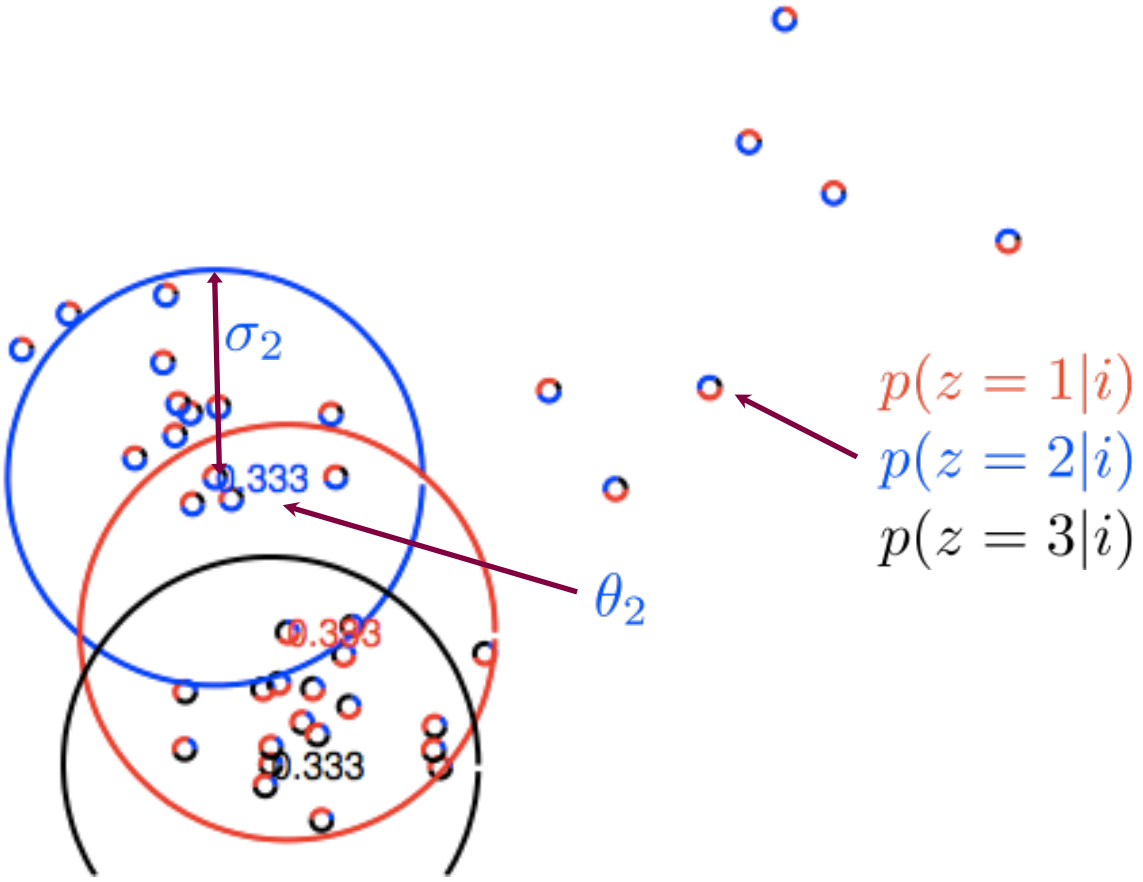
Mixture of Gaussians example



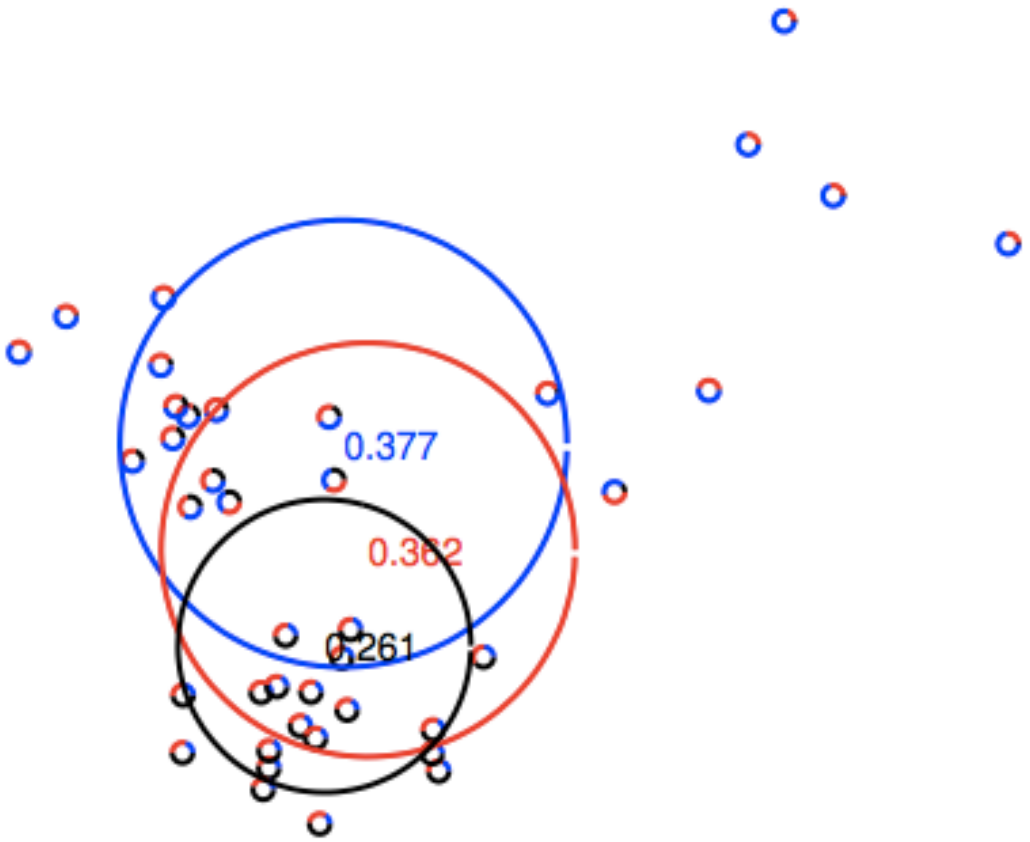
- The EM-algorithm is iterative and requires an initialization
  - $\theta_z = 1/k,\ z = 1, \ldots, k$
  - each μ_z is set to a randomly selected point
  - each σ_z^2 is set to the mean squared distance of points to the overall mean

Mixture of Gaussians example

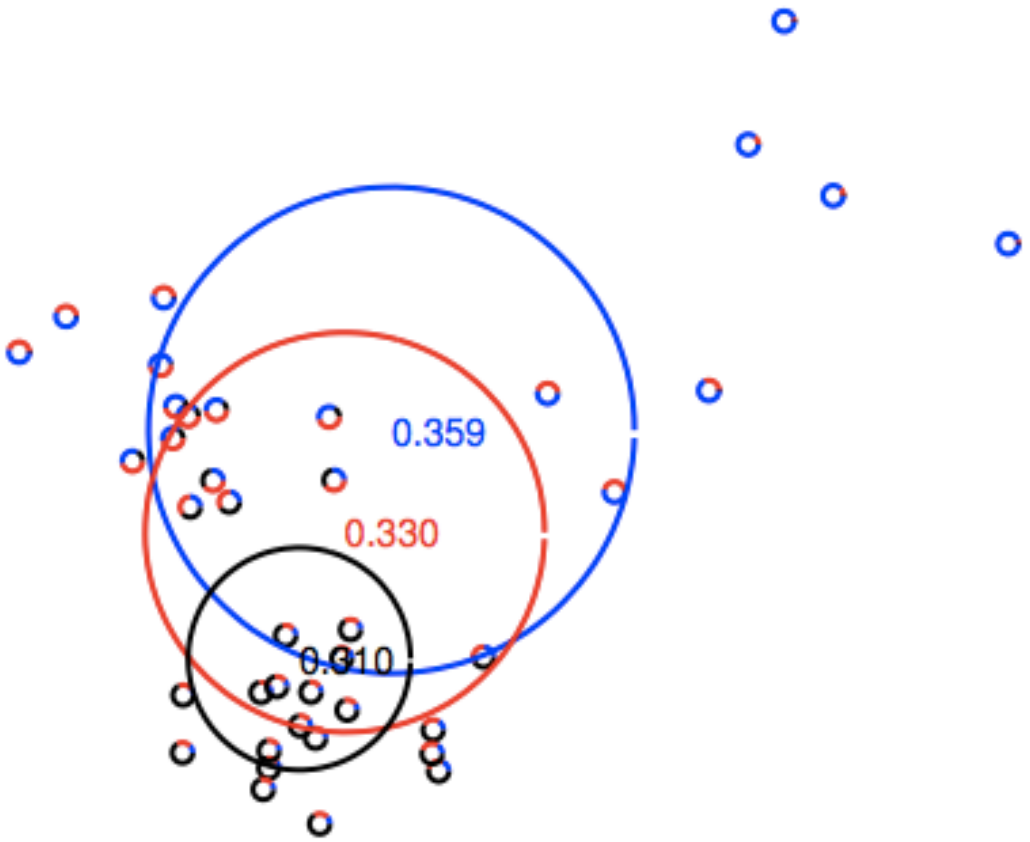
- initial 3-component mixture



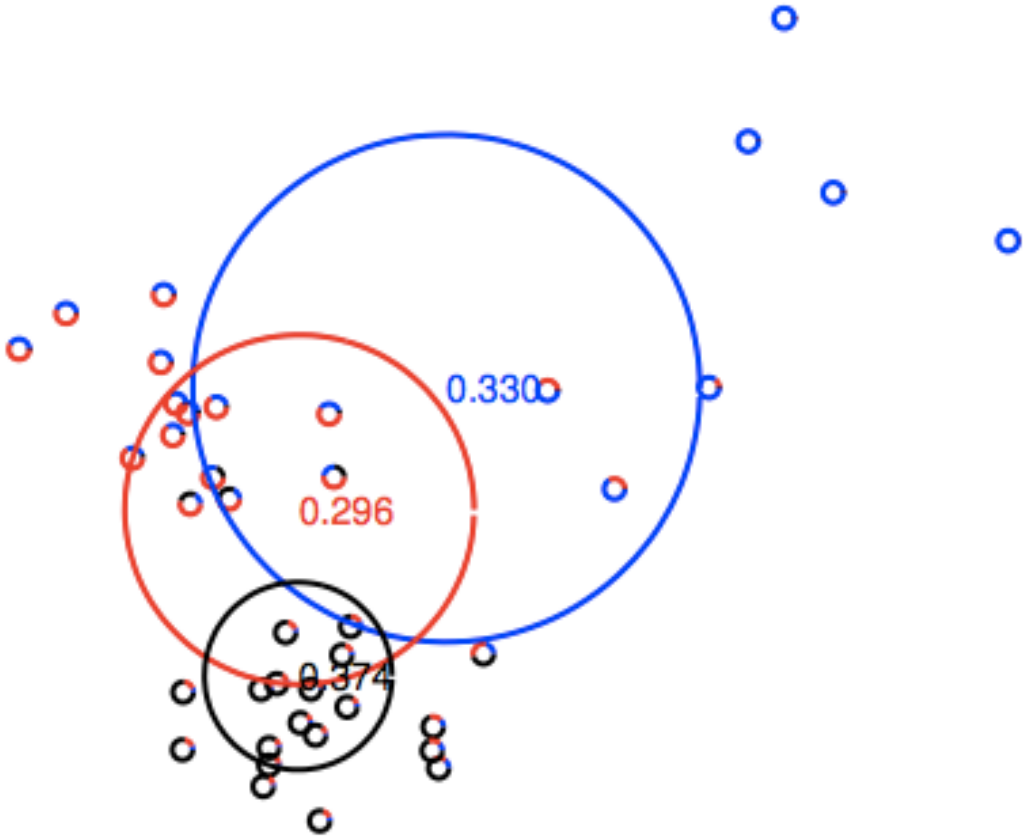
Mixture of Gaussians example



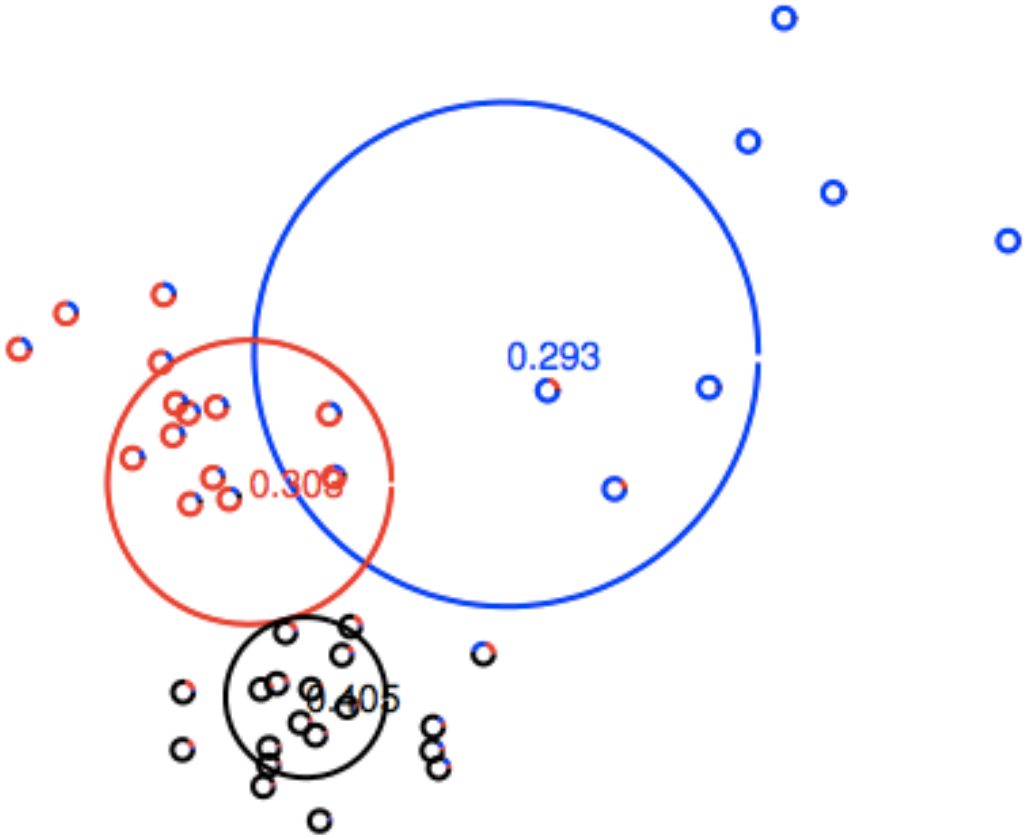
Mixture of Gaussians example



Mixture of Gaussians example



Mixture of Gaussians example



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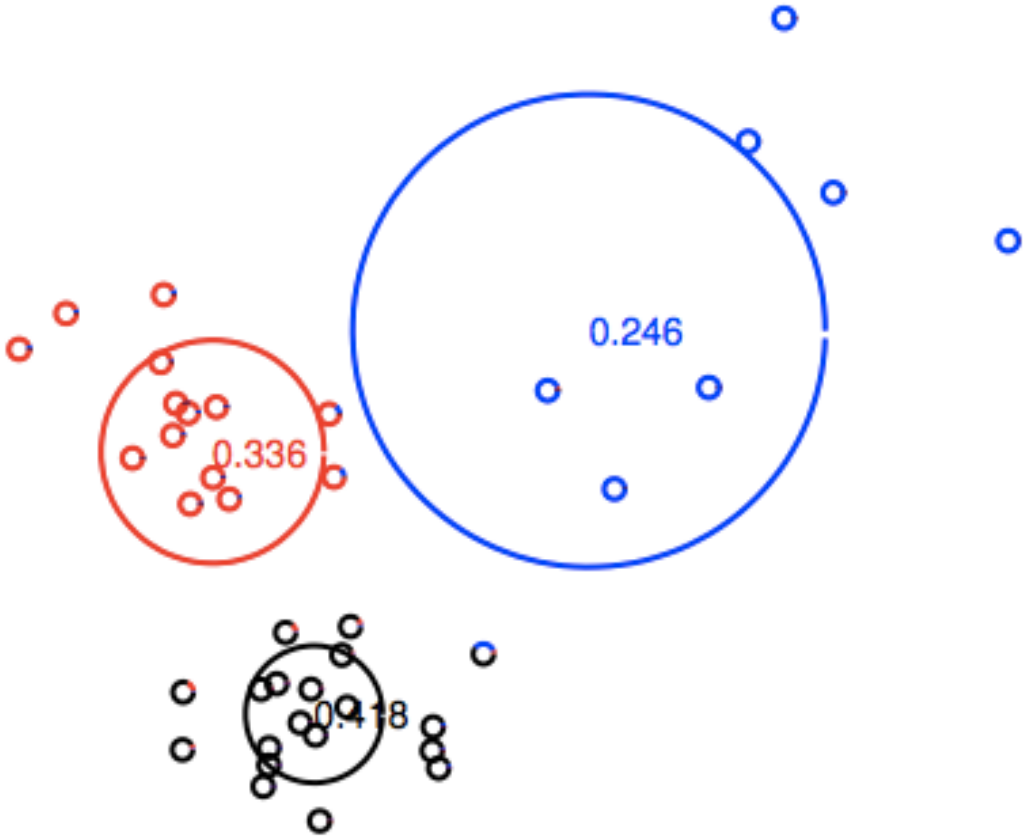
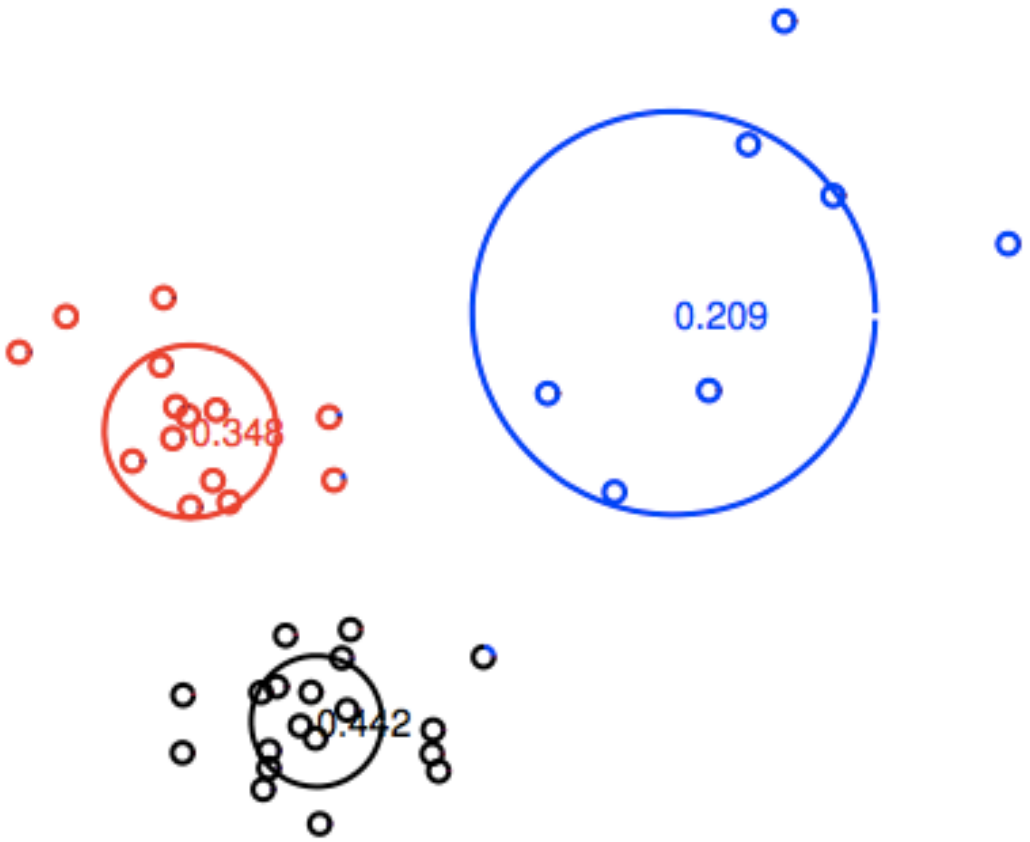
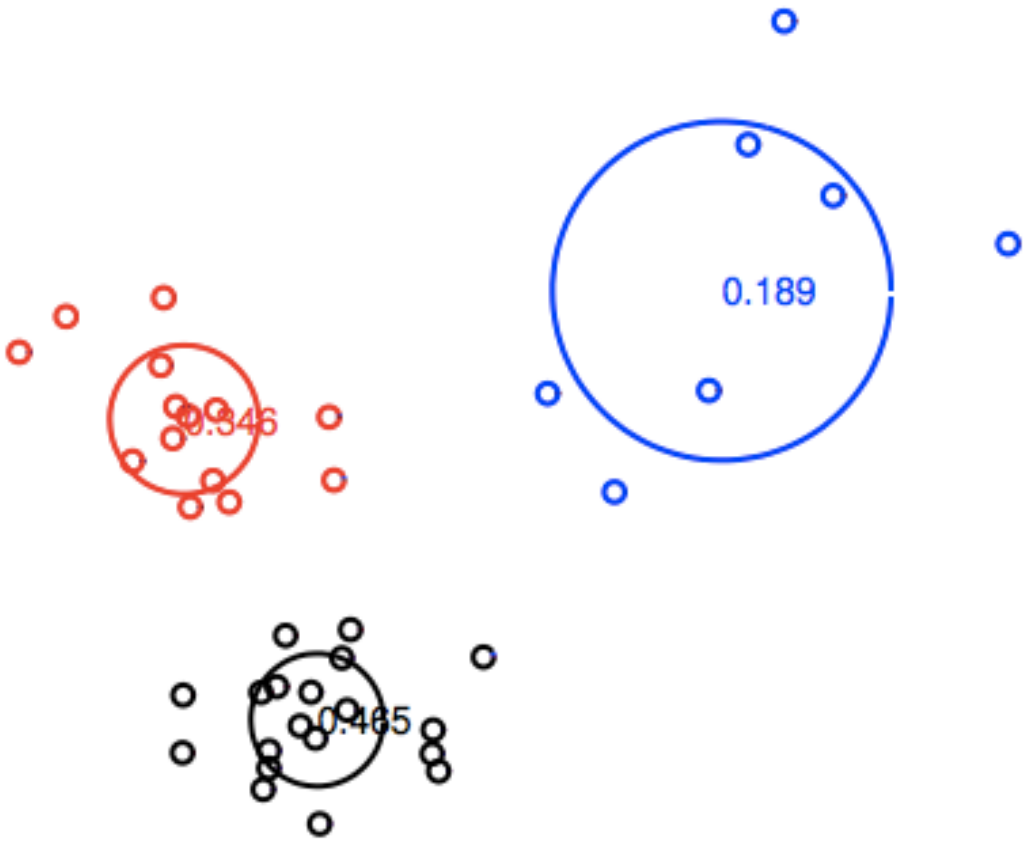


Mixture of Gaussians example

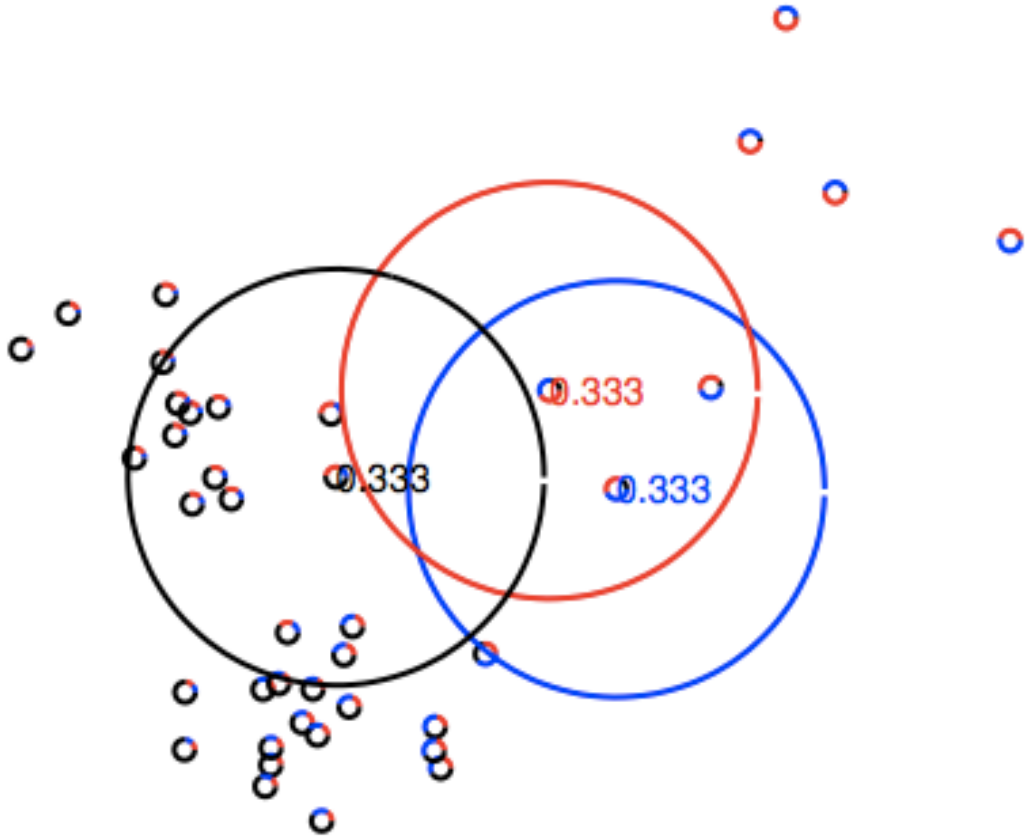


Mixture of Gaussians example

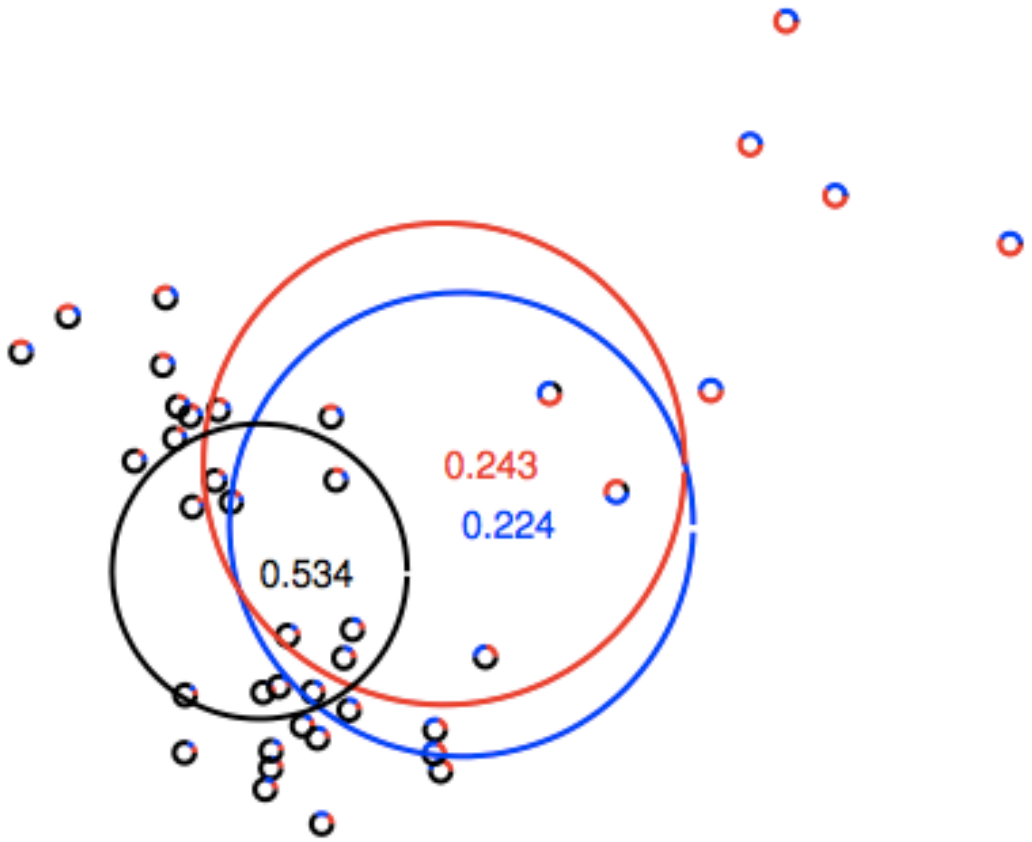


Mixture of Gaussians example

- initial 3-component mixture



Mixture of Gaussians example



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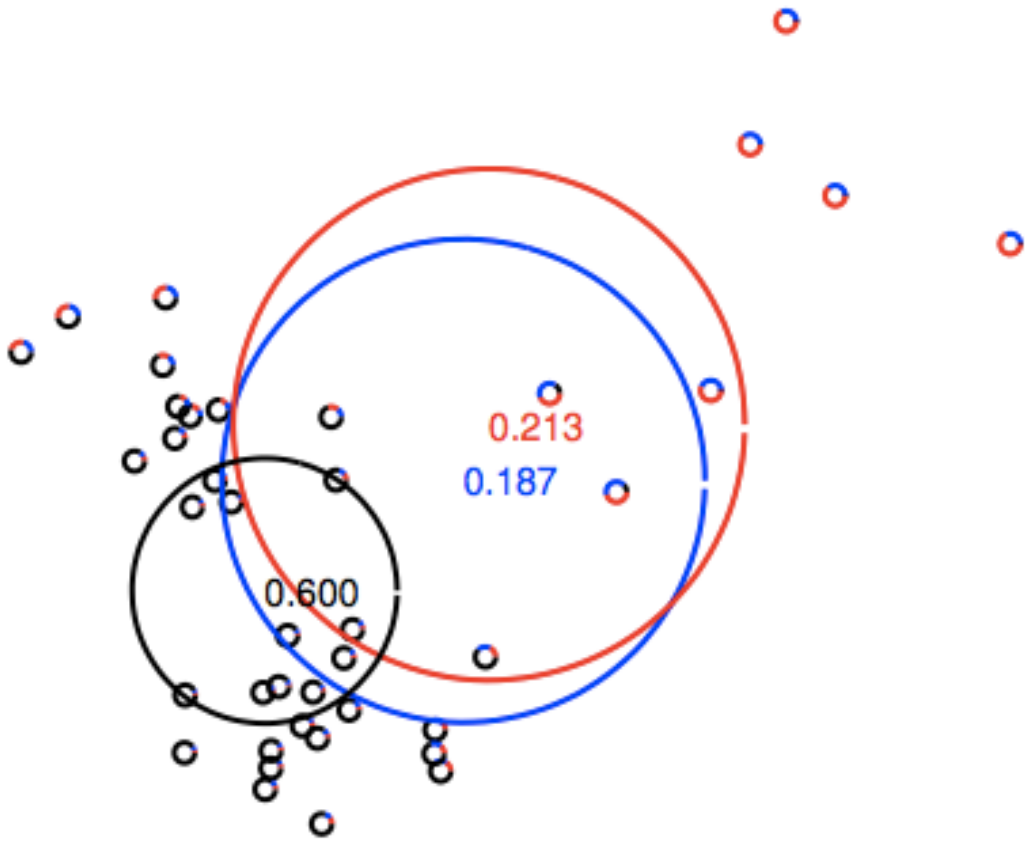

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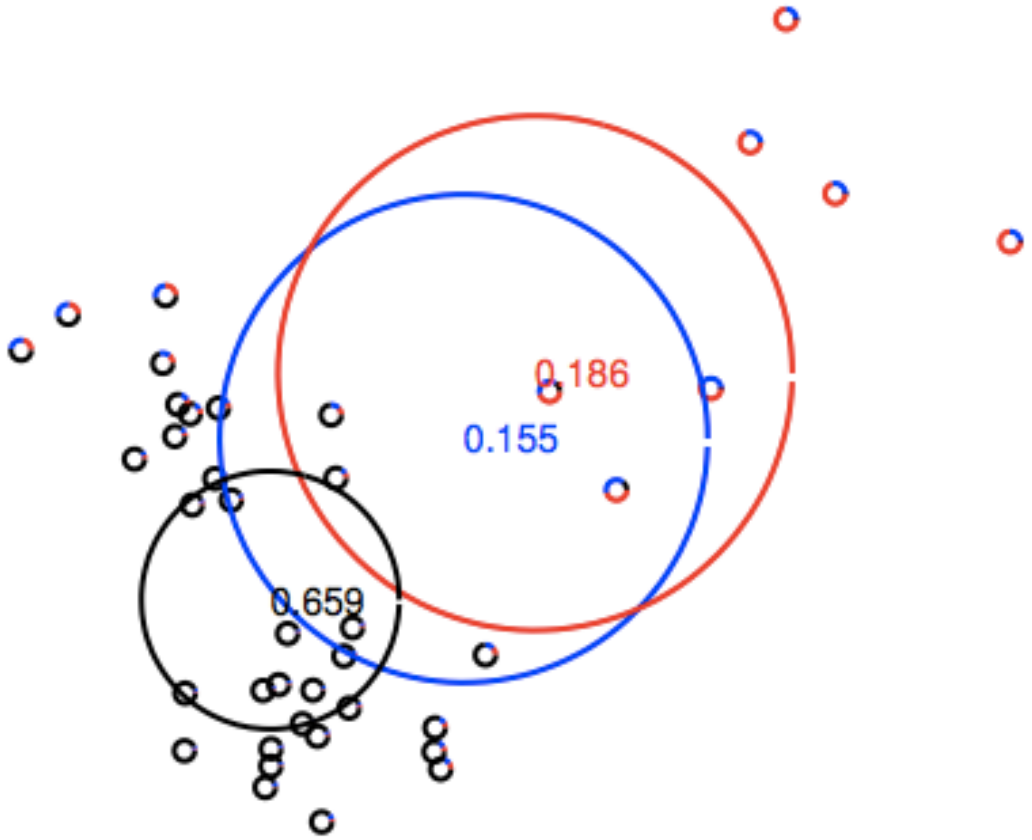

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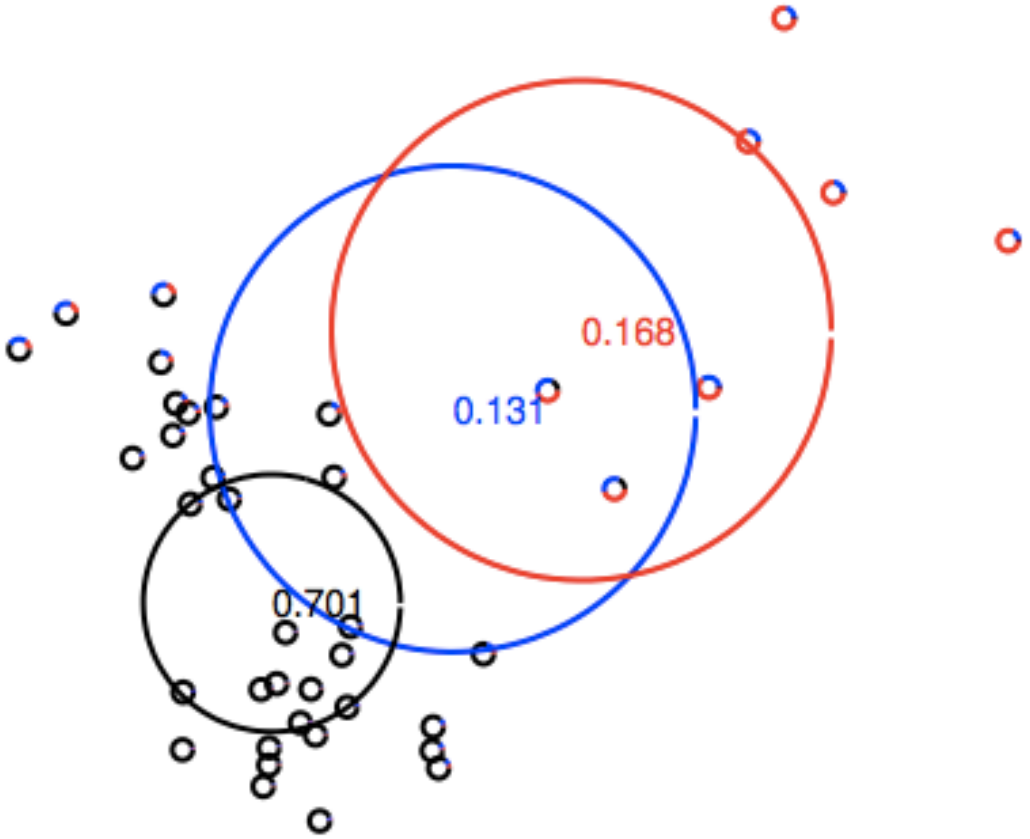

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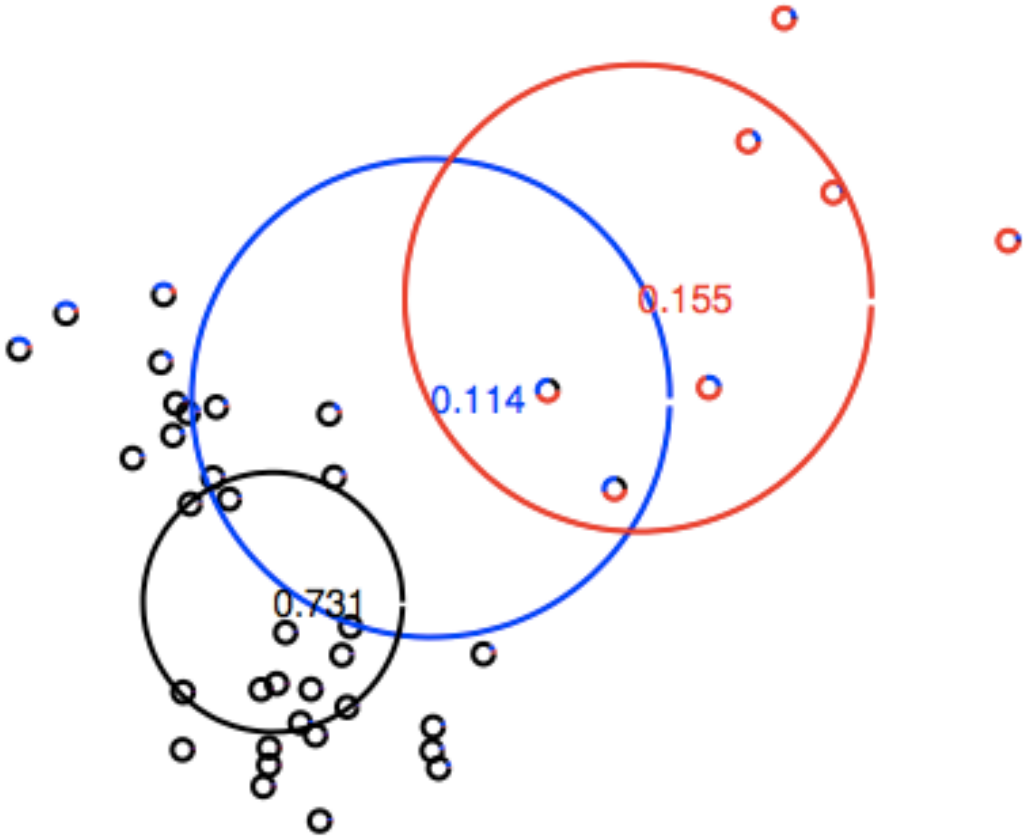

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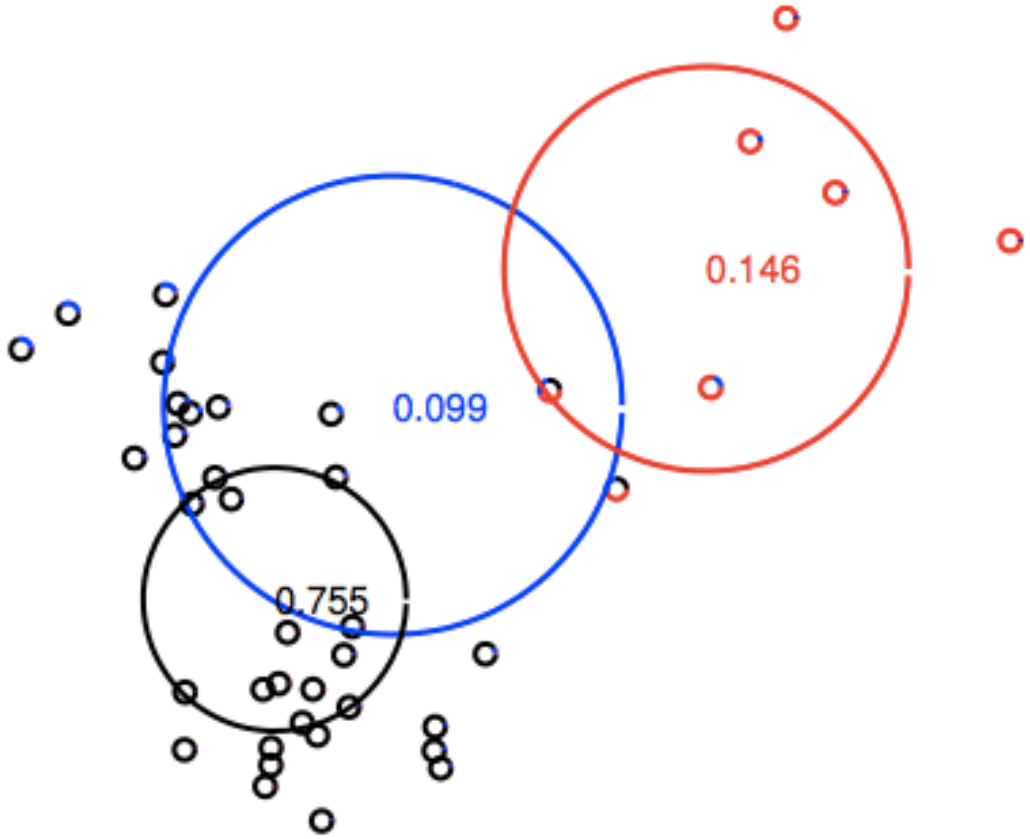

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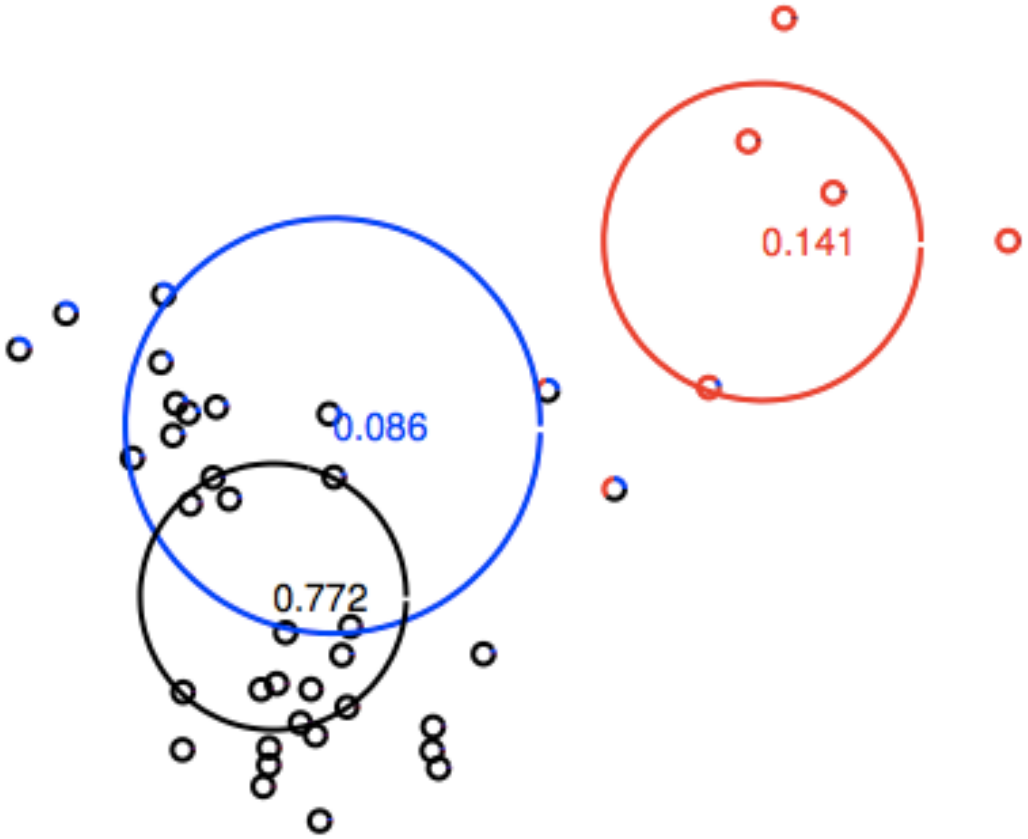

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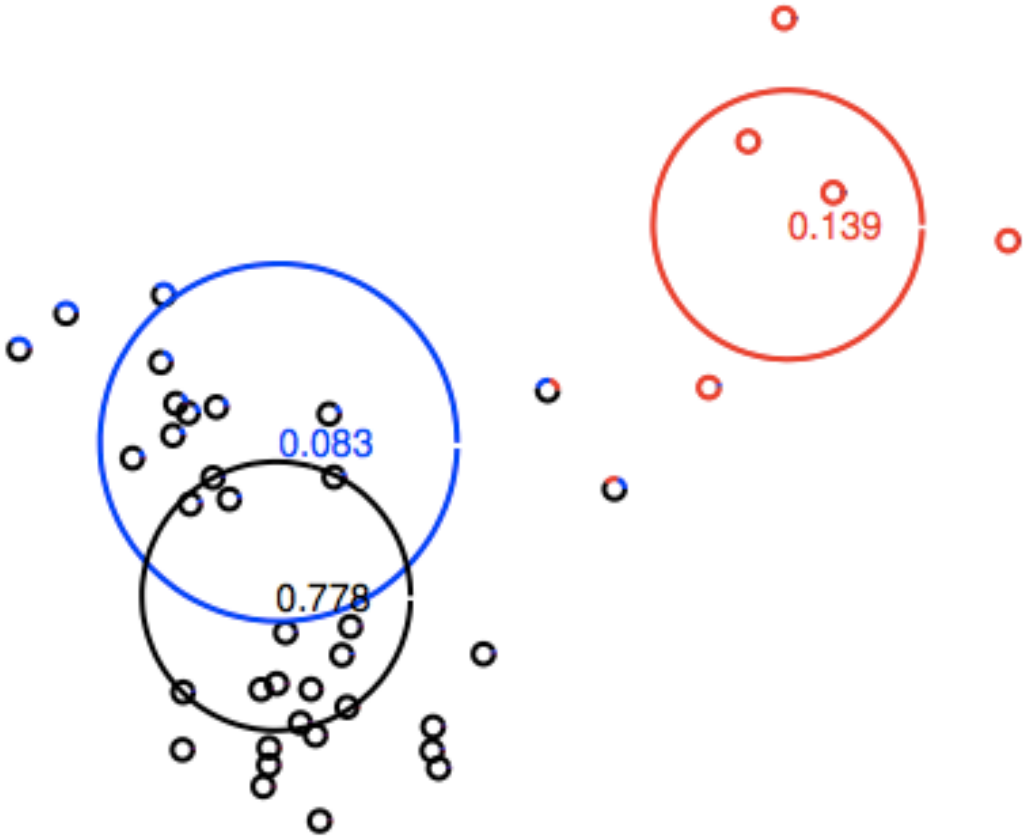

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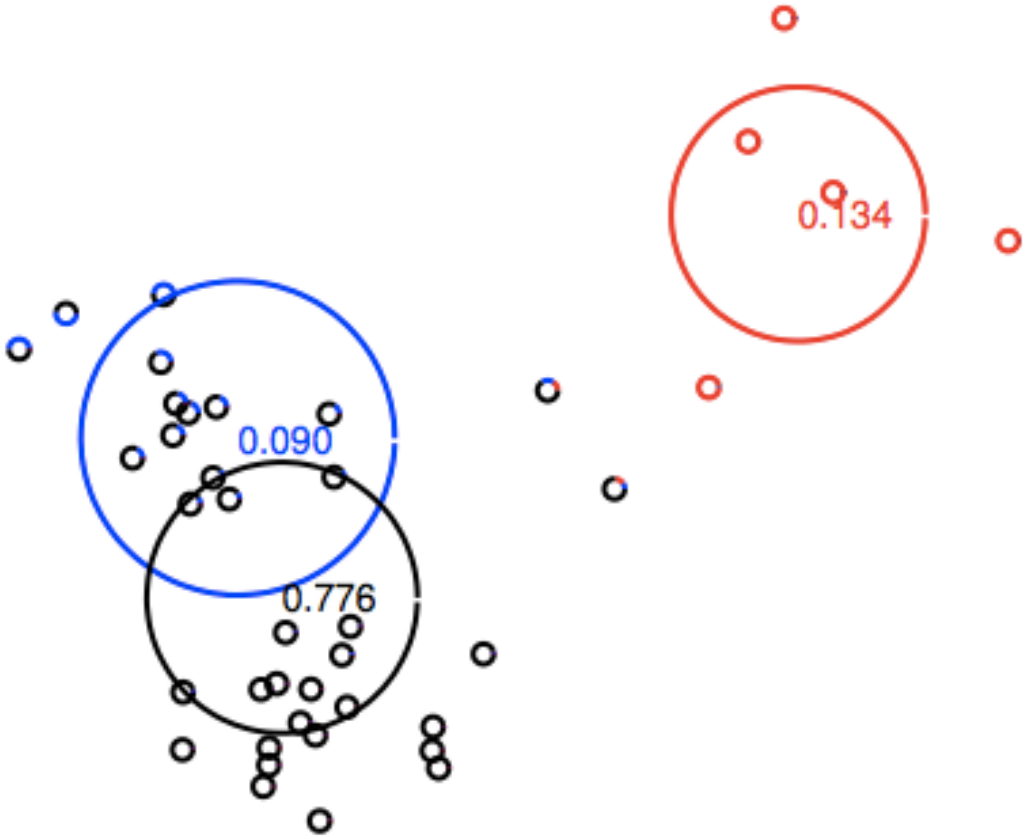

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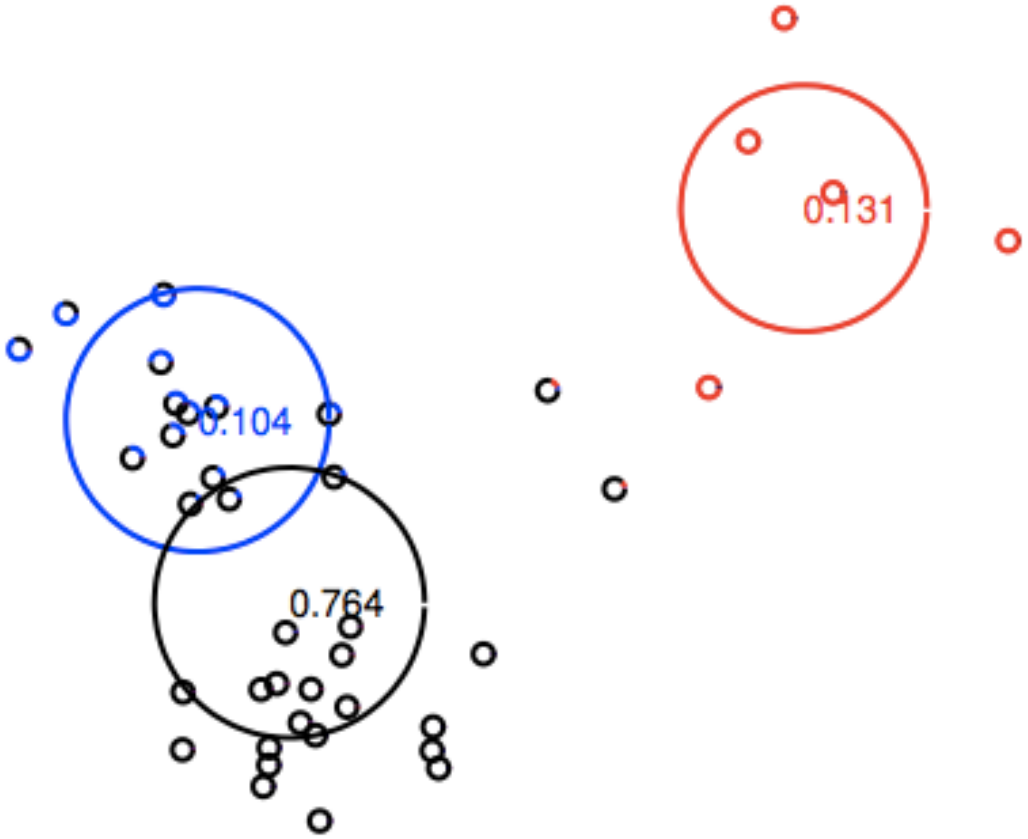

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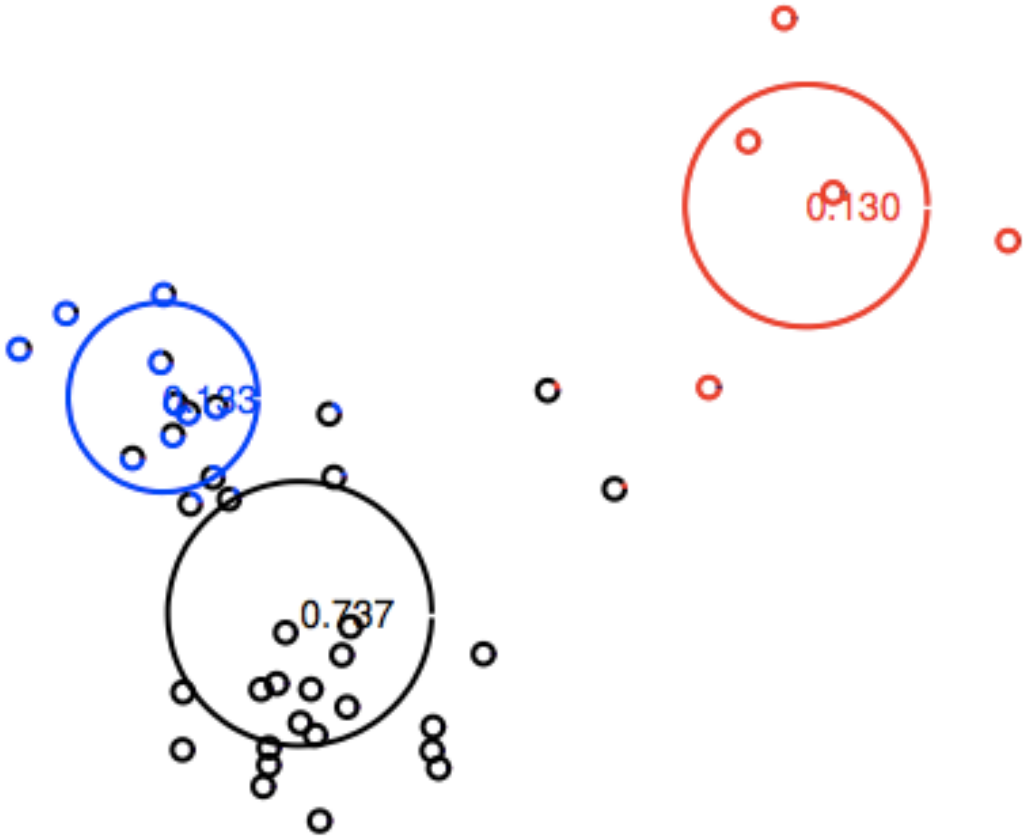

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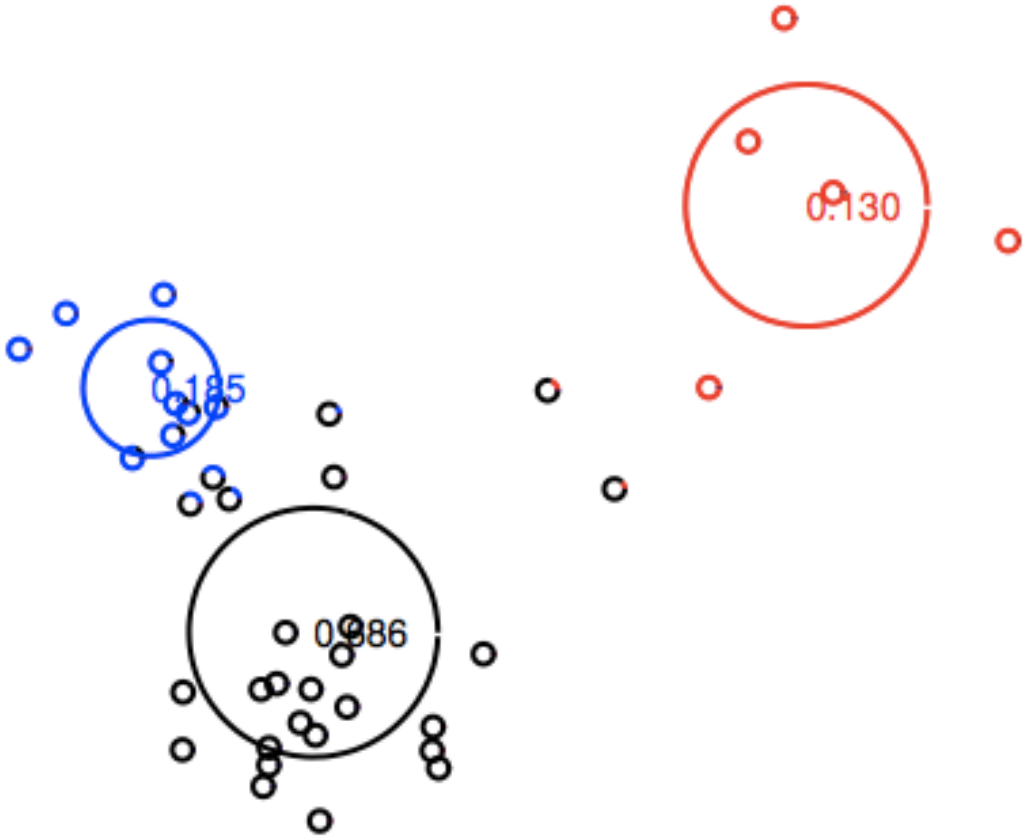
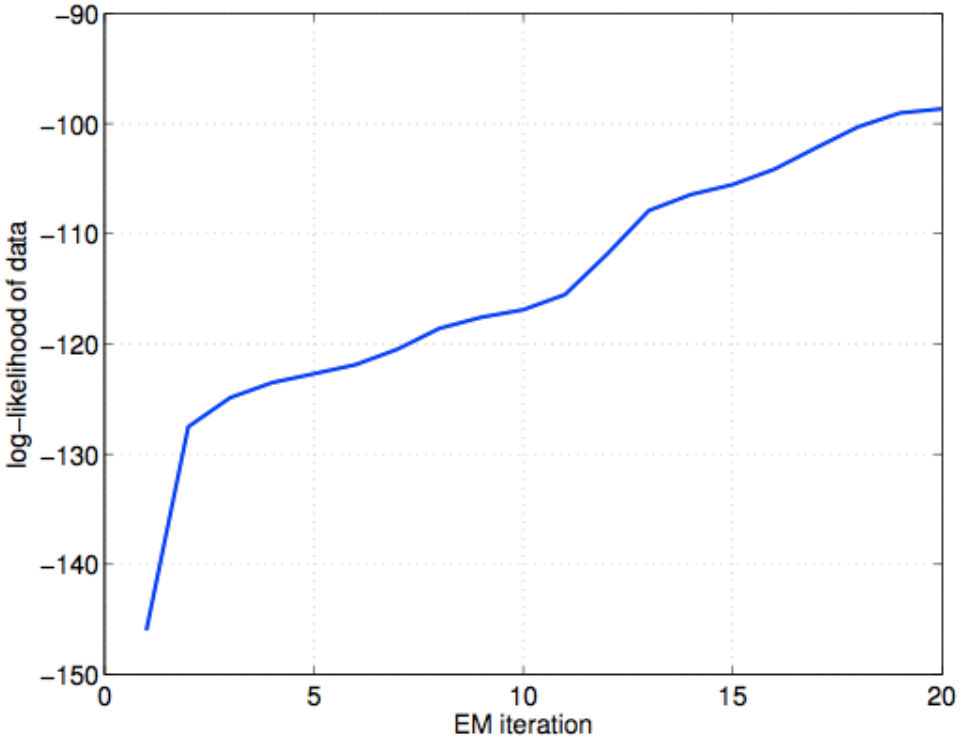


The EM algorithm



- The EM-algorithm monotonically increases the log-likelihood of the training data

$$l(D;\theta^{(0)}) < l(D;\theta^{(1)}) < \ldots < l(D;\theta^{(m)})$$

The EM-algorithm

Initialize: select the initial parameters $\theta^{(0)}$

E-step: fix the current parameters $\theta^{(m)}$, evaluate posterior assignments (divide each point softly across the mixture components)

$$p(z|i) = P(z|\underline{x}_i; \theta^{(m)}), \quad z = 1, \ldots, k, \quad i = 1, \ldots, n$$

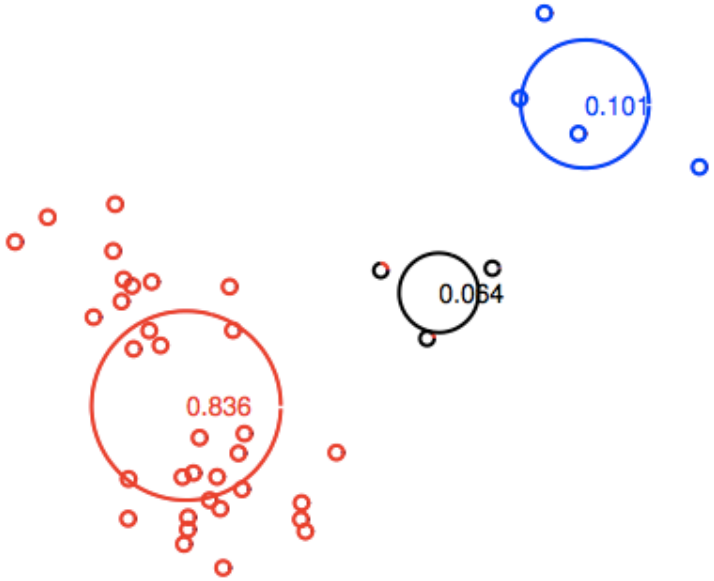
M-step: fix the posterior assignments $p(z|i)$, find new parameters $\theta^{(m+1)}$ by maximizing the expected complete log-likelihood

$$\sum_{i=1}^{n} \sum_{z=1}^{k} p(z|i) \log P(\underline{x}_i, z; \theta)$$

with respect to θ

Locally optimal solutions

- The EM-algorithm is guaranteed to find a locally optimal solution by monotonically increasing the log-likelihood (the estimation problem with respect to θ is typically not convex)
- Whether the algorithm converges to the globally optimal solution depends on the initialization



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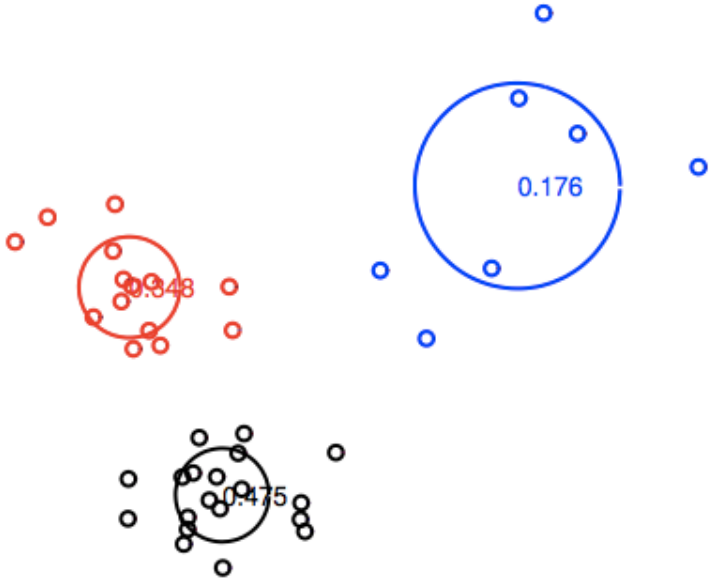
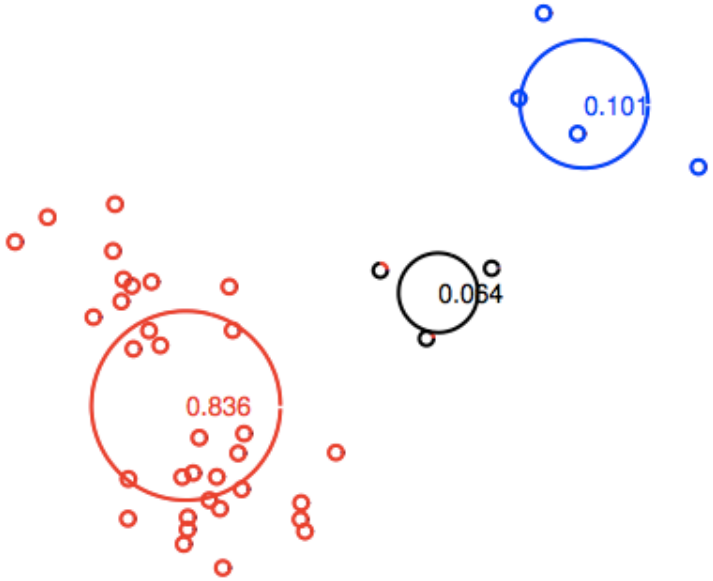


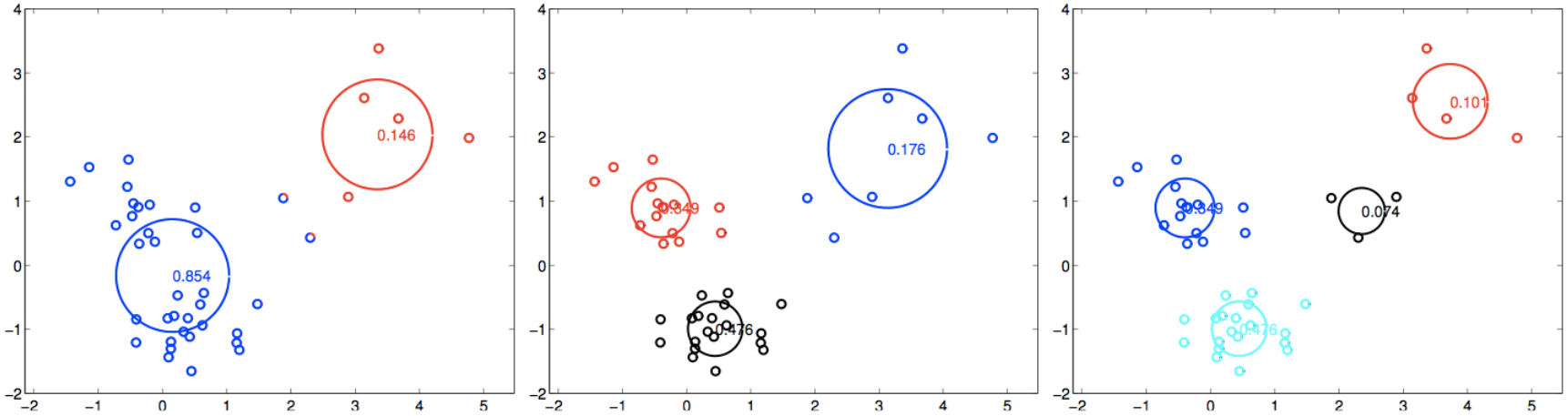
$$l(D;\hat{\theta}) = -98.64$$



$$l(D;\hat{\theta}) = -114.82$$

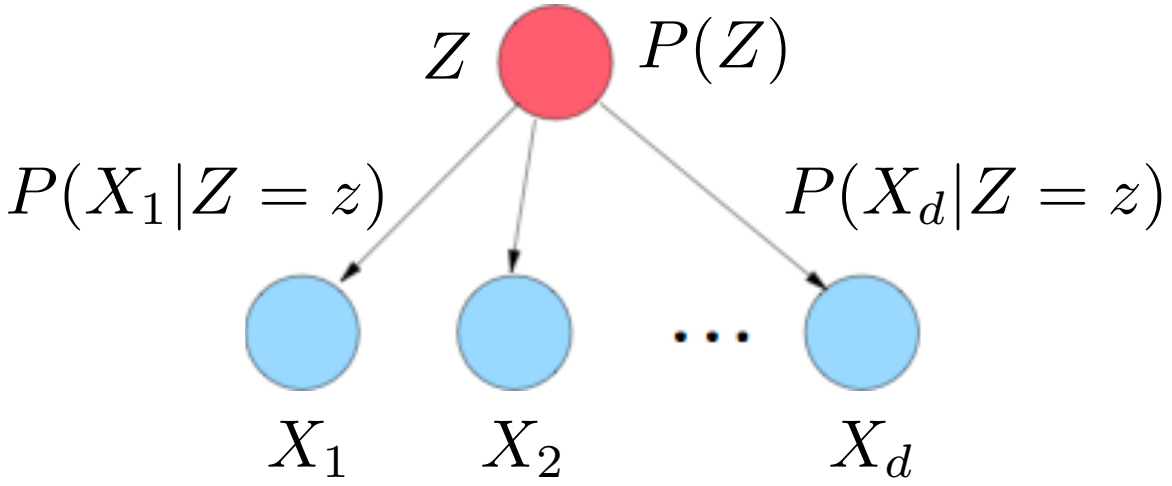
Model selection

- We can run the EM-algorithm with different numbers of components. Need to specify a criterion for selecting among the different models.



$l(D;\hat{\theta}) = -118.25$ $l(D;\hat{\theta}) = -98.64$ $l(D;\hat{\theta}) = -94.11$

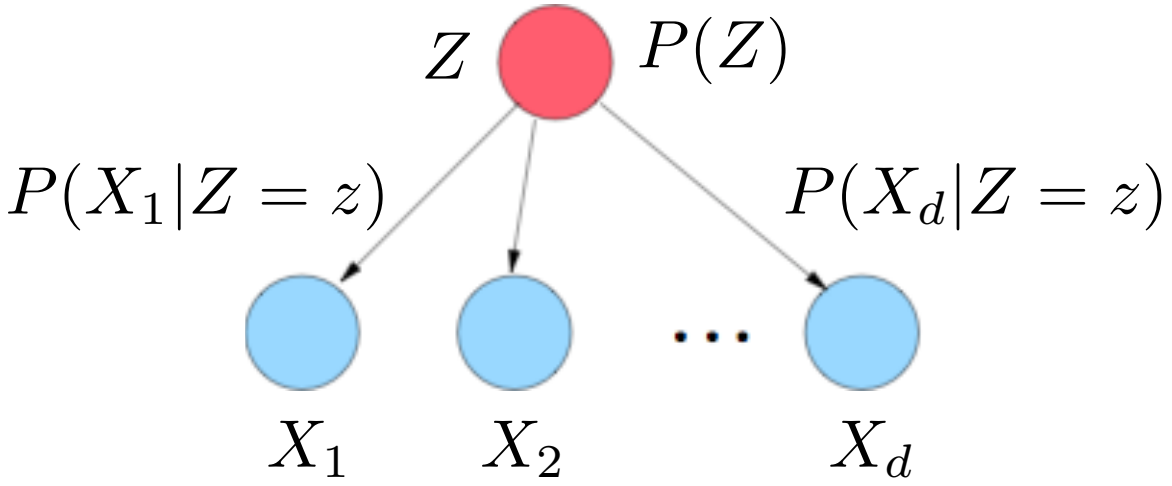
Graphical models / Bayes Nets



This is an example of a Graphical Model (a.k.a. Bayesian Network, Bayes Net, Probabilistic Graphical Model)

- Nodes are random variables
- Edges are conditional probability distributions

Graphical models / Bayes Nets

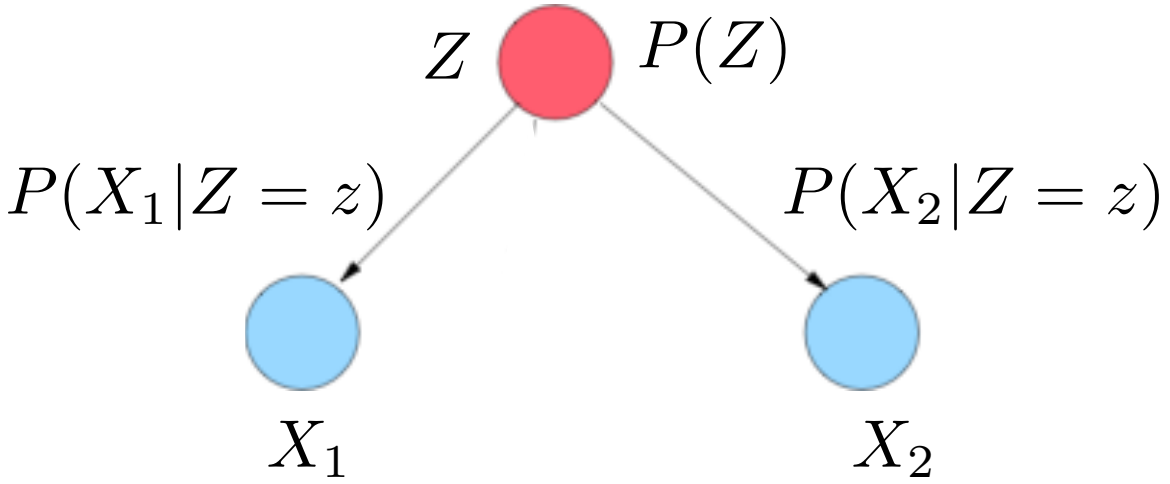


A graphical model factors the joint probability distribution (over all random variables)

→ Much fewer table entries are needed than in the full joint!

This is subject to the (conditional) independence assumptions specified by the graph.

Graphical models / Bayes Nets



Example: Binary random variables: $z, x_i, x_2 \in \{0, 1\}$

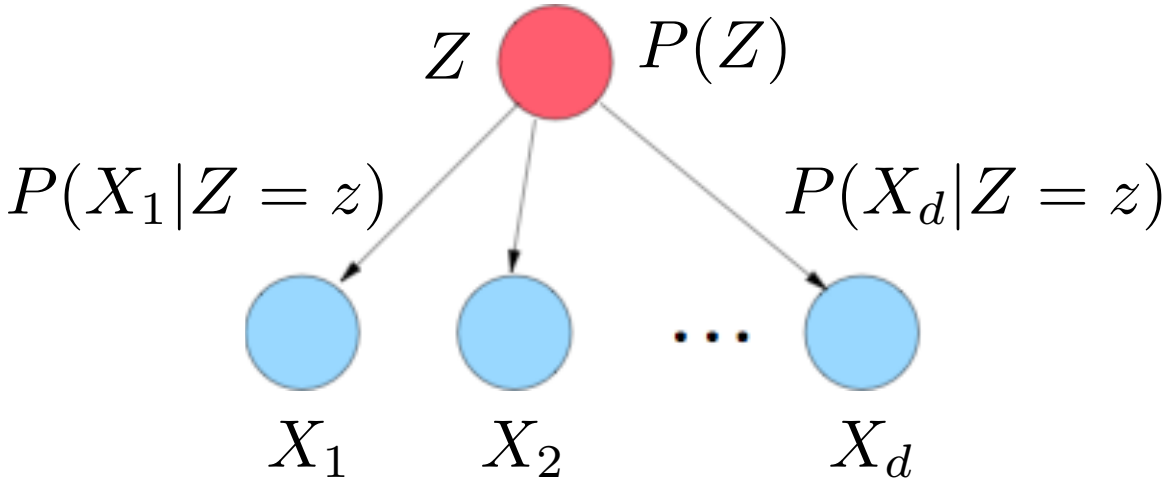
- The joint probability table $P(X_1, X_2, Z)$ has $2^3 = 8$ entries.
- Assuming the graph's independence structure, the joint factors into:

$$P(X_1, X_2, Z) = P(Z)P(X_1|Z)P(X_2|Z)$$

- To specify this Bayes Net requires only 5 parameters:

$$p(Z = 1)\, p(X_1 = 1|Z = 1), p(X_1 = 1|Z = 0)$$
$$p(X_2 = 1|Z = 1), p(X_2 = 1|Z = 0)$$

Naïve Bayes model



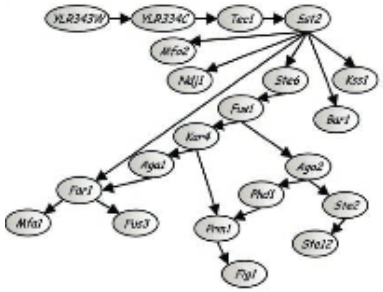
A k-component mixture over d features X_i that assumes conditional independence among the X_i's, given Z:

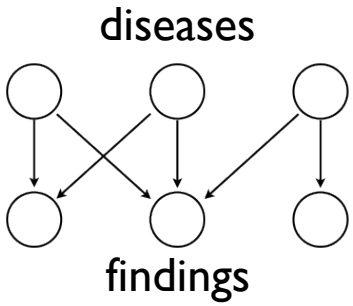
Fix the value of Z = z,

then X_i is independent of X_j for all i,j $\in \{1, \ldots, d\}$

Bayesian networks

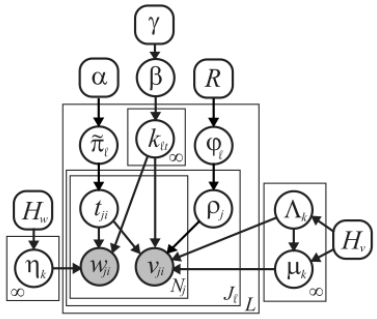
- Bayesian networks provide a simple language for succinctly expressing, using, and learning probabilistic information
- In a Bayesian network, nodes correspond to random variables and directed edges indicate dependencies
  - the graph provides a qualitative description of how the variables relate to each other
  - the probability distribution underlying the graph quantifies numerically how the variables depend on each other
- Both the graph structure and the associated distribution are important in applications
  - diagnostic tasks, medicine
  - data analysis in biology
  - etc.

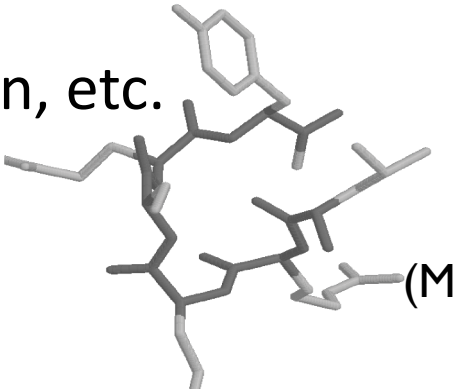




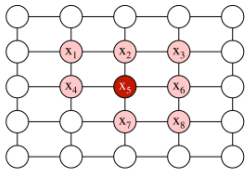
Applications of Bayes Nets

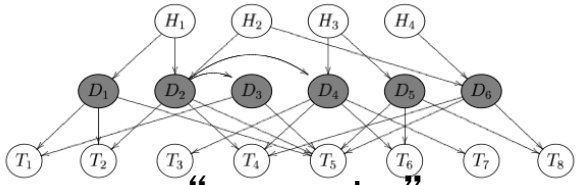
- Computer vision
  - scene analysis, stereo matching, etc.
- Molecular biology
  - networks, molecular design, etc.
- Information retrieval / NLP
  - topic models, parsing
- Diagnosis
  - fault, medical
- Signal processing
  - deconvolution, sensor networks
- Communication
  - decoding algorithms



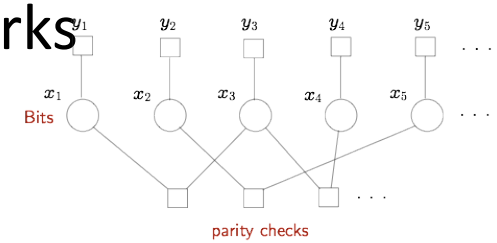


(Meltzer et al.)

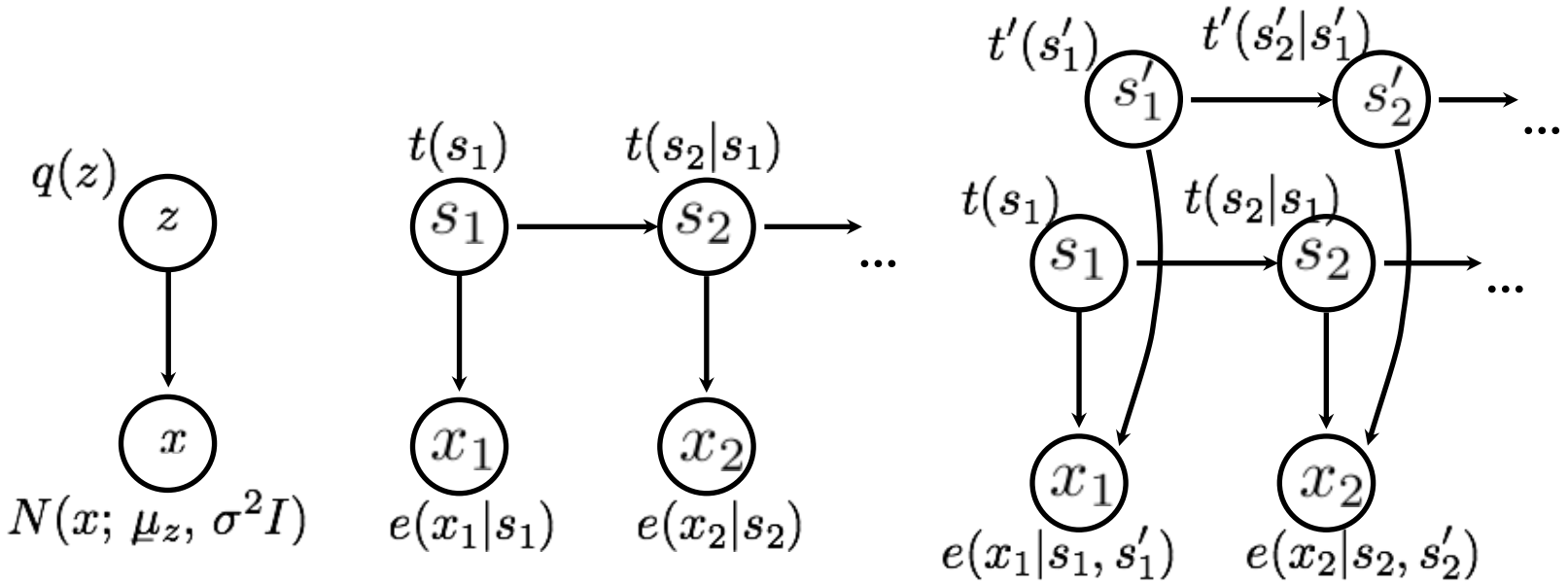




"promedas"



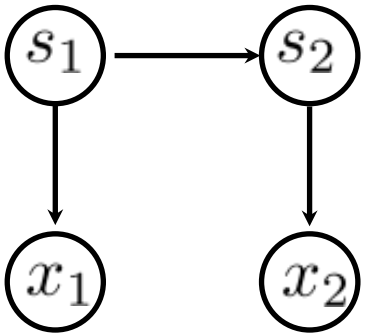
Graphs and probabilities



- Bayesian networks as probability models are represented by directed acyclic graphs (DAGs) where the nodes specify variables and the directed edges identify dependencies
- Formally, the graph encodes conditional independence properties about the variables (cf. Markov properties)
- Any probability distribution we associate with the graph has to be consistent with such independence properties

Bayesian networks

- Some basic terminology:
  - s_1 is a "parent" of x_1
  - s_1 and s_2 are "ancestors" of x_2; x_1 is not.
  - x_1 is a "child" of s_1
  - x_1, s_2 and x_2 are all "descendants" of s_1



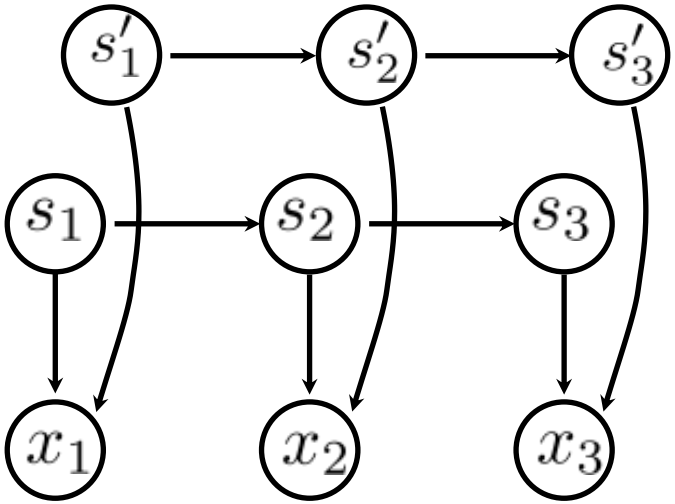
- Joint probability distribution factors as:

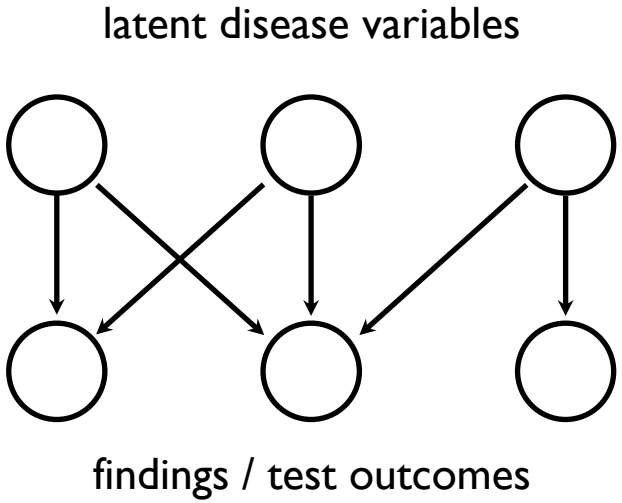
$$P(V_1, V_2, \ldots, V_k) = \prod_{i=1}^{k} P(v_i | \texttt{Parents}(V_i))$$

Bayesian networks

Examples:

- a factorial HMM, where observations depend on two Markov chains running in parallel (two speakers, one microphone)
- a two layer model for medical diagnosis





Learning Bayesian networks

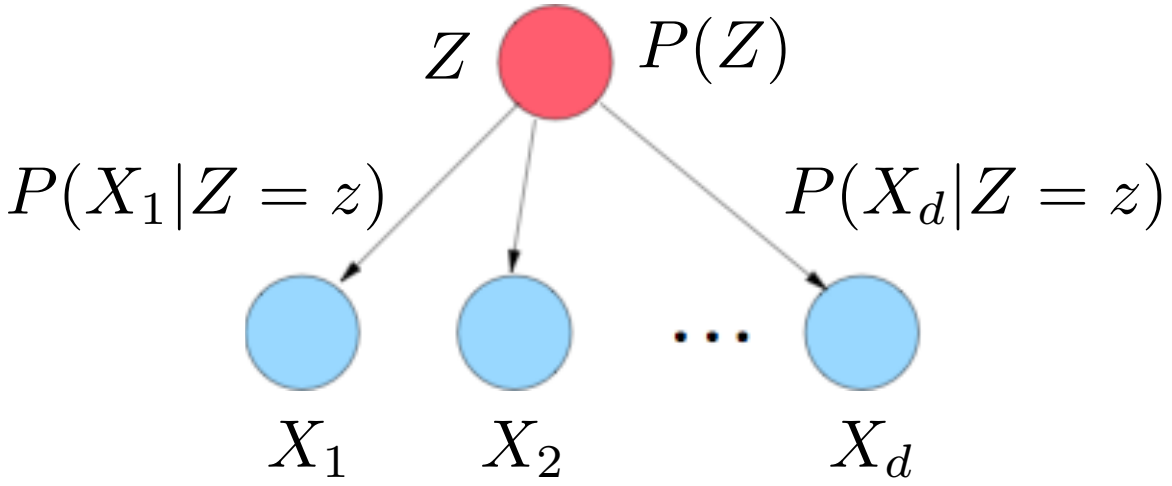
$D =$

complete data

x_1	x_2				$\cdots$					x_n
2	2	1	1	1	2	1	1	2	1	2
1	2	2	2	2	2	3	1	1	2	2
1	1	1	1	2	1	1	1	1	1	1
2	2	3	1	1	2	3	3	2	3	2
1	2	2	2	2	2	3	1	1	2	2
1	1	3	1	1	1	3	1	1	1	3
					$\cdots$					

- **Parameter estimation:** find the maximum likelihood (or Bayesian) estimates of parameters for a graph G
- **Model selection:** appropriately score each G based on its degree of fit to the data
- **Structure search:** find the highest scoring structure $\hat{G}$

Naïve Bayes model



Estimation from labeled training data: Filter the data by labels z:

For each label z, fit a probability model, $P(X_i|Z)$, for each X_i.

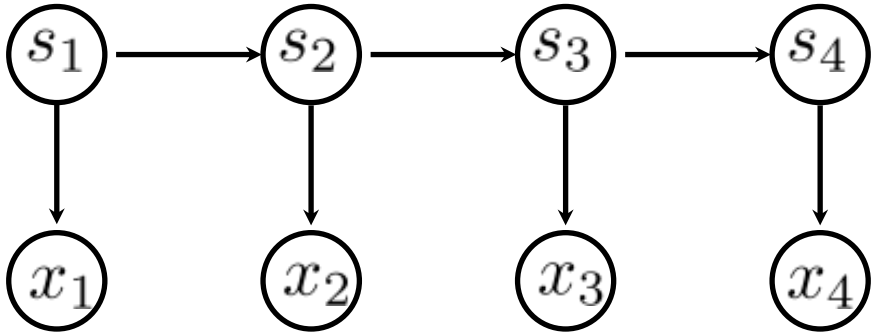
E.g. if $P(X_i|Z)$ is modeled with a Gaussian, then for each i, just need to compute $\hat{\mu}_i, \hat{\sigma}_i^2$ from the training data.

Prediction on a new example $x = (x_1, \ldots, x_d)$:

$$\hat{z} = \arg\max_z P(Z|x_1, \ldots, x_d) = \arg\max_z P(Z) \prod_{i=1}^{d} P(x_i|Z)$$

The Hidden Markov Model (HMM)

- Each node corresponds to a variable, either state s_t or observation x_t, and the arcs represent dependencies such as "s_2 depends on s_1"



HMMs

- Hidden Markov models are widely used models
- speech recognition
  - e.g., each word is a Markov sequence of phonemes which are then coupled to acoustic measurements
- computational biology
  - e.g., gene structure labels (coding region, etc.) form a Markov chain of states and each state generates a base-pair (sequence)
- natural language processing
  - e.g., part of speech tags (noun, verb, etc) form a Markov chain and the tags give rise to observed words

HMM problems

- Three problems we need to solve in the context of HMMs

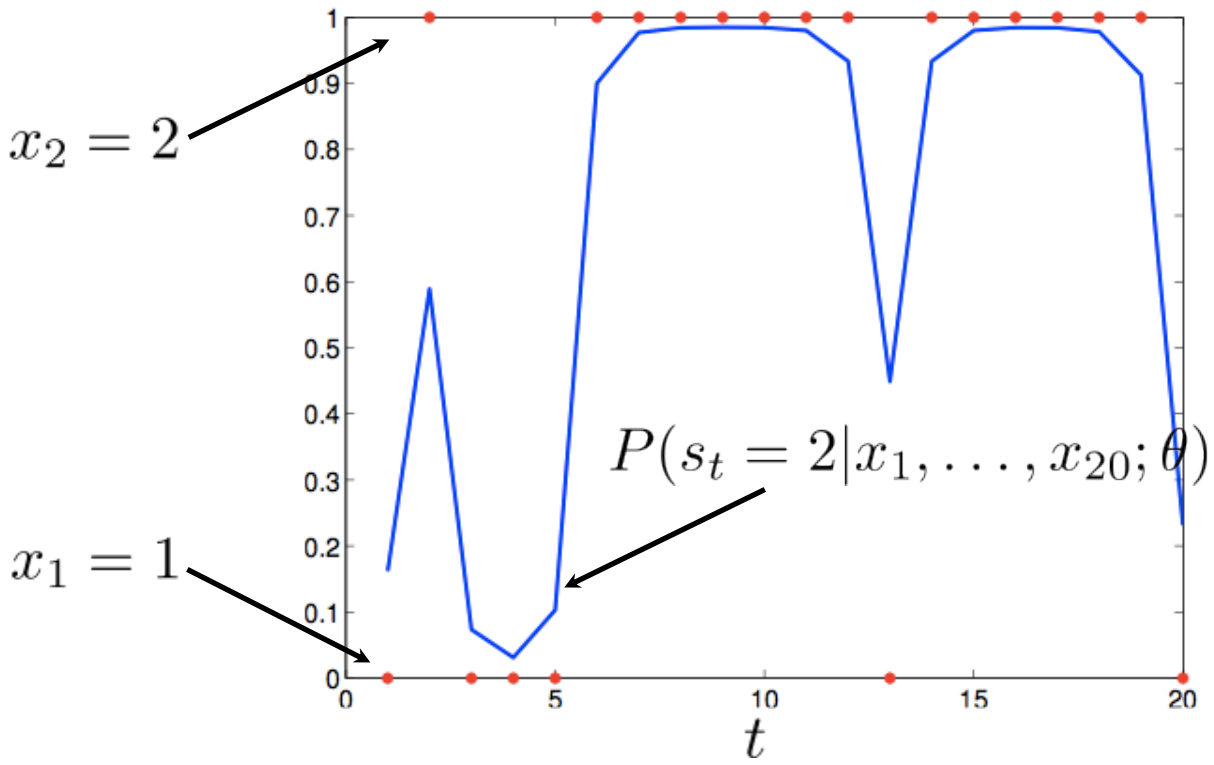
1) How to evaluate the probability of any observation sequence $P(x_1, \ldots, x_N; \theta)$
2) How to estimate the HMM parameters $\{q(s_1)\}$, $\{q(s_i|s_{i-1})\}$ and $\{q_e(x_i|s_i)\}$ on the basis of n observed sequences of varying length
3) How to find the most likely hidden state sequence $\hat{s}_1, \ldots, \hat{s}_N$ corresponding to observations $x_1, \ldots, x_N$

HMM example

- Underlying HMM

$$q(s_1) : \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}, \quad q(s_t|s_{t-1}) : \begin{bmatrix} 0.75 & 0.25 \\ 0.25 & 0.75 \end{bmatrix}$$

$$q_e(x_t|s_t) : \begin{bmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{bmatrix}$$



HMM problems: common techniques

1) Compute probability of an observation sequence: Baum-Welch, forward-backward, alpha-beta algorithms.
   - Iterative, two-stage message passing algorithms
2) Estimate HMM parameters: apply EM to iteratively maximize the likelihood of the training data given the parameters.
   - Relies on some quantities computed in 1)

3) Compute most likely hidden state sequence for an observation sequence: Viterbi Algorithm: uses dynamic programming.

Optimal substructure:

- Due to the Markov property: the most probable path (through the hidden states) for the rest of any sequence, only depends on the state in which it starts.

→ For each state, only need to keep track of most probable path that ends in that state (not all possible paths to that state).