



COMPUTER SCIENCE

INDIANA UNIVERSITY

School of Informatics and Computing
Bloomington

Mixture models



Reminders/Comments

- Thought questions due today
- Assignment 3 due on Wednesday
- After Thanksgiving, we will switch to review of the course material
- Let's take a poll for concepts/sections that are particularly confusing to you



Feedback form Q2

- Assuming that $p(y | x)$ is Bernoulli would be a reasonable choice
- Implementation/meta-parameter choices:
 - initialization of parameters
 - number of random restarts, or other optimization improvements to escape from local minima
 - number of hidden nodes
 - number of hidden layers
 - transfers on the layers
 - step-size selection and/or decay schedule



Hidden variable models

- Probabilistic PCA and factor analysis
 - common in psychology
- Mixture models
- Hidden Markov Models
 - commonly used for NLP and modeling dynamical systems



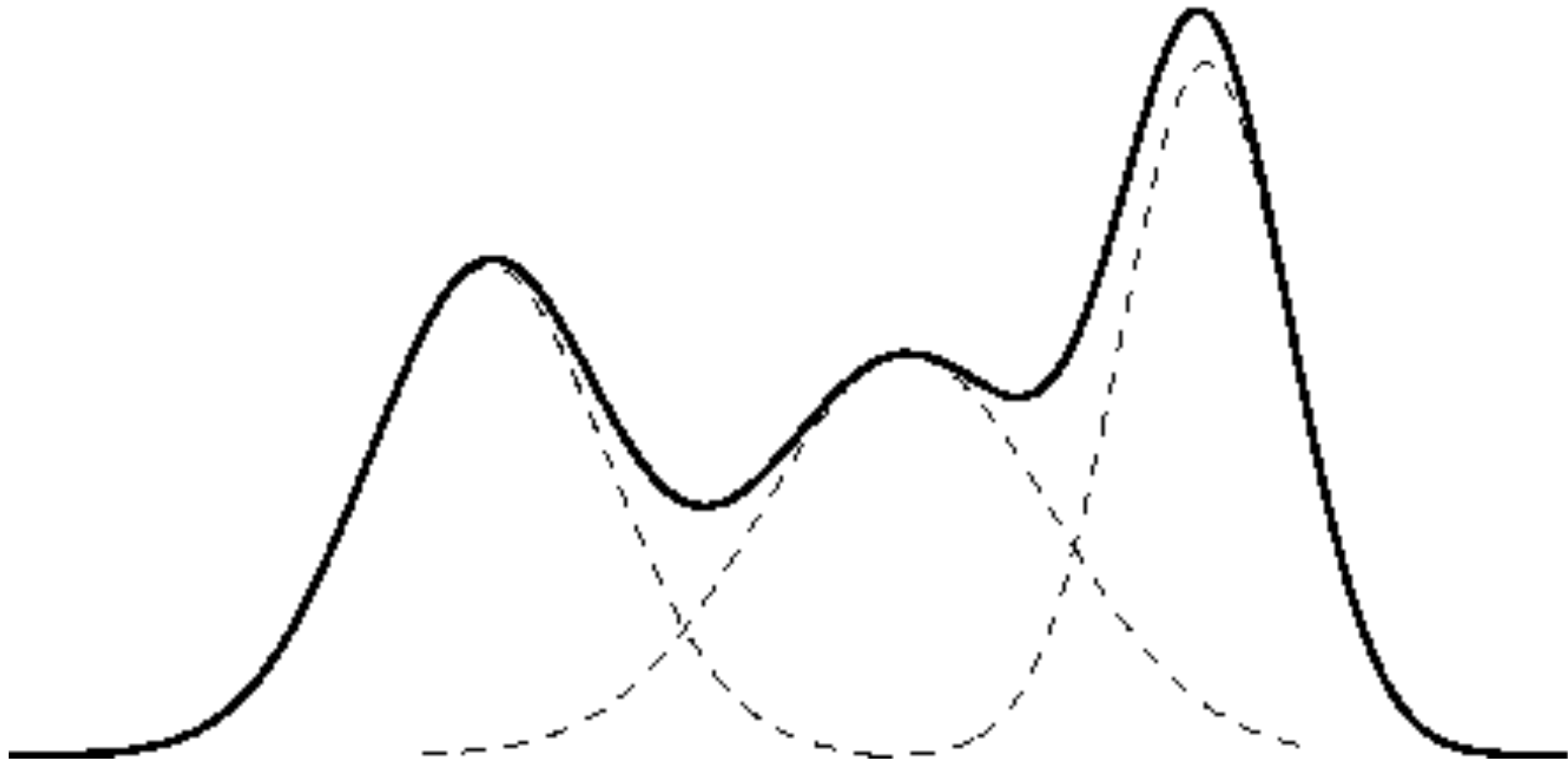
Probabilistic PCA

- In PCA, we learned $p(\mathbf{x} | \mathbf{D}, \mathbf{h})$
 - What were the assumptions on $p(\mathbf{x} | \mathbf{D}, \mathbf{h})$?
- For Probabilistic PCA, we learn $p(\mathbf{x} | \mathbf{D})$
- Given some prior $p(\mathbf{h})$, we have

$$p(\mathbf{x} | \mathbf{D}) = \int_{\mathcal{H}} p(\mathbf{x} | \mathbf{D}, \mathbf{h}) p(\mathbf{h}) d\mathbf{h}$$



Gaussian mixture model



$$\mathcal{N}(\mathbf{x}|\underset{\substack{\uparrow \\ \text{mean}}}{\boldsymbol{\mu}}, \underset{\substack{\uparrow \\ \text{covariance}}}{\boldsymbol{\Sigma}}) = \frac{1}{(2\pi)^{d/2} |\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

$$p(x|\theta) = \sum_{j=1}^m w_j p(x|\theta_j).$$



Differences to PPCA

- Hidden variable is a discrete number in set $\{1, \dots, k\}$:
represents the cluster/label that a sample could belong too
- In PPCA, hidden variable was the right singular vector, of continuous values
- The same lower bound applies, but we use a sum for mixture models (to sum over h) and an integral for PPCA

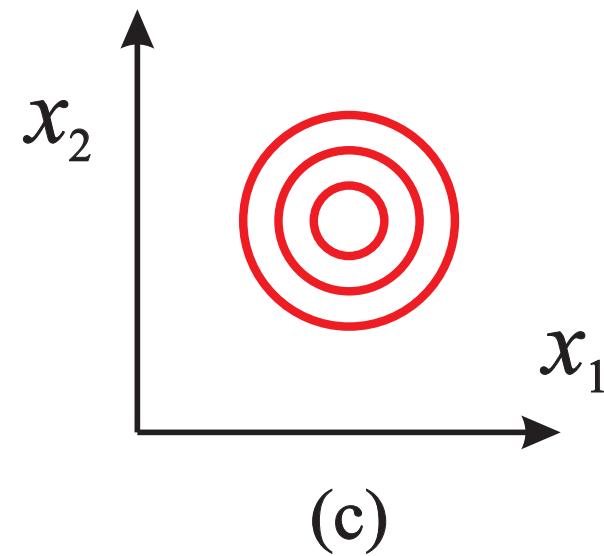
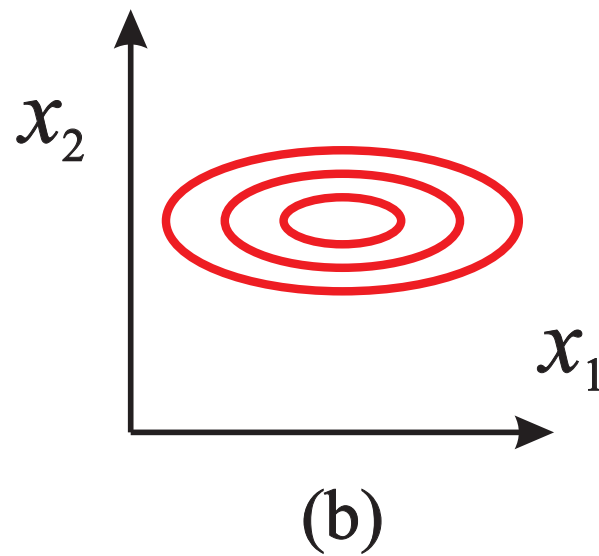
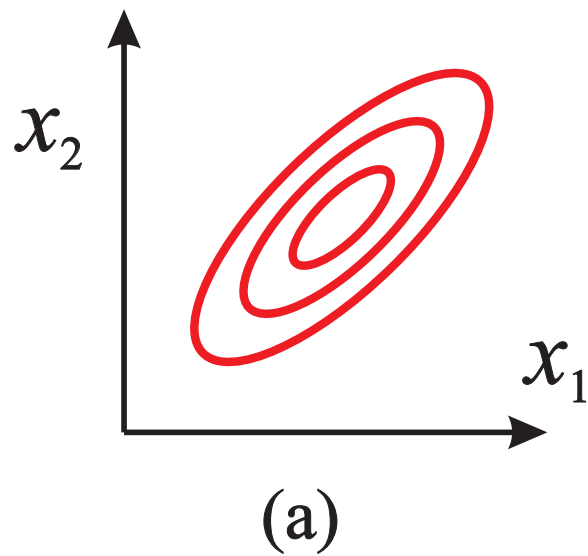


Gaussian distribution

- Multivariate Gaussian

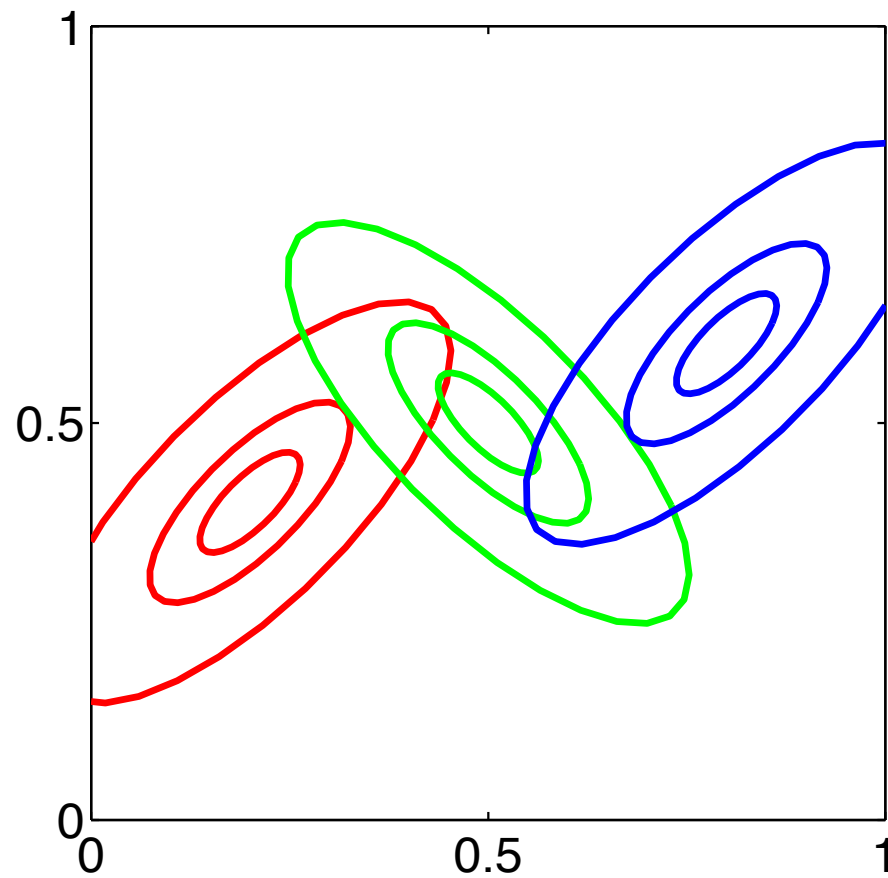
$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{d/2} |\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

mean covariance



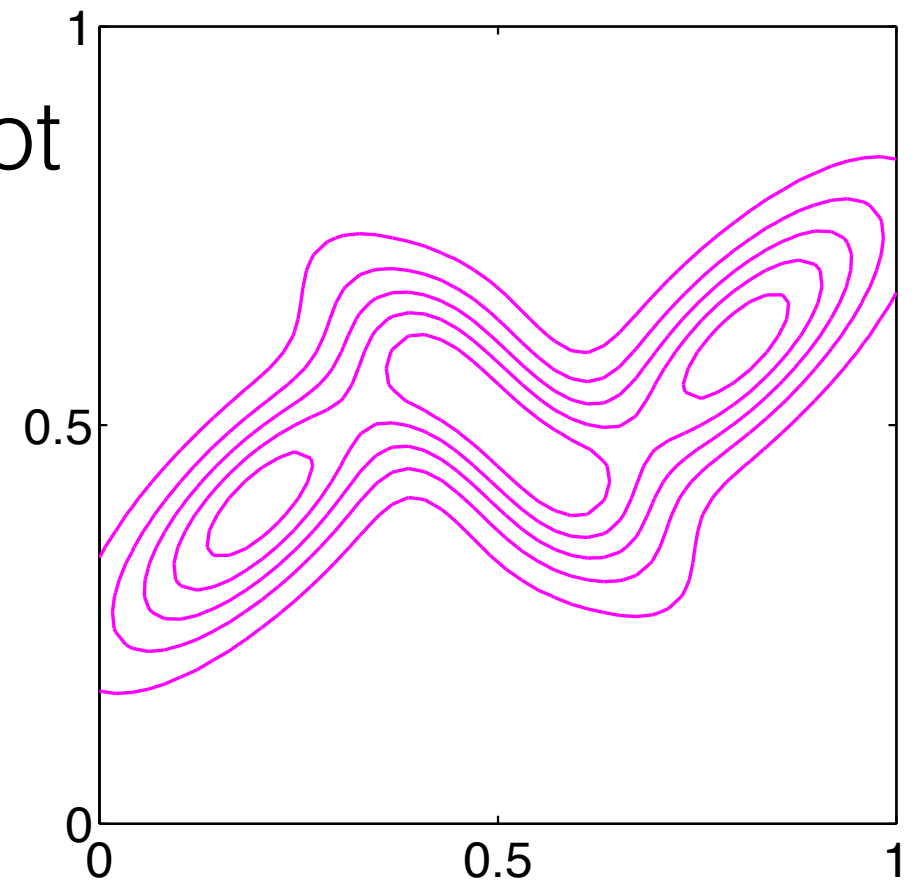


Mixture of 3 Gaussians

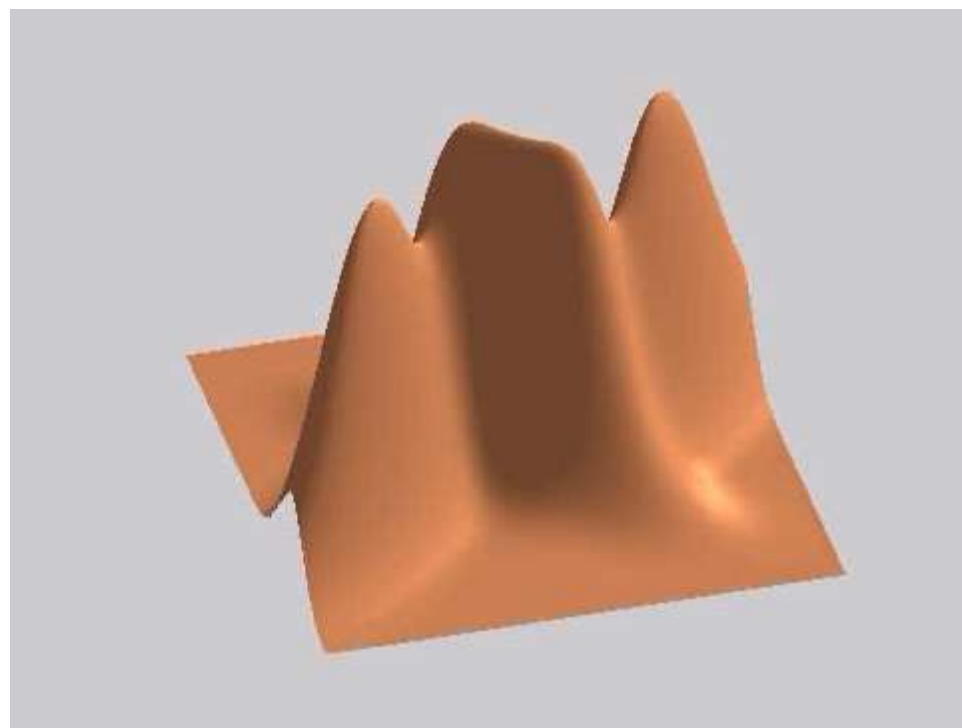


3 contours

Contour plot



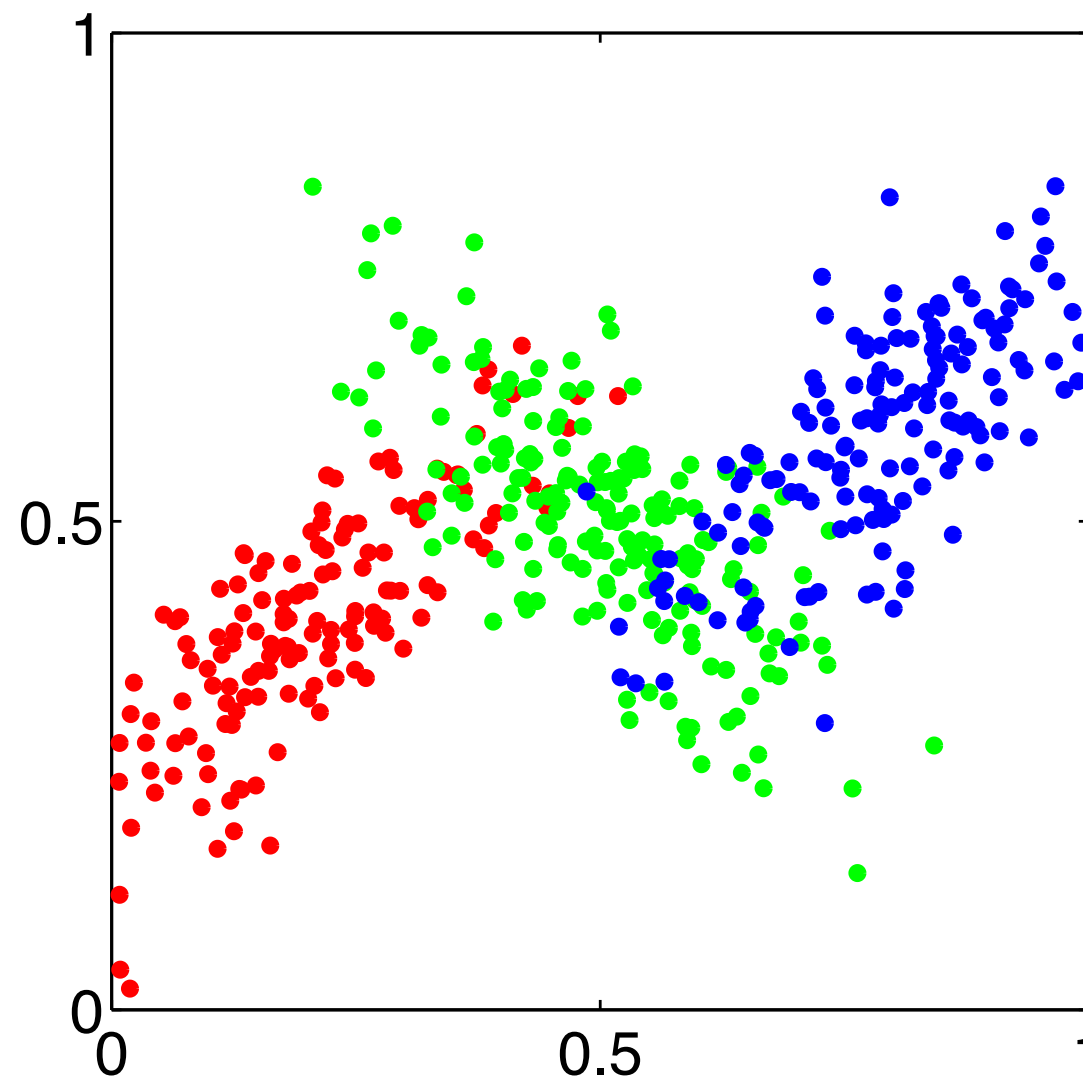
Surface plot





Generating synthetic data

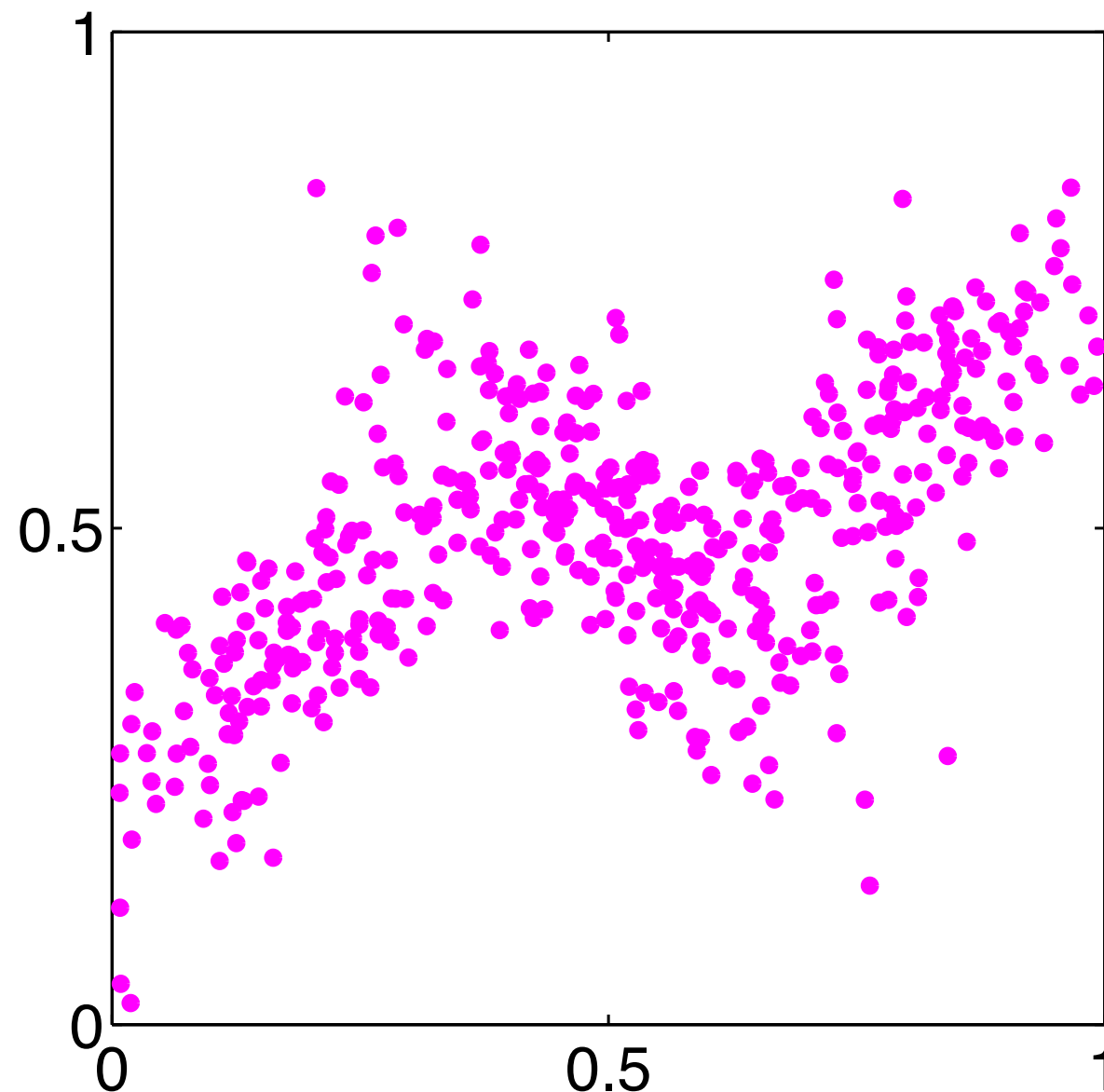
- To generate a point:
 - pick one of the components with probability w_i (e.g., using `np.random.choice`)
 - draw a sample x from that component (e.g., using `np.random.normal`)





Other direction: estimation

- Given parameters, easy to see how data generated
- Given data, now want to learn/estimate parameters



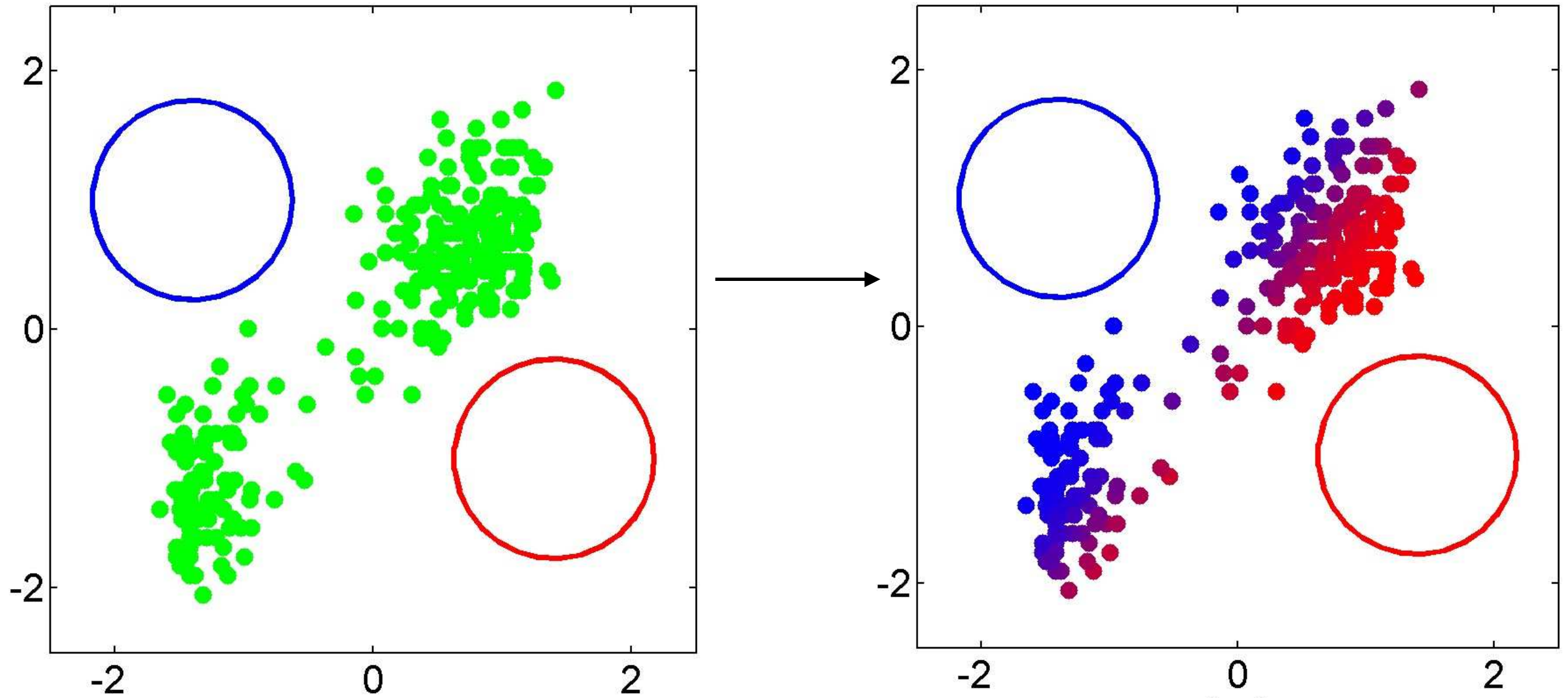


EM algorithm for mixtures

- We will use EM to obtain an algorithm for estimating the parameters
- Procedure: initialize parameters to some initial guess/random
- Alternate between:
 - E-step: fix parameter, approximate $p(h \mid x, \theta)$
 - M-step: fix $p(h \mid x, \theta)$ obtaining maximum likelihood parameters for means, covariances and weights on each distribution
- Each cycle guaranteed not to decrease likelihood, converge to a local minimum

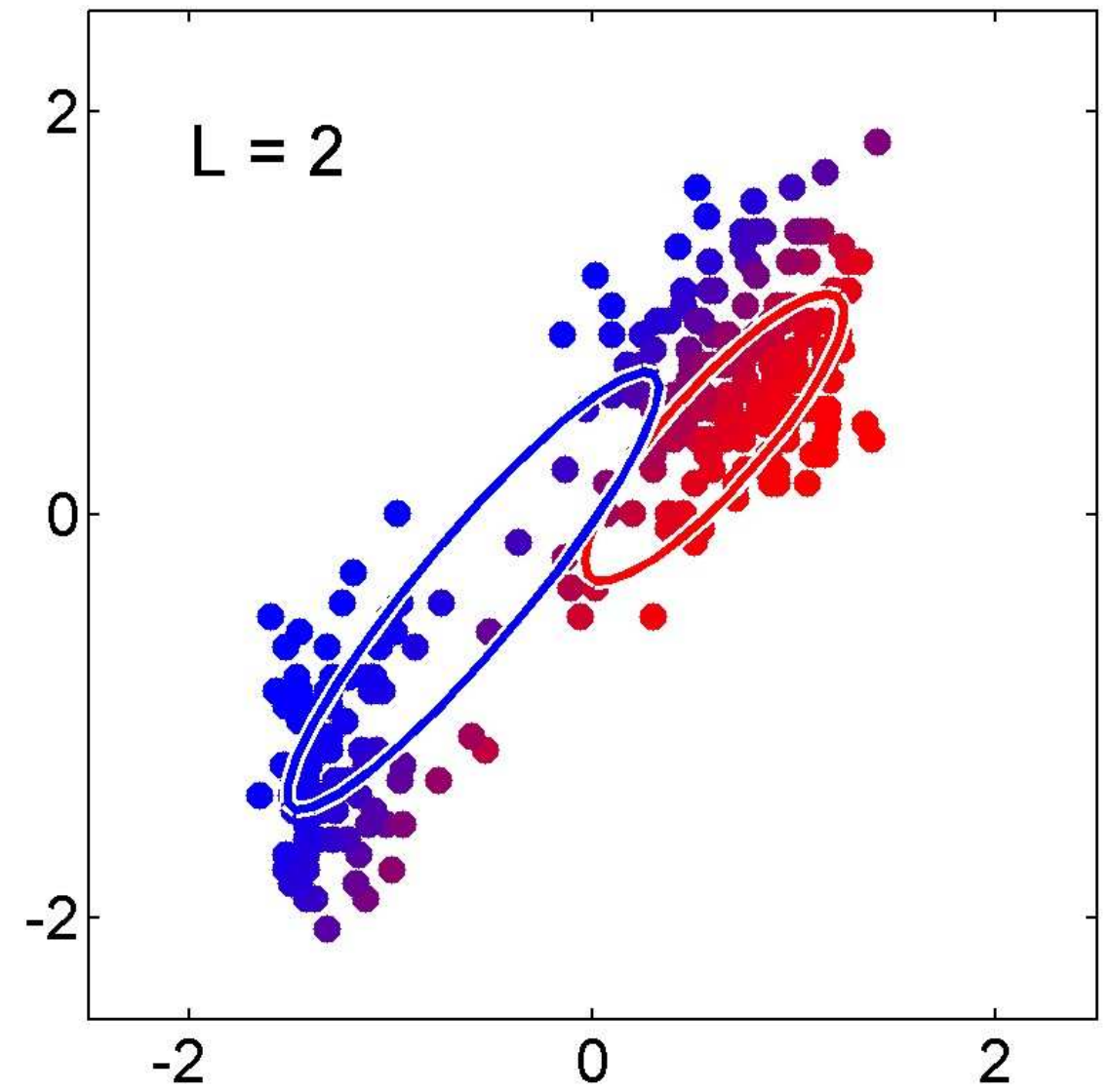
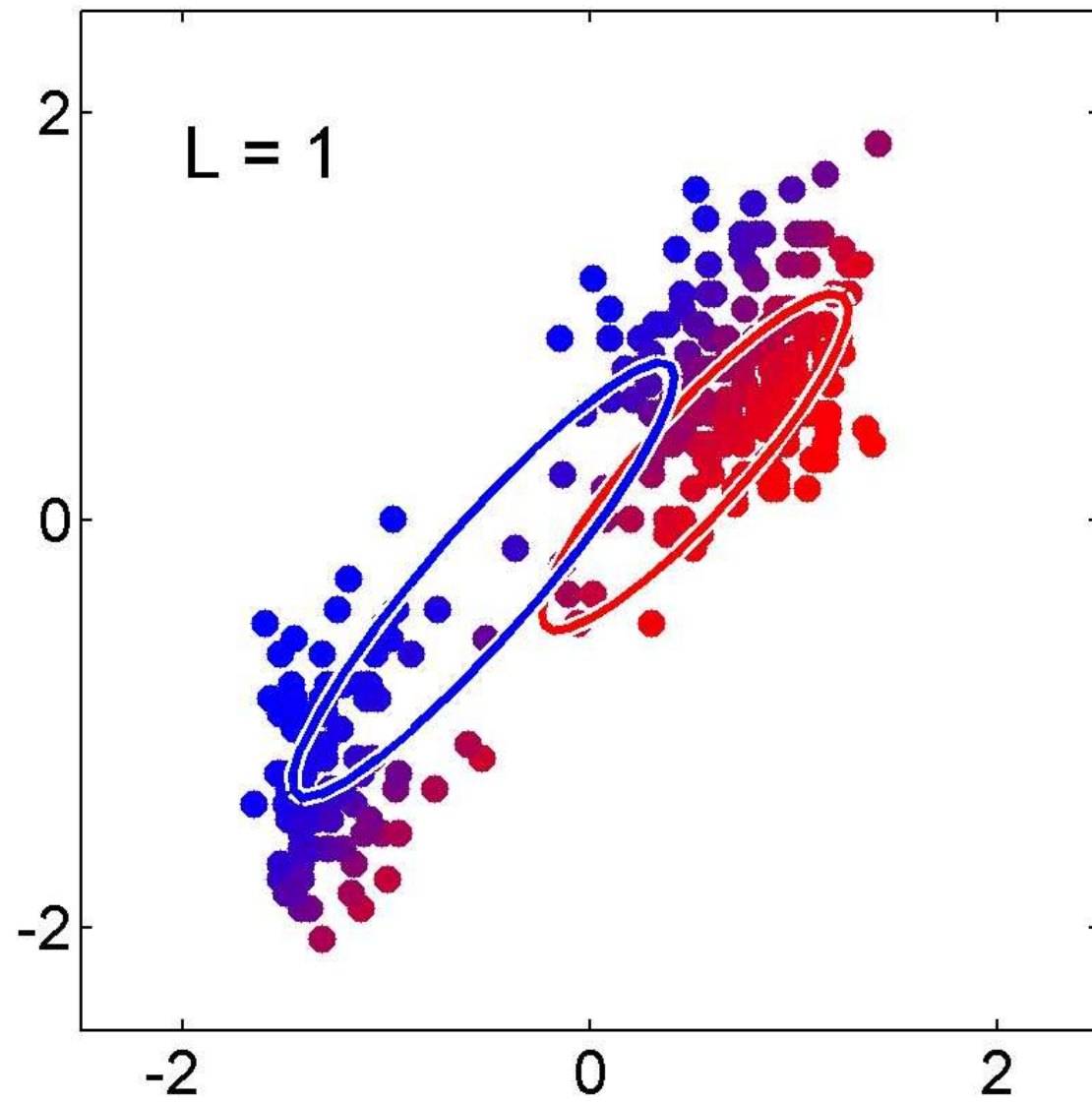


Simulation of EM for mixtures



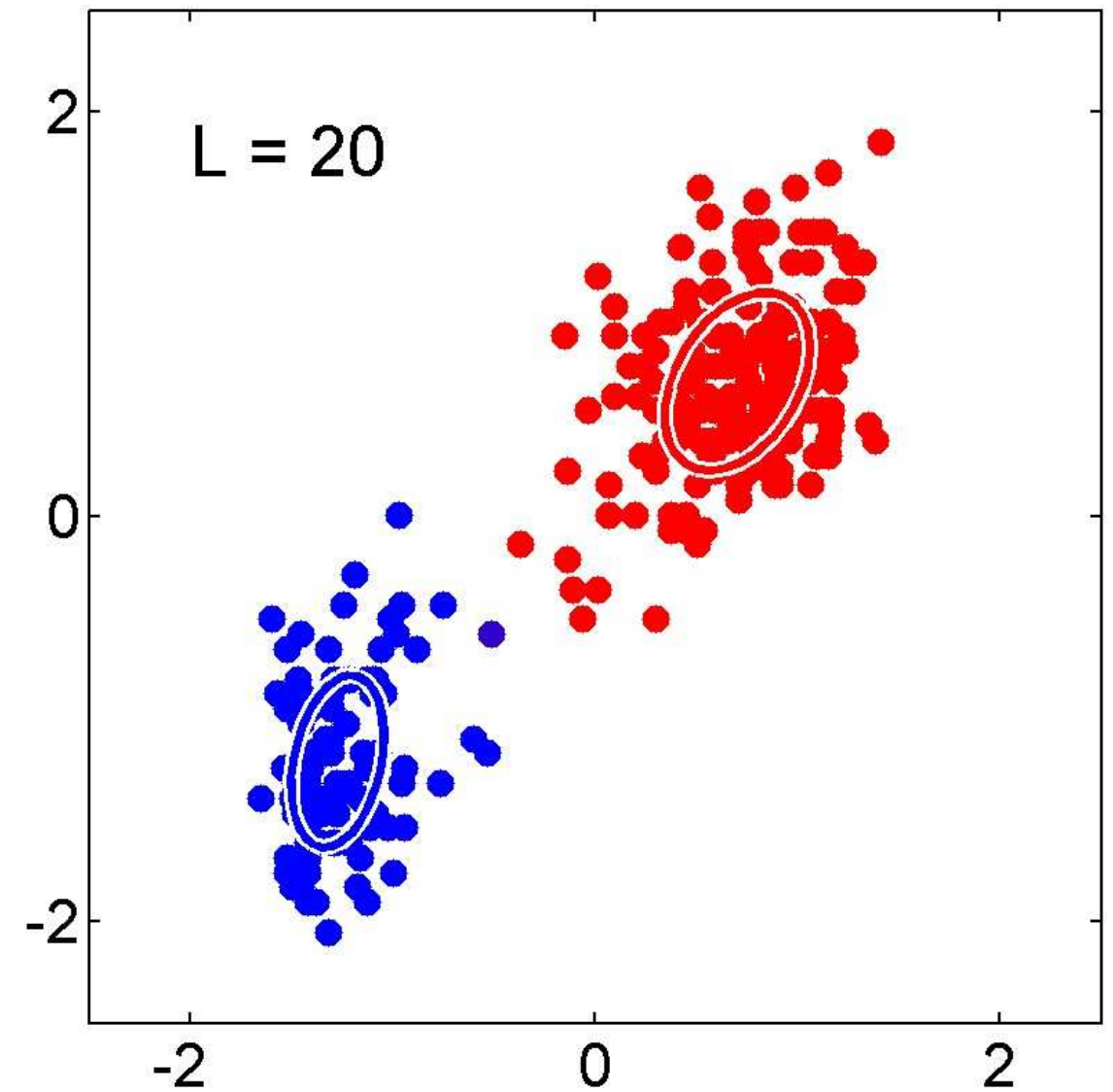
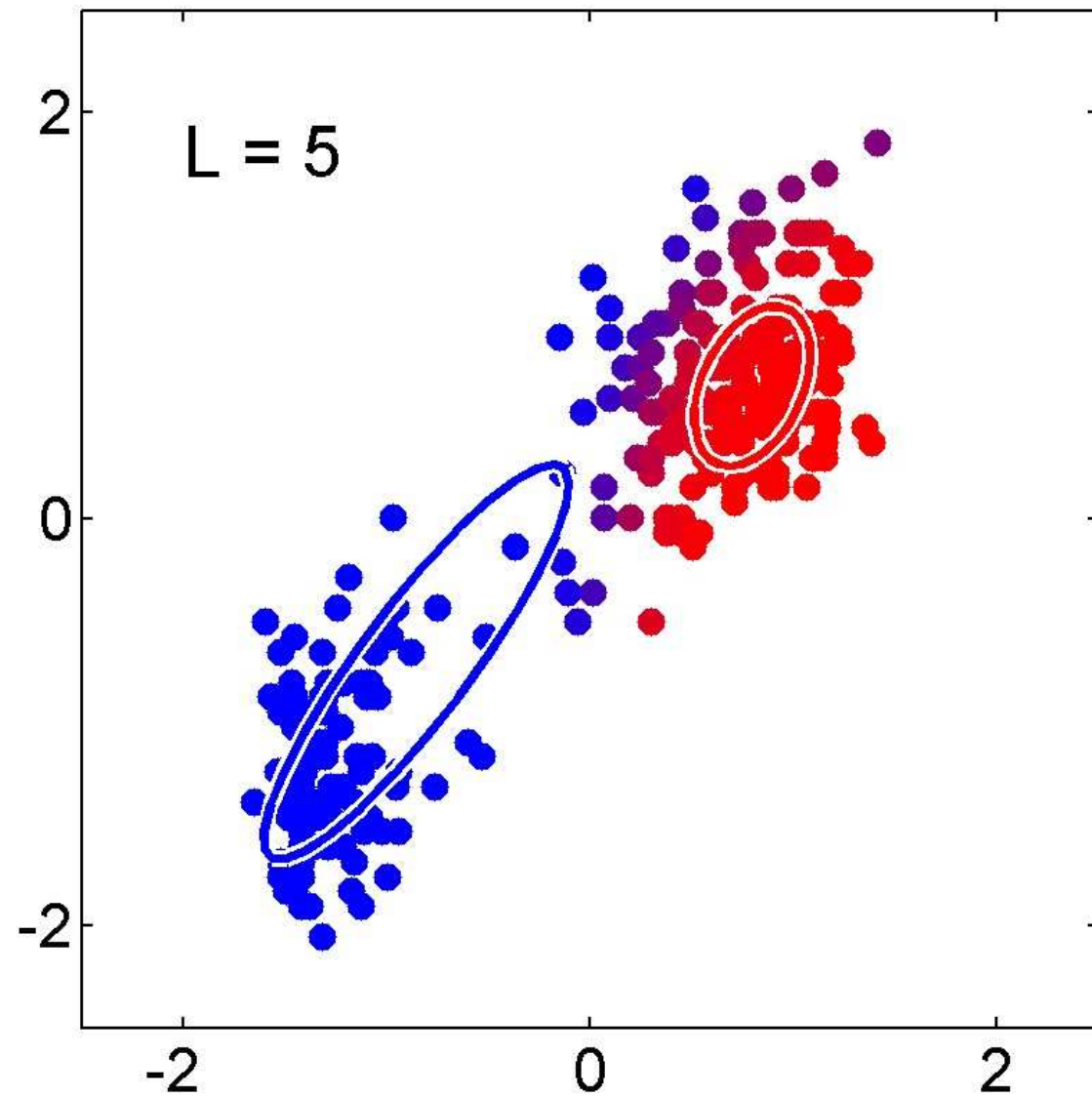


Simulation of EM for mixtures





Simulation of EM for mixtures





Mixture models

- In general, we can take mixtures of other types of distributions
- Example: mixture of exponential distributions
- The algorithm itself will be different, as start with different distributions and then obtain different E and M steps



Demo

- Estimate parameters for the Gaussian mixture models
- Can formulate as k-means problem, learning only means and assuming fixed, unit covariances
 - using Lloyd's algorithm
- Can formulate more generally as to learn means, covariances and weights
 - can learn these parameters using an EM-approach
 - EM is a general solution approach (like gradient-descent), rather than an algorithm specifically for mixture models



Motivation for summing rather than maximizing

- Could simple pick the maximum/best hidden variable, as is done for the factorizations we looked at and k-means
- Summing over values can give better performance, and is solving for the parameters to a distribution
- Depends on your assumptions/needs
 - for representations, we want the “best” representation
 - for generative models, we want to appropriately approximate the model we have specified that integrates out the variables
- In some cases, it is worth the speed of the approximate solution for estimating distributions (hard EM or viterbi EM)



Whiteboard

- Expectation-maximization for mixture models
- Expectation-maximization for probabilistic PCA