Clustering
Lecture 5: Mixture Model

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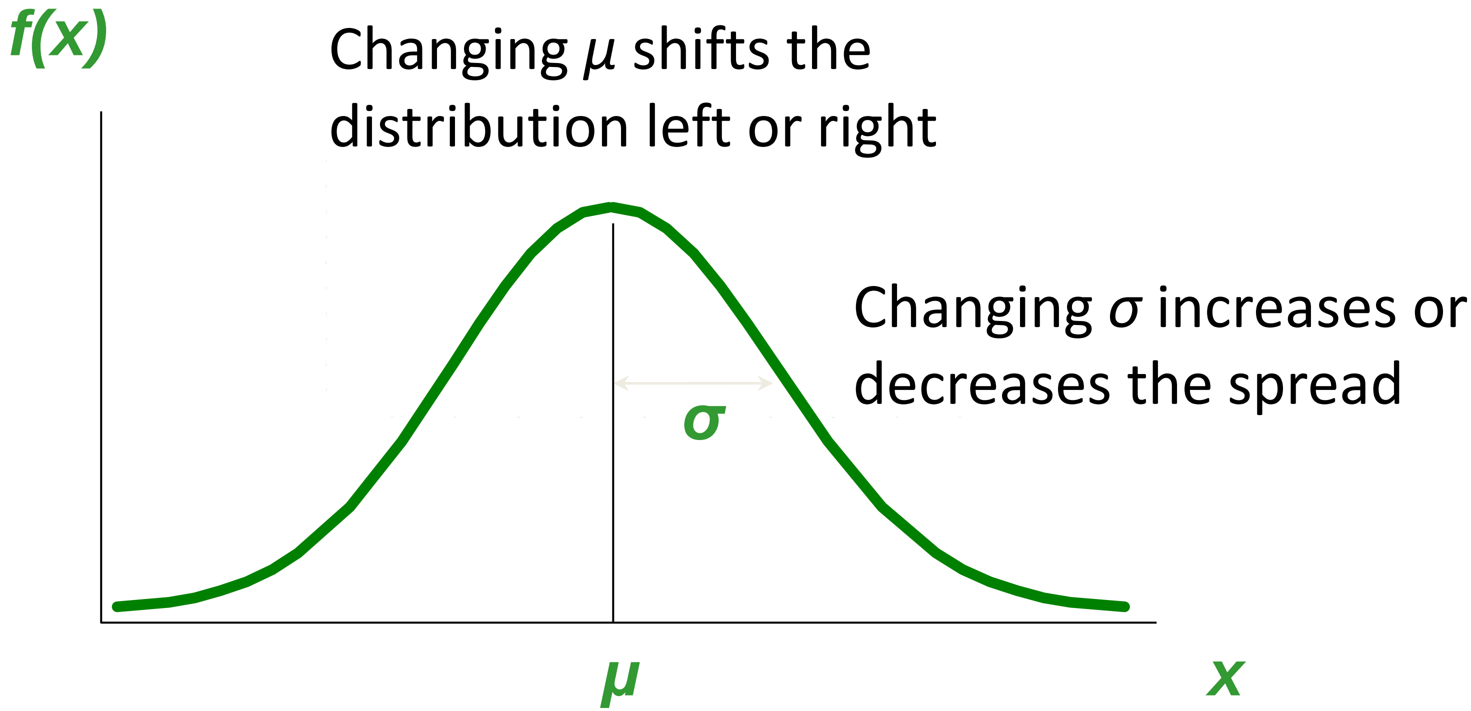
Outline

- **Basics**
  - Motivation, definition, evaluation
- **Methods**
  - Partitional
  - Hierarchical
  - Density-based
  - Mixture model
  - Spectral methods
- **Advanced topics**
  - Clustering ensemble
  - Clustering in MapReduce
  - Semi-supervised clustering, subspace clustering, co-clustering, etc.

Using Probabilistic Models for Clustering

- **Hard vs. soft clustering**
  - Hard clustering: Every point belongs to exactly one cluster
  - Soft clustering: Every point belongs to several clusters with certain degrees
- **Probabilistic clustering**
  - Each cluster is mathematically represented by a parametric distribution
  - The entire data set is modeled by a mixture of these distributions

Gaussian Distribution

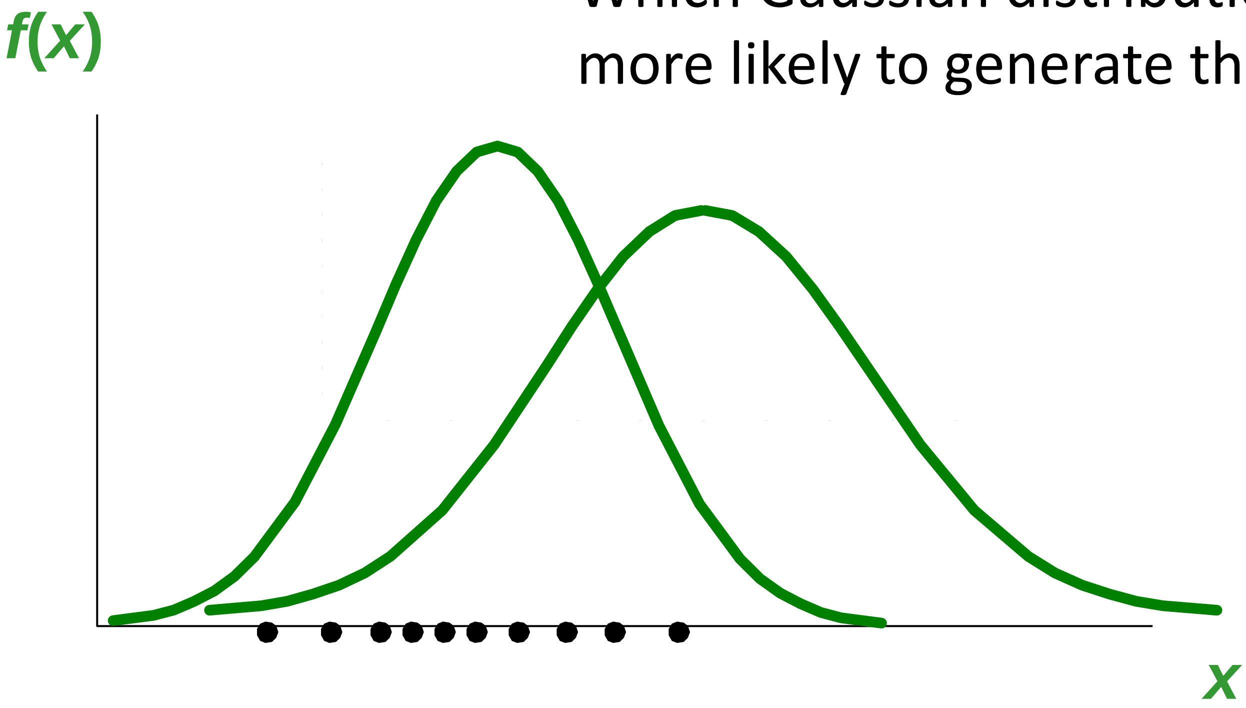


Probability density function $f(x)$ is a function of x given μ and σ

$$N(x \mid \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$$

Likelihood

Which Gaussian distribution is more likely to generate the data?



Define likelihood as a function of μ and σ given x_1, x_2, …, x_n

$$\prod_{i=1}^{n} N(x_i \mid \mu, \sigma^2)$$

Gaussian Distribution

- Multivariate Gaussian

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

mean

covariance

- Log likelihood

$$L(\mu,\Sigma) = \sum_{i=1}^{n} \ln N(x_i|\mu,\Sigma) = \sum_{i=1}^{n} (-\frac{1}{2}(x_i-\mu)^T \Sigma^{-1}(x_i-\mu)) - \pi \ln|\Sigma|)$$

Maximum Likelihood Estimate

- MLE
  - Find model parameters μ, Σ that maximize log likelihood

$$L(\mu, \Sigma)$$

- MLE for Gaussian

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

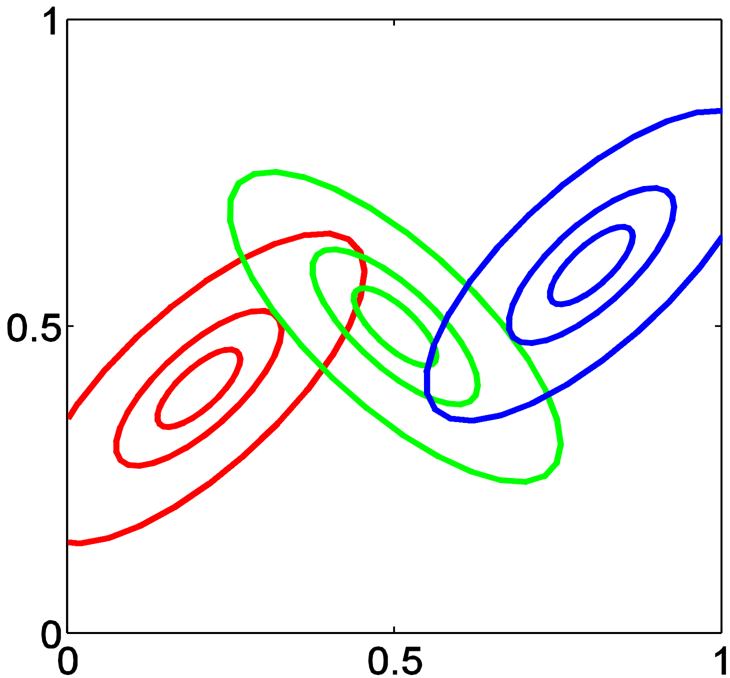
$$\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \hat{\mu})(x_i - \hat{\mu})^T$$

Gaussian Mixture

- Linear combination of Gaussians

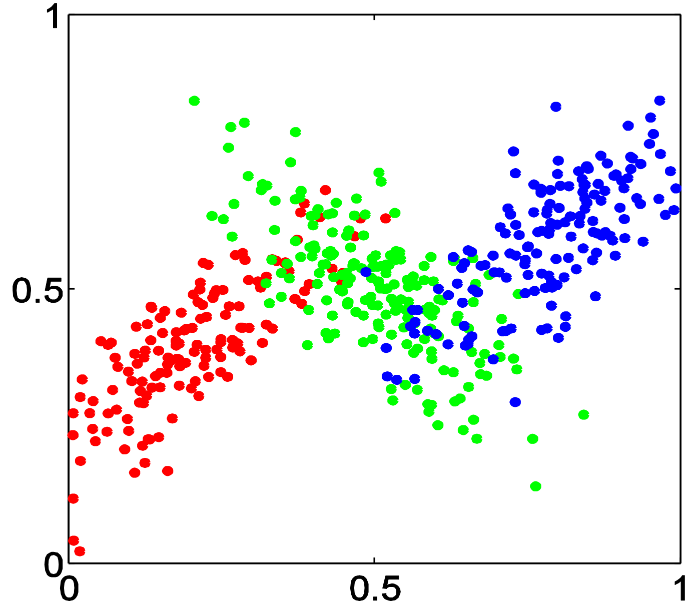
$$p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k) \quad \text{where} \quad \sum_{k=1}^{K} \pi_k = 1, \quad 0 \leqslant \pi_k \leqslant 1$$

parameters to be estimated



Gaussian Mixture

- To generate a data point:
  - first pick one of the clusters with probability π_k
  - then draw a sample x_i from that cluster distribution



Gaussian Mixture

- Maximize log likelihood

$$\ln p(x|\pi, \mu, \Sigma) = \sum_{i=1}^{n} \ln\{\sum_{k=1}^{K} \pi_k \mathcal{N}(x_i|\mu_k, \Sigma_k)\}$$

- Each data point is generated by one of *K* clusters, a latent variable $z_i = (z_{i1}, \ldots, z_{iK})$ is associated with each x_i

$$\sum_{k=1}^{K} z_{ik} = 1 \text{ and } p(z_{ik} = 1) = \pi_k$$

- Regard the values of latent variables as missing

Expectation-Maximization (EM) Algorithm

- E-step: for given parameter values we can compute the expected values of the latent variables

$$
\begin{aligned}
r_{ik} \equiv E(z_{ik}) &= p(z_{ik} = 1 | x_i, \pi, \mu, \Sigma) \\
&= \frac{p(z_{ik} = 1) p(x_i | z_{ik} = 1, \pi, \mu, \Sigma)}{\sum_{k=1}^{K} p(z_{ik} = 1) p(x_i | z_{ik} = 1, \pi, \mu, \Sigma)} \\
&= \frac{\pi_k \mathcal{N}(x_i | u_k, \Sigma_k)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(x_i | u_k, \Sigma_k)}
\end{aligned}
$$

  - Note that $r_{ik} \in [0, 1]$ instead of $\{0, 1\}$ but we still have $\sum_{k=1}^{K} r_{ik} = 1 \text{ for all } i$

Expectation-Maximization (EM) Algorithm

- M-step: maximize the expected complete log likelihood

$$E[\ln p(x, z|\pi, \mu, \Sigma)] = \sum_{i=1}^{n} \sum_{k=1}^{K} r_{ik} \{\ln \pi_k + \ln \mathcal{N}(x_i|\mu_k, \Sigma_k)\}$$

- Parameter update:

$$\pi_k = \frac{\sum_i r_{ik}}{n} \qquad \mu_k = \frac{\sum_i r_{ik} x_i}{\sum_i r_{ik}}$$

$$\Sigma_k = \frac{\sum_i r_{ik}(x_i - \mu_k)(x_i - \mu_k)^T}{\sum_i r_{ik}}$$

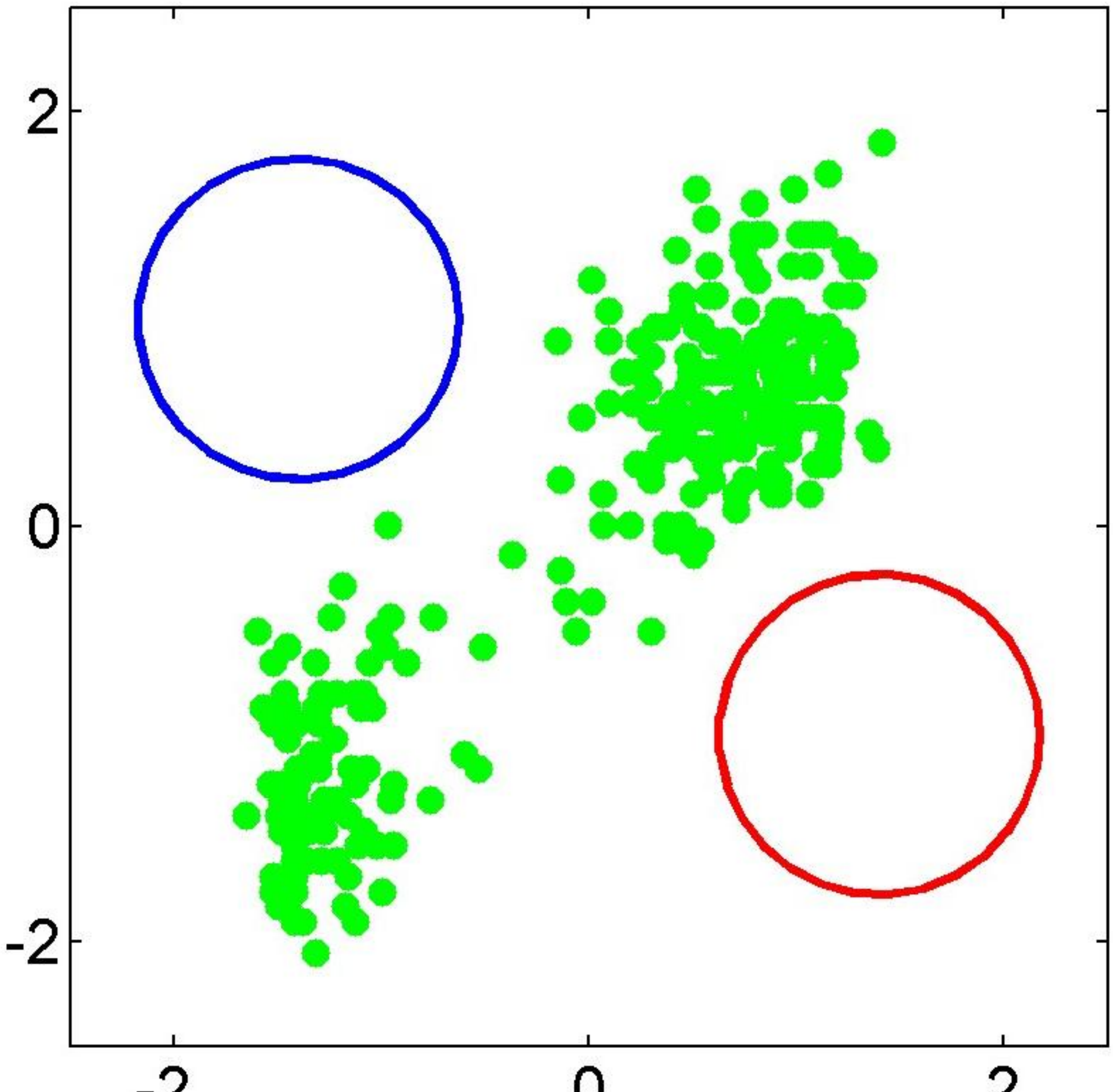
EM Algorithm

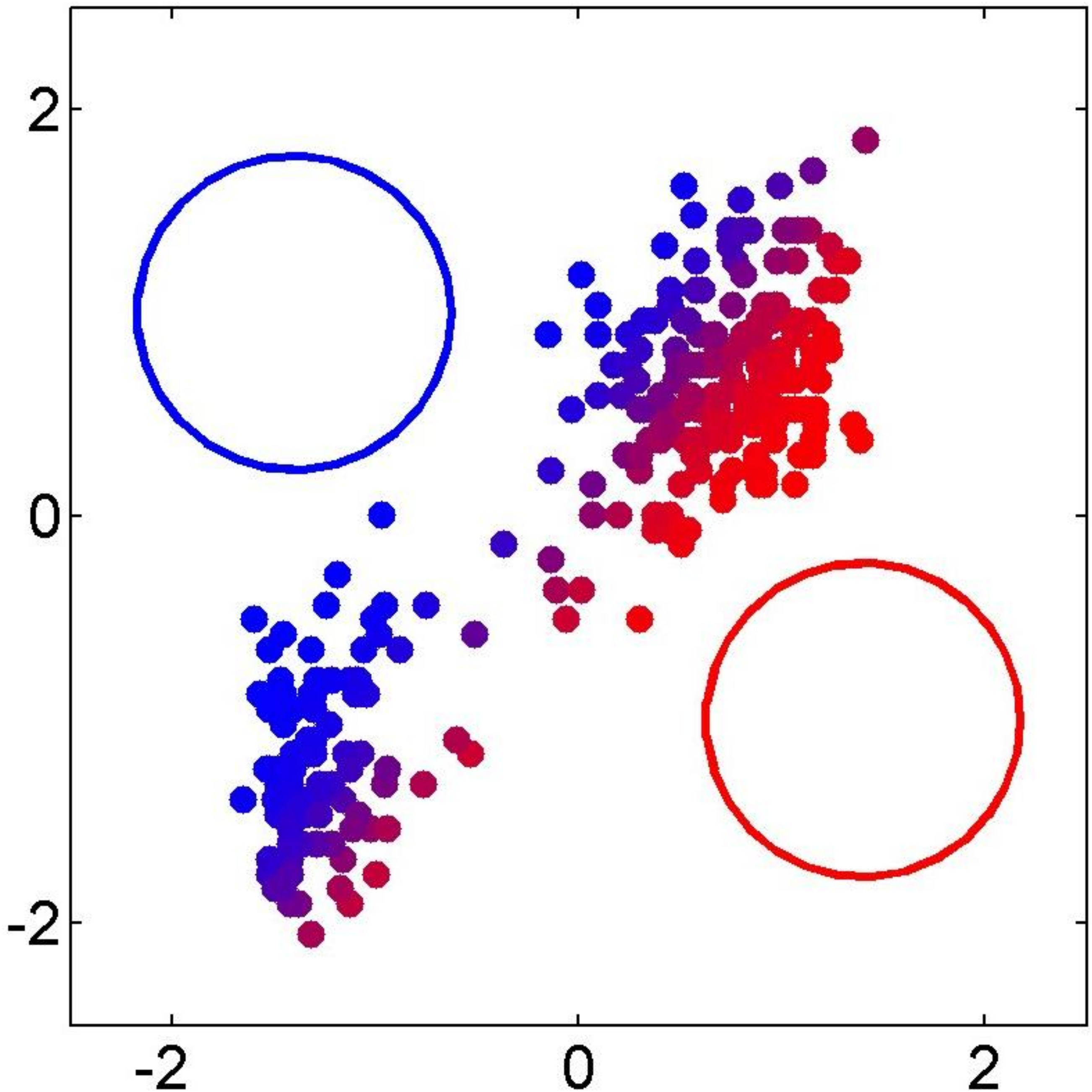
- Iterate E-step and M-step until the log likelihood of data does not increase any more.
  - Converge to local optimal
  - Need to restart algorithm with different initial guess of parameters (as in *K*-means)

- Relation to K-means
  - Consider GMM with common covariance

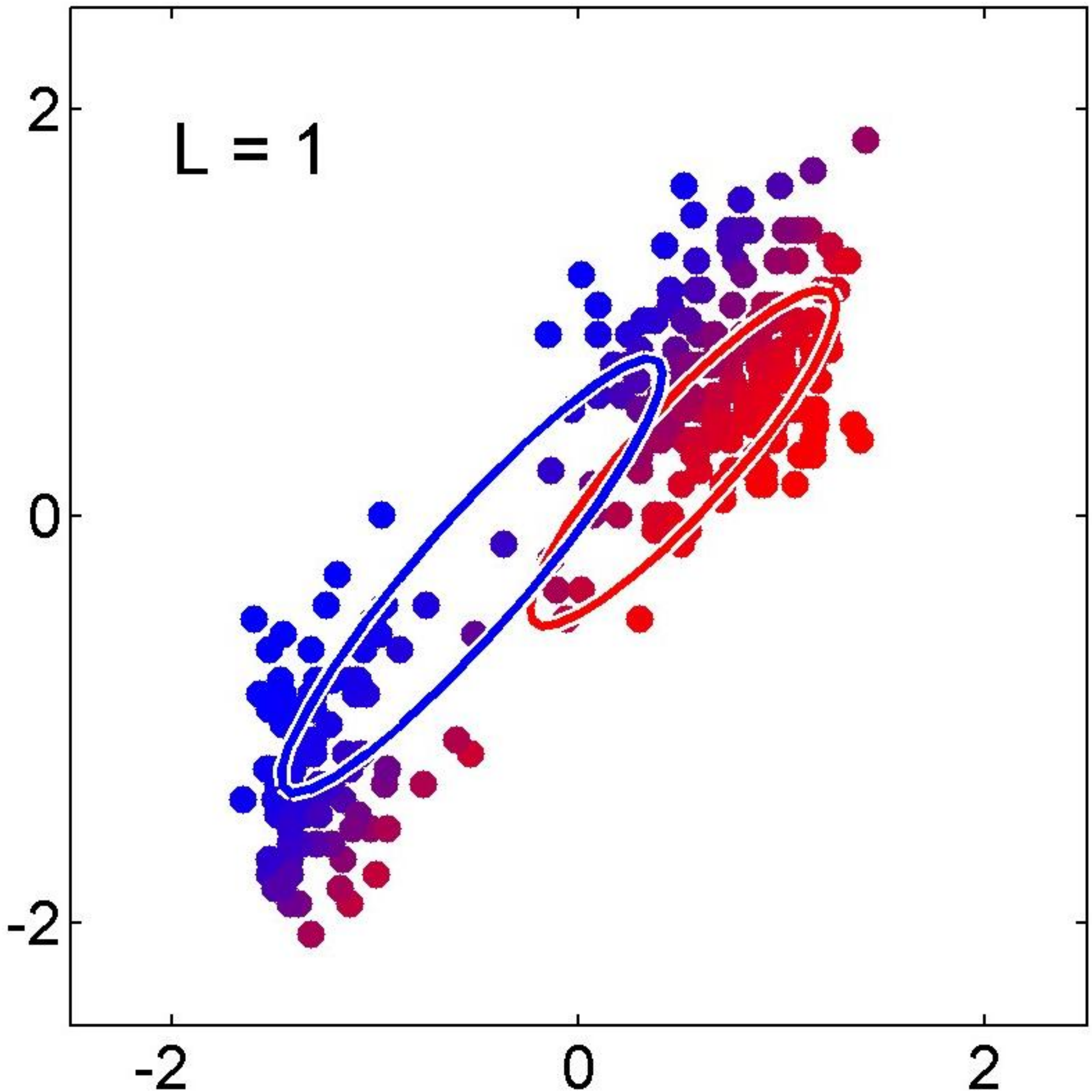
$$\Sigma_k = \delta^2 I$$

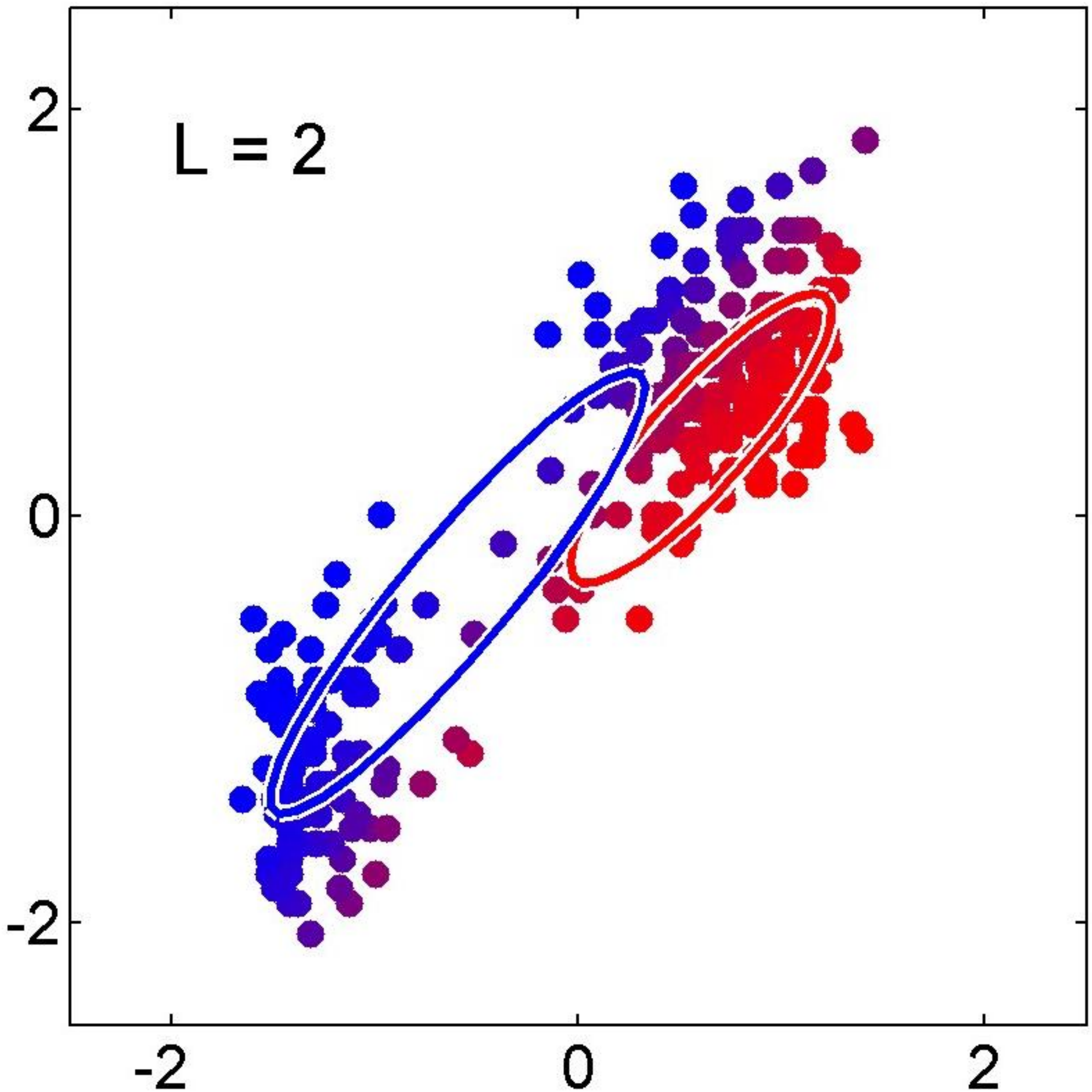
  - As $\delta^2 \to 0, r_{ik} \to 0 \text{ or } 1$, two methods coincide

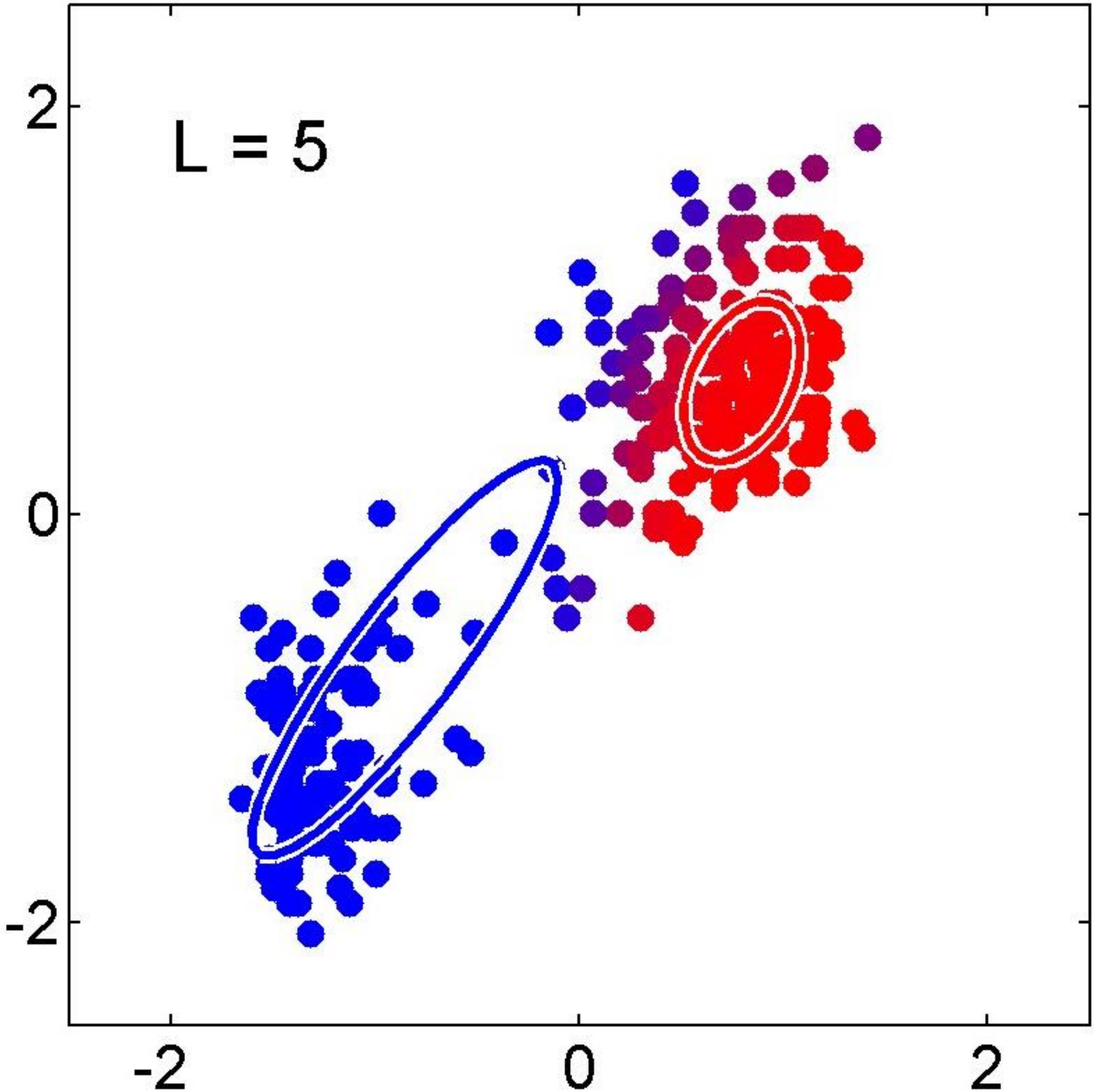

2
0
-2
-2
0
2

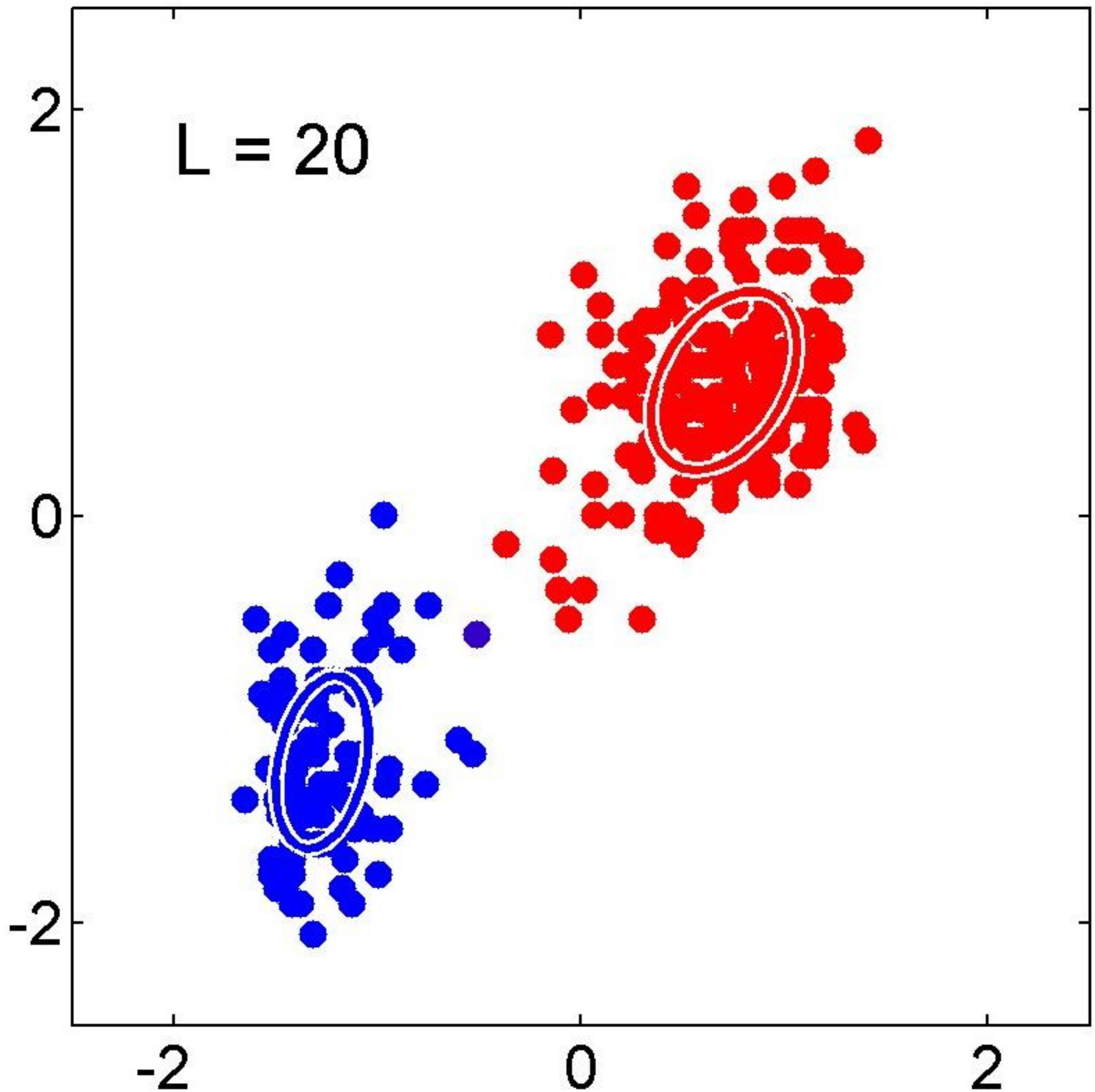


2
0
-2
-2
0
2


L = 1
2
0
-2
-2
0
2


L = 2
2
0
-2
-2
0
2


L = 5
2
0
-2
-2
0
2


L = 20
2
0
-2
-2
0
2

K-means vs GMM

- Objective function
  - Minimize sum of squared error
- Can be optimized by an EM algorithm
  - E-step: assign points to clusters
  - M-step: optimize cluster centers
  - Performs hard assignment during E-step
- Assumes spherical clusters with equal probability of a cluster

- Objective function
  - Maximize log-likelihood
- EM algorithm
  - E-step: Compute posterior probability of membership
  - M-step: Optimize parameters
  - Perform soft assignment during E-step
- Can be used for non-spherical clusters
- Can generate clusters with different probabilities

Mixture Model

- **Strengths**
  - Give probabilistic cluster assignments
  - Have probabilistic interpretation
  - Can handle clusters with varying sizes, variance etc.
- **Weakness**
  - Initialization matters
  - Choose appropriate distributions
  - Overfitting issues

Take-away Message

- Probabilistic clustering
- Maximum likelihood estimate
- Gaussian mixture model for clustering
- EM algorithm that assigns points to clusters and estimates model parameters alternatively
- Strengths and weakness