Machine Learning (CS 181): 14. Mixture Models

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Review: Unsupervised Learning

- Data $D = \{\mathbf{x}\}_{i=1}^{n}$. No target values.
- Typical goals: understand data, summarize data, identify concepts.
- Last lecture: clustering
  - K-means (simple approach, but inflexible— linear decision boundaries)
  - HAC (flexible, provides dendrograms, but poor performance in high dimensions)

Application: K-means on Image Data

CIFAR-100 color. 50,000 images. 32 x 32 x 3 (RGB), each 0-255.

(a) Cluster Centers (b) Cluster 1 (c) Cluster 2 (d) Cluster 3 (e) Cluster 4

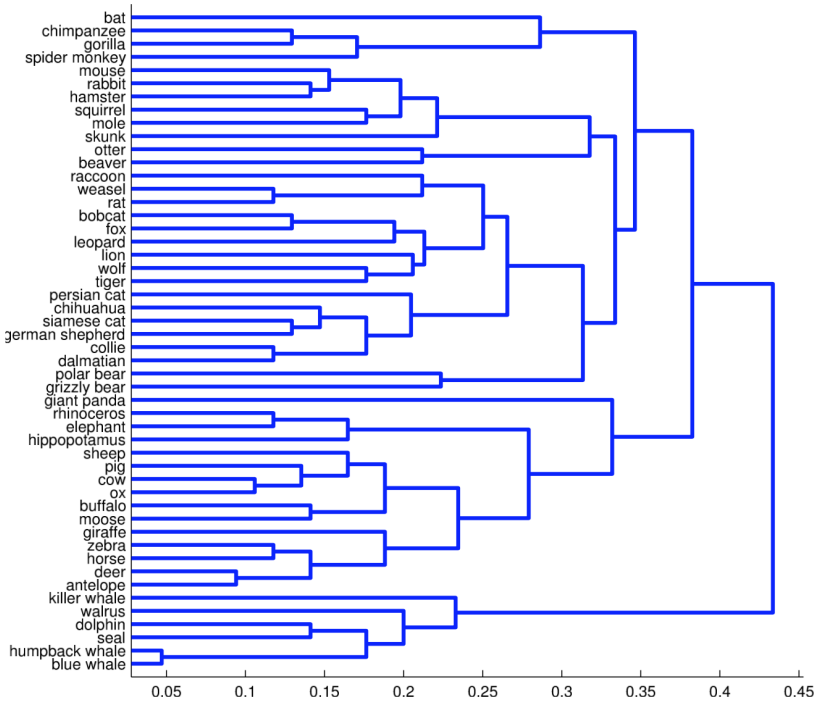
(f) Cluster 5 (g) Cluster 6 (h) Cluster 7 (i) Cluster 8 (j) Cluster 9 (k) Cluster 10

(l) Cluster 11 (m) Cluster 12 (n) Cluster 13 (o) Cluster 14 (p) Cluster 15 (q) Cluster 16

(R.Adams; $K = 16$. Clusters pick up on low-freq color variations)

Application: HAC on Animal Data

Data set of 50 animals, 85 binary features (e.g., longneck, water, smelly)



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A concern about K-means, HAC

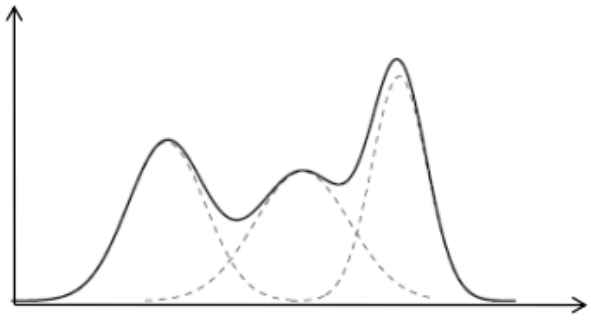
Both seem a bit ad hoc:

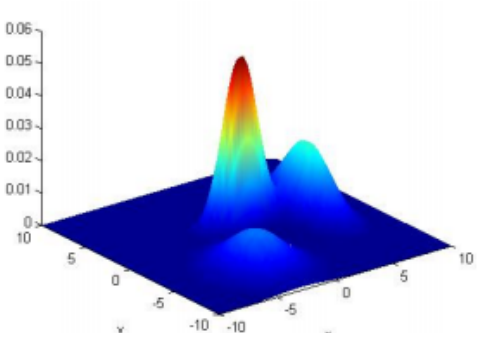
- K-means: finds an assignment of examples to clusters, and cluster prototypes to minimize the total, Euclidean distance between examples and cluster prototypes.
- HAC: adopts a pointwise distance between examples, (e.g., Euclidean or edit distance), and a "group linkage" distance (e.g., min, max, average ...).

Why are these distance measures the right way to think about what makes a good clustering?

How else can we cluster data?

- We can view data as coming from a]mixture over different components of a distribution.





D. Ogreniyorum ($m = 1, m = 2$)

- Use data D to estimate the parameters of this "mixture model." Each component will correspond to a class, or cluster. Given this, can predict the most likely cluster (or class) for each example.

Mixture Models

- Observed data (given): $\mathbf{x}_i \in \mathbb{R}^m$ (features)
- Represent the class of each example as $\mathbf{z}_i$, a one-hot vector. This is latent (unobserved.)
- Generative model (parameters $\mathbf{w}$): first sample a class, then conditioned on the class, generate features

$$p(\mathbf{x}, \mathbf{z}; \mathbf{w}) = p(\mathbf{z}; \mathbf{w}) p(\mathbf{x} \,|\, \mathbf{z}; \mathbf{w})$$

- Given parameters $\mathbf{w}$, we can predict a class via Bayes rule

$$p(\mathbf{z} \,|\, \mathbf{x}; \mathbf{w}) \propto p(\mathbf{x} \,|\, \mathbf{z}; \mathbf{w}) p(\mathbf{z}; \mathbf{w})$$

The Gaussian Mixture Model

- Observed data (given): $\mathbf{x}_i \in \mathbb{R}^m$
- Latent variable (not given): $\mathbf{z}_i \in \{C_k\}_{k=1}^c$, for c clusters
- Class distribution (generalized Bernoulli):

$$p(\mathbf{z} = C_k) = \theta_k, \quad \text{for } k \in \{1, \ldots, c\}$$

- Class conditional distribution (Normal):

$$p(\mathbf{x}|\mathbf{z} = C_k) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_k, \Sigma_k), \quad \text{for } k \in \{1, \ldots, c\}$$

- Parameters of the model: $\boldsymbol{\theta}, \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^c$
- Given estimated parameters, predict a class via Bayes rule

$$p(\mathbf{z} = C_k \,|\, \mathbf{x}) \propto \theta_k \, \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

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Maximum Likelihood Estimation

- Observed data (given) $\mathbf{x}_i \in \mathbb{R}^m$. Latent variable $\mathbf{z}_i$ (not given)
- First, suppose we see $\mathbf{z}_i$ in the data. We be able to compute the complete-data log likelihood:

$$\mathcal{L}(\mathbf{w}) = \sum_{i=1}^{n} \ln(p(\mathbf{x}_i, \mathbf{z}_i; \mathbf{w}))$$

- But: $\mathbf{z}_i$s are latent. Cannot maximize this! Rather, we need to maximize the log likelihood on observed data:

$$\sum_{i=1}^{n} \ln(p(\mathbf{x}_i; \mathbf{w})) = \sum_{i=1}^{n} \ln \left(\sum_{k=1}^{c} \theta_k \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right)$$

Aside: What if we did know the class labels?

Can write out the probability:

$$p(\mathbf{x}_i, \mathbf{z}_i) = p(\mathbf{z}_i) p(\mathbf{x}_i \mid \mathbf{z}_i)$$

$$p(\mathbf{z}_i) = \prod_{k=1}^{c} \theta_k^{z_{ik}}, \quad p(\mathbf{x}_i \mid \mathbf{z}_i) = \prod_{k=1}^{c} \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_{ik}}$$

The complete-data log likelihood is:

$$\sum_{i=1}^{n} \ln(p(\mathbf{x}_i, \mathbf{z}_i; \mathbf{w})) = \sum_{i=1}^{n} \sum_{k=1}^{c} z_{ik} \ln \theta_k + \sum_{i=1}^{n} \sum_{k=1}^{c} z_{ik} \ln \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

We could solve this MLE problem analytically (c.f., HW2):

$$\hat{\theta}_k = \frac{n_k}{n}, \quad \hat{\boldsymbol{\mu}}_k = \frac{1}{n_k} \sum_{i=1}^{n} z_{ik} \mathbf{x}_i, \quad \hat{\boldsymbol{\Sigma}}_k = \frac{1}{n_k} \sum_{i=1}^{n} z_{ik} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)^\top$$

where $n_k = \sum_i z_{ik}$. Very nice!

The Estimation Problem for Gaussian Mixture Model

But we don't know the $\mathbf{z}_i$ values. Rather, we need to maximize:

$$\sum_{i=1}^{n} \ln(p(\mathbf{x}_i; \mathbf{w})) = \sum_{i=1}^{n} \ln \left(\sum_{k=1}^{c} \theta_k \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right),$$

where we marginalize out over latent classes.

This does not have an analytical solution. The log of the sum prevents it decomposing by parameters $\boldsymbol{\theta}$ and $\{\boldsymbol{\mu}, \boldsymbol{\Sigma}\}$.

Even computing a gradient is tricky (note: $\frac{d}{dx} \ln(f(x)) = \frac{1}{f(x)} \frac{df}{dx}$, we end up with a sum of fractions).

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How to proceed?

Iteratively! Guess the class assignments for the data given current parameters, and then improve the estimate of parameters.

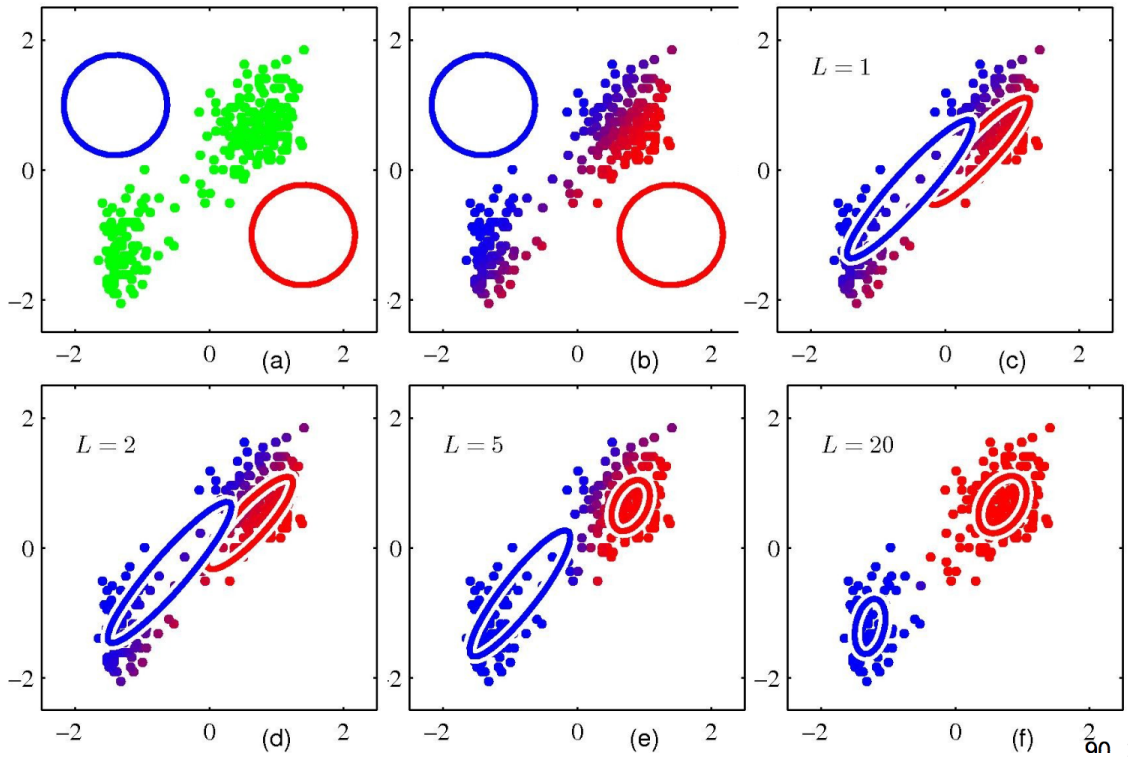
Initialize parameters, then repeat the following two steps:

- (E step) Use the current parameters to predict the assignments $\mathbf{z}_i$, in particular, a distribution on the class for each example.
- (M step) Update the parameters: maximize the "expected complete data log likelihood" using the predicted assignments.

This is the EM algorithm. It is a very powerful, general method to maximize likelihood for models with latent variables. M-step often has an analytical solution.

Illustration: EM on Mixture of Gaussians

(Bishop. Old Faithful data. 1 st. dev. contours. (b) E step. (c) M step; 2, 5, 20 interations.)



The Expected Complete-Data Log Likelihood

(E-step): Given current parameters, estimate "soft class assignments"

$$p(z_i = C_k \,|\, \mathbf{x}_i) = q_{ik} \propto \theta_k \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k),$$

the probability that example $\mathbf{x}_i$ is assigned to class k.

Recall $\mathcal{L}(\mathbf{w})$ is complete-data log likelihood. Define the expected complete-data log likelihood as

$$\begin{aligned}\mathbf{E}_{\mathbf{Z}}[\mathcal{L}(\mathbf{w})] &= \mathbf{E}_{\mathbf{Z}}[\sum_{i=1}^{n} \ln(p(\mathbf{x}_i, \mathbf{z}_i; \mathbf{w}))] \\ &= \sum_{i=1}^{n}\sum_{k=1}^{c} q_{ik} \ln \theta_k + \sum_{i=1}^{n}\sum_{k=1}^{c} q_{ik} \ln \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).\end{aligned}$$

The M-Step: Use the Soft Assignment

For complete-data log likelihood, we had the following MLE estimator:

$$\hat{\theta}_k = \frac{n_k}{n}, \quad \hat{\boldsymbol{\mu}}_k = \frac{1}{n_k}\sum_{i=1}^{n} z_{ik}\mathbf{x}_i, \quad \hat{\boldsymbol{\Sigma}}_k = \frac{1}{n_k}\sum_{i=1}^{n} z_{ik}(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)^\top$$

where $n_k = \sum_i z_{ik}$.

Computing our M-step leads to the following modification:

$$\hat{\theta}_k = \frac{n_k}{n}, \quad \hat{\boldsymbol{\mu}}_k = \frac{1}{n_k}\sum_{i=1}^{n} q_{ik}\mathbf{x}_i, \quad \hat{\boldsymbol{\Sigma}}_k = \frac{1}{n_k}\sum_{i=1}^{n} q_{ik}(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)^\top$$

where $n_k = \sum_i q_{ik}$. Still has a nice, analytical solution!

The Expectation Maximization algorithm

Initialize parameters. Then repeat:

- Expectation step: estimate class distribution conditioned on $\mathbf{x}_i$, $p(\mathbf{z}_i \mid \mathbf{x}_i)$, for each latent variable. This is the posterior over the latent variables $\mathbf{z}_i$ conditioned on the observed data $\mathbf{x}_i$, and computed with the current model parameters.
- Maximization step: update parameters $\boldsymbol{\theta}$, $\{\boldsymbol{\mu}, \boldsymbol{\Sigma}\}$, to maximize the expected complete-data log likelihood.

Until convergence. Alternate between predicting the class for each example, and updating the parameters of the model.

A general and powerful idea: not specific to mixture of Gaussians (see this for topic models in next class.)

Convergence of EM algorithm

- At each step, the EM algorithm adjusts the parameter values to improve the likelihood of the (observed) data:

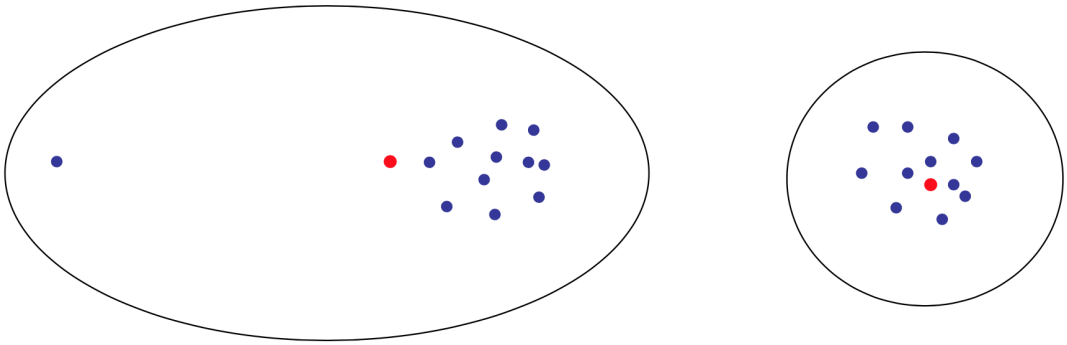
$$p(D; \mathbf{w}^{(0)}) < p(D; \mathbf{w}^{(1)}) < \ldots <$$

- This means that the EM algorithm will converge to a local optimum. Can be usefully combined with random restarts.

Global vs Local optima

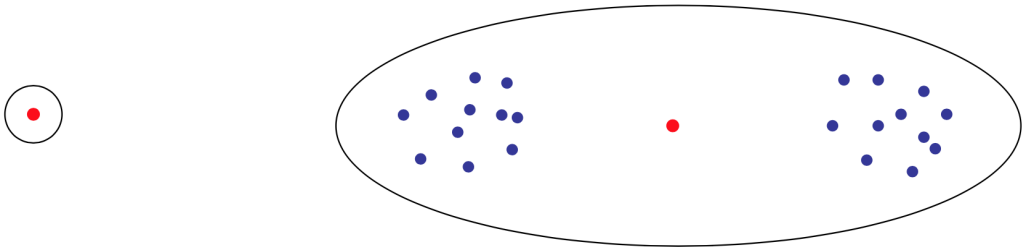
Example: Global vs Local optima

Global optimum ($c = 2$):



Example: Global vs Local optima

Local optimum ($c = 2$):



Note: Initialization of EM for Mixture of Gaussians

E-step:

$$p(z_i = C_k \,|\, \mathbf{x}_i) = q_{ik} \propto \theta_k \, \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

M-step:

$$\hat{\theta}_k = \frac{n_k}{n}, \quad \hat{\boldsymbol{\mu}}_k = \frac{1}{n_k} \sum_{i=1}^{n} q_{ik} \mathbf{x}_i, \quad \hat{\boldsymbol{\Sigma}}_k = \frac{1}{n_k} \sum_{i=1}^{n} q_{ik} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)^\top$$

where $n_k = \sum_i q_{ik}$.

Need asymmetric initialization. What happens if:

- class probability $\hat{\theta}_k = 1/c$, and $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ equal for each class?
- class probability $\hat{\theta}_1 > \max_{j \neq 1} \hat{\theta}_j$, and $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ equal for each class?

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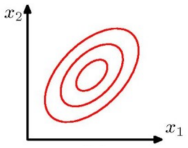
Variations on Mixture of Gaussians model

- Mixture of Gaussians (General)

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

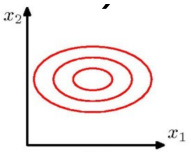


O(m^2) *parameters*

- Mixture of Gaussians (Diagonal)

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k),$$

where $\boldsymbol{\Sigma}_k$ is diagonal.

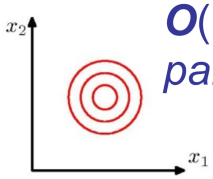


O(m) *parameters*

- Mixture of Gaussians (isotropic, or spherical)

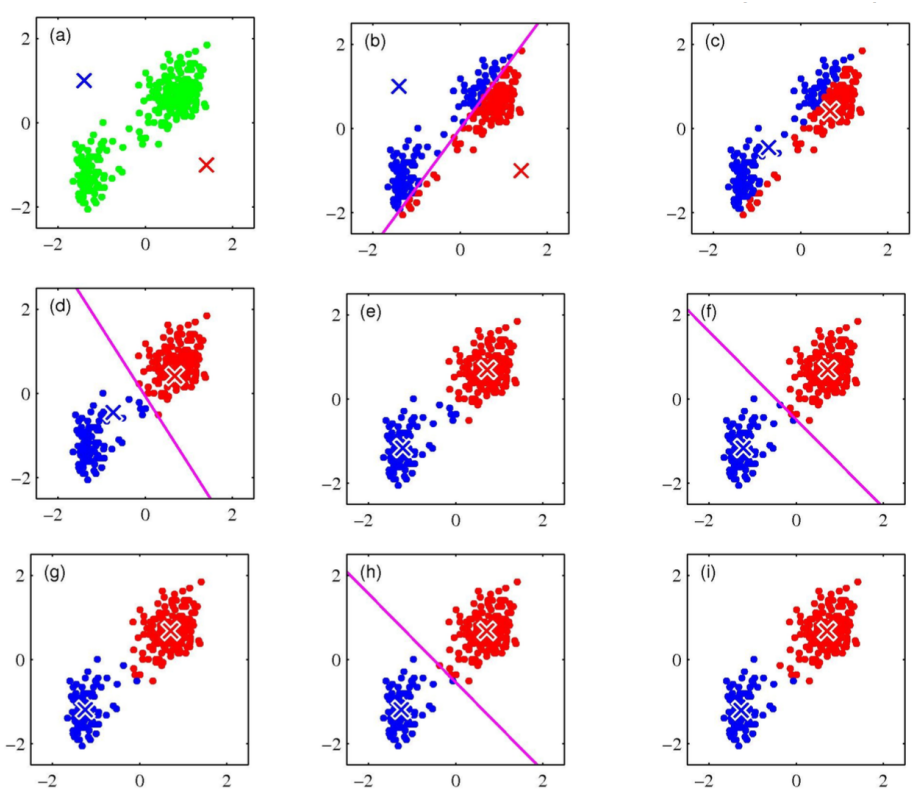
$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \sigma^2\mathbf{I}),$$

where $\mathbf{I}$ is the identity matrix. (Linear decision boundaries.)



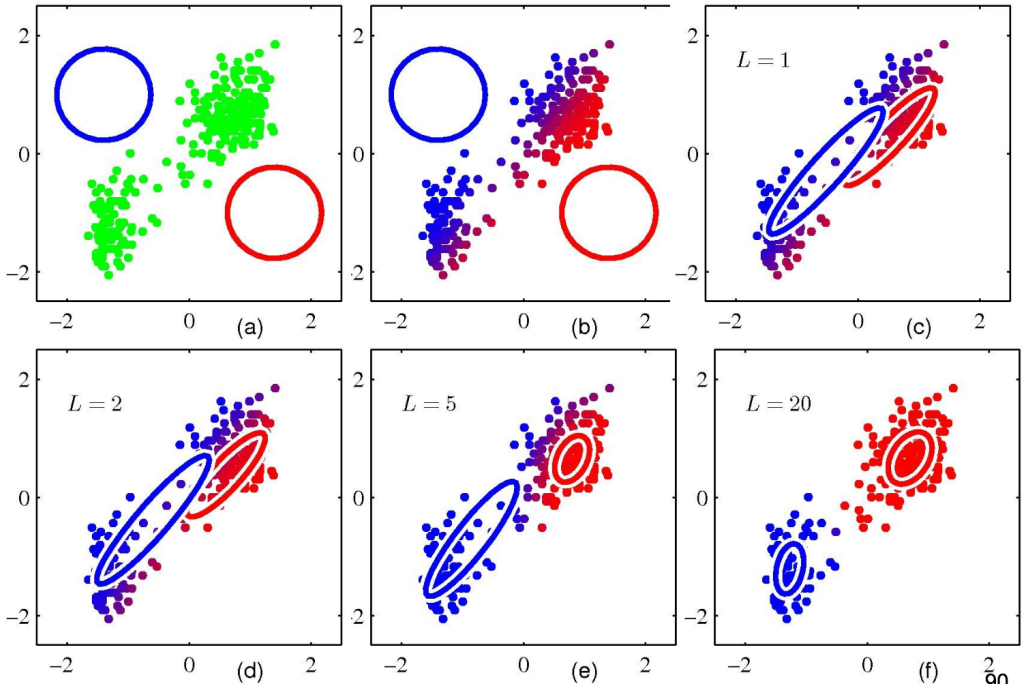
O(m) *parameters*

Recall: K-Means on Old Faithful Eruptions (Bishop)



Compare: EM (Gaussian Mixture) on Old Faithful

(Bishop. Old Faithful data. 1 st. dev. contours. (b) E step. (c) M step; 2, 5, 20 interations.)



Connecting EM and K-Means (Lloyd's algorithm)

K-means:

- (E-step): assign each example to the closest prototype
- (M-step): for each k, update each prototype to the centroid of assigned examples

This is a special case of EM:

- Class probabilities fixed at $1/c$; spherical Gaussians, each with the same, fixed covariance $\epsilon\mathbf{I}$, for small $\epsilon > 0$.
- (E-step) produces a hard assignment (why?)
- (M-step) the centroid maximizes the expected complete-data log likelihood given spherical noise

See that K-means is the limit of EM on Gaussian mixture in which variance parameter $\epsilon \to 0$.

Next class

- Naive Bayes with latent variables (i.e., clustering with discrete features).
- Topic models: each example is a proportion of different 'topics,' and each topic has a topic-conditional distribution on features.
- Graphical representations: a convenient language with which to describe probabilistic models.

Summary

- A mixture model describes a distribution as the average over a number of component distributions.
- The Gaussian mixture model is useful for clustering.
- The MLE problem has no analytical solution because the class variables are latent (unobserved). Ugly expression for log likelihood.
- But: by guessing classes, we can repeatedly update parameters to maximize the expected, complete-data log likelihood.
- This is an application of the EM algorithm. A useful, widely-applicable method for MLE estimation.