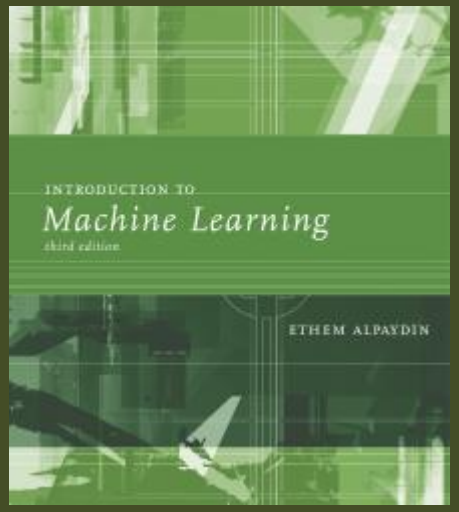

Lecture Slides for

INTRODUCTION TO MACHINE LEARNING

3RD EDITION

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CHAPTER 7:

CLUSTERING

Semiparametric Density Estimation

- Parametric: Assume a single model for $p(\mathbf{x} \mid C_i)$ (Chapters 4 and 5)
- Semiparametric: $p(\mathbf{x} \mid C_i)$ is a mixture of densities

  Multiple possible explanations/prototypes:

  Different handwriting styles, accents in speech
- Nonparametric: No model; data speaks for itself (Chapter 8)

Mixture Densities

$$p(\mathbf{x}) = \sum_{i=1}^{k} p(\mathbf{x} \mid G_i) P(G_i)$$

where G_i the components/groups/clusters,

$P(G_i)$ mixture proportions (priors),

$p(\mathbf{x} \mid G_i)$ component densities

Gaussian mixture where $p(\mathbf{x} \mid G_i) \sim N(\boldsymbol{\mu}_i, \sum_i)$

parameters $\Phi = \{P(G_i), \boldsymbol{\mu}_i, \sum_i\}_{i=1}^{k}$

unlabeled sample $X = \{\mathbf{x}^t\}_t$ (unsupervised learning)

Classes vs. Clusters

- Supervised: $X = \{\mathbf{x}^t, r^t\}_t$
- Classes C_i $i=1,\ldots,K$

$$p(\mathbf{x}) = \sum_{i=1}^{K} p(\mathbf{x} \mid C_i) P(C_i)$$

where $p(\mathbf{x} \mid C_i) \sim N(\boldsymbol{\mu}_i, \sum_i)$

- $\Phi = \{P(C_i), \boldsymbol{\mu}_i, \sum_i\}_{i=1}^{K}$

$$\hat{P}(C_i) = \frac{\sum_t r_i^t}{N} \quad \mathbf{m}_i = \frac{\sum_t r_i^t \mathbf{x}^t}{\sum_t r_i^t}$$

$$\mathbf{S}_i = \frac{\sum_t r_i^t (\mathbf{x}^t - \mathbf{m}_i)(\mathbf{x}^t - \mathbf{m}_i)^T}{\sum_t r_i^t}$$

- Unsupervised : $X = \{\mathbf{x}^t\}_t$
- Clusters G_i $i=1,\ldots,k$

$$p(\mathbf{x}) = \sum_{i=1}^{k} p(\mathbf{x} \mid G_i) P(G_i)$$

where $p(\mathbf{x} \mid G_i) \sim N(\boldsymbol{\mu}_i, \sum_i)$

- $\Phi = \{P(G_i), \boldsymbol{\mu}_i, \sum_i\}_{i=1}^{k}$

Labels r_i^t ?

k-Means Clustering

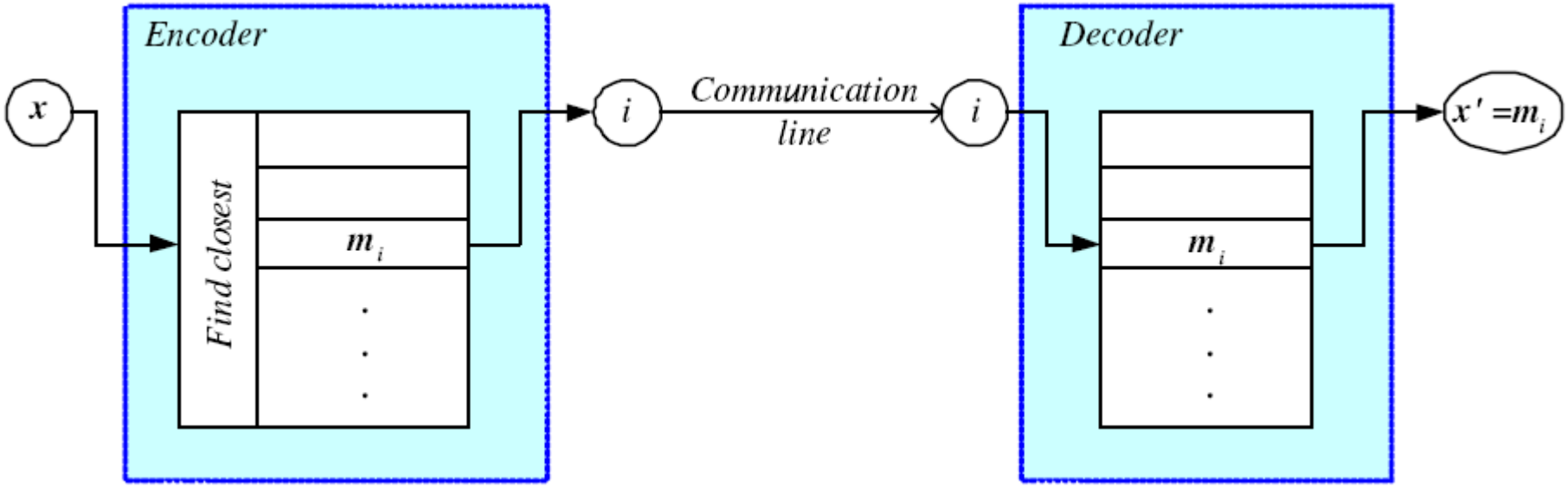
- Find *k* reference vectors (prototypes/codebook vectors/codewords) which best represent data
- Reference vectors, $\boldsymbol{m}_i$, $i = 1,\ldots,k$
- Use nearest (most similar) reference:

$$\left\|\mathbf{x}^t - \mathbf{m}_i\right\| = \min_j \left\|\mathbf{x}^t - \mathbf{m}_j\right\|$$

- Reconstruction error $E\left(\{\mathbf{m}_i\}_{i=1}^k | \mathcal{X}\right) = \sum_t \sum_i b_i^t \left\|\mathbf{x}^t - \mathbf{m}_i\right\|$

$$b_i^t = \begin{cases} 1 & \text{if } \left\|\mathbf{x}^t - \mathbf{m}_i\right\| = \min_j \left\|\mathbf{x}^t - \mathbf{m}_j\right\| \\ 0 & \text{otherwise} \end{cases}$$

Encoding/Decoding



k-means Clustering

Initialize $\boldsymbol{m}_i, i = 1, \ldots, k$, for example, to k random $\boldsymbol{x}^t$

Repeat

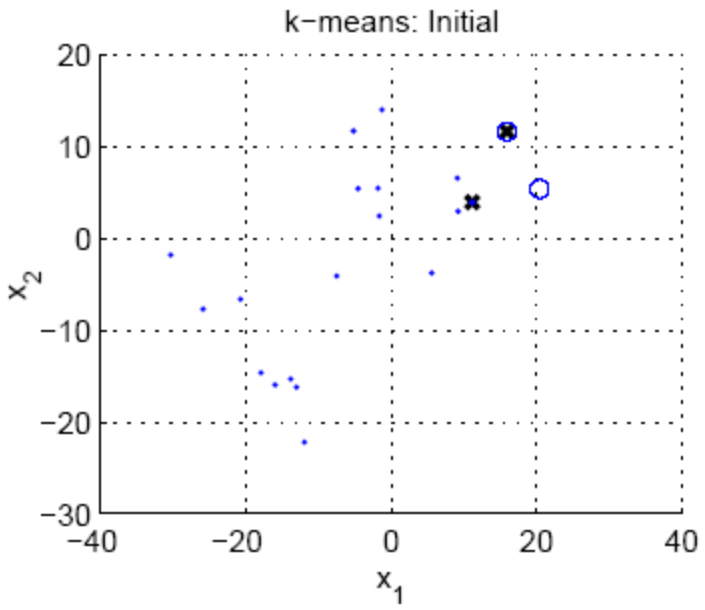
For all $\boldsymbol{x}^t \in \mathcal{X}$

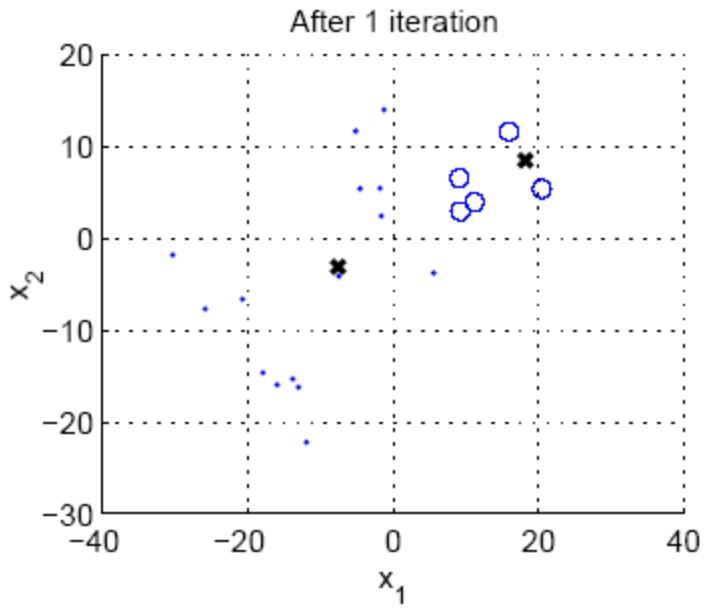
$$b_i^t \leftarrow \begin{cases} 1 & \text{if } \|\boldsymbol{x}^t - \boldsymbol{m}_i\| = \min_j \|\boldsymbol{x}^t - \boldsymbol{m}_j\| \\ 0 & \text{otherwise} \end{cases}$$

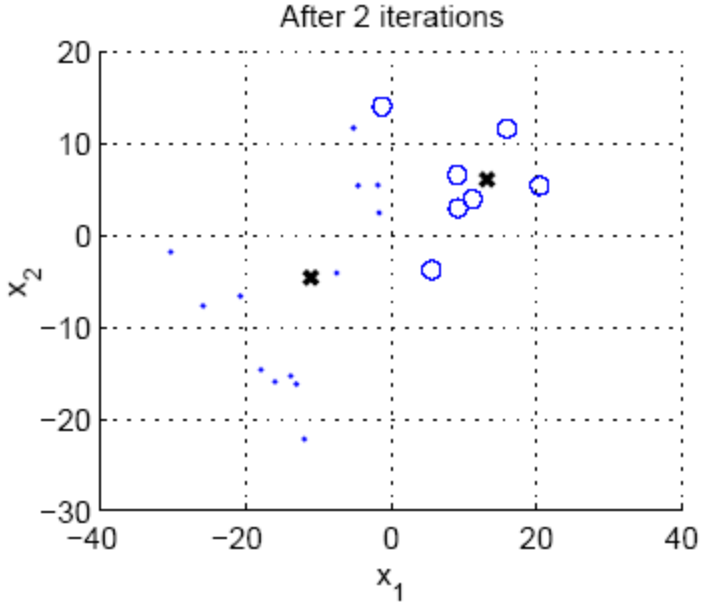
For all $\boldsymbol{m}_i, i = 1, \ldots, k$

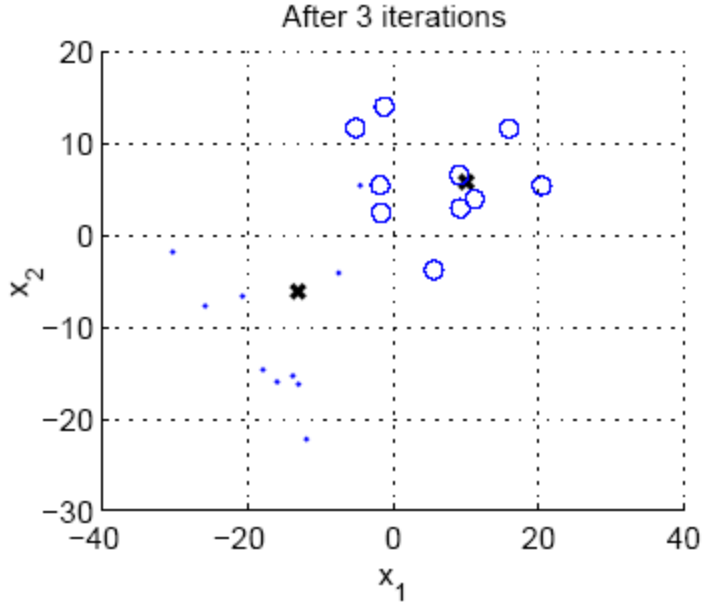
$$\boldsymbol{m}_i \leftarrow \sum_t b_i^t \boldsymbol{x}^t / \sum_t b_i^t$$

Until $\boldsymbol{m}_i$ converge


k−means: Initial
20
10
0
−10
−20
−30
−40
−20
0
20
40
x2
x1


After 1 iteration
20
10
0
−10
−20
−30
−40
−20
0
20
40
x2
x1


After 2 iterations
20
10
0
−10
−20
−30
−40
−20
0
20
40
x2
x1


After 3 iterations
20
10
0
−10
−20
−30
−40
−20
0
20
40
x2
x1

Expectation-Maximization (EM)

- Log likelihood with a mixture model

$$\mathcal{L}(\Phi \mid \mathcal{X}) = \log \prod_t p\left(\mathbf{x}^t \mid \Phi\right)$$

$$= \sum_t \log \sum_{i=1}^{k} p\left(\mathbf{x}^t \mid G_i\right) P\left(G_i\right)$$

- Assume hidden variables z, which when known, make optimization much simpler
- Complete likelihood, $L_c(\Phi \mid X,Z)$, in terms of ***x*** and ***z***
- Incomplete likelihood, $L(\Phi \mid X)$, in terms of ***x***

E- and M-steps

Iterate the two steps

1. E-step: Estimate *z* given X and current Φ
2. M-step: Find new Φ' given *z*, X, and old Φ.

$$\text{E-step: } \mathcal{Q}\left(\Phi \mid \Phi^{l}\right) = E\left[\mathcal{L}_c(\Phi \mid \mathcal{X}, \mathcal{Z}) \mid \mathcal{X}, \Phi^{l}\right]$$

$$\text{M-step: } \Phi^{l+1} = \underset{\Phi}{\operatorname{argmax}}\, \mathcal{Q}\left(\Phi \mid \Phi^{l}\right)$$

An increase in Q increases incomplete likelihood

$$\mathcal{L}\left(\Phi^{l+1} \mid \mathcal{X}\right) \geq \mathcal{L}\left(\Phi^{l} \mid \mathcal{X}\right)$$

EM in Gaussian Mixtures

- $z^t_i = 1$ if $\mathbf{x}^t$ belongs to G_i, 0 otherwise (labels $\mathbf{r}^t_i$ of supervised learning); assume $p(\mathbf{x} | G_i) \sim N(\boldsymbol{\mu}_i, \sum_i)$
- E-step:

$$E\left[z_i^t | \mathcal{X}, \Phi^l\right] = \frac{p\left(\mathbf{x}^t | G_i, \Phi^l\right) P\left(G_i\right)}{\sum_j p\left(\mathbf{x}^t | G_j, \Phi^l\right) P\left(G_j\right)}$$

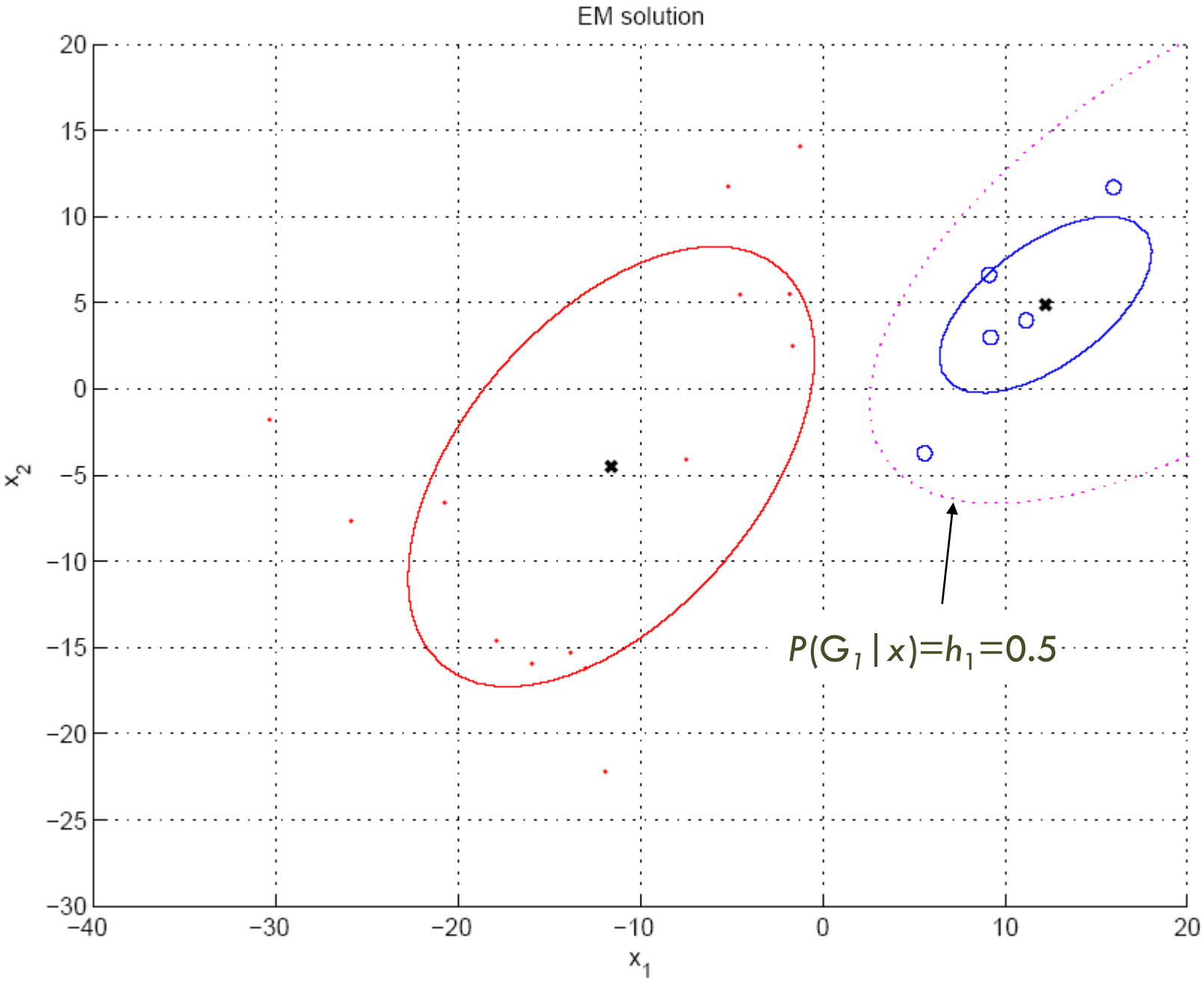
$$= P\left(G_i | \mathbf{x}^t, \Phi^l\right) \equiv h_i^t$$

- M-step:

$$P\left(G_i\right) = \frac{\sum_t h_i^t}{N} \qquad \mathbf{m}_i^{l+1} = \frac{\sum_t h_i^t \mathbf{x}^t}{\sum_t h_i^t}$$

$$\mathbf{S}_i^{l+1} = \frac{\sum_t h_i^t \left(\mathbf{x}^t - \mathbf{m}_i^{l+1}\right)\left(\mathbf{x}^t - \mathbf{m}_i^{l+1}\right)^T}{\sum_t h_i^t}$$

Use estimated labels in place of unknown labels


EM solution
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−40
−30
−20
−10
0
10
20
x2
x1
P(G1 | x)=h1=0.5

Mixtures of Latent Variable Models

Regularize clusters

1. Assume shared/diagonal covariance matrices
2. Use PCA/FA to decrease dimensionality: Mixtures of PCA/FA

$$p(\mathbf{x}_t \mid G_i) = \mathcal{N}(\mathbf{m}_i, \mathbf{V}_i\mathbf{V}_i^T + \boldsymbol{\psi}_i)$$

Can use EM to learn $\mathbf{V}_i$ (Ghahramani and Hinton, 1997; Tipping and Bishop, 1999)

After Clustering

- Dimensionality reduction methods find correlations between features and group features
- Clustering methods find similarities between instances and group instances
- Allows knowledge extraction through
  - number of clusters,
  - prior probabilities,
  - cluster parameters, i.e., center, range of features.

  Example: CRM, customer segmentation

Clustering as Preprocessing

- Estimated group labels h_i (soft) or b_i (hard) may be seen as the dimensions of a new k dimensional space, where we can then learn our discriminant or regressor.
- Local representation (only one b_i is 1, all others are 0; only few h_i are nonzero) vs

  Distributed representation (After PCA; all z_i are nonzero)

Mixture of Mixtures

- In classification, the input comes from a mixture of classes (supervised).
- If each class is also a mixture, e.g., of Gaussians, (unsupervised), we have a mixture of mixtures:

$$p(\mathbf{x}|C_i) = \sum_{j=1}^{k_i} p(\mathbf{x}|G_{ij}) P(G_{ij})$$

$$p(\mathbf{x}) = \sum_{i=1}^{K} p(\mathbf{x}|C_i) P(C_i)$$

Spectral Clustering

- Cluster using predefined pairwise similarities B_{rs} instead of using Euclidean or Mahalanobis distance
- Can be used even if instances not vectorially represented
- Steps:
  I. Use Laplacian Eigenmaps (chapter 6) to map to a new $\mathbf{z}$ space using B_{rs}
  II. Use k-means in this new $\mathbf{z}$ space for clustering

Hierarchical Clustering

- Cluster based on similarities/distances
- Distance measure between instances $\mathbf{x}^r$ and $\mathbf{x}^s$

  Minkowski (L_p) (Euclidean for $p = 2$)

$$d_m\left(\mathbf{x}^r, \mathbf{x}^s\right) = \left[\sum_{j=1}^{d}\left(x_j^r - x_j^s\right)^p\right]^{1/p}$$

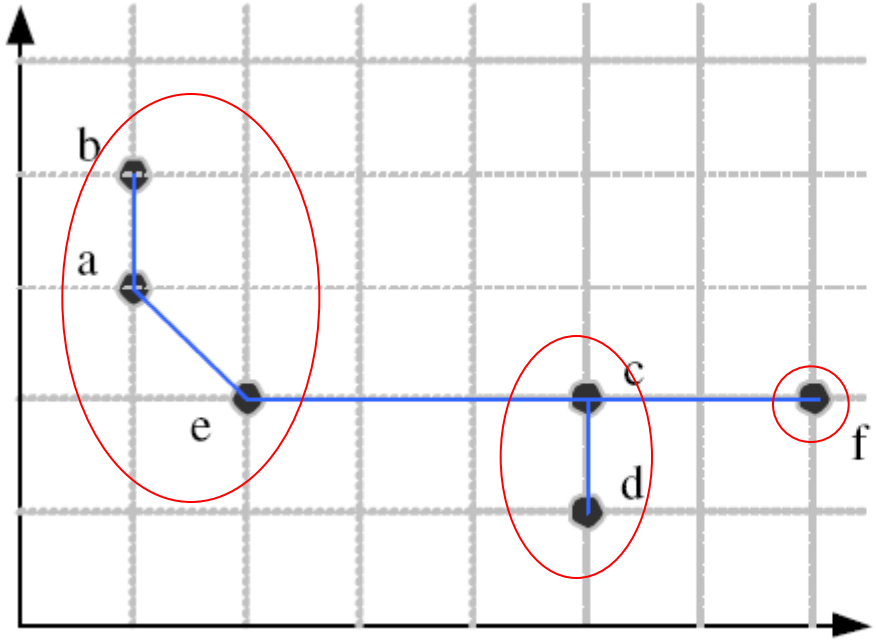
  City-block distance

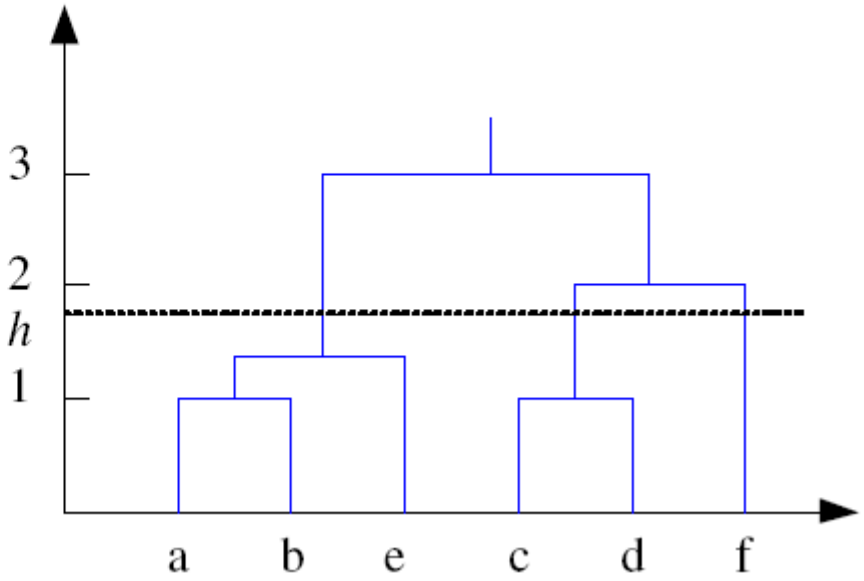
$$d_{cb}\left(\mathbf{x}^r, \mathbf{x}^s\right) = \sum_{j=1}^{d}\left|x_j^r - x_j^s\right|$$

Agglomerative Clustering

- Start with *N* groups each with one instance and merge two closest groups at each iteration
- Distance between two groups G_i and G_j:
  - Single-link:
$$d(G_i, G_j) = \min_{\mathbf{x}^r \in G_i, \mathbf{x}^s \in G_j} d(\mathbf{x}^r, \mathbf{x}^s)$$
  - Complete-link:
$$d(G_i, G_j) = \max_{\mathbf{x}^r \in G_i, \mathbf{x}^s \in G_j} d(\mathbf{x}^r, \mathbf{x}^s)$$
  - Average-link, centroid
$$d(G_i, G_j) = \text{ave}_{\mathbf{x}^r \in G_i, \mathbf{x}^s \in G_j} d(\mathbf{x}^r, \mathbf{x}^s)$$

Example: Single-Link Clustering





Dendrogram

Choosing *k*

- Defined by the application, e.g., image quantization
- Plot data (after PCA) and check for clusters
- Incremental (leader-cluster) algorithm: Add one at a time until "elbow" (reconstruction error/log likelihood/intergroup distances)
- Manually check for meaning