Lecture Slides for

INTRODUCTION TO

Machine Learning

2nd Edition

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CHAPTER 7:

Clustering

Semiparametric Density Estimation

- Parametric: Assume a single model for $p\ (\boldsymbol{x} \mid C_i)$ (Chapters 4 and 5)
- Semiparametric: $p\ (\boldsymbol{x} \mid C_i)$ 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),

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

Gaussian mixture where $p(\boldsymbol{x}|G_i) \sim N(\boldsymbol{\mu}_i, \sum_i)$ parameters $\Phi = \{P(G_i), \boldsymbol{\mu}_i, \sum_i\}_{i=1}^{k}$

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

Classes vs. Clusters

- Supervised: X = { $\boldsymbol{x}^t, \boldsymbol{r}^t$ }$_t$
- Classes C$_i$ i=1,...,K

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

where p ($\boldsymbol{x}$ | C$_i$) ~ N ($\boldsymbol{\mu}_i$, $\boldsymbol{\Sigma}_i$)

- Φ = {P (C$_i$), $\boldsymbol{\mu}_i$, $\boldsymbol{\Sigma}_i$ }$^K_{i=1}$

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

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

- Unsupervised : X = { $\boldsymbol{x}^t$ }$_t$
- Clusters G$_i$ i=1,...,k

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

where p ($\boldsymbol{x}$ | G$_i$) ~ N ($\boldsymbol{\mu}_i$, $\boldsymbol{\Sigma}_i$)

- Φ = {P (G$_i$), $\boldsymbol{\mu}_i$, $\boldsymbol{\Sigma}_i$ }$^k_{i=1}$

Labels, $\boldsymbol{r}^t_i$?

k-Means Clustering

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

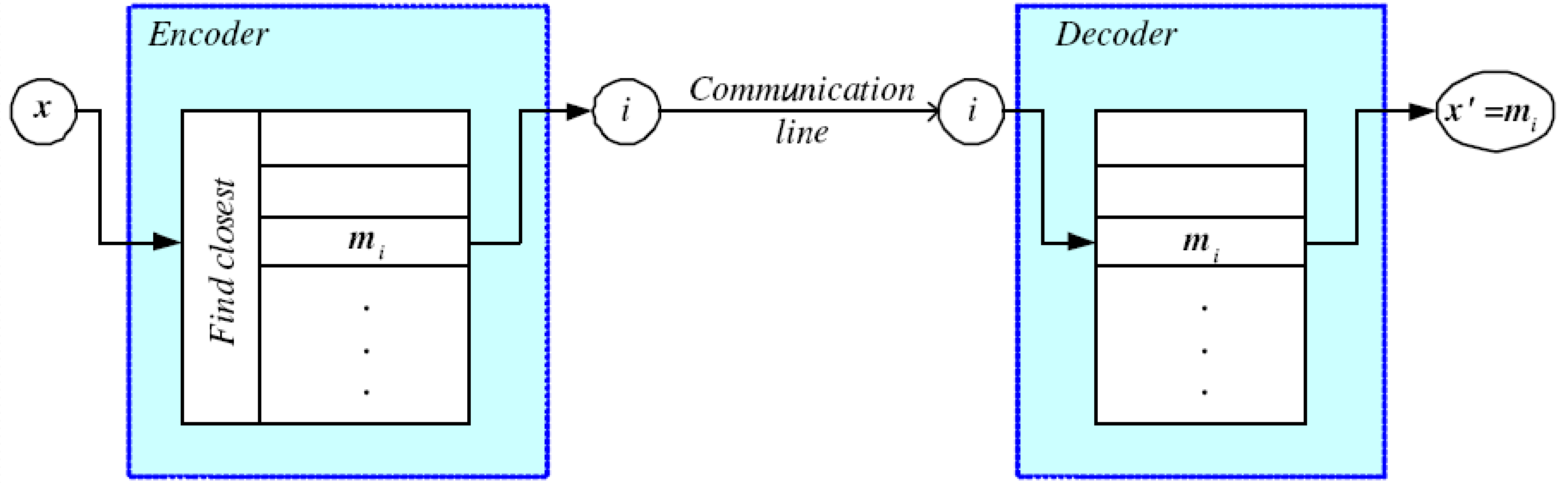
$$\left\|\mathbf{x}^t - \mathbf{m}_i\right\| = \min_j \left\|\mathbf{x}^t - \mathbf{m}_j\right\|$$

- Reconstruction error

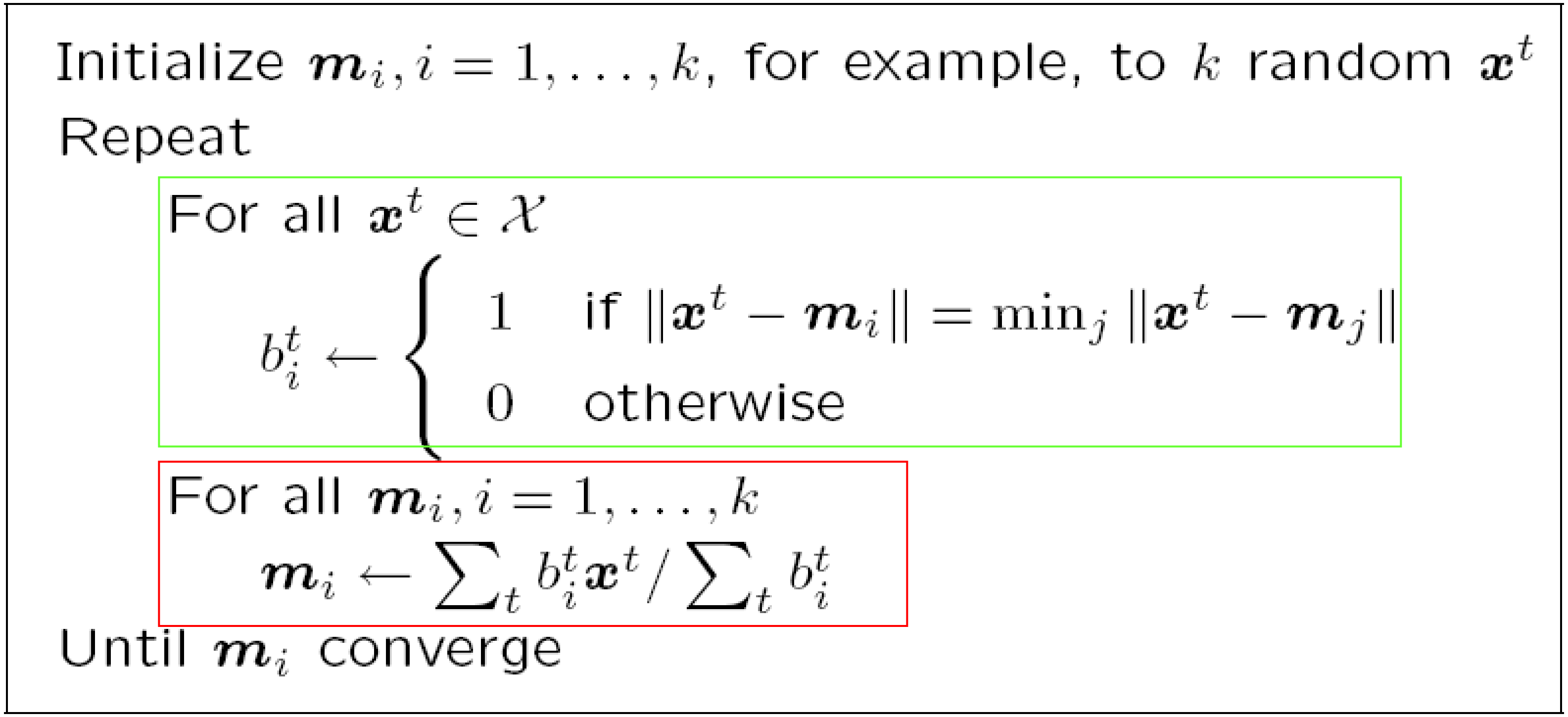
$$E\left(\{\mathbf{m}_i\}_{i=1}^k \middle| \mathcal{X}\right) = \sum_t \sum_i b_i^t \left\|\mathbf{x}^t - \mathbf{m}_i\right\|$$

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

Encoding/Decoding



k-means Clustering



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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
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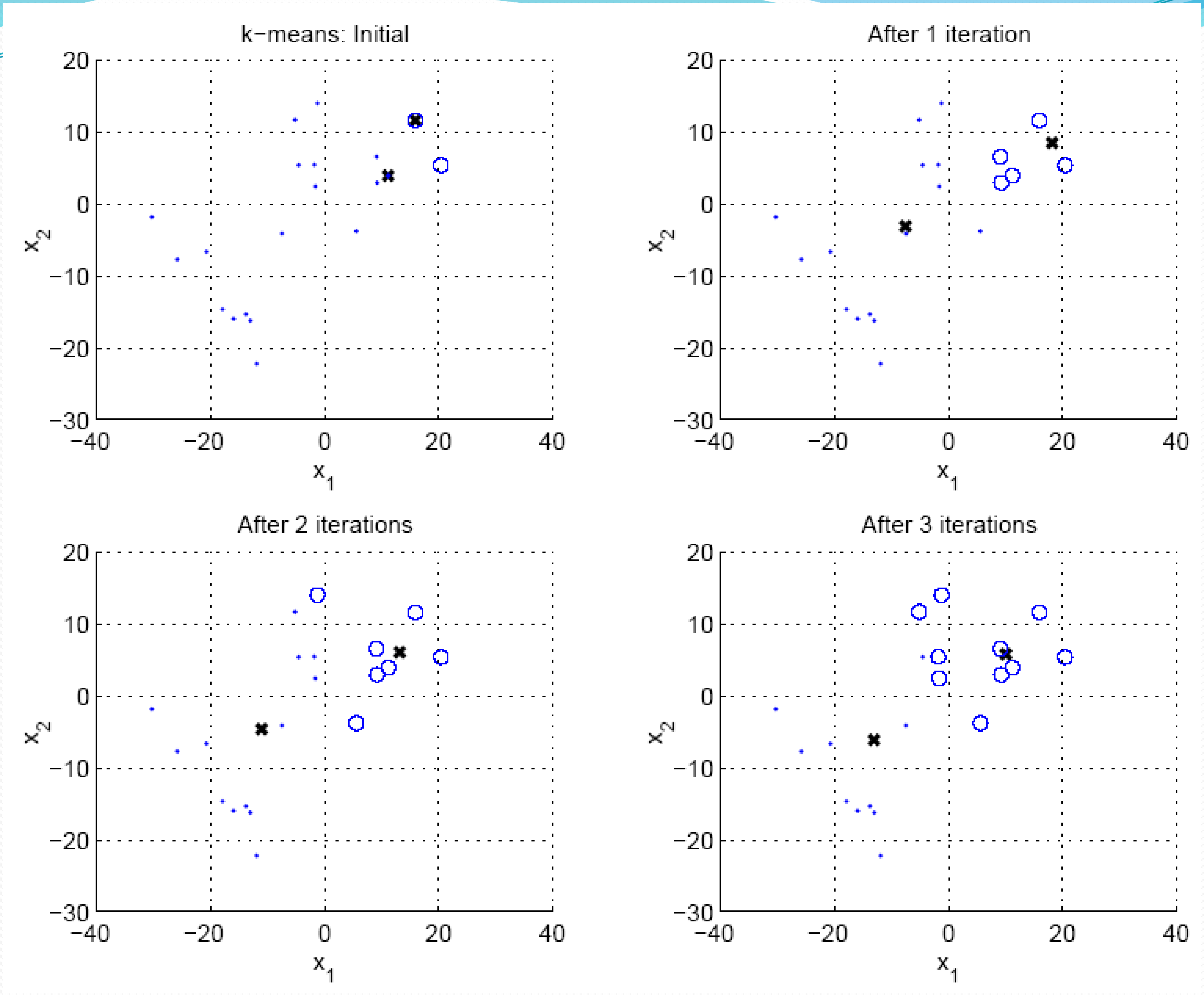

k−means: Initial
After 1 iteration
After 2 iterations
After 3 iterations
20
10
0
−10
−20
−30
−40
−20
0
20
40
x_1
x_2

Expectation-Maximization (EM)

- Log likelihood with a mixture model

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

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

- 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.

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

$$\text{M-step: } \Phi^{l+1} = \arg\max_{\Phi} \mathcal{Q}\left(\Phi \mid \Phi^l\right)$$

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

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

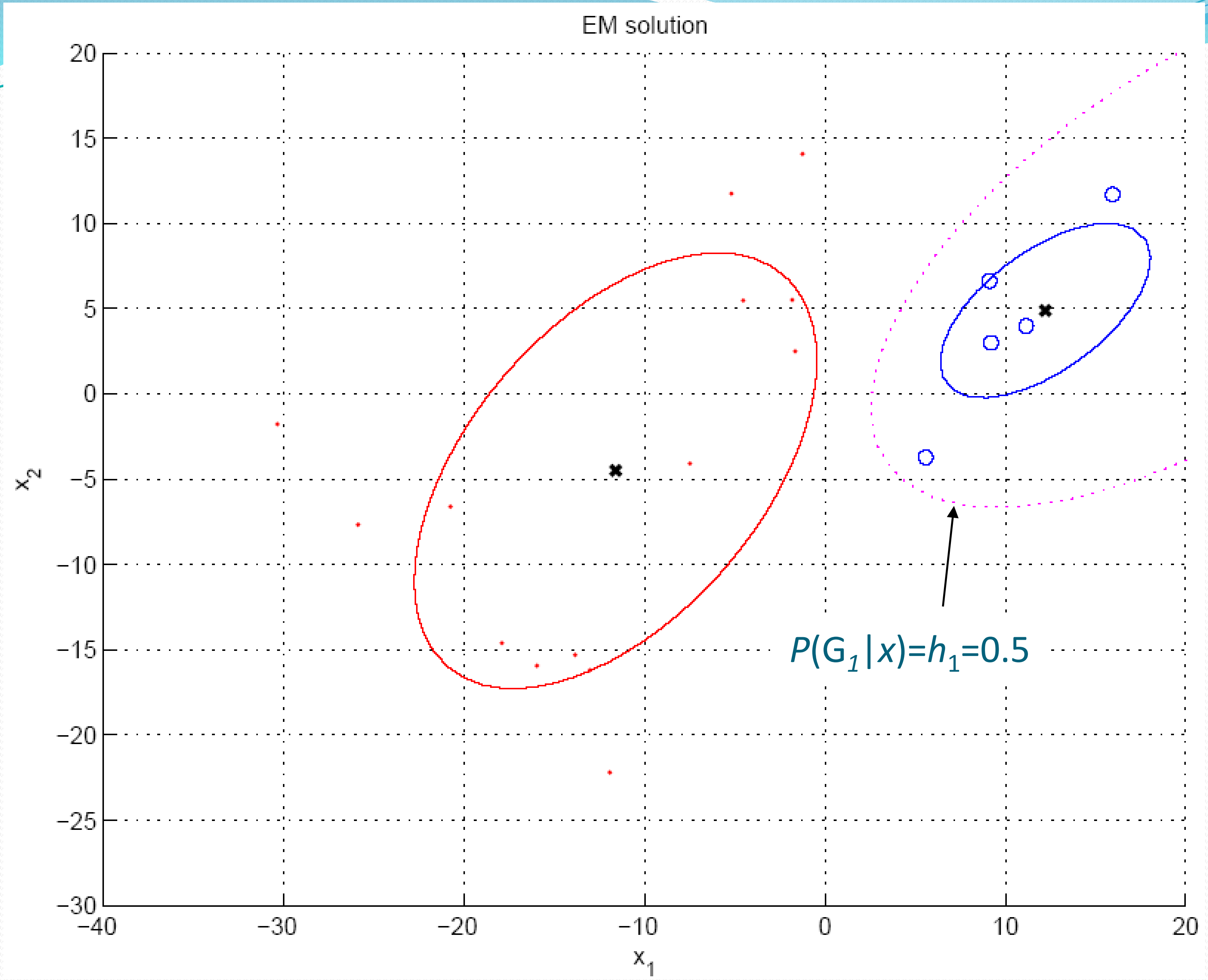
$$=P\left(G_i \mid \mathbf{x}^t,\Phi^l\right)\equiv h_i^t$$

- M-step:

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

Use estimated labels in place of unknown labels

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



$P(G_1|x)=h_1=0.5$

Mixtures of Latent Variable Models

- Regularize clusters

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

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

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_j (soft) or b_j (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_j is 1, all others are 0; only few h_j are nonzero) vs

  Distributed representation (After PCA; all z_j 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:

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

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

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:

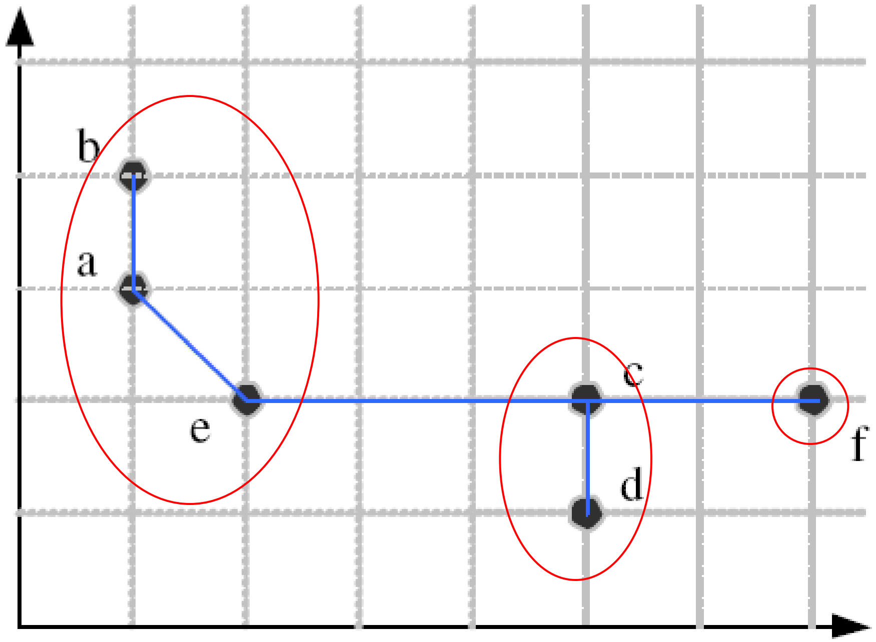
$$d(G_i,G_j)=\min_{\mathbf{x}^r\in\mathcal{G}_i,\mathbf{x}^s\in\mathcal{G}_j} d(\mathbf{x}^r,\mathbf{x}^s)$$

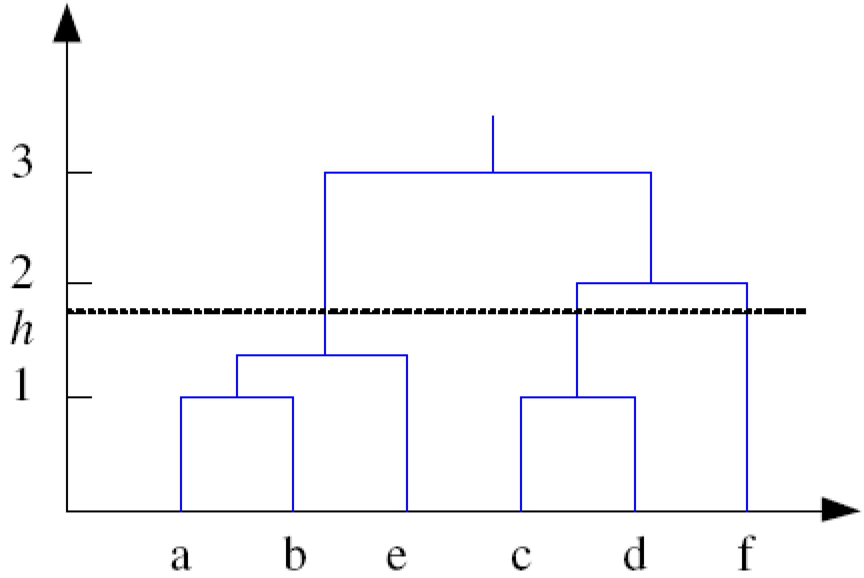
  - Complete-link:

$$d(G_i,G_j)=\max_{\mathbf{x}^r\in\mathcal{G}_i,\mathbf{x}^s\in\mathcal{G}_j} d(\mathbf{x}^r,\mathbf{x}^s)$$

  - Average-link, centroid

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