

# Probabilistic Principal Component Analysis

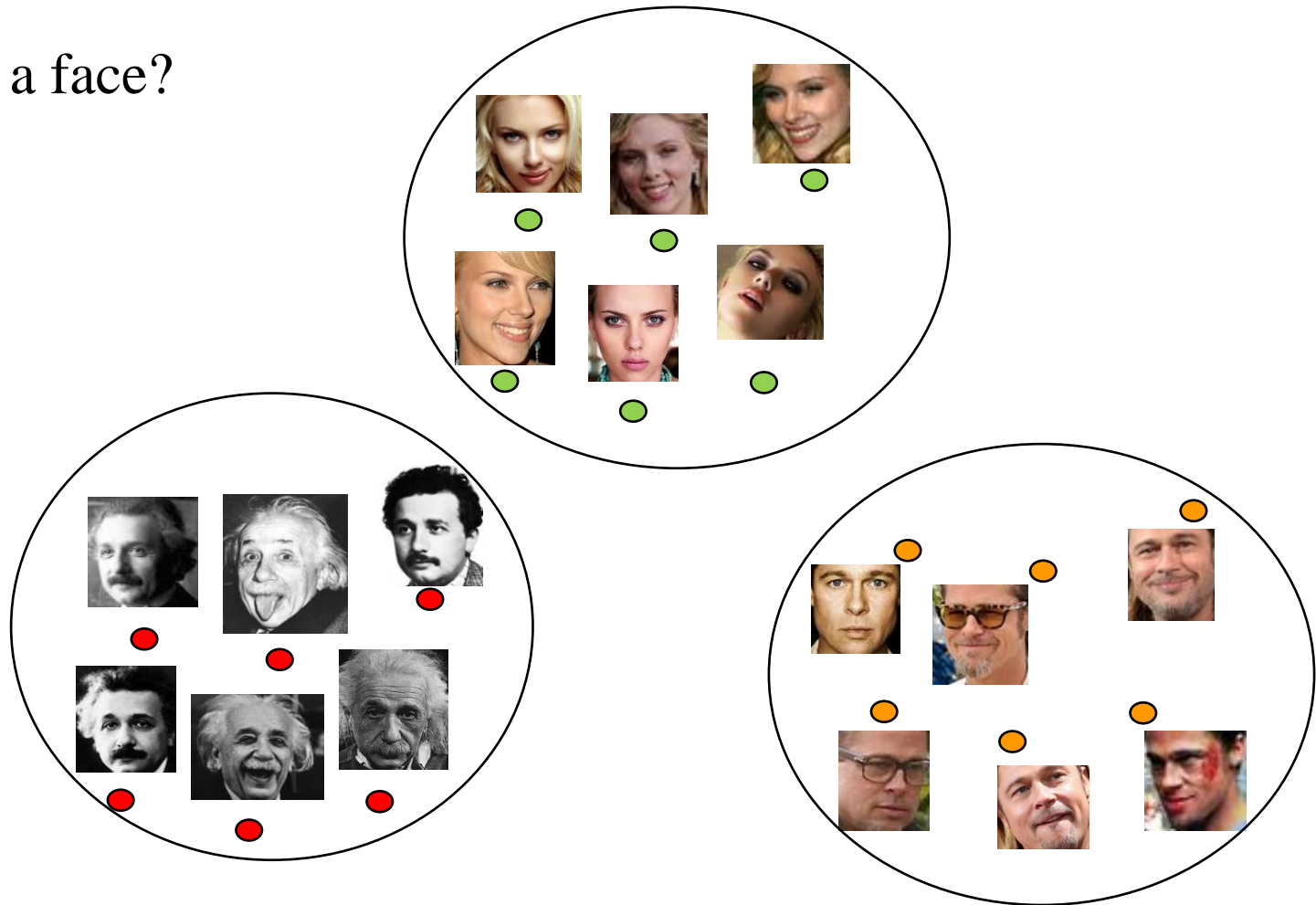
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*Mixtures of Principal Component Analyzers*

# Why do we need mixtures?

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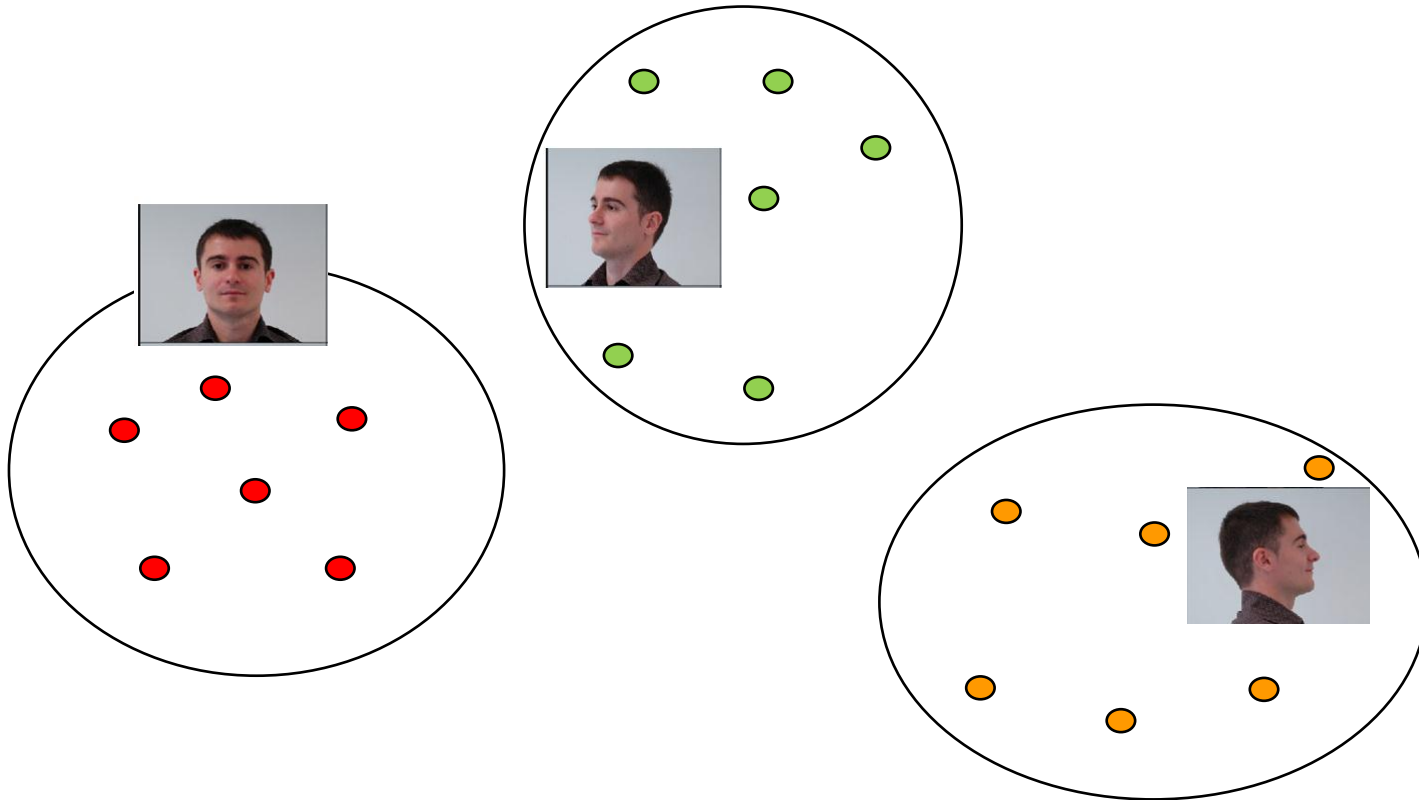
What is a face?



# Why do we need mixtures?

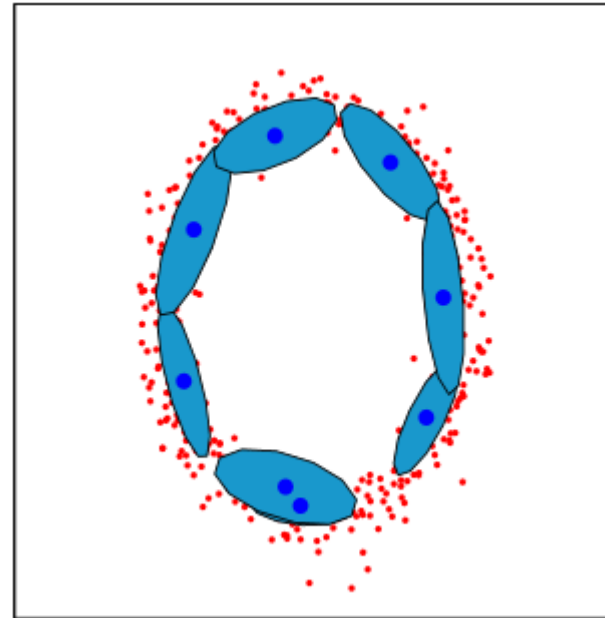
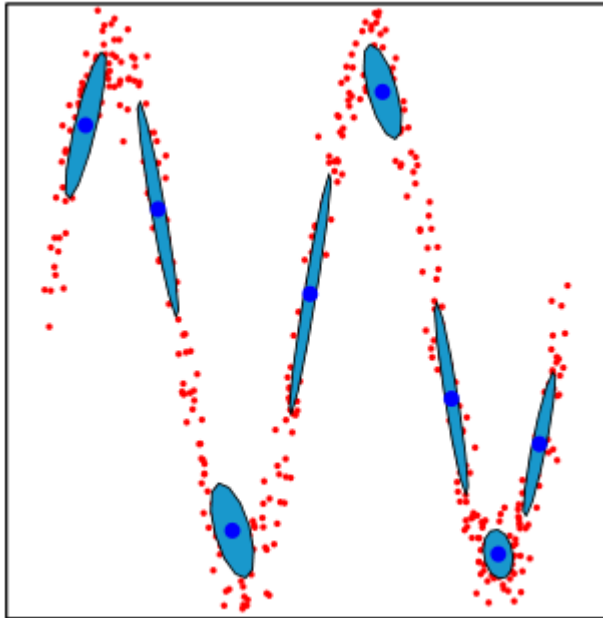
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What is a particular face?



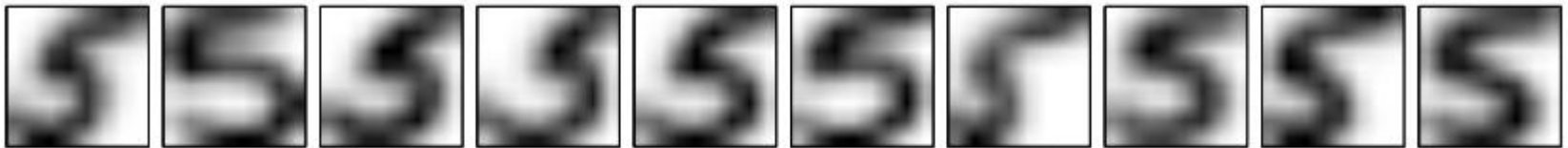
# Why do we need mixtures?

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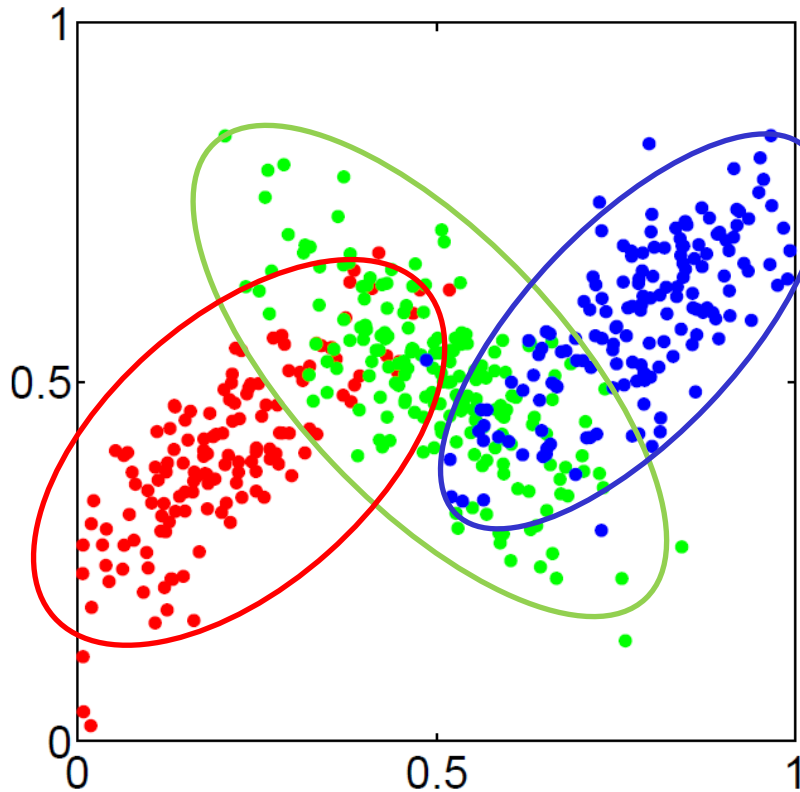
# Why do we need mixtures?

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# Mixtures of PPCA

Parameters  $\theta_x = \{\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\mu}_3, \sigma_1^2, \sigma_2^2, \sigma_3^2\}$



$$\pi_1 = p(k = 1)$$

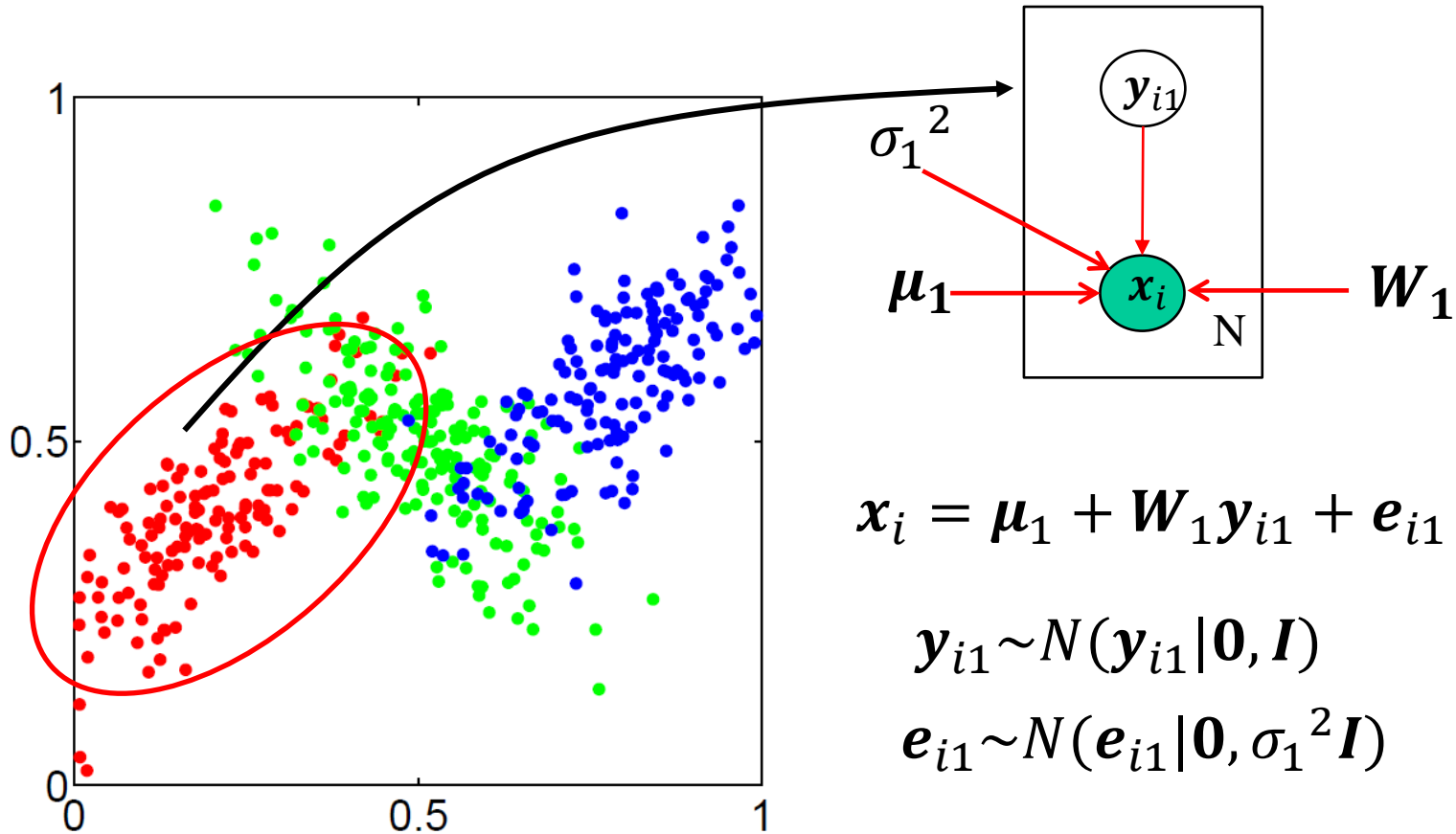
$$\pi_2 = p(k = 2)$$

$$\pi_3 = p(k = 3)$$

$$\theta_z = \{\pi_1, \pi_2, \pi_3\}$$

$$\mathbf{z}_i = \begin{bmatrix} z_{i1} \\ z_{i2} \\ z_{i3} \end{bmatrix} \in \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$$

# Mixtures of PPCA



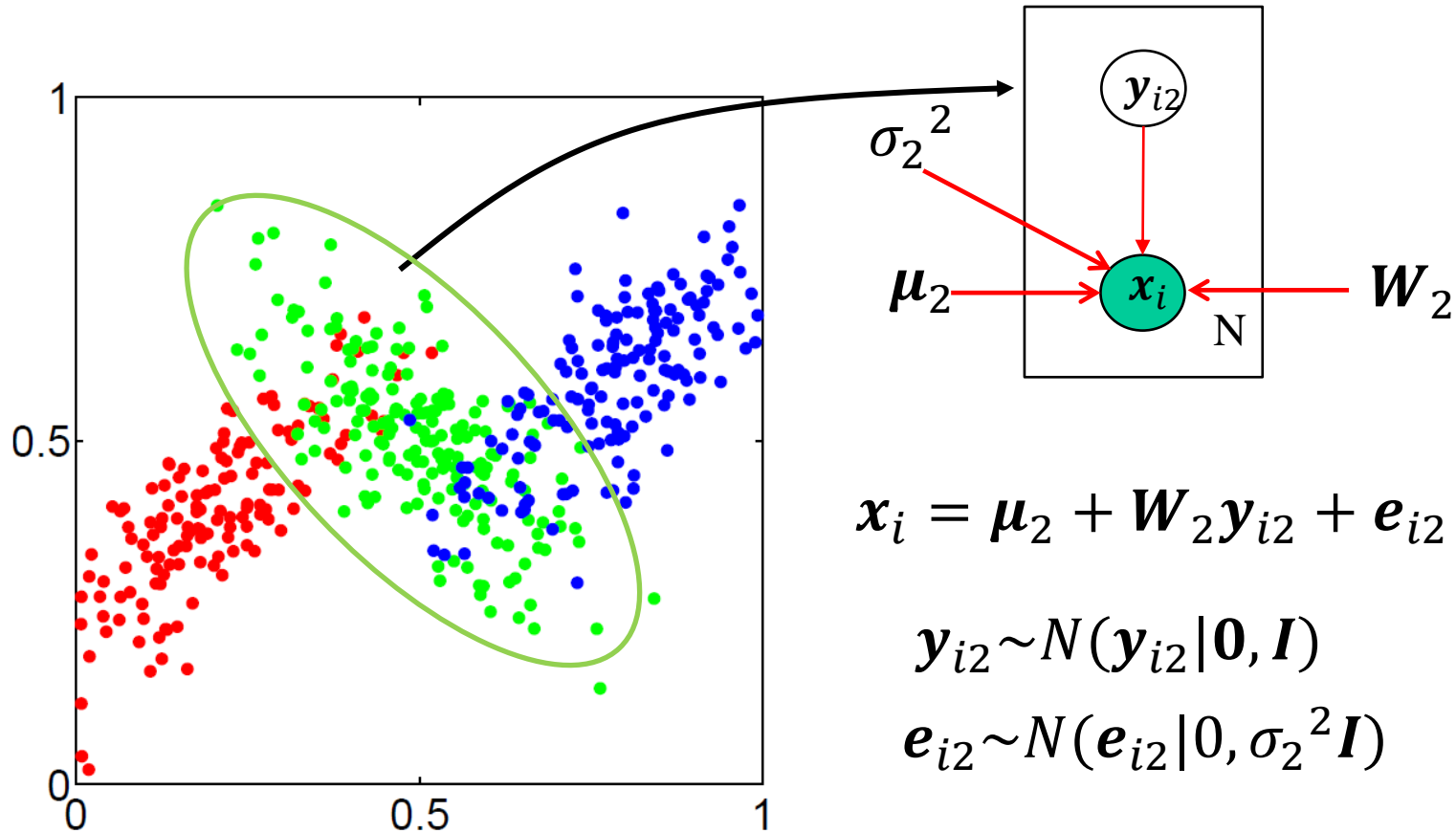
$$x_i = \mu_1 + W_1 y_{i1} + e_{i1}$$

$$y_{i1} \sim N(y_{i1} | \mathbf{0}, I)$$

$$e_{i1} \sim N(e_{i1} | \mathbf{0}, \sigma_1^2 I)$$

$$p(x_i | z_{ik} = 1, y_{i1}, W_1, \mu_1, \sigma_1^2) = N(x_i | W_1 y_{i1} + \mu_1, \sigma_1^2 I)$$

# Mixtures of PPCA



$$\mathbf{x}_i = \boldsymbol{\mu}_2 + \mathbf{W}_2 \mathbf{y}_{i2} + \mathbf{e}_{i2}$$

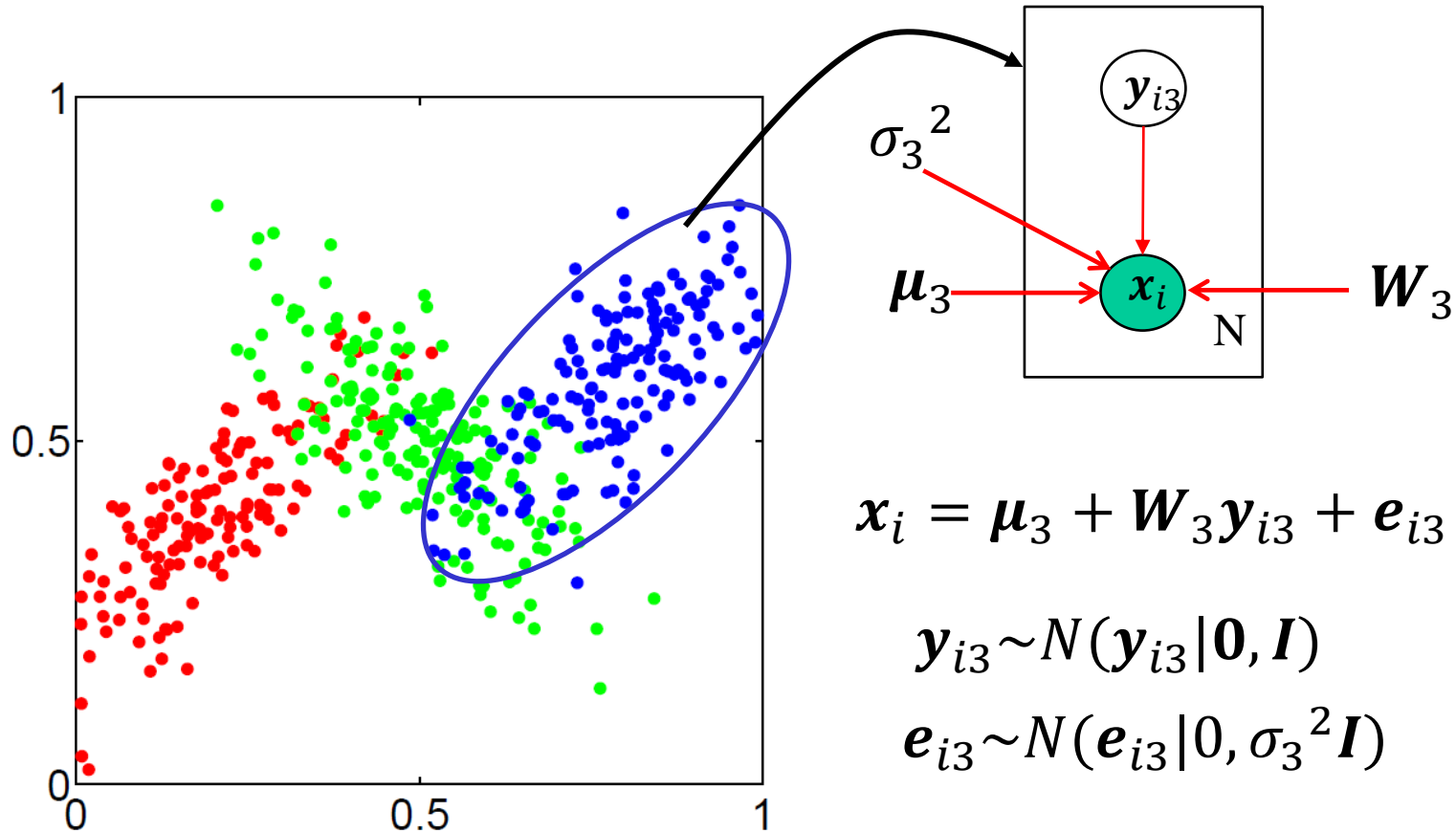
$$\mathbf{y}_{i2} \sim N(\mathbf{y}_{i2} | \mathbf{0}, \mathbf{I})$$

$$\mathbf{e}_{i2} \sim N(\mathbf{e}_{i2} | \mathbf{0}, \sigma_2^2 \mathbf{I})$$

$$p(\mathbf{x}_i | \mathbf{z}_{i2} = 1, \mathbf{y}_{i1}, \mathbf{W}_2, \boldsymbol{\mu}_2, \sigma_2^2) = N(\mathbf{x}_i | \mathbf{W}_2 \mathbf{y}_{i2} + \boldsymbol{\mu}_2, \sigma_2^2 \mathbf{I})$$



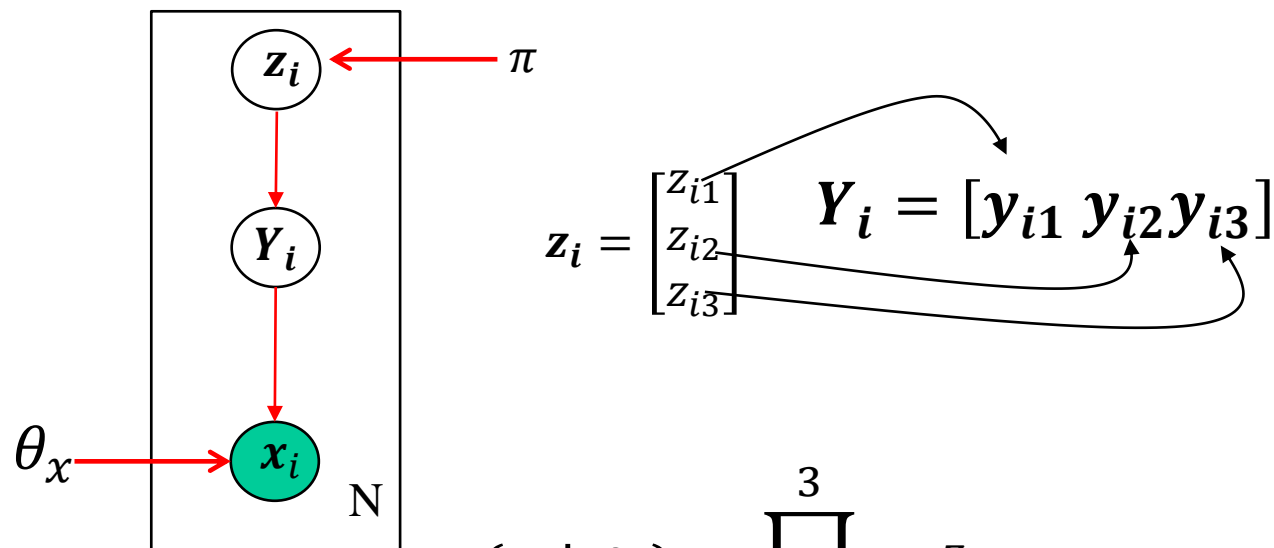
# Mixtures of PPCA



$$p(\mathbf{x}_i | \mathbf{z}_{i3} = 1, \mathbf{y}_{i3}, \mathbf{W}_3, \boldsymbol{\mu}_3, \sigma_3^2) = N(\mathbf{x}_{i3} | \mathbf{W}_3 \mathbf{y}_{i3} + \boldsymbol{\mu}_3, \sigma_3^2 \mathbf{I})$$

# Modelling the problem

## Graphical model



(1) Priors

$$p(\mathbf{z}_i | \theta_z) = \prod_{k=1}^3 \pi_k^{z_{ik}}$$

$$p(\mathbf{Y}_i | \mathbf{z}_i, \theta_z) = \prod_{k=1}^3 p(y_{ki})^{z_{ik}} = \prod_{k=1}^3 N(y_{ki} | 0, I)^{z_{ik}}$$

# Modelling the problem

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## (2) Conditional distribution

$$\begin{aligned} p(\mathbf{x}_i | \mathbf{z}_i, \mathbf{Y}_i, \boldsymbol{\theta}_x) &= \prod_{k=1}^3 p(\mathbf{x}_i | \mathbf{z}_{ik} = 1, \mathbf{y}_{ik}, \mathbf{W}_k, \boldsymbol{\mu}_k, \sigma_k^2 \mathbf{I})^{z_{ik}} \\ &= \prod_{k=1}^3 \text{N}(\mathbf{x}_{ik} | \mathbf{W}_k \mathbf{y}_{ik} + \boldsymbol{\mu}_k, \sigma_k^2 \mathbf{I})^{z_{ik}} \end{aligned}$$

# Modelling the problem

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(3) Marginal distributions per cluster

$$p(\mathbf{x}_i | \mathbf{z}_{ik} = 1, \mathbf{W}_k, \boldsymbol{\mu}_k, \sigma_k^2) = \mathbf{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \mathbf{D}_k)$$

$$\mathbf{D}_k = \mathbf{W}_k \mathbf{W}_k^T + \sigma_k^2 \mathbf{I}$$

Exercise: Show that indeed

$$p(\mathbf{x}_i | \mathbf{z}_{ik} = 1, \mathbf{W}_k, \boldsymbol{\mu}_k, \sigma_k^2) = \mathbf{N}(\mathbf{x}_i | \mathbf{D}_k, \boldsymbol{\mu}_k, \sigma_k^2)$$

Tip:

$$p(\mathbf{x}_i | \mathbf{z}_{ik} = 1, \mathbf{W}_k, \boldsymbol{\mu}_k, \sigma_k^2) = \int_{\mathbf{y}_{ik}} p(\mathbf{x}_i, \mathbf{y}_{ik} | \mathbf{z}_{ik} = 1, \mathbf{W}_k, \boldsymbol{\mu}_k, \sigma_k^2) d\mathbf{y}_{ik}$$

# Modelling the problem

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(4) Full marginal distributions:

$$\begin{aligned} p(\mathbf{x}_i|\theta) &= \sum_{k=1}^3 p(z_{ik} = 1) p(\mathbf{x}_i|z_{ik} = 1, \theta_x) \\ &= \pi_1 N(\mathbf{x}_i|\boldsymbol{\mu}_1, \mathbf{D}_1) + \pi_2 N(\mathbf{x}_i|\boldsymbol{\mu}_2, \mathbf{D}_2) + \pi_3 N(\mathbf{x}_i|\boldsymbol{\mu}_2, \mathbf{D}_2) \\ &= \sum_{k=1}^3 \pi_k N(\mathbf{x}_i|\boldsymbol{\mu}_k, \mathbf{D}_k) \end{aligned}$$

# Modelling the problem

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(5a) Posteriors on  $\mathbf{y}_{ik}$

$$\begin{aligned} p(\mathbf{y}_{ik} | \mathbf{x}_i, z_{ik} = 1, \mathbf{W}_k, \boldsymbol{\mu}_k, \sigma_k^2) \\ = N(\mathbf{y}_{ik} | \mathbf{M}_k^{-1} \mathbf{W}_k^T (\mathbf{x}_i - \boldsymbol{\mu}_k), \sigma_k^2 \mathbf{M}_k^{-1}) \end{aligned}$$

$$\mathbf{M}_k = \mathbf{W}_k^T \mathbf{W}_k + \sigma_k^2 \mathbf{I}$$

Exercise: Show the above

Tip (use the Bayes rule):

$$\begin{aligned} p(\mathbf{y}_{ik} | \mathbf{x}_i, z_{ik} = 1, \mathbf{W}_k, \boldsymbol{\mu}_k, \sigma_k^2) \\ = \frac{p(\mathbf{x}_i | \mathbf{y}_{ik}, z_{ik} = 1, \mathbf{W}_k, \boldsymbol{\mu}_k, \sigma_k^2) p(\mathbf{y}_{ik} | z_{ik} = 1)}{p(\mathbf{x}_i | z_{ik} = 1, \mathbf{W}_k, \boldsymbol{\mu}_k, \sigma_k^2)} \end{aligned}$$

# Expectation-Step

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(5a) Posteriors expectations on  $\mathbf{y}_{ik}$

$$\begin{aligned} E(\mathbf{y}_{ik}) &= E\left[\mathcal{N}(\mathbf{y}_{ik} \mid \mathbf{M}_k^{-1} \mathbf{W}_k^T (\mathbf{x}_i - \boldsymbol{\mu}_k), \sigma_k^2 \mathbf{M}_k^{-1})\right] \\ &= \mathbf{M}_k^{-1} \mathbf{W}_k^T (\mathbf{x}_i - \boldsymbol{\mu}_k) \end{aligned}$$

$$E(\mathbf{y}_{ik} \mathbf{y}_{ik}^T) = \sigma_k^2 \mathbf{M}_k^{-1} + E(\mathbf{y}_{ik}) E(\mathbf{y}_{ik})^T$$

# Expectation-Step

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(1) Posteriors on  $\mathbf{z}_i$

$$\begin{aligned} p(\mathbf{z}_i | \mathbf{x}_i, \theta) &= \frac{p(\mathbf{x}_i, \mathbf{z}_i | \theta)}{p(\mathbf{x}_i | \theta)} = \frac{p(\mathbf{x}_i | \mathbf{z}_i, \theta) p(\mathbf{z}_i | \theta)}{p(\mathbf{x}_i | \theta)} \\ &= \frac{\prod_{k=1}^3 \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \mathbf{D}_k)^{z_{ik}} \pi_k^{z_{ik}}}{\sum_{l=1}^3 \pi_l \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_l, \mathbf{D}_l)} \\ E(z_{ik}) &= \sum_{z_{ik}=0,1} z_{ik} \frac{\prod_{k=1}^3 \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \mathbf{D}_k)^{z_{ik}} \pi_k^{z_{ik}}}{\sum_{l=1}^3 \pi_l \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_l, \mathbf{D}_l)} \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \mathbf{D}_k)}{\sum_{l=1}^3 \pi_l \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_l, \mathbf{D}_l)} \end{aligned}$$



# Formulating the EM

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Now we have everything we need

to set the joint likelihood:

$$\begin{aligned} p(\mathbf{X}, \mathbf{Z}, \mathbf{Y} | \theta) &= p(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N, \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N, \mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_N | \theta) \\ &= p(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N | \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N, \mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_N, \theta_x) \end{aligned}$$

Conditional probability  $p(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N, \mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_N | \theta_z)$

Prior probability

# Formulating the EM

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$$p(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N, \mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_N | \theta_z) = p(\mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_N | \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N) p(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N | \theta_z)$$

$$\begin{aligned} p(\mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_N | \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N) &= \prod_{i=1}^N p(\mathbf{Y}_i | \mathbf{z}_i, \theta_z) = \prod_{i=1}^N \prod_{k=1}^3 p(\mathbf{y}_{ik})^{z_{ik}} \\ &= \prod_{i=1}^N \prod_{k=1}^3 N(\mathbf{y}_{ki} | 0, I)^{z_{ik}} \end{aligned}$$

$$p(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N | \theta_z) = \prod_{i=1}^N \prod_{k=1}^3 \pi_k^{z_{ik}}$$

# Formulating the EM

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$$\begin{aligned} p(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N | \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N, \mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_N, \theta_x) &= \prod_{i=1}^N p(\mathbf{x}_i | \mathbf{z}_i, \mathbf{Y}_i, \theta_x) \\ &= \prod_{i=1}^N \prod_{k=1}^3 N(\mathbf{x}_i | \mathbf{W}_k \mathbf{y}_{ik} + \boldsymbol{\mu}_k, \sigma_k^2)^{z_{ik}} \end{aligned}$$

Hence the likelihood becomes:

$$\begin{aligned} p(\mathbf{X}, \mathbf{Z}, \mathbf{Y} | \theta) &= \prod_{i=1}^N \prod_{k=1}^3 N(\mathbf{x}_i | \mathbf{W}_k \mathbf{y}_{ik} + \boldsymbol{\mu}_k, \sigma_k^2)^{z_{ik}} \prod_{i=1}^N \prod_{k=1}^3 N(\mathbf{y}_{ki} | \mathbf{0}, \mathbf{I})^{z_{ik}} \\ &\quad \prod_{i=1}^N \prod_{k=1}^3 \pi_k^{z_{ik}} \end{aligned}$$

# Formulating the EM

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$$\begin{aligned}\ln p(\mathbf{X}, \mathbf{Z}, \mathbf{Y} | \theta) &= \sum_{i=1}^N \sum_{k=1}^3 z_{ik} \ln N(\mathbf{x}_i | \mathbf{W}_k \mathbf{y}_{ik} + \boldsymbol{\mu}_k, \sigma_k^2) + \\ &\quad + \sum_{i=1}^N \sum_{k=1}^3 z_{ik} \ln N(\mathbf{y}_{ik} | 0, I) + \sum_{i=1}^N \sum_{k=1}^3 z_{ik} \ln \pi_k \\ &= \sum_{i=1}^N \sum_{k=1}^3 z_{ik} \left[ -\frac{1}{2\sigma_k^2} (\mathbf{x}_i - \boldsymbol{\mu}_k - \mathbf{W}_k \mathbf{y}_{ik})^T (\mathbf{x}_i - \boldsymbol{\mu}_k - \mathbf{W}_k \mathbf{y}_{ik}) - \frac{F}{2} \ln 2\pi - F \ln \sigma \right] \\ &\quad + \sum_{i=1}^N \sum_{k=1}^3 z_{ik} \left[ -\frac{1}{2} \mathbf{y}_{ik}^T \mathbf{y}_{ik} - \frac{d}{2} \ln 2\pi \right] + \sum_{i=1}^N \sum_{k=1}^3 z_{ik} \ln \pi_k\end{aligned}$$

# Formulating the EM

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Taking the expectations:

$$E[\ln p(\mathbf{X}, \mathbf{Z}, \mathbf{Y}|\theta)]$$

$$\begin{aligned} &= \sum_{i=1}^N \sum_{k=1}^3 E[z_{ik}] \left[ -\frac{1}{2\sigma_k^2} (\|x_i - \mu_k\|^2 - E[y_{ik}]^T W_k^T (x_i - \mu_k) \right. \\ &\quad \left. + \text{tr}(W_k^T W_k E[y_{ik} y_{ik}^T]) - \frac{F}{2} \ln 2\pi - F \ln \sigma \right] \\ &\quad + \sum_{i=1}^N \sum_{k=1}^3 E[z_{ik}] \left[ -\frac{1}{2} \text{tr}(E[y_{ik} y_{ik}^T]) - \frac{d}{2} \ln 2\pi \right] + \sum_{i=1}^N \sum_{k=1}^3 E[z_{ik}] \ln \pi_k \end{aligned}$$

# Maximization Step

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$$\pi_k = \frac{\sum_{i=1}^N E(z_{ik})}{N}$$

$$\mu_k = \frac{\sum_{i=1}^N E(z_{ik})(x_i - W_k E(y_{ik}))}{\sum_{i=1}^N E(z_{ik})}$$

$$W_k = \left[ \sum_{i=1}^N E(z_{ik})(x_i - \mu_k)E[y_{ik}]^T \right] \left[ \sum_{i=1}^N E(z_{ik})E[y_{ik}y_{ik}^T] \right]^{-1}$$

$$\sigma_k^2 = \frac{1}{F \sum_{i=1}^N E(z_{ik})} \sum_{i=1}^N E(z_{ik}) ( \|x_i - \mu_k\|^2 - E[y_{ik}]^T W_k^T (x_i - \mu_k) + \text{tr}(W_k^T W_k E[y_{ik}y_{ik}^T]) )$$

# Summary

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Initialize  $\theta_x = \{\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\mu}_3, \sigma_1^2, \sigma_2^2, \sigma_3^2\}$

$$\theta_z = \{\pi_1, \pi_2, \pi_3\}$$

E-Step:

$$E[z_{ik}] = \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \mathbf{D}_k)}{\sum_{l=1}^3 \pi_l \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_l, \mathbf{D}_l)} \quad \mathbf{D}_k = \mathbf{W}_k \mathbf{W}_k^T + \sigma_k^2 \mathbf{I}$$

$$E(\mathbf{y}_{ik}) = \mathbf{M}_k^{-1} \mathbf{W}_k^T (\mathbf{x}_i - \boldsymbol{\mu}_k) \quad \mathbf{M}_k = \mathbf{W}_k^T \mathbf{W}_k + \sigma_k^2 \mathbf{I}$$

$$E[\mathbf{y}_{ik} \mathbf{y}_{ik}^T] = \sigma_k^2 \mathbf{M}_k^{-1} + E(\mathbf{y}_{ik}) E(\mathbf{y}_{ik}^T)$$

# Summary

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M-Step:

$$\pi_k = \frac{\sum_{i=1}^N E(z_{ik})}{N}$$

$$\boldsymbol{\mu}_k = \frac{\sum_{i=1}^N E(z_{ik})(\mathbf{x}_i - \mathbf{W}_k E(\mathbf{y}_{ik}))}{\sum_{i=1}^N E(z_{ik})}$$

$$\mathbf{W}_k = \left[ \sum_{i=1}^N E(z_{ik})(\mathbf{x}_i - \boldsymbol{\mu}_k)E[\mathbf{y}_{ik}]^T \right] \left[ \sum_{i=1}^N E(z_{ik}) E[\mathbf{y}_{ik}\mathbf{y}_{ik}^T] \right]^{-1}$$

$$\sigma_k^2 = \frac{1}{F \sum_{i=1}^N E(z_{ik})} \sum_{i=1}^N E(z_{ik}) ( \|\mathbf{x}_i - \boldsymbol{\mu}_k\|^2 - E[\mathbf{y}_{ik}]^T \mathbf{W}_k^T (\mathbf{x}_i - \boldsymbol{\mu}_k) + \text{tr}(\mathbf{W}_k^T \mathbf{W}_k E[\mathbf{y}_{ik}\mathbf{y}_{ik}^T]) )$$



# Summary

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- In the EM for single PPCA we have only one latent variable per observation  $\mathbf{y}_i$
- The EM for mixture PPCA we have a latent vector  $\mathbf{z}_i$  per sample (i.e., the identity of the cluster) and we have an latent variable  $\mathbf{y}_{ik}$  for each of the elements  $z_{ik}$  of  $\mathbf{z}_i$ .
- We need to compute the expectations  $E[z_{ik}], E(\mathbf{y}_{ik}), E[\mathbf{y}_{ik}\mathbf{y}_{ik}^T]$