

Probabilistic PCA

Course of Machine Learning
Master Degree in Computer Science
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Introduce a latent variable model to relate a d -dimensional observation vector to a corresponding d' -dimensional gaussian latent variable (with $d' < d$)

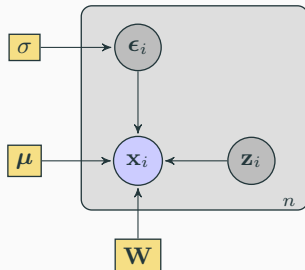
$$\mathbf{x} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$$

where

- \mathbf{z} is a d' -dimensional gaussian latent variable (the “projection” of \mathbf{x} on a lower-dimensional subspace)
- \mathbf{W} is a $d \times d'$ matrix, relating the original space with the lower-dimensional subspace
- $\boldsymbol{\epsilon}$ is a d -dimensional gaussian noise: noise covariance on different dimensions is assumed to be 0. Noise variance is assumed equal on all dimensions: hence $p(\boldsymbol{\epsilon}) = \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$
- $\boldsymbol{\mu}$ is the d -dimensional vector of the means

$\boldsymbol{\epsilon}$ and $\boldsymbol{\mu}$ are assumed independent.

Graphical model



1. $\mathbf{z} \in \mathbb{R}^{d'}, \mathbf{x}, \boldsymbol{\epsilon} \in \mathbb{R}^d, d' < d$
2. $p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
3. $p(\boldsymbol{\epsilon}) = \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$, (isotropic gaussian noise)

This can be interpreted in terms of a generative process

1. sample the latent variable $\mathbf{z} \in \mathbb{R}^{d'}$ from

$$p(\mathbf{z}) = \frac{1}{(2\pi)^{d'/2}} e^{-\frac{\|\mathbf{z}\|^2}{2}}$$

2. linearly project onto \mathbb{R}^d

$$\mathbf{y} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu}$$

3. sample the noise component $\boldsymbol{\epsilon} \in \mathbb{R}^d$ from

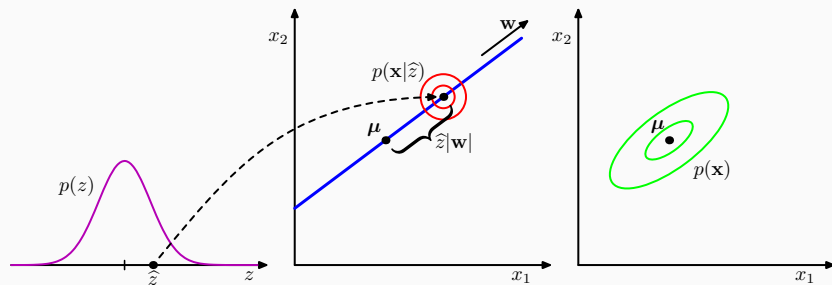
$$p(\boldsymbol{\epsilon}) = \frac{1}{(2\pi)^{d/2}} e^{-\frac{\|\boldsymbol{\epsilon}\|^2}{2\sigma^2}}$$

4. add the noise component $\boldsymbol{\epsilon}$

$$\mathbf{x} = \mathbf{y} + \boldsymbol{\epsilon}$$

This results into $p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$

Generative process



Let

$$\mathbf{x}_1 \in \mathbb{R}^r \quad \mathbf{x}_2 \in \mathbb{R}^s \quad \mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}$$

Assume \mathbf{x} is normally distributed: $p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, and let

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix} \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}$$

with

$$\boldsymbol{\mu}_1 \in \mathbb{R}^r$$

$$\boldsymbol{\mu}_2 \in \mathbb{R}^s$$

$$\boldsymbol{\Sigma}_{11} \in \mathbb{R}^{r \times r}$$

$$\boldsymbol{\Sigma}_{12} = \boldsymbol{\Sigma}_{21}^T \in \mathbb{R}^{r \times s}$$

$$\boldsymbol{\Sigma}_{22} \in \mathbb{R}^{s \times s}$$

Under the above assumptions:

- The marginal distribution $p(\mathbf{x}_1)$ is a gaussian on \mathbb{R}^r , with

$$E[\mathbf{x}_1] = \boldsymbol{\mu}_1$$

$$\text{Cov}(\mathbf{x}_1) = \boldsymbol{\Sigma}_{11}$$

- The conditional distribution $p(\mathbf{x}_1|\mathbf{x}_2)$ is a gaussian on \mathbb{R}^r , with

$$E[\mathbf{x}_1|\mathbf{x}_2] = \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)$$

$$\text{Cov}(\mathbf{x}_1|\mathbf{x}_2) = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}$$

Latent variable model

The joint distribution is

$$p\left(\begin{bmatrix} \mathbf{z} \\ \mathbf{x} \end{bmatrix}\right) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{zx}}, \boldsymbol{\Sigma})$$

Joint distribution mean

By definition,

$$\boldsymbol{\mu}_{\mathbf{zx}} = \begin{bmatrix} \boldsymbol{\mu}_{\mathbf{z}} \\ \boldsymbol{\mu}_{\mathbf{x}} \end{bmatrix}$$

- Since $p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$, then $\boldsymbol{\mu}_{\mathbf{z}} = \mathbf{0}$.
- Since $p(\mathbf{x}) = \mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$, then

$$\boldsymbol{\mu}_{\mathbf{x}} = E[\mathbf{x}] = E[\mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}] = \mathbf{W}E[\mathbf{z}] + \boldsymbol{\mu} + E[\boldsymbol{\epsilon}] = \boldsymbol{\mu}$$

Hence

$$\boldsymbol{\mu}_{\mathbf{zx}} = \begin{bmatrix} \mathbf{0} \\ \boldsymbol{\mu} \end{bmatrix}$$

Joint distribution covariance

For what concerns the distribution covariance

$$\Sigma = \begin{bmatrix} \Sigma_{zz} & \Sigma_{zx} \\ \Sigma_{zx} & \Sigma_{xx} \end{bmatrix}$$

where

$$\Sigma_{zz} = E[(\mathbf{z} - E[\mathbf{z}])(\mathbf{z} - E[\mathbf{z}])^T] = E[\mathbf{z}\mathbf{z}^T] = \mathbf{I}$$

$$\begin{aligned} \Sigma_{zx} &= E[(\mathbf{z} - E[\mathbf{z}])(\mathbf{x} - E[\mathbf{x}])^T] = E[\mathbf{z}(\mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon} - \boldsymbol{\mu})^T] \\ &= E[\mathbf{z}(\mathbf{W}\mathbf{z})^T] + E[\mathbf{z}\boldsymbol{\epsilon}^T] = E[\mathbf{z}\mathbf{z}^T \mathbf{W}^T] = \mathbf{W}^T \end{aligned}$$

$$\begin{aligned} \Sigma_{xx} &= E[(\mathbf{x} - E[\mathbf{x}])(\mathbf{x} - E[\mathbf{x}])^T] \\ &= E[(\boldsymbol{\mu} + \mathbf{W}\mathbf{z} + \boldsymbol{\epsilon} - \boldsymbol{\mu})(\boldsymbol{\mu} + \mathbf{W}\mathbf{z} + \boldsymbol{\epsilon} - \boldsymbol{\mu})^T] \\ &= E[\mathbf{W}\mathbf{z}\mathbf{z}^T \mathbf{W}^T + \boldsymbol{\epsilon}\mathbf{z}^T \mathbf{W}^T + \mathbf{W}\mathbf{z}\boldsymbol{\epsilon}^T + \boldsymbol{\epsilon}\boldsymbol{\epsilon}^T] \\ &= \mathbf{W}E[\mathbf{z}\mathbf{z}^T] \mathbf{W}^T + E[\boldsymbol{\epsilon}\mathbf{z}^T] \mathbf{W}^T + \mathbf{W}E[\mathbf{z}\boldsymbol{\epsilon}^T] + E[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T] \\ &= \mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I} \end{aligned}$$

Joint distribution

As a consequence, we get

$$\boldsymbol{\mu}_{\mathbf{z}|\mathbf{x}} = \begin{bmatrix} \mathbf{0} \\ \boldsymbol{\mu} \end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} \mathbf{I} & \mathbf{W}^T \\ \mathbf{W} & \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I} \end{bmatrix}$$

Marginal distribution

The marginal distribution of \mathbf{x} is then $p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})$

Conditional distribution

The conditional distribution of \mathbf{z} given \mathbf{x} is $p(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{z}|\mathbf{x}}, \boldsymbol{\Sigma}_{\mathbf{z}|\mathbf{x}})$ with

$$\begin{aligned} \boldsymbol{\mu}_{\mathbf{z}|\mathbf{x}} &= \mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1}(\mathbf{x} - \boldsymbol{\mu}) \\ \boldsymbol{\Sigma}_{\mathbf{z}|\mathbf{x}} &= \mathbf{I} - \mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1}\mathbf{W} = \sigma^2(\sigma^2\mathbf{I} + \mathbf{W}^T\mathbf{W})^{-1} \end{aligned}$$

Maximum likelihood for PCA

Setting $\mathbf{C} = \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}$, the log-likelihood of the dataset in the model is

$$\begin{aligned}\log p(\mathbf{X}|\mathbf{W}, \boldsymbol{\mu}, \sigma^2) &= \sum_{i=1}^n \log p(\mathbf{x}_i|\mathbf{W}, \boldsymbol{\mu}, \sigma^2) \\ &= -\frac{nd}{2} \log(2\pi) - \frac{n}{2} \log |\mathbf{C}| - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \boldsymbol{\mu}) \mathbf{C}^{-1} (\mathbf{x}_i - \boldsymbol{\mu})^T\end{aligned}$$

Setting the derivative wrt $\boldsymbol{\mu}$ to zero results into

$$\boldsymbol{\mu} = \bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$$

and, substituting into the log-likelihood formula,

$$\log p(\mathbf{X}|\mathbf{W}, \boldsymbol{\mu}, \sigma^2) = -\frac{nd}{2} \log(2\pi) + \log |\mathbf{C}| + \text{tr}(\mathbf{C}^{-1}\mathbf{S})$$

where \mathbf{S} is the data covariance matrix

$$\mathbf{S} = \frac{1}{n} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T$$

Maximum likelihood for PCA

Maximization wrt \mathbf{W} and σ^2 is more complex: however, a closed form solution exists:

$$\mathbf{W} = \mathbf{U}_{d'}(\mathbf{L}_{d'} - \sigma^2\mathbf{I})^{1/2}\mathbf{R}$$

where

- $\mathbf{U}_{d'}$ is the $d \times d'$ matrix whose columns are the eigenvectors corresponding to the d' largest eigenvalues
- $\mathbf{L}_{d'}$ is the $d' \times d'$ diagonal matrix of the largest eigenvalues
- \mathbf{R} is an arbitrary $d' \times d'$ orthogonal matrix, corresponding to a rotation in the latent space

\mathbf{R} can be interpreted as a rotation matrix in latent space.

If $\mathbf{R} = \mathbf{I}$, the columns of \mathbf{W} are the principal components eigenvectors scaled by the variance $\lambda_i - \sigma^2$

For what concerns maximization wrt σ^2 , it results

$$\sigma^2 = \frac{1}{d - d'} \sum_{i=d'+1}^d \lambda_i$$

since eigenvalues provide measures of the dataset variance along the corresponding eigenvector direction, this corresponds to the average variance along the discarded directions.

The conditional distribution

$$p(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1}(\mathbf{x} - \boldsymbol{\mu}), \sigma^2(\sigma^2\mathbf{I} + \mathbf{W}^T\mathbf{W})^{-1})$$

can be applied.

In particular, the conditional expectation

$$E[\mathbf{z}|\mathbf{x}] = \mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1}(\mathbf{x} - \boldsymbol{\mu})$$

can be assumed as the latent space point corresponding to \mathbf{x} .

The projection onto the d' -dimensional subspace can then be performed as

$$\mathbf{x}' = \mathbf{W}E[\mathbf{z}|\mathbf{x}] + \boldsymbol{\mu} = \mathbf{W}\mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1}(\mathbf{x} - \boldsymbol{\mu}) + \boldsymbol{\mu}$$

Even if the log-likelihood has a closed form maximization, applying EM can be useful in high-dimensional spaces.

The complete dataset log-likelihood is considered

$$\log p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\mu}, \mathbf{W}, \sigma^2) = \sum_{i=1}^n (\log p(\mathbf{x}_i | \mathbf{z}_i) + \log p(\mathbf{z}_i))$$

Since

$$p(\mathbf{z}_i) = \mathcal{N}(0, \mathbf{I}) \quad p(\mathbf{x}_i | \mathbf{z}_i) = \mathcal{N}(\mathbf{W}\mathbf{z}_i + \boldsymbol{\mu}, \sigma^2 \mathbf{I})$$

it turns out that the expectation of $p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\mu}, \mathbf{W}, \sigma^2)$ wrt $p(\mathbf{Z} | \mathbf{X}, \boldsymbol{\mu}, \mathbf{W}, \sigma^2)$ is given by

$$\begin{aligned} \sum_{i=1}^n p(\mathbf{z}_i | \mathbf{x}_i) \log p(\mathbf{x}_i, \mathbf{z}_i) &= -\frac{nd}{2} \log(2\pi\sigma^2) - \frac{1}{2} \sum_{i=1}^n \text{tr}(E[\mathbf{z}_i \mathbf{z}_i^T | \mathbf{x}_i]) \\ &\quad - \frac{1}{2\sigma^2} \sum_{i=1}^n \|\mathbf{x}_i - \boldsymbol{\mu}\|^2 + \frac{1}{\sigma^2} \sum_{i=1}^n E[\mathbf{z}_i | \mathbf{x}_i]^T \mathbf{W}^T (\mathbf{x}_i - \boldsymbol{\mu}) \\ &\quad - \frac{1}{2\sigma^2} \sum_{i=1}^n \text{tr}(E[\mathbf{z}_i \mathbf{z}_i^T | \mathbf{x}_i] \mathbf{W}^T \mathbf{W}) \end{aligned}$$

The conditional expectations are estimated in the E-step as

$$E[\mathbf{z}_i | \mathbf{x}_i] = \mathbf{W}^T (\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} (\mathbf{x} - \boldsymbol{\mu}) = \mathbf{W}^T (\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} (\mathbf{x} - \bar{\mathbf{x}})$$

(since the maximum likelihood estimation of $\boldsymbol{\mu}$ is $\bar{\mathbf{x}}$), and

$$E[\mathbf{z}_i \mathbf{z}_i^T | \mathbf{x}_i] = \text{cov}(\mathbf{z}_i) + E[\mathbf{z}_i] E[\mathbf{z}_i]^T = \sigma^2 (\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} + E[\mathbf{z}_i] E[\mathbf{z}_i]^T$$

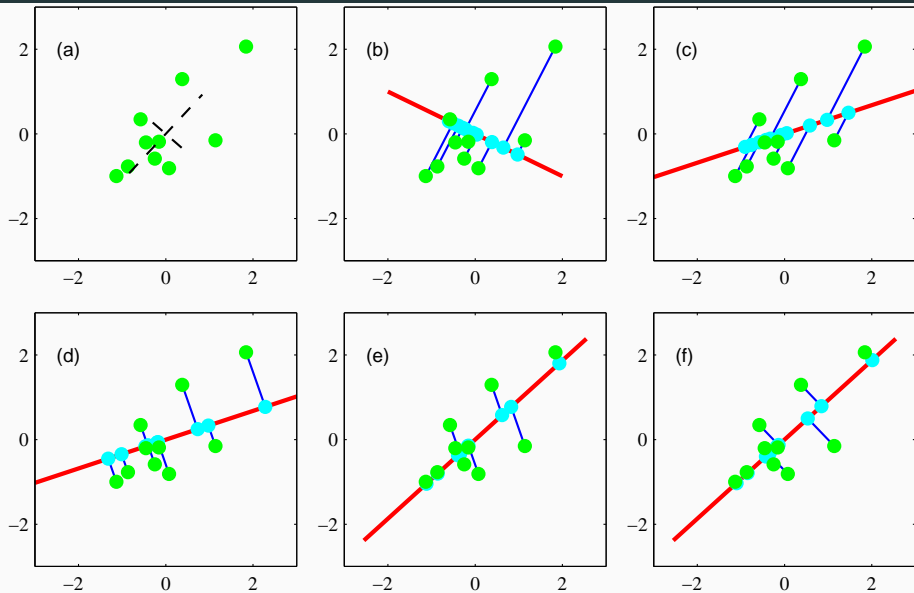
The new estimates of parameters \mathbf{W} and σ^2 are obtained through maximization of the expectation of $p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\mu}, \mathbf{W}, \sigma^2)$ wrt $p(\mathbf{Z} | \mathbf{X}, \boldsymbol{\mu}, \mathbf{W}, \sigma^2)$ (as already observed, the maximum likelihood estimate of $\boldsymbol{\mu}$ is $\bar{\mathbf{x}}$).

The following equations result

$$\mathbf{W}_{new} = \left(\sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}}) E[\mathbf{z}_i | \mathbf{x}_i]^T \right) \left(\sum_{i=1}^n E[\mathbf{z}_i \mathbf{z}_i^T | \mathbf{x}_i] \right)^{-1}$$

$$\sigma_{new}^2 = \frac{1}{nd} \sum_{i=1}^n \left(\|\mathbf{x}_i - \bar{\mathbf{x}}\|^2 - 2E[\mathbf{z}_i | \mathbf{x}_i]^T \mathbf{W}_{new}^T (\mathbf{x}_i - \bar{\mathbf{x}}) + \text{tr}(E[\mathbf{z}_i \mathbf{z}_i^T | \mathbf{x}_i] \mathbf{W}_{new}^T \mathbf{W}_{new}) \right)$$

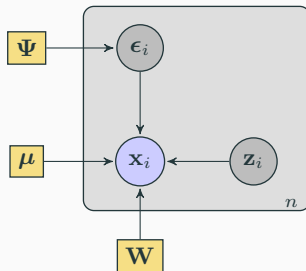
EM for PCA



Factor analysis

Graphical model

Noise components still gaussian and independent, but with different variance.



1. $\mathbf{z} \in \mathbb{R}^d, \mathbf{x}, \epsilon \in \mathbb{R}^D, d \ll D$
2. $p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
3. $p(\epsilon) = \mathcal{N}(\mathbf{0}, \Psi)$, Ψ diagonal (independent gaussian noise)

Model distribution are modified accordingly.

Joint distribution

$$p\left(\begin{bmatrix} \mathbf{z} \\ \mathbf{x} \end{bmatrix}\right) = \mathcal{N}\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{W} \end{bmatrix}, \begin{bmatrix} \mathbf{I} & \mathbf{W}^T \\ \mathbf{\Lambda} & \mathbf{W}\mathbf{W}^T + \mathbf{\Psi} \end{bmatrix}\right)$$

Marginal distribution

$$p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \mathbf{W}\mathbf{W}^T + \mathbf{\Psi})$$

Conditional distribution

The conditional distribution of \mathbf{z} given \mathbf{x} is now $p(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{z}|\mathbf{x}}, \Sigma_{\mathbf{z}|\mathbf{x}})$ with

$$\begin{aligned}\boldsymbol{\mu}_{\mathbf{z}|\mathbf{x}} &= \mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \mathbf{\Psi})^{-1}(\mathbf{x} - \boldsymbol{\mu}) \\ \Sigma_{\mathbf{z}|\mathbf{x}} &= \mathbf{I} - \mathbf{W}^T(\mathbf{W}\mathbf{W}^T + \mathbf{\Psi})^{-1}\mathbf{W}\end{aligned}$$

The log-likelihood of the dataset in the model is now

$$\begin{aligned}\log p(\mathbf{X}|\mathbf{W}, \boldsymbol{\mu}, \boldsymbol{\Psi}) &= \sum_{i=1}^n \log p(\mathbf{x}_i|\mathbf{W}, \boldsymbol{\mu}, \boldsymbol{\Psi}) \\ &= -\frac{nd}{2} \log(2\pi) - \frac{n}{2} \log |\mathbf{W}\mathbf{W}^T + \boldsymbol{\Psi}| - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \boldsymbol{\mu})(\mathbf{W}\mathbf{W}^T + \boldsymbol{\Psi})^{-1}(\mathbf{x}_i - \boldsymbol{\mu})\end{aligned}$$

Setting the derivative wrt $\boldsymbol{\mu}$ to zero results in

$$\boldsymbol{\mu} = \bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$$

Estimating parameters through log-likelihood maximization does not provide a closed form solution for \mathbf{W} and $\boldsymbol{\Psi}$. Iterative techniques such as EM must be applied.

The conditional expectations are estimated in the E-step as

$$E[\mathbf{z}_i | \mathbf{x}_i] = (\mathbf{I} + \mathbf{W}^T \mathbf{\Psi} \mathbf{W})^{-1} \mathbf{W}^T \mathbf{\Psi}^{-1} (\mathbf{x} - \bar{\mathbf{x}})$$

(since the maximum likelihood estimation of $\boldsymbol{\mu}$ is, again, $\bar{\mathbf{x}}$), and

$$E[\mathbf{z}_i \mathbf{z}_i^T | \mathbf{x}_i] = (\mathbf{I} + \mathbf{W}^T \mathbf{\Psi} \mathbf{W})^{-1} + E[\mathbf{z}_i] E[\mathbf{z}_i]^T$$

The new estimates of parameters \mathbf{W} and σ^2 are obtained through maximization of the expectation of $p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\mu}, \mathbf{W}, \sigma^2)$ wrt $p(\mathbf{Z} | \mathbf{X}, \boldsymbol{\mu}, \mathbf{W}, \sigma^2)$ (as already observed, the maximum likelihood estimate of $\boldsymbol{\mu}$ is $\bar{\mathbf{x}}$).

The following equations result

$$\mathbf{W}_{new} = \left(\sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}}) E[\mathbf{z}_i | \mathbf{x}_i]^T \right) \left(\sum_{i=1}^n E[\mathbf{z}_i \mathbf{z}_i^T | \mathbf{x}_i] \right)^{-1}$$

$$\boldsymbol{\Psi}_{new} = \text{diag} \left(\mathbf{S} - \mathbf{W}_{new} \frac{1}{n} \sum_{i=1}^n E[\mathbf{z}_i | \mathbf{x}_i] (\mathbf{x}_i - \bar{\mathbf{x}})^T \right)$$

Where the *diag* operator sets to 0 all non diagonal elements and, as usual,

$$\mathbf{S} = \frac{1}{n} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}}) (\mathbf{x}_i - \bar{\mathbf{x}})^T$$