Probabilistic PCA

Course of Machine Learning
Master Degree in Computer Science
University of Rome ``Tor Vergata''

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Idea

Introduce a latent variable model to relate a d-dimensional observation vector to a corresponding d'-dimensional gaussian latent variable (with $d' < d$)

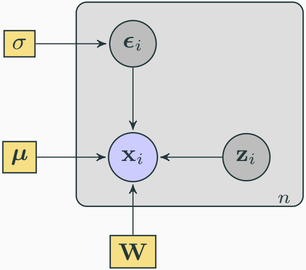
$$\mathbf{x} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$$

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)

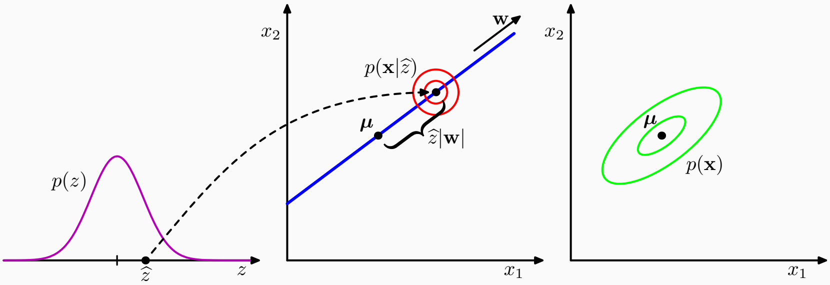
Generative process

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



Probability recall

Let

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

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

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

with

$$\begin{aligned} \boldsymbol{\mu}_1 &\in \mathbb{R}^r \\ \boldsymbol{\mu}_2 &\in \mathbb{R}^s \\ \boldsymbol{\Sigma}_{11} &\in \mathbb{R}^{r \times r} \\ \boldsymbol{\Sigma}_{12} &= \boldsymbol{\Sigma}_{21}^T \in \mathbb{R}^{r \times s} \\ \boldsymbol{\Sigma}_{22} &\in \mathbb{R}^{s \times s} \end{aligned}$$

Probability recall

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

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

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 $\boldsymbol{\mu}_{\mathbf{z}} = 0$.
- 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

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

where

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

Joint distribution

As a consequence, we get

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

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 $p(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{z}|\mathbf{x}}, \Sigma_{\mathbf{z}|\mathbf{x}})$ with

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

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

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

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

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

and, substituting into the log-likelihood formula,

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

where $\mathbf{S}$ is the data covariance matrix

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

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 $\lambda_i - \sigma^2$

Rotations in latent space

Observe that solutions are invariant wrt rotations in latent space: in particular, if we consider a rotation $\mathbf{R}$, then the matrix $\mathbf{W}$ mapping from latent to data space turns out to be $\tilde{\mathbf{W}} = \mathbf{W}\mathbf{R}$. Since $\mathbf{R}\mathbf{R}^T = \mathbf{I}$ by the orthogonality of $\mathbf{R}$, and

$$\Sigma_{\mathbf{x}} = \mathbf{W}\mathbf{R}(\mathbf{W}\mathbf{R})^T + \sigma^2\mathbf{I} = \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}$$

the same marginal distribution results. Thus, applying a rotation $\mathbf{R}$ has no effect on the model.

Maximum likelihood for PCA

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.

Mapping points to subspace

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

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

EM for PCA

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

$$p(\mathbf{z}_i) = \mathcal{N}(0, 1) \qquad\qquad p(\mathbf{x}_i|\mathbf{z}_i) = \mathcal{N}(\mathbf{W}\mathbf{z}_i + \boldsymbol{\mu}, \sigma^2\mathbf{I})$$

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

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

The conditional expectations are estimated in the E-step as

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

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

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

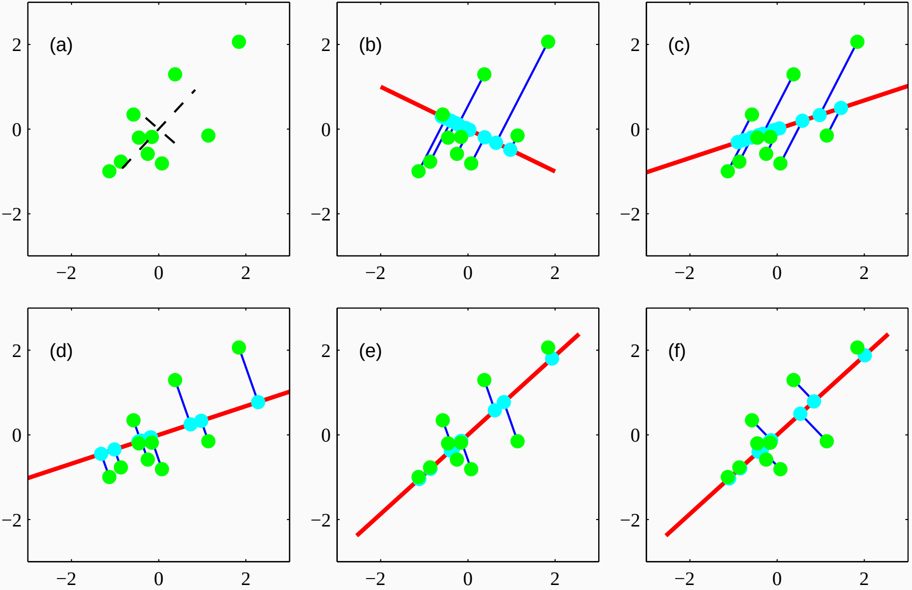
The new estimates of parameters $\mathbf{W}$ and σ^2 are obtained through maximization of the expectation of $p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \mathbf{W}, \sigma^2)$ wrt $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\mu}, \mathbf{W}, \sigma^2)$ (as already observed, the maximum likelihood estimate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

The following equations result

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

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

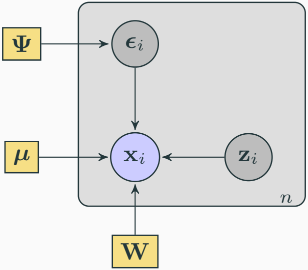
EM for PCA



Factor analysis

Graphical model

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



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

Model distribution are modified accordingly.

Joint distribution

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

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

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

Maximum likelihood for FA

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

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

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

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

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

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

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

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

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 $\overline{\mathbf{x}}$).

The following equations result

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

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

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

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