Lecture 8: Principle Component Analysis and Factor Analysis

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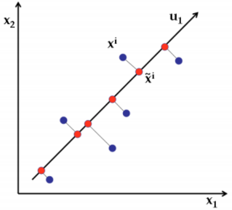
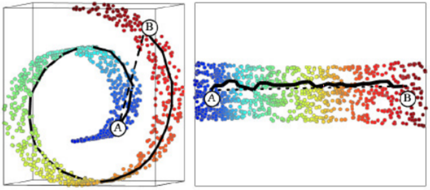
Outline

Dimensionality Reduction

- Usually considered an unsupervised learning method
- Used for learning the low-dimensional structures in the data

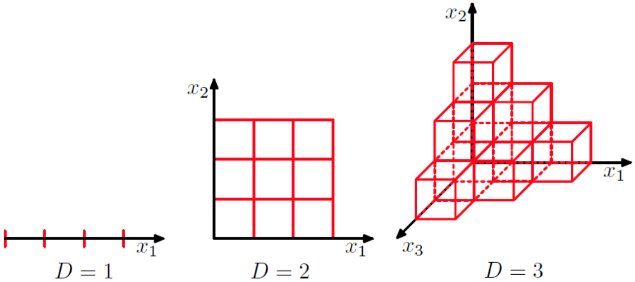




- Also useful for "feature learning" or "representation learning" (learning a better, often smaller-dimensional, representation of the data), e.g.,
  - Documents using topic vectors instead of bag-of-words vectors
  - Images using their constituent parts (faces - eigenfaces)
- Can be used for speeding up learning algorithms

Dimensionality Reduction (Contd.)

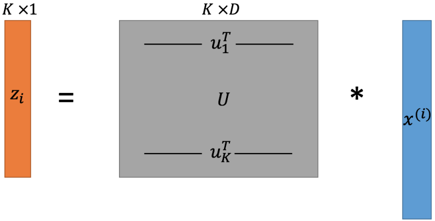
- Exponentially large # of examples required to "fill up" high-dim spaces



- Fewer dimensions $\Rightarrow$ Less chances of overfitting $\Rightarrow$ Better generalization
- Dimensionality reduction is a way to beat the curse of dimensionality

Linear Dimensionality Reduction

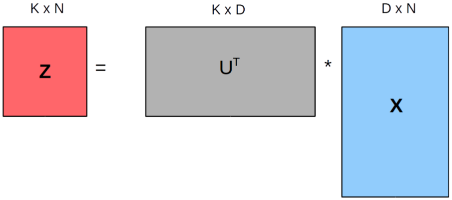
- A projection matrix $U = [u_1 u_2 \cdots u_K]$ of size $D \times K$ defines K linear projection direction
- Use U to transform $x^{(i)} \in \mathbb{R}^D$ into $z^{(i)} \in \mathbb{R}^K$



- $z^{(i)} = U^T x^{(i)} = [u_1^T x^{(i)},\ u_2^T x^{(i)},\ \cdots u_K^T x^{(i)}]^T$ is a K-dim projection of $x^{(i)}$
  - $z^{(i)} \in \mathbb{R}^K$ is also called low-dimensional "embeding" of $x^{(i)} \in \mathbb{R}^D$

Linear Dimensionality Reduction

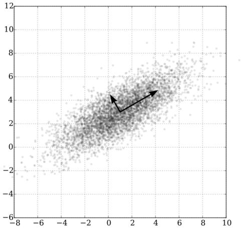
- $X = [x^{(1)} \; x^{(2)} \cdots x^{(N)}]$ is $D \times N$ matrix deoting all the N data points
- $Z = [z^{(1)} \; z^{(2)} \cdots z^{(N)}]$ is $K \times N$ matrix denoting embeddings of the data points
- With this notation, the figure on previous slide can be re-drawn as



- How do we learn the "best" projection matrix U?
- What criteria should we optimize for when learning U
- Principle Component Analysis (PCA) is an algorithm for doing this

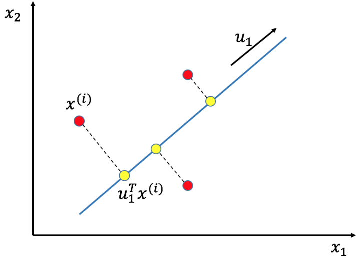
Principle Component Analysis (PCA)

- PCA is a technique widely used for applications such as dimensionality reduction, lossy data compression, feature extraction, and data visualization
- Two commonly used definitions
  - Learning projection directions that capture maximum variance in data
  - Learning projection directions that result in smallest reconstruction error
- Can also be seen as changing the basis in which the data is represented (and transforming the features such that new features become decorrelated)



Variance Captured by Projections

- Consider $x^{(i)} \in \mathbb{R}^D$ on a one-dim subspace defined by $u_1 \in \mathbb{R}^D$ ($\|u_1\| = 1$)
- Projection of $x^{(i)}$ along a one-dim subspace



- Mean of projections of all the data ($\mu = \frac{1}{N}\sum_{i=1}^{N} x^{(i)}$)

$$\frac{1}{N}\sum_{i=1}^{N} u_1^T x^{(i)} = u_1^T \frac{1}{N}\sum_{i=1}^{N} x^{(i)} = u_1^T \mu$$

Variance Captured by Projections

- Variance of the projected data

$$\frac{1}{N}\sum_{i=1}^{N}(u_1^T x^{(i)} - u_1^T \mu)^2 = \frac{1}{N}\sum_{i=1}^{N}[u_1^T (x^{(i)} - \mu)]^2 = u_1^T S u_1$$

- S is the $D \times D$ data covariance matrix

$$S = \frac{1}{N}\sum_{i=1}^{N}(x^{(i)} - \mu)(x^{(i)} - \mu)^T$$

  - Variance of the projected data ("spread" of the yellow points)
  - If data already centered at $\mu = 0$, then $S = \frac{1}{N}\sum_{i=1}^{N} x^{(i)}(x^{(i)})^T$

Optimization Problem

- We want u_1 s.t. the variance of the projected data is maximized

$$\max_{u_1} \quad u_1^T S u_1$$
$$s.t. \quad u_1^T u_1 = 1$$

- The method of Lagrange multipliers

$$\mathcal{L}(u_1, \lambda_1) = u_1^T S u_1 - \lambda_1 (u_1^T u_1 - 1)$$

where λ_1 is a Lagrange multiplier

Direction of Maximum Variance

- Taking the derivative w.r.t. u_1 and setting to zero gives

$$Su_1 = \lambda_1 u_1$$

- Thus u_1 is an eigenvector of S (with corresponding eigenvalue λ_1)
- But which of S's eigenvectors it is?
- Note that since $u_1^T u_1 = 1$, the variance of projected data is

$$u_1^T S u_1 = \lambda_1$$

- Var. is maximized when u_1 is the top eigenvector with largest eigenvalue
- The top eigenvector u_1 is also known as the first Principle Component (PC)
- Other directions can also be found likewise (with each being orthogonal to all previous ones) using the eigendecomposition of S (this is PCA)

Steps in Principle Component Analysis

- Center the data (subtract the mean $\mu = \frac{1}{N}\sum_{i=1}^{N} x^{(i)}$ from each data point)
- Compute the covariance matrix

$$S = \frac{1}{N}\sum_{i=1}^{N} x^{(i)} {x^{(i)}}^T = \frac{1}{N} X X^T$$

- Do an eigendecomposition of the covariance matrix S
- Take first K leading eigenvectors $\{u_l\}_{l=1,\cdots,K}$ with eigenvalues $\{\lambda_l\}_{l=1,\cdots,K}$
- The final K dim. projection of data is given by

$$Z = U^T X$$

where U is $D \times K$ and Z is $K \times N$

PCA as Minimizing the Reconstruction Error

- Assume complete orthonormal basis vector $u_1, u_2, \cdots, u_D$, each $u_l \in \mathbb{R}^D$
- We can represent each data point $x^{(i)} \in \mathbb{R}^D$ exactly using the new basis

$$x^{(i)} = \sum_{l=1}^{D} z_l^{(i)} u_l$$

$$\begin{bmatrix} x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_D^{(i)} \end{bmatrix} = \begin{bmatrix} u_1 & u_2 & \cdots & u_D \end{bmatrix} * \begin{bmatrix} z_1^{(i)} \\ z_2^{(i)} \\ \vdots \\ z_D^{(i)} \end{bmatrix}$$

- Denoting $z^{(i)} = [z_1^{(i)} \cdots z_D^{(i)}]^T$, $U = [u_1 \cdots u_D]$, and using $U^T U = I$

$$x^{(i)} = Uz^{(i)} \text{ and } z^{(i)} = U^T x^{(i)}$$

- Also note that each component of vector $z^{(i)}$ is $z_l^{(i)} = u_l^T x^{(i)}$

Reconstruction of Data from Projections

- Reconstruction of $x^{(i)}$ from $z^{(i)}$ will be exact if we use all D basis vectors
- Will be approximate if we only use $K < D$ basis vectors:

$$x^{(i)} \approx \sum_{l=1}^{K} z_l^{(i)} u_l$$

- Let's use $K = 1$ basis vector. Then, the one-dim embedding of $x^{(i)}$ is

$$z^{(i)} = u_1^T x^{(i)} \quad (z^{(i)} \in \mathbb{R})$$

- We can now try to "reconstruct" $x^{(i)}$ from its embedding $z^{(i)}$ as follows

$$\tilde{x}^{(i)} = u_1 z^{(i)} = u_1 u_1^T x^{(i)}$$

- Total error or "loss" in reconstructing all the data points

$$\ell(u_1) = \sum_{i=1}^{N} \|x^{(i)} - \tilde{x}^{(i)}\|^2 = \sum_{i=1}^{N} \|x^{(i)} - u_1 u_1^T x^{(i)}\|^2$$

Direction with Best Reconstruction

- We want to find u_1 that minimize the reconstruction error

$$\ell(u_1) = \sum_{i=1}^{N} \|x^{(i)} - u_1 u_1^T x^{(i)}\|^2 = \sum_{i=1}^{N} \left(-u_1^T x^{(i)} (x^{(i)})^T u_1 + (x^{(i)})^T x^{(i)} \right)$$

  by using $u_1^T u_1 = 1$

- Minimizing the error of reconstructing all the data points is equivalent to

$$\max_{u_1 : \|u_1\|^2 = 1} u_1^T \left(\sum_{n=1}^{N} x^{(i)} (x^{(i)})^T \right) u_1 = \max_{u_1 : \|u_1\|^2 = 1} u_1^T S u_1$$

  where S is the covariance matrix of the data (which are assumed to be centered)

- It is the same objective that we had when we maximized the variance

Revisiting Gaussian

- Gaussian distribution with a single variable

$$\mathcal{N}(x;\mu,\sigma^2)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

  where μ is the mean and σ^2 is the variance

- n-dimensional multivariate Gaussian distribution

$$\mathcal{N}(x;\mu,\Sigma)=\frac{1}{(2\pi)^{\frac{n}{2}}|\Sigma|^{\frac{1}{2}}}\exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

  where μ is the n-dimensional mean vector and Σ is the $n\times n$-dimensional covariance matrix

Revisiting Gaussian (Contd.)

- Central limit theorem
  - Subject to certain mild conditions, the sum of a set of random variables has a distribution increasingly approaching Gaussian as the number of the variables increases

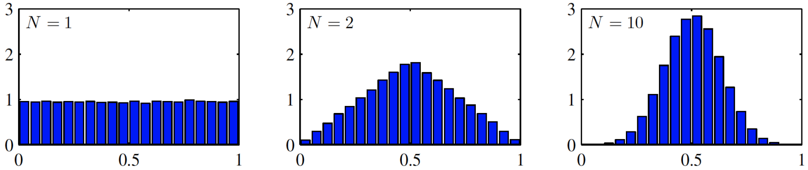


Figure: Consider N random variables $x_1, x_2, \cdots, x_N$ each of which has a uniform distribution over $[0, 1]$. The distribution of their mean $\frac{1}{N}\sum_{i=1}^{N} x_i$ tends to a Gaussian as $N \to \infty$

Revisiting Gaussian (Contd.)

- The following Gaussian integrals have closed-form solutions

$$
\begin{aligned}
&\int_{\mathbb{R}^n} \mathcal{N}(x;\mu,\Sigma)dx = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathcal{N}(x;\mu,\Sigma)dx_1 \cdots dx_n = 1 \\
&\int_{\mathbb{R}^n} x_i \mathcal{N}(x;\mu,\Sigma)dx = \mu_i,\ \forall i = 1,2,\cdots,n \\
&\int_{\mathbb{R}^n} (x_i - \mu_i)(x_j - \mu_j)\mathcal{N}(x;\mu,\Sigma)dx = \Sigma_{ij}
\end{aligned}
$$

Revisiting Gaussian (Contd.)

- The functional dependence of the Gaussian on x is through the quadratic form

$$\Delta^2 = (x - \mu)^T \Sigma (x - \mu)$$

  where Δ is called the Mahalanobis distance from x to μ
- Σ is *symmetric* such that
  - All eigenvalues of Σ, i.e., $\lambda_1, \lambda_2, \cdots, \lambda_D$, are real
  - Eigenvectors (i.e., u_1, u_2, u_D) corresponding to distinct eigenvalues are orthogonal

Conditional Gaussian and Marginal Gaussian

An important property

- If two sets of variables are jointly Gaussian, then the conditional distribution of one set conditioned on the other is again Gaussian

$$\begin{aligned} \mu_{a|b} &= \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b) \\ \Sigma_{a|b} &= \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba} \end{aligned}$$

- Similarly, the marginal distribution of either set is also Gaussian

$$\begin{aligned} \mathbb{E}[x_a] &= \mu_a \\ \mathrm{cov}[x_a] &= \Sigma_{aa} \end{aligned}$$

Conditional Gaussian Distribution

- $x \sim \mathcal{N}(\mu, \Sigma)$
- Partition x into two disjoint subsets x_a and x_b

$$x = \begin{bmatrix} x_a \\ x_b \end{bmatrix}, \quad \mu = \begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}, \quad \Sigma = \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}$$

- Precision matrix

$$\Lambda := \Sigma^{-1} = \begin{bmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{bmatrix}$$

where $\Lambda_{ab}^T = \Lambda_{ba}$

Conditional Gaussian Distribution (Contd.)

- n-dimensional multivariate Gaussian distribution

$$\mathcal{N}(x;\mu,\Sigma)=\frac{1}{(2\pi)^{\frac{n}{2}}|\Sigma|^{\frac{1}{2}}}\exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

where μ is the n-dimensional mean vector and Σ is the $n\times n$-dimensional covariance matrix

- If the conditional probability of x_a conditioned on x_b is a Gaussian

$$\begin{aligned} & \mathcal{N}(x_a \mid x_b;\mu_{a|b},\Sigma_{a|b}) \\ = \quad & \frac{1}{(2\pi)^{\frac{n}{2}}|\Sigma_{a|b}|^{\frac{1}{2}}}\exp\left(-\frac{1}{2}(x-\mu_{a|b})^T\Sigma_{a|b}^{-1}(x-\mu_{a|b})\right)\end{aligned}$$

where $\mu_{a|b}$ is the n_a-dimensional conditional mean vector of x_a and $\Sigma_{a|b}$ is the $n_a\times n_a$-dimensional conditional covariance matrix

Conditional Gaussian Distribution (Contd.)

- A quadratic form of x_a

$$
\begin{aligned}
& -\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu) \\
= & -\frac{1}{2}\left(\begin{bmatrix} x_a \\ x_b \end{bmatrix} - \begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}\right)^T \begin{bmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{bmatrix} \left(\begin{bmatrix} x_a \\ x_b \end{bmatrix} - \begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}\right) \\
= & -\frac{1}{2}(x_a-\mu_a)^T\Lambda_{aa}(x_a-\mu_a) - (x_a-\mu_a)^T\Lambda_{ab}(x_b-\mu_b) \\
& -\frac{1}{2}(x_b-\mu_b)^T\Lambda_{bb}(x_b-\mu_b) \\
= & -\frac{1}{2}x_a^T\Lambda_{aa}x_a + x_a^T(\Lambda_{aa}\mu_a - \Lambda_{ab}(x_b-\mu_b)) + const
\end{aligned}
$$

Conditional Gaussian Distribution (Contd.)

- A quadratic form of x_a

$$
\begin{aligned}
& -\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu) \\
= \quad & -\frac{1}{2}x_a^T\Lambda_{aa}x_a + x_a^T(\Lambda_{aa}\mu_a - \Lambda_{ab}(x_b-\mu_b)) + const
\end{aligned}
$$

- Referring to

$$
-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu) = -\frac{1}{2}x^T\Sigma^{-1}x + x^T\Sigma^{-1}\mu + const
$$

- The covariance of $p(x_a \mid x_b)$ is given by

$$
\Sigma_{a|b} = \Lambda_{aa}^{-1}
$$

Conditional Gaussian Distribution (Contd.)

- A quadratic form of x_a

$$\begin{aligned} & -\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu) \\ = \quad & -\frac{1}{2}x_a^T\Lambda_{aa}x_a + x_a^T(\Lambda_{aa}\mu_a - \Lambda_{ab}(x_b-\mu_b)) + const \end{aligned}$$

- Referring to

$$-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu) = -\frac{1}{2}x^T\Sigma^{-1}x + x^T\Sigma^{-1}\mu + const$$

- The mean of $p(x_a \mid x_b)$ is given by

$$\mu_{a|b} = \Sigma_{a|b}(\Lambda_{aa}\mu_a - \Lambda_{ab}(x_b-\mu_b)) = \mu_a - \Lambda_{aa}^{-1}\Lambda_{ab}(x_b-\mu_b)$$

Conditional Gaussian Distribution (Contd.)

- Since

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} M & -MBD^{-1} \\ -D^{-1}CM & D^{-1} + D^{-1}CMBD^{-1} \end{bmatrix}$$

where $M = (A - BD^{-1}C)^{-1}$ is known as the *Schur complement*

- Then

$$\begin{aligned} \Lambda_{aa} &= (\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba})^{-1} \\ \Lambda_{ab} &= -(\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba})^{-1}\Sigma_{ab}\Sigma_{bb}^{-1} \end{aligned}$$

- All in all,

$$\begin{aligned} \mu_{a|b} &= \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b) \\ \Sigma_{a|b} &= \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba} \end{aligned}$$

- Check the normalization item by yourselves

Marginal Gaussian Distribution

- n-dimensional multivariate Gaussian distribution

$$\mathcal{N}(x;\mu,\Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}}|\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

  where μ is the n-dimensional mean vector and Σ is the $n \times n$-dimensional covariance matrix

- Marginal Gaussian

$$p(x_a) = \int_{\mathbb{R}^{n_b}} p(x_a, x_b) dx_b$$

- If the marginal probability of x_a is a Gaussian

$$\mathcal{N}(x_a;\bar{\mu}_a,\Sigma_a) = \frac{1}{(2\pi)^{\frac{n}{2}}|\Sigma_a|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x-\bar{\mu}_a)^T\Sigma_a^{-1}(x-\bar{\mu}_a)\right)$$

Marginal Gaussian Distribution (Contd.)

- Recalling the quadratic form of x_a

$$\begin{aligned}-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu) &= -\frac{1}{2}(x_a-\mu_a)^T\Lambda_{aa}(x_a-\mu_a) \\ &\quad -(x_a-\mu_a)^T\Lambda_{ab}(x_b-\mu_b) \\ &\quad -\frac{1}{2}(x_b-\mu_b)^T\Lambda_{bb}(x_b-\mu_b)\end{aligned}$$

- Picking out all items involving x_b

$$-\frac{1}{2}x_b^T\Lambda_{bb}x_b + x_b^T m = -\frac{1}{2}(x_b-\Lambda_{bb}^{-1}m)^T\Lambda_{bb}(x_b-\Lambda_{bb}^{-1}m) + \frac{1}{2}m^T\Lambda_{bb}^{-1}m$$

where $m = \Lambda_{bb}\mu_b - \Lambda_{ba}(x_a-\mu_a)$

Marginal Gaussian Distribution (Contd.)

- Taking the exponential of this quadratic form, the integration over x_b can be defined as

$$\int \exp\left(-\frac{1}{2}(x_b - \Lambda_{bb}^{-1}m)^T \Lambda_{bb}(x_b - \Lambda_{bb}^{-1}m)\right) dx_b$$

- It is the integral over an unnormalized Gaussian, and hence the result will be the reciprocal of the normalization coefficient which depends only on the determinant of the covariance matrix

Marginal Gaussian Distribution (Contd.)

- Combining $\frac{1}{2}m^T\Lambda_{bb}^{-1}m$ with the remaining terms depending on x_a

$$
\begin{aligned}
& \frac{1}{2}[\Lambda_{bb}\mu_b - \Lambda_{ba}(x_a - \mu_a)]^T\Lambda_{bb}^{-1}[\Lambda_{bb}\mu_b - \Lambda_{ba}(x_a - \mu_a)] \\
& -\frac{1}{2}x_a^T\Lambda_{aa}x_a + x_a^T(\Lambda_{aa}\mu_a + \Lambda_{ab}\mu_b) + const \\
= & -\frac{1}{2}x_a^T(\Lambda_{aa} - \Lambda_{ab}\Lambda_{bb}^{-1}\Lambda_{ba})x_a \\
& +x_a^T(\Lambda_{aa} - \Lambda_{ab}\Lambda_{bb}^{-1}\Lambda_{ba})\mu_a + const
\end{aligned}
$$

- Therefore

$$
\begin{aligned}
\Sigma_a &= (\Lambda_{aa} - \Lambda_{ab}\Lambda_{bb}^{-1}\Lambda_{ba})^{-1} = \Sigma_{aa} \\
\bar{\mu}_a &= \Sigma_a(\Lambda_{aa} - \Lambda_{ab}\Lambda_{bb}^{-1}\Lambda_{ba})\mu_a
\end{aligned}
$$

Factor Analysis Model

- $x = \mu + \Lambda z + \varepsilon$
  - $x \in \mathbb{R}^n$, $\mu \in \mathbb{R}^n$, $\Lambda \in \mathbb{R}^{n \times k}$, $z \in \mathbb{R}^k$, $\varepsilon \in \mathbb{R}^n$
  - Λ is the factor loading matrix
  - $z \sim \mathcal{N}(0, I)$ (zero-mean independent normals, with unit variance)
  - $\varepsilon \sim \mathcal{N}(0, \Psi)$ where Ψ is a diagonal matrix (the observed variables are independent given the factors)
- How do we get the training data $\{x^{(i)}\}_i$?
  - Generate $\{z^{(i)}\}_i$ according to a multivariate Gaussian distribution $\mathcal{N}(0, I)$
  - Map $\{z^{(i)}\}_i$ into a n-dimensional affine space by Λ and μ
  - Generate $\{x^{(i)}\}_i$ by sampling the above affine space with noise ε
- Equivalently,

$$
\begin{aligned}
z &\sim \mathcal{N}(0, I) \\
x|z &\sim \mathcal{N}(\mu + \Lambda z, \Psi)
\end{aligned}
$$

Higher Dimension But Less Data

- Consider a case with $n \gg m$
  - The given training data span only a low-dimensional subspace of $\mathbb{R}^n$
- If we Model the data as Gaussian and estimate the mean and covariance using MLE

$$\mu = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}$$

$$\Sigma = \frac{1}{m}\sum_{i=1}^{m}(x^{(i)} - \mu)(x^{(i)} - \mu)^T$$

we may observe that Σ may be singular such that Σ^{-1} does not exist and $1/|\Sigma|^{1/2} = 1/0$

$$p(x;\mu,\Sigma) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

Factor Analysis Model (Contd.)

- z and x have a joint Gaussian distribution

$$\begin{bmatrix} z \\ x \end{bmatrix} \sim \mathcal{N}(\mu_{zx}, \Sigma)$$

- Question: How to calculate μ_{zx} and Σ?
- Since $E[z] = 0$, we have

$$E[x] = E[\mu + \Lambda z + \epsilon] = \mu + \Lambda E[z] + E[\epsilon] = \mu$$

and then

$$\mu_{zx} = \begin{bmatrix} \vec{0} \\ \mu \end{bmatrix}$$

Factor Analysis Model (Contd.)

- Since $z \sim \mathcal{N}(0, I)$, $\mathbb{E}[zz^T] = \mathrm{Cov}(z)$, and $\mathbb{E}[z\epsilon^T] = \mathbb{E}[z]\mathbb{E}[\epsilon^T] = 0$,

$$
\begin{aligned}
\Sigma_{zz} &= \mathbb{E}[(z - E[z])(z - E[z])^T] = \mathrm{Cov}(z) = I \\
\Sigma_{xx} &= \mathbb{E}[(x - \mathbb{E}[x])(x - \mathbb{E}[x])^T] \\
&= \mathbb{E}[(\mu + \Lambda z + \epsilon - \mu)(\mu + \Lambda z + \epsilon - \mu)^T] \\
&= \mathbb{E}[\Lambda z z^T \Lambda^T + \epsilon z^T \Lambda^T + \Lambda z \epsilon^T + \epsilon\epsilon^T] \\
&= \Lambda \mathbb{E}[zz^T]\Lambda^T + \mathbb{E}[\epsilon\epsilon^T] \\
&= \Lambda\Lambda^T + \Psi \\
\Sigma_{zx} &= \mathbb{E}[(z - \mathbb{E}[z])(x - \mathbb{E}[x])^T] \\
&= \mathbb{E}[z(\mu + \Lambda z + \epsilon - \mu)^T] \\
&= \mathbb{E}[zz^T]\Lambda^T + \mathbb{E}[z\epsilon^T] \\
&= \Lambda^T
\end{aligned}
$$

Factor Analysis Model (Contd.)

- Putting everything together, we therefore have

$$\begin{bmatrix} z \\ x \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \vec{0} \\ \mu \end{bmatrix}, \begin{bmatrix} I & \Lambda^T \\ \Lambda & \Lambda\Lambda^T + \Psi \end{bmatrix} \right)$$

- Then, $x \sim \mathcal{N}(\mu, \Lambda\Lambda^T + \Psi)$
- Log-likelihood function

$$\ell(\mu, \Lambda, \Psi) = \log \prod_{i=1}^{m} \frac{1}{(2\pi)^{n/2} |\Sigma_{xx}|^{1/2}} \exp\left(-\frac{1}{2} (x^{(i)} - \mu)^T \Sigma_{xx}^{-1} (x^{(i)} - \mu) \right)$$

EM Algorithm Review

- Repeat the following step until convergence
  - (E-step) For each i, set

$$Q_i(z^{(i)}) := p(z^{(i)} \mid x^{(i)}; \theta)$$

  - (M-step) set

$$\theta := \arg\max_{\theta} \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}$$

EM Algorithm for Factor Analysis

- Recall that if

$$\begin{bmatrix} x_a \\ x_b \end{bmatrix} \sim \mathcal{N}\left(\mu = \begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}, \Sigma = \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}\right)$$

we then have

$$x_a | x_b \sim \mathcal{N}(\mu_{a|b}, \Sigma_{a|b})$$

where

$$\begin{aligned} \mu_{a|b} &= \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b) \\ \Sigma_{a|b} &= \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba} \end{aligned}$$

EM Algorithm for Factor Analysis (Contd.)

- Since

$$\begin{bmatrix} z \\ x \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \vec{0} \\ \mu \end{bmatrix}, \begin{bmatrix} I & \Lambda^T \\ \Lambda & \Lambda\Lambda^T + \Psi \end{bmatrix}\right)$$

we have

$$z^{(i)}|x^{(i)}; \mu, \Lambda, \Psi \sim \mathcal{N}(\mu_{z^{(i)}|x^{(i)}}, \Sigma_{z^{(i)}|x^{(i)}})$$

where

$$\mu_{z^{(i)}|x^{(i)}} = \Lambda^T(\Lambda\Lambda^T + \Psi)^{-1}(x^{(i)} - \mu)$$
$$\Sigma_{z^{(i)}|x^{(i)}} = I - \Lambda^T(\Lambda\Lambda^T + \Psi)^{-1}\Lambda$$

- Calculate $Q_i(z^{(i)})$ in the E-step

$$Q_i(z^{(i)}) = \frac{\exp\left(-\frac{1}{2}(z^{(i)} - \mu_{z^{(i)}|x^{(i)}})^T \Sigma^{-1}_{z^{(i)}|x^{(i)}}(z^{(i)} - \mu_{z^{(i)}|x^{(i)}})\right)}{(2\pi)^{n/2}|\Sigma_{z^{(i)}|x^{(i)}}|^{1/2}}$$

EM Algorithm for Factor Analysis (Contd.)

- In M-step, we maximize the following equation with respect to μ, Λ, and Ψ

$$
\begin{aligned}
& \sum_{i=1}^{m} \int_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \mu, \Lambda, \Psi)}{Q_i(z^{(i)})} dz^{(i)} \\
= & \sum_{i=1}^{m} \mathbb{E}_{z^{(i)} \sim Q_i} \left[\log p(x^{(i)} \mid z^{(i)}; \mu, \Lambda, \Psi) + \log p(z^{(i)}) - \log Q_i(z^{(i)}) \right] \\
= & \sum_{i=1}^{m} \mathbb{E}_{z^{(i)} \sim Q_i} \left[\log \frac{1}{(2\pi)^{n/2} |\Psi|^{1/2}} \exp\left(-\frac{(x^{(i)} - \mu - \Lambda z^{(i)})^T \Psi^{-1} (x^{(i)} - \mu - \Lambda z^{(i)})}{2} \right) + \log p(z^{(i)}) - \log Q_i(z^{(i)}) \right] \\
= & \sum_{i=1}^{m} \mathbb{E}_{z^{(i)} \sim Q_i} \left[-\frac{1}{2} \log |\Psi| - \frac{n}{2} \log(2\pi) - \frac{1}{2} (x^{(i)} - \mu - \Lambda z^{(i)})^T \Psi^{-1} (x^{(i)} - \mu - \Lambda z^{(i)}) + \log p(z^{(i)}) - \log Q_i(z^{(i)}) \right]
\end{aligned}
$$

EM Algorithm for Factor Analysis (Contd.)

- Let

$$
\begin{aligned}
& \nabla_\Lambda \sum_{i=1}^{m} -\mathbb{E}[\frac{1}{2}(x^{(i)} - \mu - \Lambda z^{(i)})^T \Psi^{-1}(x^{(i)} - \mu - \Lambda z^{(i)})] \\
= & \sum_{i=1}^{m} \nabla_\Lambda \mathbb{E}_{z^{(i)} \sim Q_i}\left[-\mathrm{tr}\left(\frac{1}{2} {z^{(i)}}^T \Lambda^T \Psi^{-1} \Lambda z^{(i)}\right) + \mathrm{tr}\left({z^{(i)}}^T \Lambda^T \Psi^{-1}(x^{(i)} - \mu)\right)\right] \\
= & \sum_{i=1}^{m} \nabla_\Lambda \mathbb{E}_{z^{(i)} \sim Q_i}\left[-\mathrm{tr}\left(\frac{1}{2} \Lambda^T \Psi^{-1} \Lambda z^{(i)} {z^{(i)}}^T\right) + \mathrm{tr}\left(\Lambda^T \Psi^{-1}(x^{(i)} - \mu) {z^{(i)}}^T\right)\right] \\
= & \sum_{i=1}^{m} \mathbb{E}_{z^{(i)} \sim Q_i}\left[-\Psi^{-1} \Lambda z^{(i)} {z^{(i)}}^T + \Psi^{-1}(x^{(i)} - \mu) {z^{(i)}}^T\right] \\
= & \ 0
\end{aligned}
$$

- we have

$$
\begin{aligned}
\Lambda &= \left(\sum_{i=1}^{m} (x^{(i)} - \mu) \mathbb{E}_{z^{(i)} \sim Q_i}\left[{z^{(i)}}^T\right]\right) \left(\sum_{i=1}^{m} \mathbb{E}_{z^{(i)} \sim Q_i}\left[z^{(i)} {z^{(i)}}^T\right]\right)^{-1} \\
&= \left(\sum_{i=1}^{m} (x^{(i)} - \mu) \mu_{z^{(i)}|x^{(i)}}^T\right) \left(\sum_{i=1}^{m} \mu_{z^{(i)}|x^{(i)}} \mu_{z^{(i)}|x^{(i)}}^T + \Sigma_{z^{(i)}|x^{(i)}}\right)^{-1}
\end{aligned}
$$

EM Algorithm for Factor Analysis (Contd.)

- Maximize

$$\sum_{i=1}^{m} \int_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \mu, \Lambda, \Psi)}{Q_i(z^{(i)})} dz^{(i)}$$

  with respect to μ and Ψ

- Results are as follows

$$\mu = \frac{1}{m} \sum_{i=1}^{m} x^{(i)}$$

$$\Psi = \text{diag}(\frac{1}{m} \sum_{i=1}^{m} x^{(i)} {x^{(i)}}^T - x^{(i)} \mu_{z^{(i)}|x^{(i)}}^T \Lambda^T - \Lambda \mu_{z^{(i)}|x^{(i)}} {x^{(i)}}^T + \Lambda(\mu_{z^{(i)}|x^{(i)}} \mu_{z^{(i)}|x^{(i)}}^T + \Sigma_{z^{(i)}|x^{(i)}}) \Lambda^T)$$

Thanks!

Q & A