Deep Generative Models Probabilistic PCA

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Outline

- Probabilistic PCA: Model
  - Joint, Marginal and Conditional Distributions
  - PPCA as an Encoder-Decoder Architecture

- Linear Algebra Background
  - Singular Value Decomposition (SVD)
  - SVD Properties

- Probabilistic PCA: Learning
  - Maximum Likelihood Estimation

- Applications
  - Application of PPCA to Generating Face Images

Latent Variable Models

- X = observed variable

- Z = latent variable

- $z \sim p(z)$

- $x \sim p(x \mid z)$
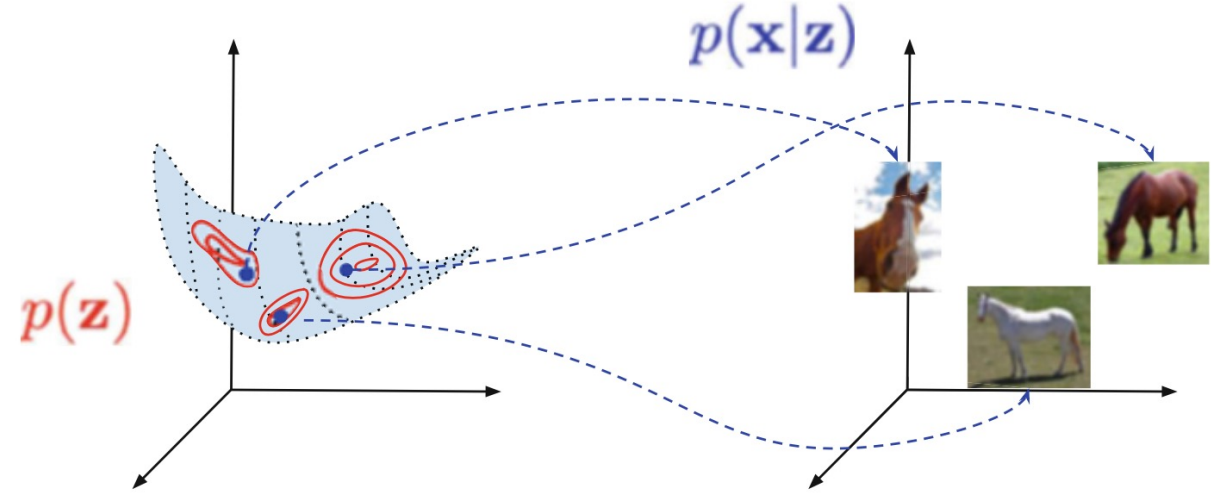
A latent variable model and a generative process. Note the low-dimensional manifold (here 2D) embedded in the high-dimensional space (here 3D)

- Factorization of the joint model

$$p(x, z) = p(x \mid z)p(z)$$

- Marginalization of the model

$$p(x) = \int p(x \mid z)p(z)dz$$

Probabilistic Principal Component Analysis: Model

- We consider continuous random variables only, i.e.,

$$\boldsymbol{z} \in \mathbb{R}^d \text{ and } \boldsymbol{x} \in \mathbb{R}^D \text{ with } d \ll D$$

- The distribution of $\boldsymbol{z}$ is the standard Gaussian, i.e.,

$$p(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{0}, \boldsymbol{I}).$$

- The dependency between $\boldsymbol{z}$ and $\boldsymbol{x}$ is linear, plus Gaussian additive noise:

$$\boldsymbol{x} = \boldsymbol{W}\boldsymbol{z} + \boldsymbol{b} + \boldsymbol{\varepsilon}$$

- Here $\boldsymbol{\varepsilon} \sim \mathcal{N}(\boldsymbol{\varepsilon} \mid \boldsymbol{0}, \sigma^2 \boldsymbol{I})$ and independent from $\boldsymbol{z}$.

Probabilistic Principal Component Analysis: Model

- PPCA model

$$x = Wz + b + \epsilon, \quad z \sim \mathcal{N}(z \mid 0, I), \quad \epsilon \sim \mathcal{N}(\epsilon \mid 0, \sigma^2 I) \,.$$

- x is a linear combination of Gaussians, thus $p(x) = \mathcal{N}(x \mid b, WW^\top + \sigma^2 I)$ because

$$\mathbb{E}[x] = \mathbb{E}[Wz] + \mathbb{E}[b] + \mathbb{E}[\epsilon] = W\mathbb{E}[z] + b + 0 = b$$
$$\mathbb{V}[x] = \mathbb{V}[Wz + b + \epsilon] = W\mathbb{V}(z)W^\top + \mathbb{V}[\epsilon] = WW^\top + \sigma^2 I$$

- $x \mid z$ is a constant + a Gaussian, thus $p(x \mid z) = \mathcal{N}(x \mid Wz + b, \sigma^2 I)$ because

$$\mathbb{E}[x \mid z] = Wz + b + \mathbb{E}[\epsilon] = Wz + b$$
$$\mathbb{V}[x \mid z] = \mathbb{V}[\epsilon] = \sigma^2 I$$

Probabilistic Principal Component Analysis: Model

- PPCA model: $x = Wz + b + \epsilon, \; p(z) = \mathcal{N}(z \mid 0, I), \; p(\epsilon) = \mathcal{N}(\epsilon \mid 0, \sigma^2 I),$

$$p(x \mid z) = \mathcal{N}(x \mid Wz + b, \sigma^2 I), \qquad p(x) = \mathcal{N}(x \mid b, WW^\top + \sigma^2 I)$$

- Let $M = W^\top W + \sigma^2 I$. We can compute the conditional distribution of $(z \mid x)$ as

$$p(z \mid x) = \frac{p(x \mid z)p(z)}{p(x)} \propto e^{-\frac{1}{2\sigma^2}\|x - Wz - b\|^2} e^{-\frac{1}{2}\|z\|^2}$$

$$p(z \mid x) \propto e^{-\frac{1}{2\sigma^2}(z^T W^T W z - 2z^T W^T (x - b) + \sigma^2 \|z\|^2)} \propto e^{-\frac{1}{2\sigma^2}(z^T M z - 2z^T W^T (x - b))}$$

$$p(z \mid x) = \mathcal{N}(z \mid M^{-1} W^\top (x - b), \sigma^2 M^{-1})$$

PPCA as an Encoder Decoder Architecture

- PPCA model: $\boldsymbol{x} = \boldsymbol{Wz} + \boldsymbol{b} + \boldsymbol{\epsilon}, \ p(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{0}, \boldsymbol{I}), \ p(\boldsymbol{\epsilon}) = \mathcal{N}(\boldsymbol{\epsilon} \mid \boldsymbol{0}, \sigma^2 \boldsymbol{I}),$

$$p(\boldsymbol{z} \mid \boldsymbol{x}) = \mathcal{N}(\boldsymbol{z} \mid M^{-1}W^{\top}(\boldsymbol{x} - \boldsymbol{b}), \sigma^{-2}M) \qquad p(\boldsymbol{x} \mid \boldsymbol{z}) = \mathcal{N}(\boldsymbol{x} \mid W\boldsymbol{z} + \boldsymbol{b}, \sigma^2 I)$$
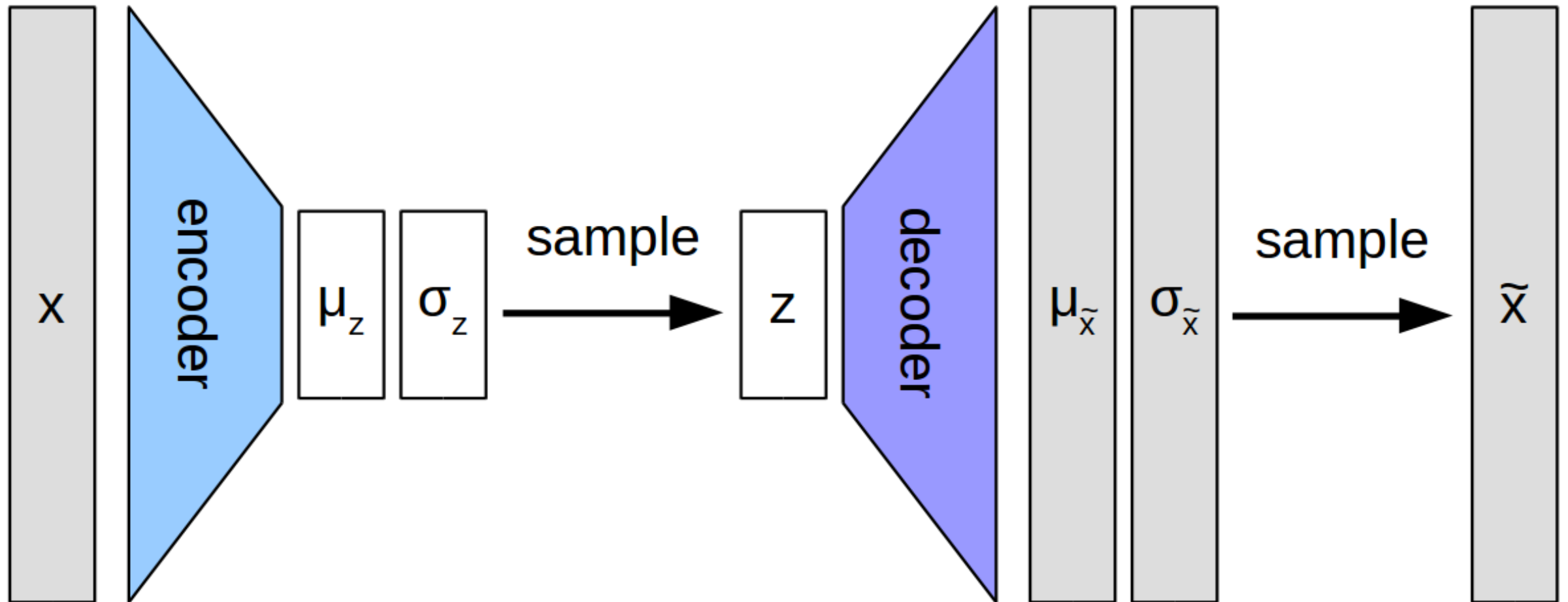
Singular Value Decomposition (SVD)

- A matrix $X \in \mathbb{R}^{m \times n}$ of rank r can be decomposed as

$$X = U\Sigma V^\top = [u_1 \cdots u_r u_{r+1} \cdots u_m] \begin{bmatrix} \sigma_1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_r & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 0 \end{bmatrix} [v_1 \cdots v_r v_{r+1} \cdots v_m]^\top$$

- $U \in \mathbb{R}^{m \times m}$ is an orthonormal matrix of left singular vectors
- $\Sigma \in \mathbb{R}^{m \times n}$ is a "diagonal" matrix with r singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$
- $V \in \mathbb{R}^{n \times n}$ is an orthonormal matrix of right singular vectors

Compact Singular Value Decomposition (SVD)

- A matrix $X \in \mathbb{R}^{m \times n}$ of rank r can be decomposed as

$$X = U\Sigma V^\top = [u_1 \cdots u_r u_{r+1} \cdots u_m] \begin{bmatrix} \sigma_1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_r & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 0 \end{bmatrix} [v_1 \cdots v_r v_{r+1} \cdots v_m]^\top$$

$$= U_1 \Sigma_1 V_1^\top = [u_1 \cdots u_r] \begin{bmatrix} \sigma_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_r \end{bmatrix} [v_1 \cdots v_r]^\top$$

- $U_1 \in \mathbb{R}^{m \times r}$ and $V \in \mathbb{R}^{n \times r}$ are orthonormal matrices singular vectors
- $\Sigma \in \mathbb{R}^{r \times r}$ is a diagonal matrix with r singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$

SVD Properties

- For any partition of the SVD, we can compute the inverse as

$$X = U_1 \Sigma_1 V_1^\top + U_2 \Sigma_2 V_2^\top \Rightarrow X^{-1} = U_1 \Sigma_1^{-1} V_1^\top + U_2 \Sigma_2^{-1} V_2^\top$$

- Moreover, we always have

$$I = U_1 V_1^\top + U_2 V_2^\top$$

Probabilistic Principal Component Analysis: Learning

- Recall the ML estimators of the parameters of a Gaussian $\mathcal{N}(x \mid \mu, \Sigma)$ are

$$\mu_N = \frac{1}{N}\sum_{i=1}^{N} x_i, \qquad \Sigma_N = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu_N)(x_i - \mu_N)^T$$

- For PPCA we need to estimate the parameters of a Gaussian with structured covariance $\Sigma = WW^T + \sigma^2 I$. The estimate of the mean is the same as before $\mu = \mu_N$. To estimate W, we need to maximize the log-likelihood w.r.t. (W, σ)

$$\ell = -\frac{N}{2}\log(\det(\Sigma)) - \frac{N}{2}\text{trace}(\Sigma^{-1}\Sigma_N)$$

- Taking derivatives w.r.t. W we get

$$\frac{\partial \ell}{\partial W} = \frac{\partial \ell}{\partial \Sigma}\frac{\partial \Sigma}{\partial W} = -\frac{N}{2}(\Sigma^{-1} - \Sigma^{-1}\Sigma_N\Sigma^{-1})2W = 0 \implies \Sigma_N\Sigma^{-1}W = W$$

Probabilistic Principal Component Analysis: Learning

- We thus need to solve the nonlinear equations
$$\boldsymbol{\Sigma}_N \boldsymbol{\Sigma}^{-1} \boldsymbol{W} = \boldsymbol{W} \text{ and } \boldsymbol{\Sigma} = \boldsymbol{W}\boldsymbol{W}^T + \sigma^2 \boldsymbol{I}$$

- A trivial solution is $(\boldsymbol{W}, \boldsymbol{\sigma}) = (\boldsymbol{0}, 0)$, but this is a minimum of the log-likelihood.

- Another solution is $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_N$, but this would require the structure of the sample covariance $\boldsymbol{\Sigma}_N$ to match the structure of $\boldsymbol{\Sigma} = \boldsymbol{W}\boldsymbol{W}^T + \sigma^2 \boldsymbol{I}$, i.e., the smallest eigenvalues would need to be all equal to each other and equal to σ^2.

- Alternatively, let
$$\boldsymbol{W} = [\boldsymbol{Z}_1 \quad \boldsymbol{Z}_2] \begin{bmatrix} \boldsymbol{\Gamma}_1 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} [\boldsymbol{V}_1 \quad \boldsymbol{V}_2]^T = \boldsymbol{Z}_1 \boldsymbol{\Gamma}_1 \boldsymbol{V}_1^T$$

- Then
$$\boldsymbol{\Sigma} = \boldsymbol{W}\boldsymbol{W}^T + \sigma^2 \boldsymbol{I} = \boldsymbol{Z}_1 \boldsymbol{\Gamma}_1^2 \boldsymbol{Z}_1^T + \sigma^2 (\boldsymbol{Z}_1 \boldsymbol{Z}_1^T + \boldsymbol{Z}_2 \boldsymbol{Z}_2^T) = \boldsymbol{Z}_1 (\boldsymbol{\Gamma}_1^2 + \sigma^2 \boldsymbol{I}) \boldsymbol{Z}_1^T + \sigma^2 \boldsymbol{Z}_2 \boldsymbol{Z}_2^T$$
$$\boldsymbol{\Sigma}^{-1} \boldsymbol{W} = (\boldsymbol{Z}_1 (\boldsymbol{\Gamma}_1^2 + \sigma^2 \boldsymbol{I})^{-1} \boldsymbol{Z}_1^T + \sigma^{-2} \boldsymbol{Z}_2 \boldsymbol{Z}_2^T) \boldsymbol{Z}_1 \boldsymbol{\Gamma}_1 \boldsymbol{V}_1^T = \boldsymbol{Z}_1 (\boldsymbol{\Gamma}_1^2 + \sigma^2 \boldsymbol{I})^{-1} \boldsymbol{\Gamma}_1 \boldsymbol{V}_1^T$$

Probabilistic Principal Component Analysis: Learning

- Therefore,

$$\Sigma_N \Sigma^{-1} W = W \Rightarrow \Sigma_N Z_1 (\Gamma_1^2 + \sigma^2 I)^{-1} \Gamma_1 V_1^T = Z_1 \Gamma_1 V_1^T \Rightarrow$$

$$\Sigma_N Z_1 (\Gamma_1^2 + \sigma^2 I)^{-1} = Z_1 \Rightarrow \Sigma_N Z_1 = Z_1 (\Gamma_1^2 + \sigma^2 I) \Rightarrow \Sigma_N z_i = (\gamma_i^2 + \sigma^2) z_i$$

  - In other words, z_i is an eigenvector of Σ_N with eigenvalue $\gamma_i^2 + \sigma^2$.

- Thus if $\Sigma_N = [U_1 \ U_2] \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix} [U_1 \ U_2]^T$, then $Z_1 = U_1, \Gamma_1^2 + \sigma^2 I = \Lambda_1$.

  - In other words, U_1 is a matrix whose d columns correspond to d singular vectors of Σ_N

- Therefore, $W = Z_1 \Gamma_1 V_1^T = U_1 (\Lambda_1 - \sigma^2 I)^{1/2} V_1^T$

- Having "almost" found W (we don't know which d columns), we now turn to finding σ.

Probabilistic Principal Component Analysis: Learning

- Recall the log-likelihood

$$\ell = -\frac{N}{2}\log(\det(\mathbf{\Sigma})) - \frac{N}{2}\text{trace}(\mathbf{\Sigma}^{-1}\mathbf{\Sigma}_N)$$

- We have $\mathbf{\Sigma} = \boldsymbol{WW^T} + \sigma^2 I$ and $\boldsymbol{W} = \boldsymbol{U}_1\boldsymbol{\Gamma}_1\boldsymbol{V}_1^T$. Thus, $\boldsymbol{WW^T} = \boldsymbol{U}_1\boldsymbol{\Gamma}_1^2\boldsymbol{U}_1^T$ and

$$\mathbf{\Sigma} = \boldsymbol{U}_1(\boldsymbol{\Gamma}_1^2 + \sigma^2\, \boldsymbol{I})\boldsymbol{U}_1^T + \sigma^2\boldsymbol{U}_2\boldsymbol{U}_2^T = \boldsymbol{U}_1\boldsymbol{\Lambda_1}\boldsymbol{U}_1^T + \sigma^2\boldsymbol{U}_2\boldsymbol{U}_2^T$$

$$\mathbf{\Sigma}^{-1}\mathbf{\Sigma}_N = \left(\boldsymbol{U}_1\boldsymbol{\Lambda_1^{-1}}\boldsymbol{U}_1^T + \sigma^{-2}\boldsymbol{U}_2\boldsymbol{U}_2^T\right)(\boldsymbol{U}_1\boldsymbol{\Lambda}_1\boldsymbol{U}_1^T + \boldsymbol{U}_2\boldsymbol{\Lambda}_2\boldsymbol{U}_2^T) = \boldsymbol{U}_1\boldsymbol{U}_1^T + \sigma^{-2}\boldsymbol{U}_2\boldsymbol{\Lambda}_2\boldsymbol{U}_2^T$$

- Substituting into the log-likelihood, we get

$$\ell = -\frac{N}{2}\log(\det(\boldsymbol{\Lambda}_1)\sigma^{2(D-d)}) - \frac{N}{2}(d + \sigma^{-2}\text{trace}(\boldsymbol{\Lambda}_2))$$

Probabilistic Principal Component Analysis: Learning

- Taking the derivative yields $\frac{\partial \ell}{\partial \sigma^2} = -\frac{N}{2}\left(\frac{D-d}{\sigma^2} - \frac{\text{trace}(\Lambda_2)}{\sigma^4}\right) = 0 \implies \sigma^2 = \frac{\text{trace}(\Lambda_2)}{D-d}$

- Final piece: we have not shown that $\mathbf{\Lambda}_1$ corresponds to **top** d eigenvalues of $\mathbf{\Sigma}_N$
  - Exercise 2.13 in GPCA textbook

- **Theorem.** The ML estimates for the parameters of the PPCA model $\boldsymbol{b}, \boldsymbol{W}$, and σ can be obtained from the ML estimates of the mean and covariance of the data, $\boldsymbol{\mu}_N$ and $\mathbf{\Sigma}_N$, respectively, as

$$\boldsymbol{b} = \boldsymbol{\mu}_N, \; \boldsymbol{W} = \boldsymbol{U}_1(\mathbf{\Lambda}_1 - \sigma^2 I)^{1/2} R \;\text{ and }\; \sigma^2 = \frac{1}{D-d} \sum_{i=d+1}^{D} \lambda_i$$

- where $\boldsymbol{U}_1$ is the matrix with the top d eigenvectors of $\mathbf{\Sigma}_N$, $\mathbf{\Lambda}_1$ is the matrix with the corresponding top d eigenvalues, $R \in \mathbb{R}^{d \times d}$ is an arbitrary orthogonal matrix, and λ_i is the ith largest eigenvalue of $\mathbf{\Sigma}_N$.

Application of PPCA to Generating Face Images

Fig. 2.2 Face images of subject 20 under 10 different illumination conditions in the extended Yale B data set. All images are frontal faces cropped to size 192 × 168.

Application of PPCA to Generating Face Images

(a) mean face   (b) first eigenface   (c) second eigenface

Fig. 2.5 Mean face and the first two eigenfaces by applying PPCA to the ten images in Figure 2.2.

Application of PPCA to Generating Face Images

(a) Variation along the first eigenface

(b) Variation along the second eigenface

Fig. 2.6 Variation of the face images along the two eigenfaces given by PPCA. Each row plots $\mu + y_i u_i$ for $y_i = -1 : \frac{1}{3} : 1, i = 1, 2$.