Dimensionality Reduction

आई आई टी हैदराबाद
IIT Hyderabad

ML Problems

	Supervised Learning	Unsupervised Learning
Discrete	classification or categorization	clustering
Continuous	regression	dimensionality reduction

Probabilistic PCA

- Maximum likelihood solution of a probabilistic latent variable model.
- Probabilistic formulation allows us to deal with missing values in the data set.
- The probabilistic PCA model can be run generatively to provide samples from the distribution.
- Probabilistic PCA can be used to model class-conditional densities and hence be applied to classification problems.
- Latent variable $\mathbf{z}$ corresponding to the principal-component subspace.
- Gaussian prior distribution $p(\mathbf{z})$ over the latent variable, together with a Gaussian conditional distribution $p(\mathbf{x}/\mathbf{z})$ for the observed variable $\mathbf{x}$ conditioned on the value of the latent variable.

आई आई टी हैदराबाद
IIT Hyderabad

Probabilistic PCA

- Maximum likelihood solution of a probabilistic latent variable model.
- latent variable **z** corresponding to the principal-component subspace.
- Gaussian prior distribution *p*(**z**) over the latent variable, together with a Gaussian conditional distribution *p*(**x**/**z**) for the observed variable **x** conditioned on the value of the latent variable.

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}).$$

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

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

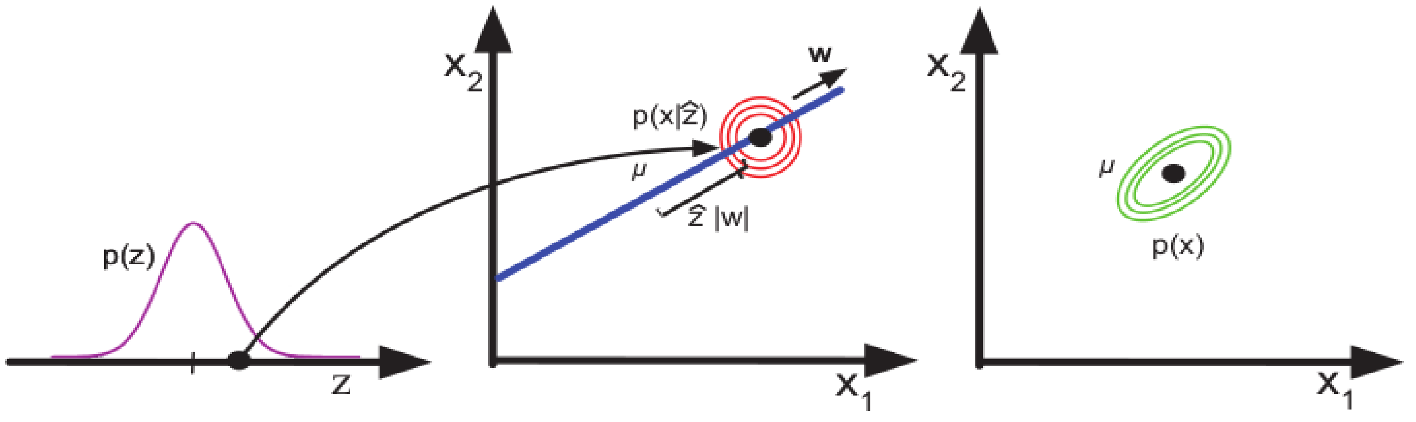
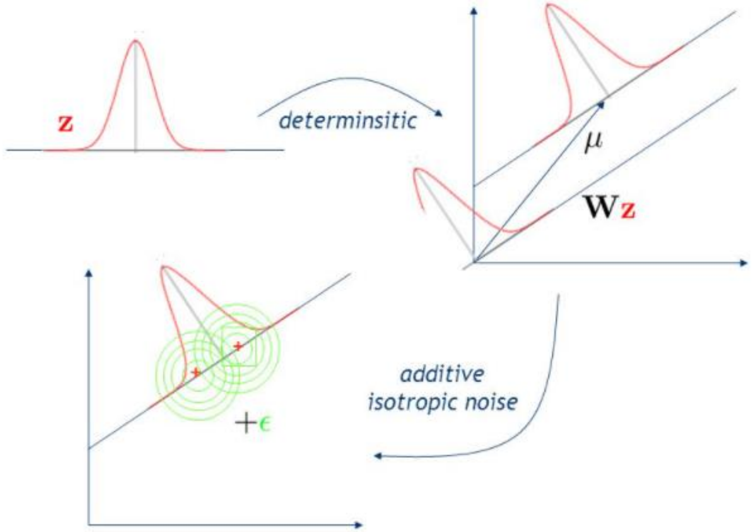


Figure 12.1 Illustration of the PPCA generative process, where we have $L = 1$ latent dimension generating $D = 2$ observed dimensions. Based on Figure 12.9 of (Bishop 2006b).



Probabilistic PCA

- Maximum likelihood solution of a probabilistic latent variable model.
- latent variable **z** corresponding to the principal-component subspace.
- Gaussian prior distribution *p*(**z**) over the latent variable, together with a Gaussian conditional distribution *p*(**x**/**z**) for the observed variable **x** conditioned on the value of the latent variable.

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

- columns of **W** span a linear subspace within the data space that corresponds to the principal subspace
- Generative view : sample a latent variable and then sampling the observed variable conditioned on this

Probabilistic PCA

- Maximum likelihood solution of a probabilistic latent variable model.
- latent variable **z** corresponding to the principal-component subspace.
- Gaussian prior distribution *p*(**z**) over the latent variable, together with a Gaussian conditional distribution *p*(**x**/**z**) for the observed variable **x** conditioned on the value of the latent variable.

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

- Parameter Estimation : maximum likelihood (marginal likelihood)

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})\,\mathrm{d}\mathbf{z}.$$

-

$$\begin{aligned}
\mathbb{E}[\mathbf{x}] &= \mathbb{E}[\mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}] = \boldsymbol{\mu} \\
\mathrm{cov}[\mathbf{x}] &= \mathbb{E}\left[(\mathbf{W}\mathbf{z} + \boldsymbol{\epsilon})(\mathbf{W}\mathbf{z} + \boldsymbol{\epsilon})^{\mathrm{T}}\right] \\
\mathbf{C} &= \mathbb{E}\left[\mathbf{W}\mathbf{z}\mathbf{z}^{\mathrm{T}}\mathbf{W}^{\mathrm{T}}\right] + \mathbb{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^{\mathrm{T}}] = \mathbf{W}\mathbf{W}^{\mathrm{T}} + \sigma^2\mathbf{I}
\end{aligned}$$

$$\boxed{p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{C})}$$

Probabilistic PCA

- Maximum likelihood solution of a probabilistic latent variable model.
- latent variable **z** corresponding to the principal-component subspace.
- Gaussian prior distribution *p*(**z**) over the latent variable, together with a Gaussian conditional distribution *p*(**x**/**z**) for the observed variable **x** conditioned on the value of the latent variable.

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}).$$

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

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

- Parameter Estimation : marginal likelihood

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})\,\mathrm{d}\mathbf{z}.$$

$$\boxed{p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{C})}$$

- Predictive distribution : finding z for an x

$$p(\mathbf{z}|\mathbf{x}) = \mathcal{N}\left(\mathbf{z}|\mathbf{M}^{-1}\mathbf{W}^{\mathrm{T}}(\mathbf{x} - \boldsymbol{\mu}), \sigma^{-2}\mathbf{M}\right).$$

Probabilistic PCA

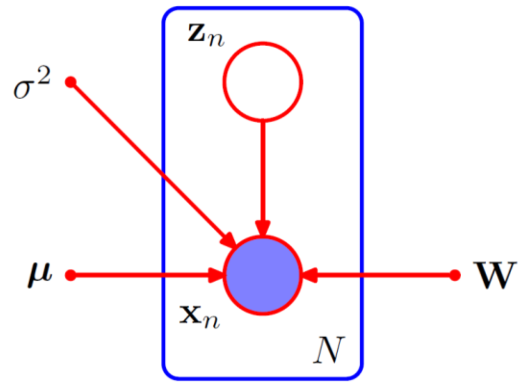
$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}).$$

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

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

$$\boxed{p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{C})}$$

$$\mathbf{C} = \mathbf{W}\mathbf{W}^{\mathrm{T}} + \sigma^2\mathbf{I}.$$



- Parameter Estimation : maximum likelihood
-

$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \mathbf{W}, \sigma^2) = \sum_{n=1}^{N} \ln p(\mathbf{x}_n|\mathbf{W}, \boldsymbol{\mu}, \sigma^2)$$

$$= \quad -\frac{ND}{2}\ln(2\pi) - \frac{N}{2}\ln|\mathbf{C}| - \frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu})^{\mathrm{T}}\mathbf{C}^{-1}(\mathbf{x}_n - \boldsymbol{\mu}).$$

$$\boldsymbol{\mu} = \overline{\mathbf{x}}$$

$$\ln p(\mathbf{X}|\mathbf{W}, \boldsymbol{\mu}, \sigma^2) = -\frac{N}{2}\left\{D\ln(2\pi) + \ln|\mathbf{C}| + \mathrm{Tr}\left(\mathbf{C}^{-1}\mathbf{S}\right)\right\}$$

$$\mathbf{S} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - \overline{\mathbf{x}})(\mathbf{x}_n - \overline{\mathbf{x}})^{\mathrm{T}}.$$

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

where $\mathbf{U}_M$ is a $D \times M$ matrix whose columns are given by top M eigenvectors of the data covariance matrix $\mathbf{S}$, the $M \times M$ diagonal matrix $\mathbf{L}_M$ has elements given by the corresponding eigenvalues λ_i, and $\mathbf{R}$ is an arbitrary $M \times M$ orthogonal matrix.