Latent Variable Models for Dimensionality Reduction

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Introduction to Machine Learning (CS771A)

October 4, 2018

Recap: Latent Variable Models, ALT-OPT, and EM

- We saw that doing MLE/MAP for latent variable models is difficult in general

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- For most models, arg max of CLL or expected CLL is usually much easier than arg max of ILL

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- ALT-OPT is an approx. of EM: Replaces posterior $p(\mathbf{Z}|\mathbf{X}, \Theta)$ by a point distribution at its mode

Brief Detour: Generative Stories

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- Note: If there are no labels or latent variables $\boldsymbol{z}_n$, then we will just have $\boldsymbol{x}_n \sim p(\boldsymbol{x}|\Theta)$

Generative Story: Some Common Examples

- Can have it if at least some part of the data is generated using a probability distribution

(Note: Generation of global parameters Θ not shown below)

Generative Classification (Gaussian Class-Conditionals)

- For $n = 1, \ldots, N$
  - Generate y_n as $y_n \sim \text{multinoulli}(\pi_1, \ldots, \pi_K)$
  - Generate $\boldsymbol{x}_n$ as $\boldsymbol{x}_n \sim \mathcal{N}(\mu_{y_n}, \Sigma_{y_n})$

Gaussian Mixture Model

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Probabilistic Dimensionality Reduction (Probabilistic PCA)
(assuming data and latent variables to be Gaussians)

- For $n = 1, \ldots, N$
  - Generate $\boldsymbol{z}_n$ as $\boldsymbol{z}_n \sim \mathcal{N}(0, \mathbf{I}_K)$
  - Generate $\boldsymbol{x}_n$ as $\boldsymbol{x}_n \sim \mathcal{N}(\mathbf{W}\boldsymbol{z}_n, \sigma^2 \mathbf{I}_D)$

Discriminative Models for Regression/Classification

- For $n = 1, \ldots, N$
  - Generate y_n as

$$y_n \sim \mathcal{N}(\boldsymbol{w}^\top \boldsymbol{x}_n, \sigma^2)$$
$$y_n \sim \text{Bernoulli}(\sigma(\boldsymbol{w}^\top \boldsymbol{x}_n))$$

x not modeled

- The model need not have latent variables (e.g. generative classification, discriminative models)

Latent Variable Models for Dimensionality Reduction

A Simple Model for Data Compression/Dimensionality-Reduction

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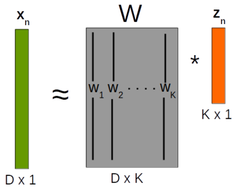

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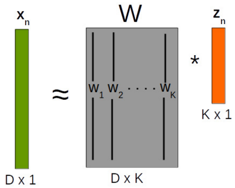

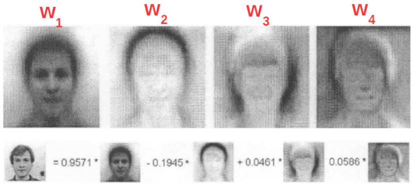

A Simple Model for Data Compression/Dimensionality-Reduction

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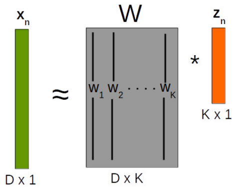

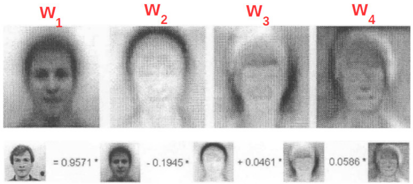

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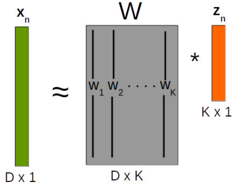

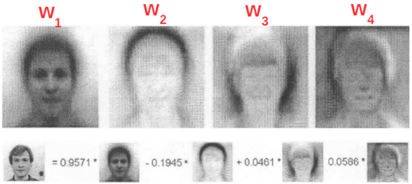

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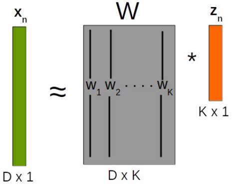

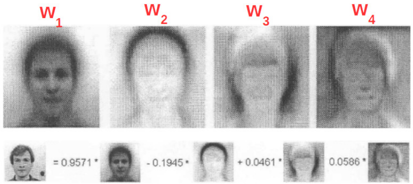

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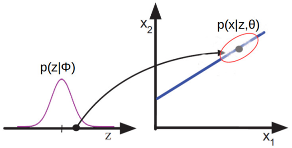

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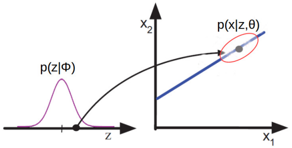

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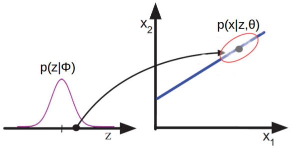

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  - The standard non-probabilistic PCA is a special case (probabilistic version has several advantages)

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- Suppose we're modeling D-dim data using a (say zero mean) Gaussian

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  - PPCA = Low-rank Gaussian. Fewer parameters to learn; less chance of overfitting

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- Many other benefits. For example, can do dim-red, even if $\boldsymbol{x}_n$ has part of it as missing.

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- Dimensionality reduction then simply boils down to solving the following problem

$$\{\hat{\mathbf{Z}}, \hat{\mathbf{W}}\} = \arg\min_{\mathbf{Z},\mathbf{W}} ||\mathbf{X} - \mathbf{Z}\mathbf{W}^\top||_F^2$$

(Alert: This is NOT doing MLE but $\arg\max \sum_{n=1}^{N} \log p(\boldsymbol{x}_n|\boldsymbol{z}_n)$)

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$$\mathcal{L}(\mathbf{Z}, \mathbf{W}, \sigma^2) = \frac{1}{2\sigma^2}\sum_{n=1}^{N}||\boldsymbol{x}_n - \mathbf{W}\boldsymbol{z}_n||^2 + \frac{ND}{2}\log(2\pi\sigma^2) \quad \text{(Exercise: Verify)}$$

$$= \frac{1}{2\sigma^2}||\mathbf{X} - \mathbf{Z}\mathbf{W}^\top||_F^2 + \frac{ND}{2}\log(2\pi\sigma^2) \quad (\mathbf{X} : N \times D, \mathbf{Z} : N \times K, \mathbf{W} : D \times K)$$

- Nice! So this loss is simply the reconstruction error. We can minimize it w.r.t. $\mathbf{Z}, \mathbf{W}, \sigma^2$
- For simplicity, let's treat σ^2 as a constant. Then the loss function will be

$$\mathcal{L}(\mathbf{Z}, \mathbf{W}) = ||\mathbf{X} - \mathbf{Z}\mathbf{W}^\top||_F^2$$

- Dimensionality reduction then simply boils down to solving the following problem

$$\{\hat{\mathbf{Z}}, \hat{\mathbf{W}}\} = \arg\min_{\mathbf{Z},\mathbf{W}} ||\mathbf{X} - \mathbf{Z}\mathbf{W}^\top||_F^2 \quad \text{(Alert: This is NOT doing MLE but } \arg\max \sum_{n=1}^{N} \log p(\boldsymbol{x}_n|\boldsymbol{z}_n)\text{)}$$

- Can solve it using ALT-OPT to solve it. Another (better) way will be to do a proper MLE using EM

Learning PPCA via ALT-OPT

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- Note that the problem is essentially a matrix factorization of $\mathbf{X}$

MLE for PPCA (or why it is hard..)

- To do MLE, we need to maximize $\log p(\mathbf{X}|\mathbf{W}, \sigma^2) = \sum_{n=1}^{N} \log p(\boldsymbol{x}_n|\mathbf{W}, \sigma^2)$ with $\boldsymbol{z}_n$ integrated out

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$$\log p(\mathbf{X}|\Theta) = -\frac{N}{2}(D \log 2\pi + \log |\mathbf{C}| + \text{trace}(\mathbf{C}^{-1}\mathbf{S}))$$

where $\mathbf{S}$ is the data covariance matrix, $\mathbf{C}^{-1} = \sigma^{-1}\mathbf{I} - \sigma^{-1}\mathbf{W}\mathbf{M}^{-1}\mathbf{W}^\top$ and $\mathbf{M} = \mathbf{W}^\top\mathbf{W} + \sigma^2\mathbf{I}$

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

$$\sigma_{ML}^2 = \frac{1}{D-K}\sum_{k=K+1}^{D}\lambda_k \quad \text{(noise variance = mean of “discarded” eigenvalues)}$$

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- Need to do eigen-decomposition of $D \times D$ data covariance matrix $\mathbf{S}$. EXPENSIVE!!!

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  - M Step: Maximize the expected complete data log-lik. (CLL) $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ w.r.t. Θ
- The CLL (and expected CLL) for PPCA has a simple expression. The CLL is

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

Learning PPCA via EM

- Instead of maximizing the ILL $\log p(\mathbf{X}|\mathbf{W},\sigma^2) = \mathcal{N}(0, \mathbf{W}\mathbf{W}^\top + \sigma^2\mathbf{I}_D)$, EM maximizes exp. CLL
- This is done by iterating between the following two steps
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- Using $p(\boldsymbol{x}_n|\boldsymbol{z}_n, \mathbf{W}, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{D/2}} \exp\left[-\frac{(\boldsymbol{x}_n - \mathbf{W}\boldsymbol{z}_n)^\top(\boldsymbol{x}_n - \mathbf{W}\boldsymbol{z}_n)}{2\sigma^2}\right]$

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$$\text{CLL} = -\sum_{n=1}^{N}\left\{\frac{D}{2}\log\sigma^2 + \frac{1}{2\sigma^2}||\boldsymbol{x}_n||^2 - \frac{1}{\sigma^2}\boldsymbol{z}_n^\top\mathbf{W}^\top\boldsymbol{x}_n + \frac{1}{2\sigma^2}\text{tr}(\boldsymbol{z}_n\boldsymbol{z}_n^\top\mathbf{W}^\top\mathbf{W}) + \frac{1}{2}\text{tr}(\boldsymbol{z}_n\boldsymbol{z}_n^\top)\right\} \quad \text{(Exercise: Verify)}$$

Learning PPCA via EM

- The expected complete data log-likelihood $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\mathbf{W}, \sigma^2)]$

$$= -\sum_{n=1}^{N}\left\{\frac{D}{2}\log\sigma^2 + \frac{1}{2\sigma^2}||\boldsymbol{x}_n||^2 - \frac{1}{\sigma^2}\mathbb{E}[\boldsymbol{z}_n]^\top\mathbf{W}^\top\boldsymbol{x}_n + \frac{1}{2\sigma^2}\text{tr}(\mathbb{E}[\boldsymbol{z}_n\boldsymbol{z}_n^\top]\mathbf{W}^\top\mathbf{W}) + \frac{1}{2}\text{tr}(\mathbb{E}[\boldsymbol{z}_n\boldsymbol{z}_n^\top])\right\}$$

Learning PPCA via EM

- The expected complete data log-likelihood $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\mathbf{W}, \sigma^2)]$

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- Taking the derivative of $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\mathbf{W}, \sigma^2)]$ w.r.t. $\mathbf{W}$ and setting to zero

$$\boxed{\mathbf{W} = \left[\sum_{n=1}^{N} \boldsymbol{x}_n \mathbb{E}[\boldsymbol{z}_n]^\top \right] \left[\sum_{n=1}^{N} \mathbb{E}[\boldsymbol{z}_n \boldsymbol{z}_n^\top] \right]^{-1}}$$

(Exercise: verify; can also be done "online")

Learning PPCA via EM

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Learning PPCA via EM

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Learning PPCA via EM

- The expected complete data log-likelihood $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\mathbf{W}, \sigma^2)]$

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Learning PPCA via EM

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Learning PPCA via EM

- The expected complete data log-likelihood $\mathbb{E}[\log p(\mathbf{X},\mathbf{Z}|\mathbf{W},\sigma^2)]$

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\end{aligned}$$

Learning PPCA via EM

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- Note: The noise variance σ^2 can also be estimated (take deriv., set to zero..)

Summary: The Full EM Algorithm for PPCA

- Specify K, initialize $\mathbf{W}$ and σ^2 randomly. Also center the data $(\boldsymbol{x}_n = \boldsymbol{x}_n - \frac{1}{N}\sum_{n=1}^{N}\boldsymbol{x}_n)$

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- **M step:** Re-estimate $\mathbf{W}$ and σ^2

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\end{aligned}
$$

- **M step:** Re-estimate $\mathbf{W}$ and σ^2

$$
\mathbf{W}_{new} = \left[\sum_{n=1}^{N}\boldsymbol{x}_n\mathbb{E}[\boldsymbol{z}_n]^\top\right]\left[\sum_{n=1}^{N}\mathbb{E}[\boldsymbol{z}_n\boldsymbol{z}_n^\top]\right]^{-1}
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p(\boldsymbol{z}_n|\boldsymbol{x}_n, \mathbf{W}) &= \mathcal{N}(\mathbf{M}^{-1}\mathbf{W}^\top \boldsymbol{x}_n, \sigma^2\mathbf{M}^{-1}) \qquad \text{where } \mathbf{M} = \mathbf{W}^\top\mathbf{W} + \sigma^2\mathbf{I}_K \\
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\mathbb{E}[\boldsymbol{z}_n\boldsymbol{z}_n^\top] &= \text{cov}(\boldsymbol{z}_n) + \mathbb{E}[\boldsymbol{z}_n]\mathbb{E}[\boldsymbol{z}_n]^\top = \mathbb{E}[\boldsymbol{z}_n]\mathbb{E}[\boldsymbol{z}_n]^\top + \sigma^2\mathbf{M}^{-1}
\end{aligned}
$$

- **M step:** Re-estimate $\mathbf{W}$ and σ^2

$$
\begin{aligned}
\mathbf{W}_{new} &= \left[\sum_{n=1}^{N} \boldsymbol{x}_n \mathbb{E}[\boldsymbol{z}_n]^\top\right]\left[\sum_{n=1}^{N} \mathbb{E}[\boldsymbol{z}_n\boldsymbol{z}_n^\top]\right]^{-1} \\
\sigma^2_{new} &= \frac{1}{ND}\sum_{n=1}^{N}\left\{||\boldsymbol{x}_n||^2 - 2\mathbb{E}[\boldsymbol{z}_n]^\top \mathbf{W}_{new}^\top \boldsymbol{x}_n + \text{tr}\left(\mathbb{E}[\boldsymbol{z}_n\boldsymbol{z}_n^\top]\mathbf{W}_{new}^\top\mathbf{W}_{new}\right)\right\}
\end{aligned}
$$

Summary: The Full EM Algorithm for PPCA

- Specify K, initialize $\mathbf{W}$ and σ^2 randomly. Also center the data ($\boldsymbol{x}_n = \boldsymbol{x}_n - \frac{1}{N}\sum_{n=1}^{N}\boldsymbol{x}_n$)
- **E step:** For each n, compute $p(\boldsymbol{z}_n|\boldsymbol{x}_n)$ using current $\mathbf{W}$ and σ^2. Compute exp. for the M step

$$\begin{aligned} p(\boldsymbol{z}_n|\boldsymbol{x}_n, \mathbf{W}) &= \mathcal{N}(\mathbf{M}^{-1}\mathbf{W}^\top \boldsymbol{x}_n, \sigma^2\mathbf{M}^{-1}) \qquad \text{where } \mathbf{M} = \mathbf{W}^\top\mathbf{W} + \sigma^2\mathbf{I}_K \\ \mathbb{E}[\boldsymbol{z}_n] &= \mathbf{M}^{-1}\mathbf{W}^\top\boldsymbol{x}_n \\ \mathbb{E}[\boldsymbol{z}_n\boldsymbol{z}_n^\top] &= \text{cov}(\boldsymbol{z}_n) + \mathbb{E}[\boldsymbol{z}_n]\mathbb{E}[\boldsymbol{z}_n]^\top = \mathbb{E}[\boldsymbol{z}_n]\mathbb{E}[\boldsymbol{z}_n]^\top + \sigma^2\mathbf{M}^{-1} \end{aligned}$$

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- Set $\mathbf{W} = \mathbf{W}_{new}$ and $\sigma^2 = \sigma^2_{new}$. If not converged (monitor $p(\mathbf{X}|\Theta)$), go back to E step

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$$

- Set $\mathbf{W} = \mathbf{W}_{new}$ and $\sigma^2 = \sigma^2_{new}$. If not converged (monitor $p(\mathbf{X}|\Theta)$), go back to E step
- **Note:** For $\sigma^2 = 0$, this EM algorithm can also be used to efficiently solve standard PCA (note that this EM algorithm doesn't require any eigen-decomposition)