

Latent Variable Models for Dimensionality Reduction

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

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

$$\begin{aligned}\Theta = \arg \max_{\Theta} \log p(\mathbf{X}|\Theta) &= \arg \max_{\Theta} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) \quad (\text{if } \mathbf{Z} \text{ is discrete}) \\ &= \arg \max_{\Theta} \log \int_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) d\mathbf{Z} \quad (\text{if } \mathbf{Z} \text{ is continuous})\end{aligned}$$

- We saw that ALT-OPT and EM can be two ways to make MLE/MAP easier in such models
- At a high-level, they solve for the MLE of Θ by solving a slightly modified problem

$$\text{ALT-OPT: } \hat{\Theta} = \arg \max_{\Theta} \log p(\mathbf{X}, \hat{\mathbf{Z}}|\Theta) \quad (\text{where } \hat{\mathbf{Z}} \text{ is a "good" estimate of } \mathbf{Z})$$

$$\text{EM: } \hat{\Theta} = \arg \max_{\Theta} \mathbb{E}_{p(\mathbf{Z}|\mathbf{X}, \Theta)} [\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$$

- But since \mathbf{Z} and Θ are usually “coupled”, both ALT-OPT and EM need an **alternating procedure**
- Instead of maximizing $\log p(\mathbf{X}|\Theta)$ (**incomplete-data log-lik - ILL**), they maximize $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ (**complete-data log-lik - CLL**) or expected CLL
- For most models, $\arg \max$ of CLL or expected CLL is usually much easier than $\arg \max$ of ILL

Recap: ALT-OPT and EM

- ALT-OPT does the following
 - ① Initialize $\Theta = \hat{\Theta}$
 - ② Estimate \mathbf{Z} as $\hat{\mathbf{Z}} = \arg \max_{\mathbf{Z}} \log p(\mathbf{Z}|\mathbf{X}, \hat{\Theta})$
 - ③ Estimate Θ as $\hat{\Theta} = \arg \max_{\Theta} \log p(\mathbf{X}, \hat{\mathbf{Z}}|\Theta)$
 - ④ Go to step 2 if not converged
- Step 2 (arg max) of ALT-OPT could potentially **throw away a lot of information** about \mathbf{Z}
- EM addresses it using “soft” version of ALT-OPT
 - ① Initialize $\Theta = \hat{\Theta}$
 - ② Compute the **posterior distribution of \mathbf{Z} , i.e., $p(\mathbf{Z}|\mathbf{X}, \hat{\Theta})$**
 - ③ Estimate Θ by maximizing the expected CLL $\hat{\Theta} = \mathbb{E}_{p(\mathbf{Z}|\mathbf{X}, \hat{\Theta})}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$
 - ④ Go to step 2 if not converged
- 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



Generative Stories..

- Most probabilistic models we've seen can be described by an imaginative “generative story”
- In this story, we first generate everything that the data depends on, and then generate the data
- Here is a brief outline of what this story looks like

- 1 Generate all the global model parameters Θ

$$\Theta \sim p(\Theta)$$

- 2 For $n = 1, \dots, N$

$$\begin{aligned} z_n &\sim p(z|\Theta) && (z_n \text{ can be an observed label } y_n \text{ or a latent variable, e.g., cluster id}) \\ x_n &\sim p(x|z = z_n, \Theta) && (x_n \text{ is generated conditioned on } z_n) \end{aligned}$$

- This procedure generates $\{(x_n, z_n)\}_{n=1}^N$ from the joint distribution $p(x, z|\Theta) = p(z|\Theta)p(x|z, \Theta)$
- Note: In this story, we don't show step 1 if we aren't using any prior distribution on Θ
- Note: If there are no labels or latent variables z_n , then we will just have $x_n \sim p(x|\Theta)$



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

Gaussian Mixture Model

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

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

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

Discriminative Models for Regression/Classification

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

$$\begin{aligned} y_n &\sim \mathcal{N}(\mathbf{w}^\top \mathbf{x}_n, \sigma^2) \\ y_n &\sim \text{Bernoulli}(\sigma(\mathbf{w}^\top \mathbf{x}_n)) \end{aligned}$$

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

- Consider a set of observations $\mathbf{x}_1, \dots, \mathbf{x}_N$, with $\mathbf{x}_n \in \mathbb{R}^D$
- Let's approximate each \mathbf{x}_n by a **linear combination** of K vectors $\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_K$ ($K \ll D$)

$$\mathbf{x}_n \approx \sum_{k=1}^K z_{nk} \mathbf{w}_k \quad \text{or} \quad \mathbf{x}_n \approx \mathbf{W} \mathbf{z}_n$$

where $\mathbf{W} = [\mathbf{w}_1 \dots \mathbf{w}_K]$ is $D \times K$, each $\mathbf{w}_k \in \mathbb{R}^D$, and $\mathbf{z}_n = [z_{n1} \dots z_{nK}] \in \mathbb{R}^K$



- z_{nk} tell us much of “component” \mathbf{w}_k is present in the observation \mathbf{x}_n
- Can think of $\mathbf{z}_n \in \mathbb{R}^K$ as a “**compressed**” latent representation of $\mathbf{x}_n \in \mathbb{R}^D$
- A good compression \mathbf{z}_n will be one for which \mathbf{x}_n is as close as possible to $\mathbf{W} \mathbf{z}_n$

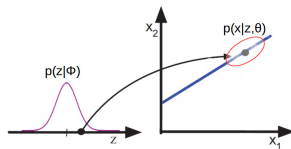
Dimensionality Reduction: The Probabilistic/Generative View

- In the linear model, we represented \mathbf{x}_n approximately as $\mathbf{x}_n \approx \mathbf{W}\mathbf{z}_n$
- The probabilistic view: Model \mathbf{x}_n by a D -dim Gaussian with mean vector $\mathbf{W}\mathbf{z}_n$

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

$$\text{Equivalently: } \mathbf{x}_n = \mathbf{W}\mathbf{z}_n + \epsilon_n \text{ where } \epsilon_n \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_D)$$

- Let's assume a prior $p(\mathbf{z}_n) = \mathcal{N}(\mathbf{0}, \mathbf{I}_K)$ on the latent variable \mathbf{z}_n
- A low-dim latent variable \mathbf{z}_n transformed to “generate” a high-dim observation \mathbf{x}_n
- This is a “reverse” way of thinking: A generative model for dimensionality reduction



- This model is popularly known as Probabilistic Principal Component Analysis (PPCA)
 - The standard non-probabilistic PCA is a special case (probabilistic version has several advantages)

Some More Motivation for PPCA..

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

$$p(\mathbf{x}) = \mathcal{N}(0, \mathbf{\Sigma})$$

where $\mathbf{\Sigma}$ is a $D \times D$ p.s.d. cov. matrix, $\mathcal{O}(D^2)$ parameters needed

- Consider modeling the same data using PPCA: $p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{W}\mathbf{z}, \sigma^2\mathbf{I}_D)$, $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}_K)$
- For this Gaussian PPCA, the marginal distribution $p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z})d\mathbf{z}$ is

$$p(\mathbf{x}|\mathbf{W}, \sigma^2) = \mathcal{N}(0, \mathbf{W}\mathbf{W}^\top + \sigma^2\mathbf{I}_D) \quad (\text{using Gaussian marginal results})$$

- Cov. matrix is close to low-rank as $\sigma^2 \rightarrow 0$. Only $(DK + 1)$ parameters needed (nice when $D \gg N$)
 - PPCA = Low-rank Gaussian. Fewer parameters to learn; less chance of overfitting



Benefits of Generative Models for Dimensionality Reduction

- One benefit: Once the model parameters are learned, we can even **generate new data**, e.g.,
 - Generate a random \mathbf{z} using the distribution $\mathcal{N}(\mathbf{0}, \mathbf{I}_K)$
 - Generate \mathbf{x} conditioned on this \mathbf{z} from $\mathcal{N}(\mathbf{W}\mathbf{z}, \sigma^2 \mathbf{I}_D)$



(a) Training data



(b) Random samples

- Note: The above random samples are generated using a slightly more sophisticated latent variable model (VAE with ALI-BiGAN inference), not the simple PPCA (but it is similar in spirit to PPCA).
- Many other benefits. For example, can do dim-red, even if \mathbf{x}_n has part of it as missing.



Learning the PPCA Model

- Since we are doing dim-red, the goal is to “recover” \mathbf{z}_n (and \mathbf{W}, σ^2) given $\mathbf{x}_n, \forall n$
- The likelihood $p(\mathbf{x}_n|\mathbf{z}_n) = \mathcal{N}(\mathbf{W}\mathbf{z}_n, \sigma^2\mathbf{I}_D)$ is Gaussian. The loss function = NLL will be

$$\begin{aligned}\mathcal{L}(\mathbf{Z}, \mathbf{W}, \sigma^2) &= \frac{1}{2\sigma^2} \sum_{n=1}^N \|\mathbf{x}_n - \mathbf{W}\mathbf{z}_n\|^2 + \frac{ND}{2} \log(2\pi\sigma^2) \quad (\text{Exercise: Verify}) \\ &= \frac{1}{2\sigma^2} \|\mathbf{X} - \mathbf{Z}\mathbf{W}^\top\|_F^2 + \frac{ND}{2} \log(2\pi\sigma^2) \quad (\mathbf{X} : N \times D, \mathbf{Z} : N \times K, \mathbf{W} : D \times K)\end{aligned}$$

- 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

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

- 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

- We saw that the PPCA problem reduced to

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

- The ALT-OPT algorithm for PPCA will alternate between the following two steps

- 1 Initialize $\mathbf{Z} = \hat{\mathbf{Z}}$
 - 2 Solve $\hat{\mathbf{W}} = \arg \min_{\mathbf{W}} \|\mathbf{X} - \hat{\mathbf{Z}}\mathbf{W}^T\|_F^2$
 - 3 Solve $\hat{\mathbf{Z}} = \arg \min_{\mathbf{Z}} \|\mathbf{X} - \mathbf{Z}\hat{\mathbf{W}}^T\|_F^2$
 - 4 Go to step 2 if not yet converged
- Step 2 is just like **multi-output regression** with $\hat{\mathbf{Z}}$ as **feature matrix** and \mathbf{X} as **label matrix**
 - Step is also like multi-output regression
 - 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 $\log p(\mathbf{X}|\mathbf{W}, \sigma^2) = \sum_{n=1}^N \log p(\mathbf{x}_n|\mathbf{W}, \sigma^2)$ with \mathbf{z}_n integrated out
- MLE on the objective $p(\mathbf{x}_n|\mathbf{W}, \sigma^2)$ can be done but turns out to be a bit expensive. In particular:

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

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

- The MLE solution is given by (don't worry about the proof)[†]

$$\begin{aligned}\mathbf{W}_{ML} &= \mathbf{U}_K(\mathbf{L}_K - \sigma_{ML}^2\mathbf{I})^{1/2}\mathbf{R} \\ \sigma_{ML}^2 &= \frac{1}{D-K} \sum_{k=K+1}^D \lambda_k \quad (\text{noise variance} = \text{mean of "discarded" eigenvalues})\end{aligned}$$

where \mathbf{U}_K is $D \times K$ matrix of **top K eigvecs** of \mathbf{S} , \mathbf{L}_K : $K \times K$ diagonal matrix of **top K eigvals** $\lambda_1, \dots, \lambda_K$, \mathbf{R} is a $K \times K$ **arbitrary rotation matrix** (equivalent to PCA for $\mathbf{R} = \mathbf{I}$ and $\sigma^2 \rightarrow 0$)

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

[†] Probabilistic Principal Component Analysis (Tipping and Bishop, 1999)



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
 - E Step: Infer the **posterior** $p(\mathbf{z}_n|\mathbf{x}_n)$ given current estimate of $\Theta = (\mathbf{W}, \sigma^2)$ (needed for expectations)

$$p(\mathbf{z}_n|\mathbf{x}_n, \mathbf{W}, \sigma^2) = \mathcal{N}(\mathbf{M}^{-1}\mathbf{W}^\top \mathbf{x}_n, \sigma^2\mathbf{M}^{-1}) \quad (\text{where } \mathbf{M} = \mathbf{W}^\top \mathbf{W} + \sigma^2\mathbf{I}_K)$$

- 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
$$\log p(\mathbf{X}, \mathbf{Z}|\mathbf{W}, \sigma^2) = \log \prod_{n=1}^N p(\mathbf{x}_n, \mathbf{z}_n|\mathbf{W}, \sigma^2) = \log \prod_{n=1}^N p(\mathbf{x}_n|\mathbf{z}_n, \mathbf{W}, \sigma^2)p(\mathbf{z}_n) = \sum_{n=1}^N \{\log p(\mathbf{x}_n|\mathbf{z}_n, \mathbf{W}, \sigma^2) + \log p(\mathbf{z}_n)\}$$
- Using $p(\mathbf{x}_n|\mathbf{z}_n, \mathbf{W}, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{D/2}} \exp\left[-\frac{(\mathbf{x}_n - \mathbf{W}\mathbf{z}_n)^\top (\mathbf{x}_n - \mathbf{W}\mathbf{z}_n)}{2\sigma^2}\right]$ and $p(\mathbf{z}_n) \propto \exp\left[-\frac{\mathbf{z}_n^\top \mathbf{z}_n}{2}\right]$ and simplifying

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

Learning PPCA via EM

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

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

- 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

$$\mathbf{W} = \left[\sum_{n=1}^N \mathbf{x}_n \mathbb{E}[\mathbf{z}_n]^\top \right] \left[\sum_{n=1}^N \mathbb{E}[\mathbf{z}_n \mathbf{z}_n^\top] \right]^{-1} \quad (\text{Exercise: verify; can also be done "online"})$$

- To compute \mathbf{W} , we need two posterior expectations $\mathbb{E}[\mathbf{z}_n]$ and $\mathbb{E}[\mathbf{z}_n \mathbf{z}_n^\top]$
- These can be easily obtained from the posterior $p(\mathbf{z}_n|\mathbf{x}_n)$ computed in E step

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

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

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

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

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

- Set $\mathbf{W} = \mathbf{W}_{new}$ and $\sigma^2 = \sigma_{new}^2$. 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)

