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Mixture Models

A mixture model is a probabilistic clustering model with the following marginal distribution over the observed data:

$$P(\mathbf{X} = \mathbf{x}|\theta) = \sum_{z=1}^{K} P(\mathbf{X} = \mathbf{x}|Z = z, \theta_z) P(Z = z|\pi)$$

■ Here, $Z \in \{1, ..., K\}$ is a discrete random variables that takes one of K discrete values.

Mixture Models and Clusters

- Mixture models are well suited to modeling data that matches the cluster assumption.
- The parameters of basic mixture component distributions $P(\mathbf{X} = \mathbf{x}|Z = z, \theta_z)$ can typically be thought of as "prototypes" for data generated from the corresponding cluster.
- In a Gaussian mixture model, for example, data are generated by selecting a mixture component z, and then adding (correlated) noise to the mean parameters.
- This generates clumps of data around the mean of each component.

Mixture Models and Manifolds

- When data instead fall on a low dimensional manifold instead of around a discrete collection of prototypes, mixture models can still be used as universal density models.
- However, it may take a very large number of mixture components to adequately approximate a probability density defined on a manifold.
- In these cases, models designed specifically for manifolds typically give better results.
- We will begin with the case of linear manifolds.

Factor Analysis

- Factor analysis is a classical statistical model for linear manifolds based on the multivariate normal distribution.
- The model asserts that real-valued data $\mathbf{x} \in \mathbb{R}^D$ are generated in a two stage process that starts by first generating a low-dimensional latent factor vector $\mathbf{z} \in \mathbb{R}^K$ from a multivariate normal distribution.
- The observed x's are then generated by a linear combination of basis vectors weighted by the latent factor values: Wz with independent Gaussian noise added.

Factor Analysis: Probabilistic Model

■ The probabilistic model for factor analysis is shown below:

$$\begin{split} P(\mathbf{X} = \mathbf{x}, \mathbf{Z} = \mathbf{z}) &= P(\mathbf{X} = \mathbf{x} | \mathbf{Z} = \mathbf{z}) P(\mathbf{Z} = \mathbf{z}) \\ P(\mathbf{Z} = \mathbf{z}) &= \mathcal{N}(\mathbf{z}; \mu_0, \Sigma_0) \\ P(\mathbf{X} = \mathbf{x} | \mathbf{Z} = \mathbf{z}) &= \mathcal{N}(\mathbf{x}; \mathbf{W}\mathbf{z} + \mu, \Psi) \end{split}$$

- We typically assume that the latent mean $\mu_0 = 0$, and that the latent covariance matrix Σ_0 is the identity matrix.
- We also typically assume that Ψ is a postive, diagonal matrix and that the data set mean has been removed so that $\mu = 0$.

Factor Analysis: Marginal Distribution

■ The marginal distribution of **X** is is given by:

$$P(\mathbf{X} = \mathbf{x}) = \int \mathcal{N}(\mathbf{x}; \mathbf{Wz}, \Psi) \mathcal{N}(\mathbf{z}; 0, I) d\mathbf{z}$$
$$= \mathcal{N}(\mathbf{x}; 0, \mathbf{WW}^T + \Psi)$$

Thus, to learn the factor analysis model, we need to maximize the log marginal likelihood:

$$\mathcal{L}(\mathcal{D}, \theta) = -\frac{N}{2} \log(|2\pi (\mathbf{W}\mathbf{W}^T + \Psi)|) - \frac{1}{2} \mathbf{x}_n^T (\mathbf{W}\mathbf{W}^T + \Psi)^{-1} \mathbf{x}_n$$

Factor Analysis: Learning

- As with mixture models, we can simply maximize the sum of the log marginal likelihoods over a data set to learn the model parameters μ , Ψ and **W**. However, we can again obtain an EM algorithm based on Jensen's inequality and lower bound optimization.
- The E-step again requires the posterior over the latent variables $q_n(\mathbf{z}) = P(\mathbf{Z} = \mathbf{z} | \mathbf{X} = \mathbf{x}_n)$. We have:

$$P(\mathbf{z}|\mathbf{x}_n) = \mathcal{N}(\mathbf{z}; \mathbf{m}_n, \Sigma_n)$$

$$\Sigma_n = (I + \mathbf{W}^T \Psi \mathbf{W})^{-1}$$

$$\mathbf{m}_n = \Sigma_n \mathbf{W}^T \Psi^{-1}(\mathbf{x}_n - \mu)$$

Factor Analysis: Learning

■ The M-Step updates are given by:

$$\mathbf{W} = \left(\sum_{n=1}^{N} \mathbf{x}_{n} \mathbf{m}_{n}^{T}\right) \left(\sum_{n=1}^{N} \mathbb{E}_{q_{n}}[\mathbf{z} \mathbf{z}^{T} | \mathbf{x}_{n}]\right)^{-1}$$

$$\Psi = \frac{1}{N} \operatorname{diag} \left(\sum_{n=1}^{N} (\mathbf{x}_{n} - \mathbf{W} \mathbf{m}_{n}) \mathbf{x}_{n}^{T}\right)$$

Latent Linear Models for Real Data

■ The basic model architecture for factor analysis is shown below.

Generalizing Inputs 00000

$$P(\mathbf{Z} = \mathbf{z}) = \mathcal{N}(\mathbf{z}; \mu_0, \Sigma_0)$$

$$P(\mathbf{X} = \mathbf{x} | \mathbf{Z} = \mathbf{z}) = \mathcal{N}(\mathbf{x}; \mathbf{W}\mathbf{z} + \mu, \Psi)$$

- The next question is, how can we model data that are not real-valued?
- One answer is to merge ideas from latent linear models with ideas from generalized linear models.

Generalized Latent Linear Models

■ This model class retains the normal distribution on **Z**, but models $\mathbf{X} = [X_1, ..., X_D]$ using generalized linear models.

Generalizing Inputs 00000

For example, we can model Binary data using a Bernoulli-Logistic model for $P(X_d = x_d | \mathbf{Z} = \mathbf{z})$:

$$\theta_{d|z} = \frac{1}{1 + \exp(-\mathbf{W}_d \mathbf{z})}$$

$$P(x_d|\mathbf{z}) = \theta_{d|z}^{x_d} (1 - \theta_{d|z})^{(1 - x_d)}$$

$$P(\mathbf{x}|\mathbf{z}) = \prod_{d=1}^{D} P(x_d|\mathbf{z})$$

Exponential Family Factor Analysis

- In general, we can let $P(X_d = x_d | \mathbf{Z} = \mathbf{z})$ be an exponential family GLM of a type that matches x_d .
- The resulting model is called *Exponential Family Factor* Analysis or Exponential Family Principal Components Analysis.

Generalizing Inputs 00000

■ However, this model class has several significant issues that derive from the fact that $P(\mathbf{X} = \mathbf{x})$ can often not be computed analytically due to the intractability of the following integral:

$$P(\mathbf{X} = \mathbf{x}) = \int \prod_{d=1}^{D} P(\mathbf{x}_{d} | \mathbf{z}) \mathcal{N}(\mathbf{z}; 0, I) d\mathbf{z}$$

As a result, $P(\mathbf{Z}|\mathbf{X} = \mathbf{x})$ is not computable and direct marginal likelihood maximization and exact EM break.

Learning Exponential Family Factor Analysis

As a result, it is generally only possible to approximately learn an exponential family factor analysis model using maximum likelihood.

Generalizing Inputs 00000

Another approach is to modify the learning criteria. Instead of aiming to optimize $\mathcal{L}(\mathcal{D}, \theta) = \sum_{n=1}^{N} \log P(\mathbf{X} = \mathbf{x}_n | \theta)$, we can optimize the function below over $\mathbf{z}_{1:N}$ and θ :

$$\mathcal{J}(\mathcal{D}, \mathbf{z}_{1:N}, \theta) = \sum_{n=1}^{N} \log P(\mathbf{X} = \mathbf{x}_n, \mathbf{Z} = \mathbf{z}_n | \theta)$$

Learning Exponential Family Factor Analysis

■ The loss function $\mathcal{J}(\mathcal{D}, \mathbf{z}_{1:N}, \theta)$ treats the latent variables $\mathbf{z}_{1:N}$ as another set of model parameters to learn and optimizes them.

Generalizing Inputs 00000

- This removes the issues with integrating over **z**, generally making the objective function easy to learn with off-the-shelf optimization tools.
- However, optimizing the **z**'s instead of integrating over them has the downside of collapsing uncertainty.
- Effectively, learning concentrates on the most likely value of each \mathbf{z}_n only.

■ The basic model architecture for generalized factor analysis is shown below.

$$P(\mathbf{Z} = \mathbf{z}) = \mathcal{N}(\mathbf{z}; \mu_0, \Sigma_0)$$

 $P(\mathbf{X} = \mathbf{x} | \mathbf{Z} = \mathbf{z}) = \prod_{d=1}^{D} P(x_d | \mathbf{z})$

• We can easily change the model to use different types of latent variables by changing $P(\mathbf{Z} = \mathbf{z})$ to a different probability distribution.

As in factor analysis, we keep the latent variables independent of each other resulting in the following generalized model:

$$P(\mathbf{Z} = \mathbf{z}) = \prod_{k=1}^{K} P(z_k)$$

$$P(\mathbf{X} = \mathbf{x} | \mathbf{Z} = \mathbf{z}) = \prod_{d=1}^{D} P(x_d | \mathbf{z})$$

- For example, we can let $P(z_k) = \pi_k^{z_k} (1 \pi_k)^{(1 z_k)}$ to obtain a model with binary latent factors.
- If we let $P(z_k)$ be a Laplace distribution and $P(x_d|\mathbf{z})$ be a normal distribution, the model is equivalent to Sparse Coding.

Latent Linear Models with Alternate Latent Variables

- For real-valued latent factors, the marginal likelihood and posterior may or may not be computable in closed form.
- When the marginal likelihood and posterior are not computable in closed form, optimization of the latent variables can be used (this is what the sparse coding learning algorithm does).
- A different problem arises with finite discrete latent variables (binary, categorical) where the marginal probability switches from an integral to a sum:

$$P(\mathbf{X} = \mathbf{x}) = \sum_{z_1 \in \mathcal{Z}} \cdots \sum_{z_K \in \mathcal{Z}} \prod_{d=1}^D P(x_d | \mathbf{z}) \prod_{k=1}^K P(z_k)$$

- This sum is computable in theory, but can take exponential time to compute.
- Note that we can't use the trick of optimizing the z's because that is now a discrete optimization problem that also requires exponential time.
- In this model class, with discrete \mathbf{z} 's, the posterior $P(\mathbf{Z}|\mathbf{X} = \mathbf{x})$ also typically takes exponential time to compute.
- For all of these reasons, learning in this model class is quite difficult and requires some significant approximations.
- As a result, other model structures are typically used when discrete latent variables are of interest.