CEE 616: Probabilistic Machine Learning

M5 Unsupervised Learning:
5B: Factor Analysis and Autoencoders

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Outline

1. Factor analysis
2. FA Estimation
3. Autoencoders
4. AE variants
5. Outlook

Factor analysis model

- Basic idea: there are latent (hidden) **common factors** $\boldsymbol{z}$ underlying some multivariate observations $\boldsymbol{x}_n \in \mathbb{R}^D$

Factor analysis (FA) is a latent variable generative model specified as:

$$
\begin{aligned}
p(\boldsymbol{z}) &= \mathcal{N}(\boldsymbol{z}|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0) &(1)\\
p(\boldsymbol{x}|\boldsymbol{z}, \boldsymbol{\theta}) &= \mathcal{N}(\boldsymbol{x}|\boldsymbol{W}\boldsymbol{z} + \boldsymbol{\mu}, \boldsymbol{\Psi}) &(2)
\end{aligned}
$$

where:

- $\boldsymbol{z}$: latent vector
- $\boldsymbol{W}$: factor loading matrix, $D \times L$
- $\boldsymbol{\Psi}$: diagonal covariance matrix, $D \times D$

Induced marginal distribution

$$
\begin{aligned}
p(\boldsymbol{x}|\boldsymbol{\theta}) &= \int \mathcal{N}(\boldsymbol{x}|\boldsymbol{W}\boldsymbol{z} + \boldsymbol{\mu}, \boldsymbol{\Psi})\mathcal{N}(\boldsymbol{z}|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)d\boldsymbol{z} & (3)\\
&= \mathcal{N}(\boldsymbol{x}|\underbrace{\boldsymbol{W}\boldsymbol{\mu}_0 + \boldsymbol{\mu}}_{\text{mean}}, \underbrace{\boldsymbol{\Psi} + \boldsymbol{W}\boldsymbol{\Sigma}_0\boldsymbol{W}^\top}_{\text{variance}}) & (4)
\end{aligned}
$$

Simplifications:

- $\boldsymbol{\mu}_0 \to \boldsymbol{0}$
- $\boldsymbol{\Sigma}_0 \to \boldsymbol{I}$

The simplified marginal distribution then becomes:

$$
p(\boldsymbol{x}|\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{\Psi}) \tag{5}
$$

Generative model simplified

$$
\begin{aligned}
\text{[Prior]} \quad p(\boldsymbol{z}) &= \mathcal{N}(\boldsymbol{z}|\mathbf{0}, \boldsymbol{I}) && (6) \\
\text{[Likelihood]} \quad p(\boldsymbol{x}|\boldsymbol{z}) &= \mathcal{N}(\boldsymbol{x}|\boldsymbol{W}\boldsymbol{z} + \boldsymbol{\mu}, \boldsymbol{\Psi}) && (7) \\
\text{[Evidence/marginal]} \quad p(\boldsymbol{x}) &= \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{\Psi}) && (8)
\end{aligned}
$$

What FA does

It approximates the covariance matrix of the visible/observed vector $\boldsymbol{x}$ using a low-rank decomposition:

$$\boldsymbol{C} = \mathrm{Cov}[\boldsymbol{x}] = \underbrace{\boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{\Psi}}_{\text{low-rank decomp}} \tag{9}$$

- $\boldsymbol{W}\boldsymbol{W}^\top$ is $D \times D$ (recall: $\boldsymbol{W} \in \mathbb{R}^{D\times L}$)
- $\boldsymbol{\Psi}$ is $D \times D$ (restricted to be diagonal)
- For each variable x_d, the **marginal variance** (each diagonal term in $\boldsymbol{C}$) is given by:

$$\mathbb{V}[x_d] = \sum_{k=1}^{L} \underbrace{w_{dk}^2}_{\text{common}} + \underbrace{\psi_d}_{\text{unique}} \tag{10}$$

Parameters to be estimated

The unknown parameters in FA are:

- $\boldsymbol{W}$: factor loading matrix
- $\boldsymbol{\Psi}$: covariance matrix

These can be estimated via:

- Maximum likelihood estimation (MLE)
- Expectation-maximization (EM) algorithm
- Bayesian methods (e.g., variational inference, MCMC)

Once estimated, the **posterior** of latent embeddings is given by:

$$p(\boldsymbol{z}|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{z}|\boldsymbol{W}^\top \boldsymbol{C}^{-1}(\boldsymbol{x} - \boldsymbol{\mu}), \boldsymbol{I} - \boldsymbol{W}^\top \boldsymbol{C}^{-1}\boldsymbol{W}) \tag{11}$$

- Posterior has closed-form solution under Gaussian distribution

FA model summary

$$
\begin{aligned}
\text{[Prior]} \quad p(\boldsymbol{z}) &= \mathcal{N}(\boldsymbol{z}|\boldsymbol{0}, \boldsymbol{I}) && (12)\\
\text{[Likelihood]} \quad p(\boldsymbol{x}|\boldsymbol{z}) &= \mathcal{N}(\boldsymbol{x}|\boldsymbol{W}\boldsymbol{z} + \boldsymbol{\mu}, \boldsymbol{\Psi}) && (13)\\
\text{[Evidence/marginal]} \quad p(\boldsymbol{x}) &= \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{C}) && (14)\\
\text{[Posterior]} \quad p(\boldsymbol{z}|\boldsymbol{x}) &= \mathcal{N}(\boldsymbol{z}|\boldsymbol{W}^\top \boldsymbol{C}^{-1}(\boldsymbol{x} - \boldsymbol{\mu}), \boldsymbol{I} - \boldsymbol{W}^\top \boldsymbol{C}^{-1}\boldsymbol{W}) && (15)
\end{aligned}
$$

- $\boldsymbol{z}$: latent vector, length L (assumed to be zero-mean, unit variance)
- $\boldsymbol{x}$: observed vector
- $\boldsymbol{W}$: $D \times L$ factor loading matrix
- $\boldsymbol{\Psi}$: $D \times D$ diagonal covariance matrix or **matrix of unique variances**
- $\boldsymbol{C} = \boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{\Psi}$

Unidentifiability of FA parameters

The parameters $\boldsymbol{W}$ and $\boldsymbol{\Psi}$ are unidentifiable. This can be addressed via:

- Constraining $\boldsymbol{W}$ to have orthonormal columns [PCA]
- Constraining $\boldsymbol{W}$ to be lower triangular
- Informative rotation: $\tilde{\boldsymbol{W}} = \boldsymbol{W}\boldsymbol{R}$, where $\boldsymbol{R}$ is the rotation matrix
  - Commonly used rotations: Varimax, Promax, Oblimin, Geomin, Thurstone, Equamax
- Sparsity-promoting priors on $\boldsymbol{W}$
- Non-Gaussian priors for latent factors

PCA as a special case of FA

Principal components analysis (PCA) is a special case of FA with:

$$\mathbf{\Psi} = \sigma^2 \boldsymbol{I} \tag{16}$$

where σ^2 is the isotropic noise variance. In PCA, the covariance of the observed vector is given by:

$$\boldsymbol{C} = \boldsymbol{W}\boldsymbol{W}^\top + \sigma^2 \boldsymbol{I} \tag{17}$$

Autoencoders as nonlinear PCA/FA

In PCA/FA, we learn a **linear mapping** from a high-dimensional observed space $\boldsymbol{x} \in \mathbb{R}^D$ to a low-dimensional latent space $\boldsymbol{z} \in \mathbb{R}^L$ and vice-versa.

- **Encoder** f_e: mapping from $\boldsymbol{x} \to \boldsymbol{z}$
- **Decoder** f_d: mapping from $\boldsymbol{z} \to \boldsymbol{x}$

In PCA, for example, f_e is given by:

$$\boldsymbol{z} = \boldsymbol{W}^\top \boldsymbol{x} \equiv f_e(\boldsymbol{x}) \tag{18}$$

And f_d is given by:

$$\hat{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{z} \equiv f_d(\boldsymbol{z}) \tag{19}$$

To introduce flexibility, we can specify f_e and f_e are nonlinear/more complex functions. This is best accomplished via neural network, resulting in an **autoencoder**.

Reconstruction loss

The reconstruction function is the approximation of the observation from the decoder:

$$\hat{\boldsymbol{x}} \equiv r(\boldsymbol{x}) = f_d(f_e(\boldsymbol{x})) \tag{20}$$

An autoencoder is thus trained to minimize the reconstruction loss

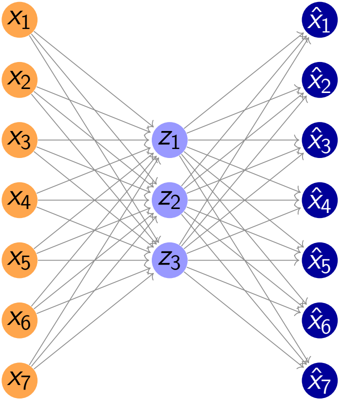
$$\mathcal{L}(\boldsymbol{\theta}) = ||r(\boldsymbol{x}) - \boldsymbol{x}||_2^2 \tag{21}$$

or equivalently, the negative log-likelihood:

$$\mathcal{L}(\boldsymbol{\theta}) = -\log p(\boldsymbol{x}|r(\boldsymbol{x})) \tag{22}$$

Basic autoencoder (AE) architecture

Autoencoder with 2 single-layer MLPS: input layer, hidden layer (latent representation) and output layer (reconstruction)

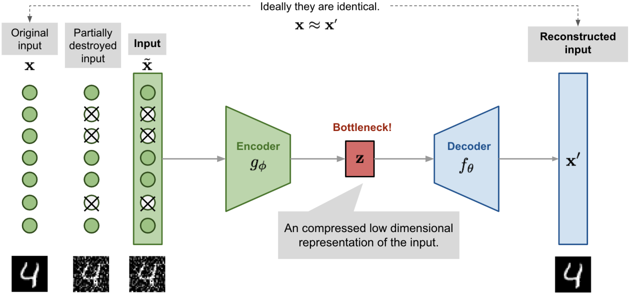


- Hidden layer (size L) is a low-dimensional **bottleneck** between input and reconstruction
- $L \ll D$: undercomplete representation
- $L \gg D$: overcomplete representation (regularize to prevent identity learning)

Denoising autoencoders

In denoising autoencoders (DAEs), the input is corrupted ($\tilde{\boldsymbol{x}}$) by:

- Gaussian noise: $p_c(\tilde{\boldsymbol{x}}|\boldsymbol{x}) = \mathcal{N}(\tilde{\boldsymbol{x}}|\boldsymbol{x}, \sigma^2 \boldsymbol{I})$
- Bernoulli dropout: randomly setting a proportion of input nodes to zero



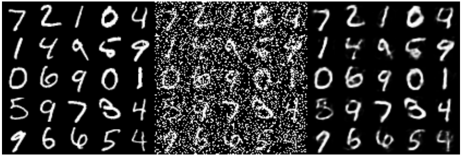
Schematic of a DAE.

Source: https://lilianweng.github.io/posts/2018-08-12-vae/

The model is then trained to minimize the loss between the reconstructed input $r(\tilde{\boldsymbol{x}})$ and its uncorrupted version $\boldsymbol{x}$

Uses of DAE

- DAEs are used for denoising images



Original, corrupted and reconstructed images from MNIST dataset.

Source: http://www.opendeep.org/v0.0.5/docs/tutorial-your-first-model

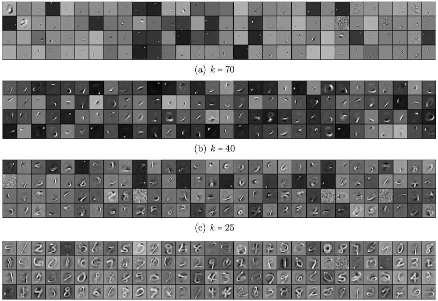
- They can also learn vector fields of input data

Sparse autoencoder (SAE)

Sparse autoencoder (SAE): sparsity penalty on latent activations

$$\Omega(\boldsymbol{z}) = \lambda ||\boldsymbol{z}||_1 \tag{23}$$

- *k*-Sparse autoencoder: use only k largest activations in training



(a) $k = 70$

(b) $k = 40$

(c) $k = 25$

(d) $k = 10$

Filters of the k -sparse autoencoder for different sparsity levels k, learnt from MNIST with 1000 hidden units.

Source: https://arxiv.org/pdf/1312.5663.pdf

Other AEs

- **Contractive autoencoder** (CAE): regularizes via penalty on reconstruction loss

$$\Omega(\boldsymbol{z}, \boldsymbol{x}) = \lambda \left\| \frac{\partial f_e(\boldsymbol{x})}{\partial \boldsymbol{x}} \right\|_F^2 \tag{24}$$

- Variational autoencoder (VAE): probablistic version of AE/generative model

Reading

- **PMLI** 20.3
- **DL** 20