Factor and Independent Component Analysis

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Recap

- Model-based learning from data
- Observed data as a sample from an unknown data generating distribution
- Learning using parametric statistical models and Bayesian models,
- Their relation to probabilistic graphical models
- Likelihood function, maximum likelihood estimation, and the mechanics of Bayesian inference
- Classical examples to illustrate the concepts
Applications of factor and independent component analysis

- Factor analysis and independent component analysis are two classical methods for data analysis.

- The origins of factor analysis (FA) are attributed to a 1904 paper by psychologist Charles Spearman. It is used in fields such as:
  - Psychology, e.g. intelligence research
  - Marketing
  - Wide range of physical and biological sciences...

- Independent component analysis (ICA) has mainly been developed in the 90s. It can be used where FA can be used. Popular applications include:
  - Neuroscience (brain imaging, spike sorting) and theoretical neuroscience
  - Telecommunications (de-convolution, blind source separation)
  - Finance (finding hidden factors)...
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Directed graphical model underlying FA and ICA

FA: factor analysis   ICA: independent component analysis

The visibles $\mathbf{v} = (v_1, \ldots, v_D)$ are independent from each other given the latents $\mathbf{h} = (h_1, \ldots, h_H)$, but generally dependent under the marginal $p(\mathbf{v})$. 
Directed graphical model underlying FA and ICA

FA: factor analysis  ICA: independent component analysis

\[ h_1 \rightarrow v_1 \]
\[ h_2 \rightarrow v_2 \]
\[ h_3 \rightarrow v_3 \]
\[ h_1 \rightarrow v_2 \]
\[ h_2 \rightarrow v_1 \]
\[ h_1 \rightarrow v_3 \]
\[ h_2 \rightarrow v_3 \]
\[ h_3 \rightarrow v_5 \]
\[ h_3 \rightarrow v_4 \]

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- Explains statistical dependencies between (observed) \( v_i \) through (unobserved) \( h_i \).
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Different assumptions on \( p(\mathbf{v}|\mathbf{h}) \) and \( p(\mathbf{h}) \) lead to different statistical models, and data analysis methods with markedly different properties.
1. Factor analysis

2. Independent component analysis
1. Factor analysis
   - Parametric model
   - Ambiguities in the model (factor rotation problem)
   - Learning the parameters by maximum likelihood estimation
   - Probabilistic principal component analysis as special case

2. Independent component analysis
In factor analysis (FA), all random variables are Gaussian.

Importantly, the number of latents $H$ is assumed smaller than the number of visibles $D$.

Latents: $p(h) = \mathcal{N}(h; 0, I)$ (uncorrelated standard normal)

Conditional $p(v|h; \theta)$ is Gaussian

$$p(v|h; \theta) = \mathcal{N}(v; Fh + c, \Psi)$$

Parameters $\theta$ are

- Vector $c \in \mathbb{R}^D$: sets the mean of $v$
- $F = (f_1, \ldots f_H)$: $D \times H$ matrix with $D > H$
  - Columns $f_i$ are called “factors”, its elements the “factor loadings”.
- $\Psi$: diagonal matrix $\Psi = \text{diag}(\Psi_1, \ldots, \Psi_D)$

Tuning parameter: the number of factors $H$
Parametric model for factor analysis

\[ p(v|h; \theta) = \mathcal{N}(v; Fh + c, \Psi) \] is equivalent to

\[ v = Fh + c + \epsilon \]

\[ = \sum_{i=1}^{H} f_i h_i + c + \epsilon \quad \epsilon \sim \mathcal{N}(\epsilon; 0, \Psi) \]

Data generation: Add \( H < D \) factors weighted by \( h_i \) to the constant vector \( c \), and corrupt the “signal” \( Fh + c \) by additive Gaussian noise.

\( Fh \) spans a \( H \) dimensional subspace of \( \mathbb{R}^D \)
Interesting structure of the data is contained in a subspace.

Example for $D = 2$, $H = 1$. 

![Plot of data points with vectors and axes labeled $v_1$ and $v_2$.]
Interesting structure of the data is contained in a subspace

Example for $D = 3, H = 2$ ("pancake" in the 3D space)

Black points: $\mathbf{Fh} + \mathbf{c}$

Red points: $\mathbf{Fh} + \mathbf{c} + \mathbf{\epsilon}$
(points below the plane not shown)

(Figures courtesy of David Barber)
Basic results that we need

- If $\mathbf{x}$ has density $\mathcal{N}(\mathbf{x}; \mu_x, \mathbf{C}_x)$, $\mathbf{z}$ density $\mathcal{N}(\mathbf{z}; \mu_z, \mathbf{C}_z)$, and $\mathbf{x} \perp \perp \mathbf{z}$ then $\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{z}$ has density

\[
\mathcal{N}(\mathbf{y}; \mathbf{A}\mu_x + \mu_z, \mathbf{A}\mathbf{C}_x\mathbf{A}^\top + \mathbf{C}_z)
\]

(see e.g. Barber Result 8.3)
Basic results that we need

- If $x$ has density $\mathcal{N}(x; \mu_x, C_x)$, $z$ density $\mathcal{N}(z; \mu_z, C_z)$, and $x \perp z$ then $y = Ax + z$ has density

$$\mathcal{N}(y; A\mu_x + \mu_z, ACA^\top + C_z)$$

(see e.g. Barber Result 8.3)

- An orthonormal (orthogonal) matrix $R$ is a symmetric matrix for which the transpose $R^\top$ equals the inverse $R^{-1}$, i.e.

$$R^\top = R^{-1} \quad \text{or} \quad R^\top R = RR^\top = I$$

(see e.g. Barber Appendix A.1)
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(see e.g. Barber Appendix A.1)

- Orthonormal matrices rotate points.
Factor rotation problem

- Using the basic results, we obtain

\[ \mathbf{v} = \mathbf{Fh} + \mathbf{c} + \epsilon \]

\[ = \mathbf{F}(\mathbf{RR}^\top)\mathbf{h} + \mathbf{c} + \epsilon \]

\[ = (\mathbf{FR})(\mathbf{R}^\top\mathbf{h}) + \mathbf{c} + \epsilon \]

\[ = (\mathbf{FR})\tilde{\mathbf{h}} + \mathbf{c} + \epsilon \]

- Since \( p(\mathbf{h}) = \mathcal{N}(\mathbf{h}; \mathbf{0}, \mathbf{I}) \) and \( \mathbf{R} \) is orthonormal, \( p(\tilde{\mathbf{h}}) = \mathcal{N}(\tilde{\mathbf{h}}; \mathbf{0}, \mathbf{I}) \), and the two models

\[ \mathbf{v} = \mathbf{Fh} + \mathbf{c} + \epsilon \]

\[ \mathbf{v} = (\mathbf{FR})\tilde{\mathbf{h}} + \mathbf{c} + \epsilon \]

produce data with exactly the same distribution.
Factor rotation problem

- Two estimates \( \hat{F} \) and \( \hat{FR} \) explain the data equally well.
Factor rotation problem

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- The columns of $F$ and $FR$ span the same subspace, so that the FA model is best understood to define a subspace of the data space.
- The individual columns of $F$ (factors) carry little meaning by themselves.
- There are post-processing methods that choose $R$ after estimation of $F$ so that the columns of $FR$ have some desirable properties to aid interpretation, e.g. that they have as many zeros as possible (sparsity).
We have seen that the FA model can be written as

\[ v = Fh + c + \epsilon \quad h \sim \mathcal{N}(h; 0, I) \quad \epsilon \sim \mathcal{N}(\epsilon; 0, \Psi) \]

with \( \epsilon \perp \perp h \)
Likelihood function

- We have seen that the FA model can be written as

\[ \mathbf{v} = \mathbf{F} \mathbf{h} + \mathbf{c} + \mathbf{\epsilon} \quad \mathbf{h} \sim \mathcal{N}(\mathbf{h}; 0, \mathbf{I}) \quad \mathbf{\epsilon} \sim \mathcal{N}(\mathbf{\epsilon}; \mathbf{0}, \mathbf{\Psi}) \]

with \( \mathbf{\epsilon} \perp \perp \mathbf{h} \)

- From the basic results on multivariate Gaussians: \( \mathbf{v} \) is Gaussian with mean and variance equal to

\[
\mathbb{E} [\mathbf{v}] = \mathbf{c} \quad \mathbb{V} [\mathbf{v}] = \mathbf{F} \mathbf{F}^\top + \mathbf{\Psi}
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Likelihood is given by likelihood for multivariate Gaussian (see Barber Section 21.1)
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From the basic results on multivariate Gaussians: \( v \) is Gaussian with mean and variance equal to

\[ \mathbb{E}[v] = c \quad \mathbb{V}[v] = FF^\top + \Psi \]

Likelihood is given by likelihood for multivariate Gaussian (see Barber Section 21.1)

But due to the form of the covariance matrix of \( v \), closed form solution is not possible and iterative methods are needed (see Barber Section 21.2, not examinable).
Probabilistic principal component analysis as special case

- In FA, the variances $\Psi_i$ of the additive noise $\epsilon$ can be different for each dimension.
- Probabilistic principal component analysis (PPCA) is obtained for
  \[ \Psi_i = \sigma^2 \quad \Psi = \sigma^2 I \]
- FA has a richer description of the additive noise than PCA.
Comparison of FA and PPCA  (Based on a slide from David Barber)

The parameters were estimated from handwritten “7s” for FA and PPCA.
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\[ \mathbf{v} = \hat{\mathbf{F}} \mathbf{h} + \hat{\mathbf{c}} + \epsilon \]

\[ \epsilon \sim \begin{cases} 
\mathcal{N}(\epsilon; \mathbf{0}; \hat{\Psi}) & \text{for FA} \\
\mathcal{N}(\epsilon; \mathbf{0}; \hat{\sigma}^2 \mathbf{I}) & \text{for PPCA} 
\end{cases} \]
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\end{cases} \]

Figures below show samples. Note how the noise variance for FA depends on the pixel, being zero for pixels on the boundary of the image.

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(f) PPCA
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   - Learning the parameters by maximum likelihood estimation
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2. Independent component analysis
1. Factor analysis

2. Independent component analysis
   - Parametric model
   - Ambiguities in the model
   - sub-Gaussian and super-Gaussian pdfs
   - Learning the parameters by maximum likelihood estimation
In ICA, unlike in FA, the latents are assumed to be non-Gaussian. (one latent can be assumed to be Gaussian)
Parametric model for independent component analysis

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- The latents $h_i$ are assumed to be statistically independent

$$p_h(h) = \prod_i p_h(h_i)$$
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Called “noisy” ICA
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The number of latents $H$ can be larger than $D$ (“overcomplete” case) or smaller (“undercomplete” case).
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The number of latents $H$ can be larger than $D$ (“overcomplete” case) or smaller (“undercomplete” case).

We here consider the widely used special case where the noise is zero and $H = D$. 
In ICA, the matrix $F$ is typically denoted by $A$ and called the “mixing” matrix. The model is

$$v = Ah$$

$$p_h(h) = \prod_{i=1}^{D} p_h(h_i)$$

where the $h_i$ are typically assumed to have zero mean and unit variance.
Ambiguities

- Denote the columns of $A$ by $a_i$. 

It follows that the ICA model has an ambiguity regarding the ordering of the columns of $A$ and their scaling.

The unit variance assumption on the latents fixes the scaling but not the ordering ambiguity.

Note: for non-Gaussian latents, there is no rotational ambiguity.
Denote the columns of $A$ by $a_i$.

From

$$v = Ah = \sum_{i=1}^{D} a_i h_i = \sum_{k=1}^{D} a_{i_k} h_{i_k} = \sum_{i=1}^{D} (a_i \alpha_i) \frac{1}{\alpha_i} h_i$$

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The unit variance assumption on the latents fixes the scaling but not the ordering ambiguity.

Note: for non-Gaussian latents, there is no rotational ambiguity.
Non-Gaussian latents: variables with sub-Gaussian pdfs

- Sub-Gaussian pdf: pdf that is less peaked at zero than a Gaussian of the same variance and mean.
- Example: pdf of a uniform distribution

Samples \((h_1, h_2)\)  
Samples \((v_1, v_2)\)

Horizontal axes: \(h_1\) and \(v_1\). Vertical axes \(h_2\) and \(v_2\). Not in the same scale

(Figures 7.5 and 7.6 from *Independent Component Analysis* by Hyvärinen, Karhunen, and Oja).
Non-Gaussian latents: variables with super-Gaussian pdfs

- Super-Gaussian pdf: pdf that is more peaked at zero than a Gaussian of the same variance and mean.
- Example: pdf of a Laplace distribution (see Def 8.24 in Barber)

\[
\text{Samples } (h_1, h_2) \quad \text{Samples } (v_1, v_2)
\]

Horizontal axes: \(h_1\) and \(v_1\). Vertical axes \(h_2\) and \(v_2\). Not in the same scale

(Figures 7.8 and 7.9 from *Independent Component Analysis* by Hyvärinen, Karhunen, and Oja).
Distribution of the visibles

The mapping $h \mapsto v = Ah$ is deterministic and invertible. By the laws of transformation of random variables

$$p(v; A) = p_h(A^{-1}v) |\det A^{-1}|$$

(see e.g. Barber Result 8.1)
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Denote the inverse of $A$ by $B$

$$A^{-1}v = Bv = \begin{pmatrix} b_1v \\ \vdots \\ b_Dv \end{pmatrix}$$

where the $b_1, \ldots, b_D$ are the row vectors of the matrix $B$. 
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where the \( b_1, \ldots, b_D \) are the row vectors of the matrix \( B \).

Given the independence of the latents, we thus have

\[
p(v; A) = p_h(A^{-1}v) | \det A^{-1} | = p_h(Bv) | \det B |
\]

\[
= \prod_{j=1}^{D} p_h(b_j v) | \det B |
\]
Likelihood function

- Since the mapping from $A$ to $B$ is invertible. We can write the likelihood function in terms of the matrix $B$, 

\[ L(B) = n \prod_{i=1}^{n} \left[ D \prod_{j=1}^{n} p_h(b_j v_i) \right] \left| \text{det} B \right| \]

The log-likelihood is given by

\[ \ell(B) = n \sum_{i=1}^{n} D \sum_{j=1}^{n} \log p_h(b_j v_i) + n \log \left| \text{det} B \right| \]

Can be optimised using gradient ascent (slow) or with more powerful methods (see Barber 21.6)
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Given iid data $\mathcal{D} = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$, we obtain

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The likelihood and the distribution of the latents

\[ \ell(B) = \sum_{i=1}^{n} \sum_{j=1}^{D} \log p_h(b_jv_i) + n \log |\det B| \]

- B and hence the mixing A can be uniquely estimated, up to the scaling and order ambiguity, as long as the \( p_h \) are non-Gaussian (see Barber 21.6) (one latent Gaussian is allowed).
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- The pdf \( p_h \) of the latents enter the (log) likelihood.
- If not known, they have to be estimated, which is difficult.
The likelihood and the distribution of the latents

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- Non-Gaussianity assumption on the latents solves the “factor rotation” problem in FA.
- The pdf \(p_h\) of the latents enter the (log) likelihood.
- If not known, they have to be estimated, which is difficult.
- It turns out that learning whether \(p_h\) is super-Gaussian or sub-Gaussian is enough. (not examinable, Section 9.1.2 of *Independent Component Analysis* by Hyvärinen, Karhunen, and Oja)
Program recap

1. Factor analysis
   - Parametric model
   - Ambiguities in the model (factor rotation problem)
   - Learning the parameters by maximum likelihood estimation
   - Probabilistic principal component analysis as special case

2. Independent component analysis
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   - Ambiguities in the model
   - sub-Gaussian and super-Gaussian pdfs
   - Learning the parameters by maximum likelihood estimation