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

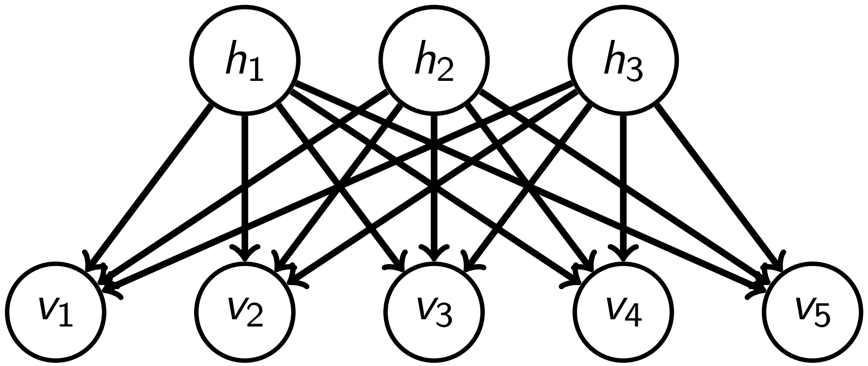
- Factor analysis and independent component analysis are two classical methods for data analysis.
- The origins of factor analysis (FA) are attributed to a 1904 paper by psychologist Charles Spearman. It is used in fields such as
  - Psychology, e.g intelligence research
  - Marketing
  - Wide range 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)

  ⋮

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 $p(\mathbf{v})$.
- Explains statistical dependencies between (observed) v_i through (unobserved) h_i.
- 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.

Program

1. Factor analysis

2. Independent component analysis

Program

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

Parametric model for factor 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: $p(\mathbf{h}) = \mathcal{N}(\mathbf{h}; \mathbf{0}, \mathbf{I})$ (uncorrelated standard normal)
- Conditional $p(\mathbf{v}|\mathbf{h}; \boldsymbol{\theta})$ is Gaussian

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

Parameters $\boldsymbol{\theta}$ are

- Vector $\mathbf{c} \in \mathbb{R}^D$: sets the mean of $\mathbf{v}$
- $\mathbf{F} = (\mathbf{f}_1, \ldots \mathbf{f}_H)$: $D \times H$ matrix with $D > H$
  Columns $\mathbf{f}_i$ are called "factors", its elements the "factor loadings".
- $\boldsymbol{\Psi}$: diagonal matrix $\boldsymbol{\Psi} = \text{diag}(\Psi_1, \ldots, \Psi_D)$

Tuning parameter: the number of factors H

Parametric model for factor analysis

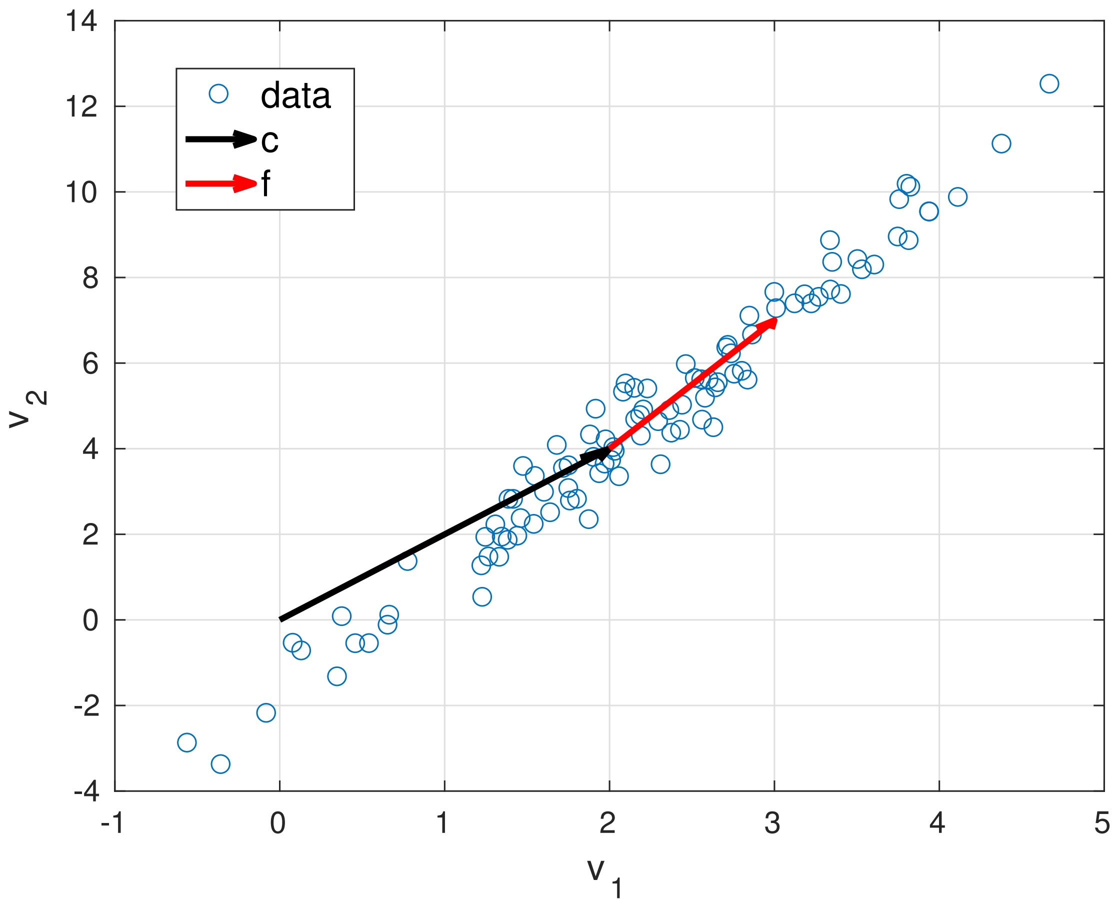
- $p(\mathbf{v}|\mathbf{h};\boldsymbol{\theta}) = \mathcal{N}(\mathbf{v};\mathbf{Fh}+\mathbf{c},\boldsymbol{\Psi})$ is equivalent to

$$\begin{aligned} \mathbf{v} &= \mathbf{Fh} + \mathbf{c} + \boldsymbol{\epsilon} \\ &= \sum_{i=1}^{H} \mathbf{f}_i h_i + \mathbf{c} + \boldsymbol{\epsilon} \qquad\qquad \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon}; 0, \boldsymbol{\Psi}) \end{aligned}$$

- Data generation: Add $H < D$ factors weighted by h_i to the constant vector $\mathbf{c}$, and corrupt the "signal" $\mathbf{Fh}+\mathbf{c}$ by additive Gaussian noise.
- $\mathbf{Fh}$ spans a H dimensional subspace of $\mathbb{R}^D$

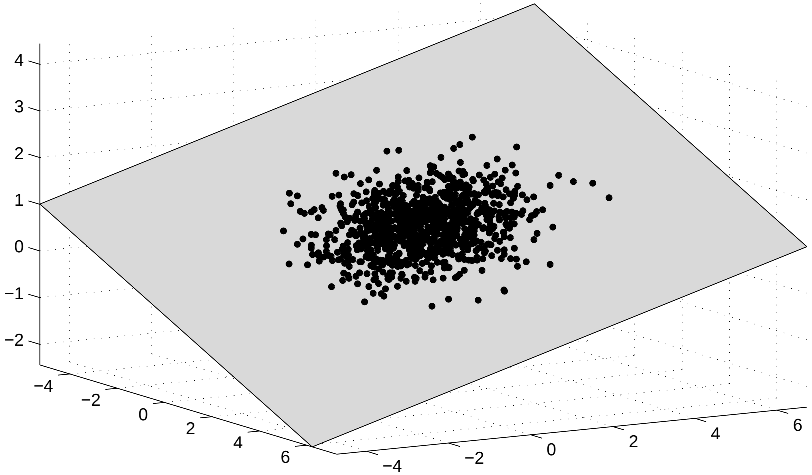
Interesting structure of the data is contained in a subspace

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

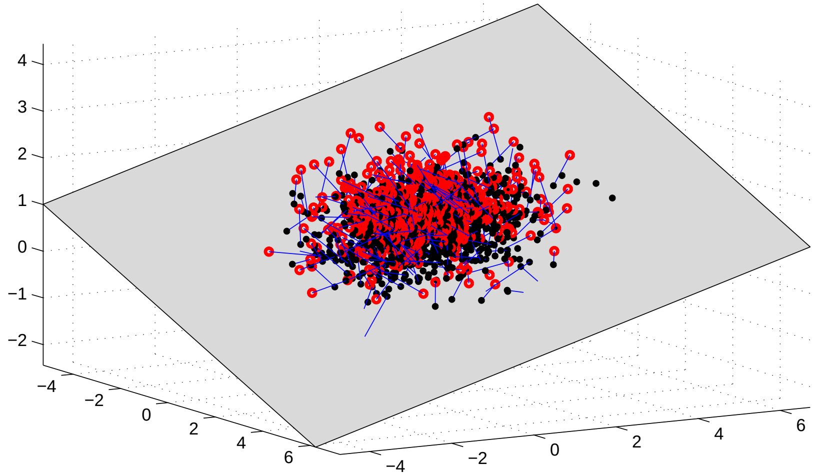


Interesting structure of the data is contained in a subspace

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



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



Red points: $\mathbf{Fh} + \mathbf{c} + \boldsymbol{\epsilon}$

(points below the plane not shown)

(Figures courtesy of David Barber)

Basic results that we need

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

$$\mathcal{N}(\mathbf{y}; \mathbf{A}\boldsymbol{\mu}_x + \boldsymbol{\mu}_z, \mathbf{A}\mathbf{C}_x\mathbf{A}^\top + \mathbf{C}_z)$$

  (see e.g. Barber Result 8.3)

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

$$\mathbf{R}^\top = \mathbf{R}^{-1} \qquad \text{or} \qquad \mathbf{R}^\top\mathbf{R} = \mathbf{R}\mathbf{R}^\top = \mathbf{I}$$

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

- Orthonormal matrices rotate points.

Factor rotation problem

- Using the basic results, we obtain

$$\begin{aligned} \mathbf{v} &= \mathbf{F}\mathbf{h} + \mathbf{c} + \boldsymbol{\epsilon} \\ &= \mathbf{F}(\mathbf{R}\mathbf{R}^\top)\mathbf{h} + \mathbf{c} + \boldsymbol{\epsilon} \\ &= (\mathbf{F}\mathbf{R})(\mathbf{R}^\top\mathbf{h}) + \mathbf{c} + \boldsymbol{\epsilon} \\ &= (\mathbf{F}\mathbf{R})\tilde{\mathbf{h}} + \mathbf{c} + \boldsymbol{\epsilon} \end{aligned}$$

- 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

$$\mathbf{v} = \mathbf{F}\mathbf{h} + \mathbf{c} + \boldsymbol{\epsilon} \qquad\qquad \mathbf{v} = (\mathbf{F}\mathbf{R})\tilde{\mathbf{h}} + \mathbf{c} + \boldsymbol{\epsilon}$$

produce data with exactly the same distribution.

Factor rotation problem

- Two estimates $\hat{\mathbf{F}}$ and $\hat{\mathbf{F}}\mathbf{R}$ explain the data equally well.
- Estimation of the factor matrix $\mathbf{F}$ is not unique.
- With the Gaussianity assumption on $\mathbf{h}$, there is a rotational ambiguity in the factor analysis model.
- The columns of $\mathbf{F}$ and $\mathbf{FR}$ span the same subspace, so that the FA model is best understood to define a subspace of the data space.
- The individual columns of $\mathbf{F}$ (factors) carry little meaning by themselves.
- There are post-processing methods that choose $\mathbf{R}$ *after* estimation of $\mathbf{F}$ so that the columns of $\mathbf{FR}$ have some desirable properties to aid interpretation, e.g. that they have as many zeros as possible (sparsity).

Likelihood function

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

$$\mathbf{v} = \mathbf{F}\mathbf{h} + \mathbf{c} + \boldsymbol{\epsilon} \qquad \mathbf{h} \sim \mathcal{N}(\mathbf{h}; \mathbf{0}, \mathbf{I}) \qquad \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon}; \mathbf{0}, \boldsymbol{\Psi})$$

  with $\boldsymbol{\epsilon} \perp\!\!\!\perp \mathbf{h}$

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

$$\mathbb{E}[\mathbf{v}] = \mathbf{c} \qquad \mathbb{V}[\mathbf{v}] = \mathbf{F}\mathbf{F}^\top + \boldsymbol{\Psi}$$

- Likelihood is given by likelihood for multivariate Gaussian (see Barber Section 21.1)
- But due to the form of the covariance matrix of $\mathbf{v}$, 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 Ψ_i of the additive noise $\boldsymbol{\epsilon}$ can be different for each dimension.
- Probabilistic principal component analysis (PPCA) is obtained for

$$\Psi_i = \sigma^2 \qquad\qquad \mathbf{\Psi} = \sigma^2 \mathbf{I}$$

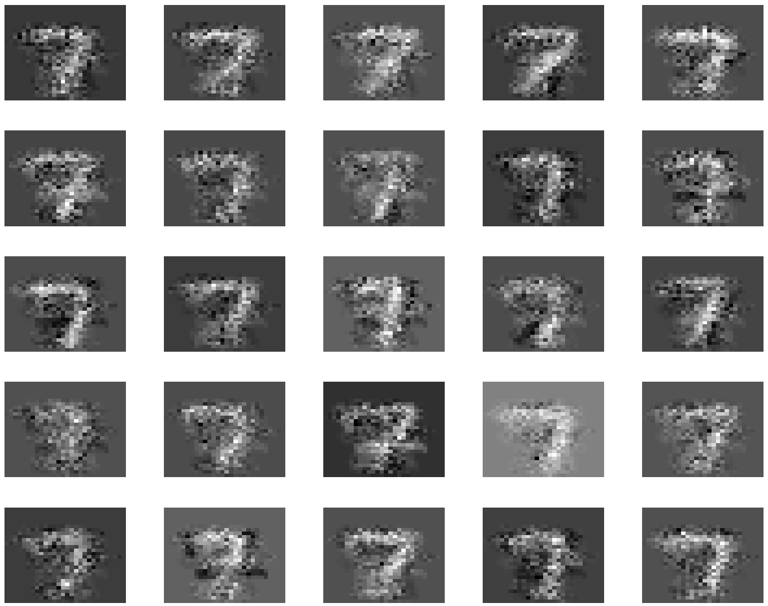
- FA has a richer description of the additive noise than PCA.

Comparison of FA and PPCA (Based on a slide from David Barber)

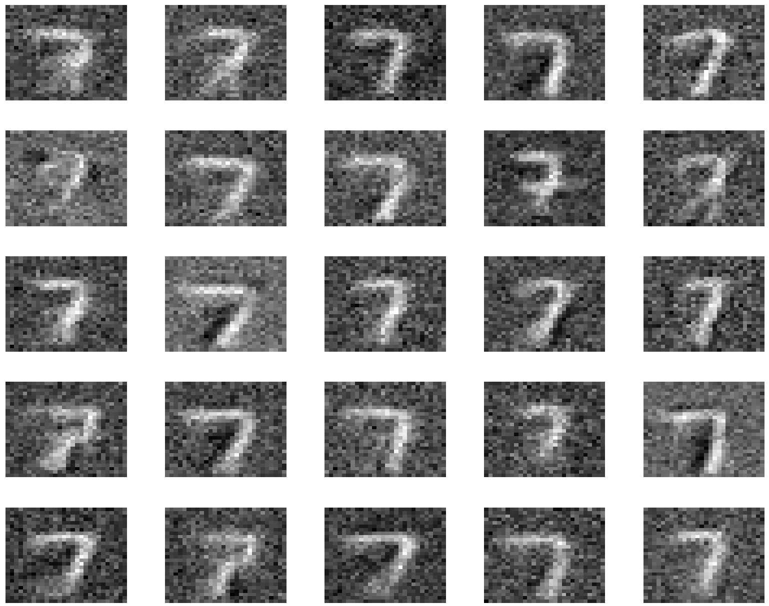
The parameters were estimated from handwritten "7s" for FA and PPCA. After learning, samples can be drawn from the model via

$$\mathbf{v} = \hat{\mathbf{F}}\mathbf{h} + \hat{\mathbf{c}} + \boldsymbol{\epsilon} \qquad \boldsymbol{\epsilon} \sim \begin{cases} \mathcal{N}(\boldsymbol{\epsilon}; \mathbf{0}; \hat{\boldsymbol{\Psi}}) & \text{for FA} \\ \mathcal{N}(\boldsymbol{\epsilon}; \mathbf{0}; \hat{\sigma}^2\mathbf{I}) & \text{for PPCA} \end{cases}$$

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.



(a) Factor Analysis



(b) PPCA

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    - Parametric model
    - Ambiguities in the model
    - sub-Gaussian and super-Gaussian pdfs
    - Learning the parameters by maximum likelihood estimation

Parametric model for independent component analysis

- In ICA, unlike in FA, the latents are assumed to be non-Gaussian. (one latent can be assumed to be Gaussian)
- The latents h_i are assumed to be statistically independent

$$p_{\mathbf{h}}(\mathbf{h}) = \prod_i p_h(h_i)$$

- Conditional $p(\mathbf{v}|\mathbf{h};\boldsymbol{\theta})$ is generally Gaussian

$$p(\mathbf{v}|\mathbf{h};\boldsymbol{\theta}) = \mathcal{N}(\mathbf{v};\mathbf{F}\mathbf{h}+\mathbf{c},\boldsymbol{\Psi}) \qquad \text{or} \qquad \mathbf{v} = \mathbf{F}\mathbf{h}+\mathbf{c}+\boldsymbol{\epsilon}$$

  Called "noisy" ICA
- 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 $H = D$.

Parametric model for independent component analysis

In ICA, the matrix $\mathbf{F}$ is typically denoted by $\mathbf{A}$ and called the "mixing" matrix. The model is

$$\mathbf{v} = \mathbf{A}\mathbf{h} \qquad\qquad p_{\mathbf{h}}(\mathbf{h}) = \prod_{i=1}^{D} p_h(h_i)$$

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

Ambiguities

- Denote the columns of $\mathbf{A}$ by $\mathbf{a}_i$.
- From

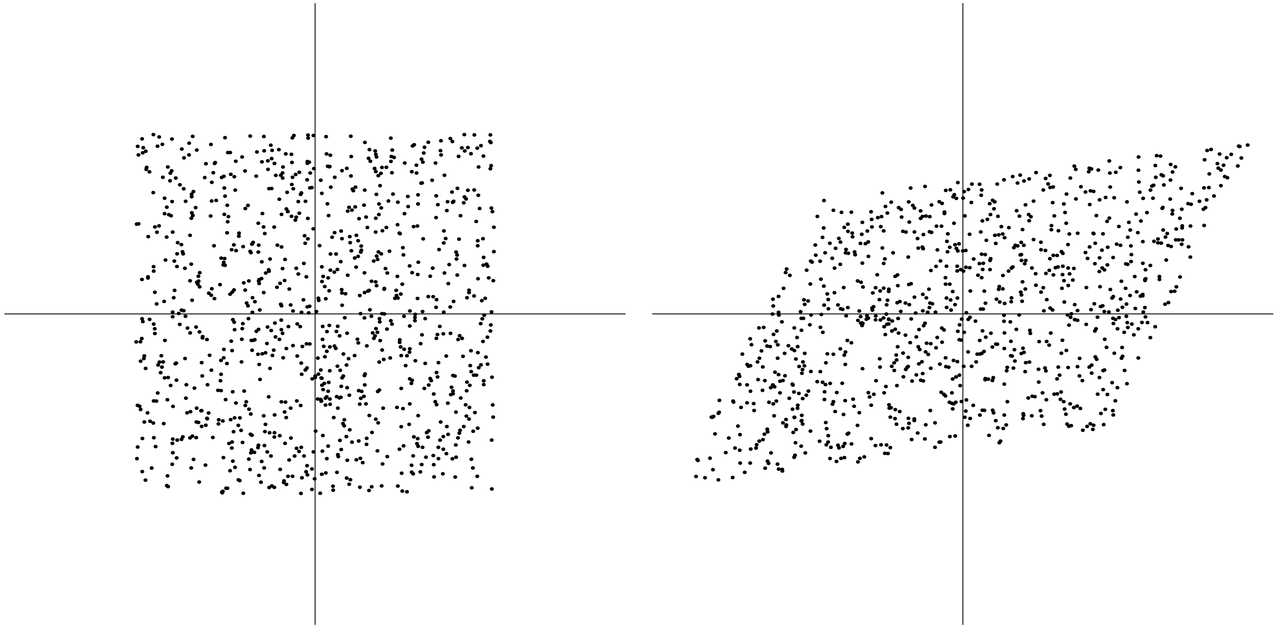
$$\mathbf{v} = \mathbf{A}\mathbf{h} = \sum_{i=1}^{D} \mathbf{a}_i h_i = \sum_{k=1}^{D} \mathbf{a}_{i_k} h_{i_k} = \sum_{i=1}^{D} (\mathbf{a}_i \alpha_i) \frac{1}{\alpha_i} h_i$$

  it follows that the ICA model has an ambiguity regarding the ordering of the columns of $\mathbf{A}$ 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.

Non-Gaussian latents: variables with sub-Gaussian pdfs

- Sub-Gaussian pdf: (assume variables have mean zero) pdf that is less peaked at zero than a Gaussian of the same variance.
- Example: pdf of a uniform distribution

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



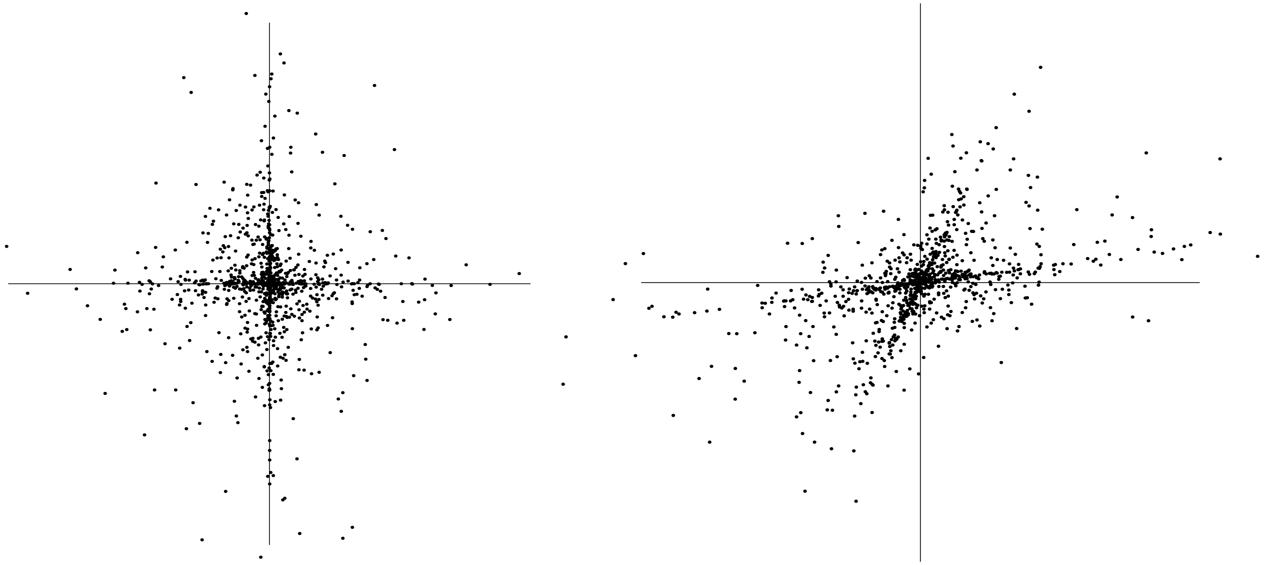
Horizontal axes: h_1 and v_1. Vertical axes h_2 and v_2. Not in the same scale

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

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 7.8 and 7.9 from *Independent Component Analysis* by Hyvärinen, Karhunen, and Oja).

Distribution of the visibles

- The mapping $\mathbf{h} \mapsto \mathbf{v} = \mathbf{A}\mathbf{h}$ is deterministic and invertible. By the laws of transformation of random variables
$$p(\mathbf{v}; \mathbf{A}) = p_{\mathbf{h}}(\mathbf{A}^{-1}\mathbf{v})|\det \mathbf{A}^{-1}|$$
(see e.g. Barber Result 8.1)
- Denote the inverse of $\mathbf{A}$ by $\mathbf{B}$
$$\mathbf{A}^{-1}\mathbf{v} = \mathbf{B}\mathbf{v} = \begin{pmatrix} \mathbf{b}_1\mathbf{v} \\ \vdots \\ \mathbf{b}_D\mathbf{v} \end{pmatrix}$$
where the $\mathbf{b}_1, \ldots, \mathbf{b}_D$ are the *row* vectors of the matrix $\mathbf{B}$.
- Given the independence of the latents, we thus have
$$\begin{aligned} p(\mathbf{v}; \mathbf{A}) &= p_{\mathbf{h}}(\mathbf{A}^{-1}\mathbf{v})|\det \mathbf{A}^{-1}| = p_{\mathbf{h}}(\mathbf{B}\mathbf{v})|\det \mathbf{B}| \\ &= \left[\prod_{j=1}^{D} p_h(\mathbf{b}_j\mathbf{v})\right]|\det \mathbf{B}| \end{aligned}$$

Likelihood function

- Since the mapping from $\mathbf{A}$ to $\mathbf{B}$ is invertible. We can write the likelihood function in terms of the matrix $\mathbf{B}$,
- Given iid data $\mathcal{D} = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$, we obtain

$$L(\mathbf{B}) = \prod_{i=1}^{n} \left[\prod_{j=1}^{D} p_h(\mathbf{b}_j \mathbf{v}_i) \right] |\det \mathbf{B}|$$

- The log-likelihood is given by

$$\ell(\mathbf{B}) = \sum_{i=1}^{n} \sum_{j=1}^{D} \log p_h(\mathbf{b}_j \mathbf{v}_i) + n \log |\det \mathbf{B}|$$

- Can be optimised using gradient ascent (slow) or with more powerful methods (see Barber 21.6)

The likelihood and the distribution of the latents

$\ell(\mathbf{B}) = \sum_{i=1}^{n} \sum_{j=1}^{D} \log p_h(\mathbf{b}_j \mathbf{v}_i) + n \log |\det \mathbf{B}|$

- $\mathbf{B}$ and hence the mixing $\mathbf{A}$ 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).
- 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

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