Introduction to Data Mining
04 - Principal Component Analysis

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WS 2023/2024, Bielefeld University

Registration for Presentations

- Registration for homework presentations is open.

Link: Registration

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- First come-first serve principle.

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- Submit other questions for the tutorials: Link

Link: Registration

Moodle

- Moodle available now in Lernraum, including groups and submissions

Moodle

- Moodle available now in Lernraum, including groups and submissions
- Voluntary for now; your feedback is appreciated!

Outline for this lecture

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- (Almost) Full derivation of PCA, based on Ren and MacKay (2019)
- Factor analysis
- Factor rotations

Motivation

- Explain data as a **linear combination** of basis vectors (or factors) $v_1, \ldots, v_n$

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Examples:

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Examples:

- Underlying skills in educational data

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Examples:

- Underlying skills in educational data
- Fourier transform
- Eigenfaces

Spooky example

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- Assume we are detectives and try to find the underlying patterns behind a serious of deaths

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mysterious loss of blood	1	1	0	1	1	1	1	1	1	1	1	0
two punctures on the neck	1	1	0	1	1	1	1	1	1	1	1	0
slash and bite wounds	0	0	1	0	0	0	0	0	0	0	0	1
paw prints	0	0	1	0	0	0	0	0	0	0	0	1
animal hair	0	0	1	0	0	0	0	0	0	0	0	1
full moon	0	0	1	0	0	0	0	0	0	0	0	1
age	78	49	44	24	29	31	50	63	73	27	62	49

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full moon	0	0	1	0	0	0	0	0	0	0	0	1
age	78	49	44	24	29	31	50	63	73	27	62	49

- Which patterns jump out at you?

Spooky example (continued)

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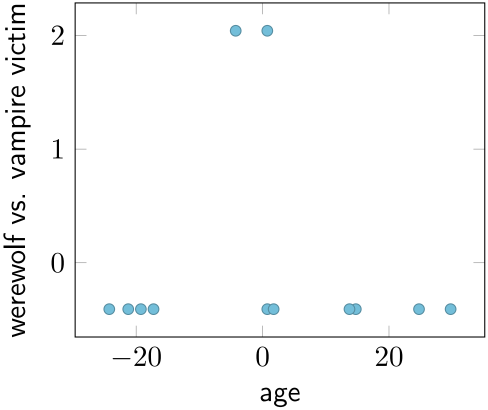
feature	v_1	v_2
mysterious loss of blood	0.00	-0.41
two punctures on the neck	0.00	-0.41
slash and bite wounds	0.00	0.41
paw prints	0.00	0.41
animal hair	0.00	0.41
full moon	0.00	0.41
age	1.00	0.00



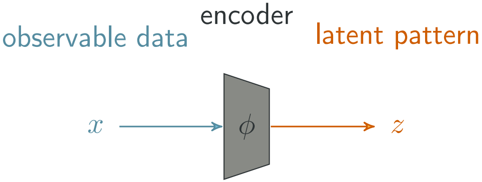
Principal Component Analysis

Setup

observable data

x

Setup



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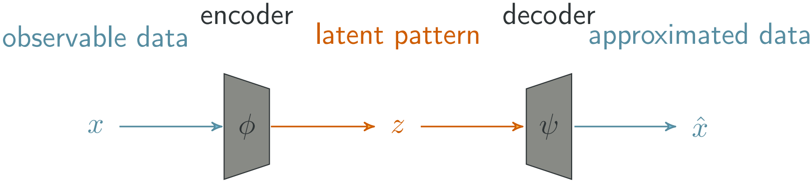
encoder
decoder
observable data
latent pattern
approximated data
x
ϕ
z
ψ
$\hat{x}$

Formalization

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$$\min_{\phi,\psi} \quad \sum_{i=1}^{N} \|\psi\Big(\phi(x_i)\Big) - x_i\|^2$$

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- **But** both ϕ and ψ are affine maps

$$z = \phi(x) = \boldsymbol{U} \cdot x + a \qquad \text{where } \boldsymbol{U} \in \mathbb{R}^{n \times m}, a \in \mathbb{R}^n$$
$$\hat{x} = \psi(z) = \boldsymbol{V} \cdot z + b \qquad \text{where } \boldsymbol{V} \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m$$

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$$\hat{x} = \psi(z) = \boldsymbol{V} \cdot z + b \qquad \text{where } \boldsymbol{V} \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m$$

- Trick question: What is the solution for $n \geq m$?

Outline for the full derivation of PCA

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6. Find optimal $\boldsymbol{V}$

Decoding: Geometric interpretation

- Assume $m = 3$ and $n = 2$, and let v_1, v_2 be the columns of $\boldsymbol{V}$.

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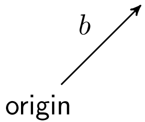

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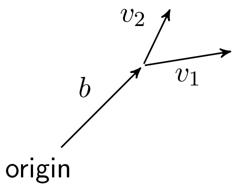

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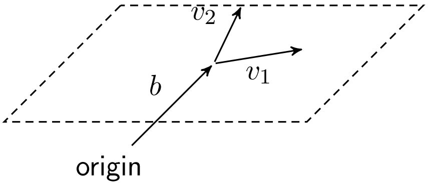

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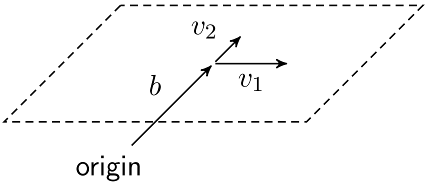

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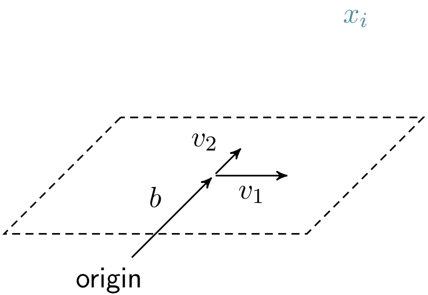

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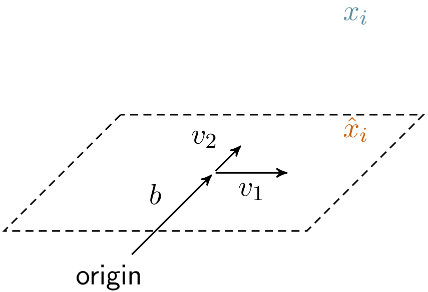

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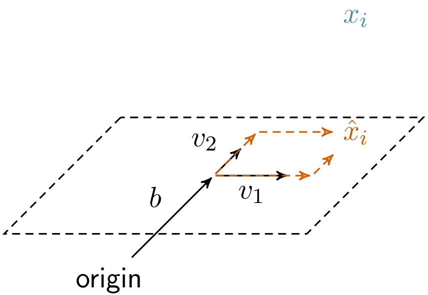

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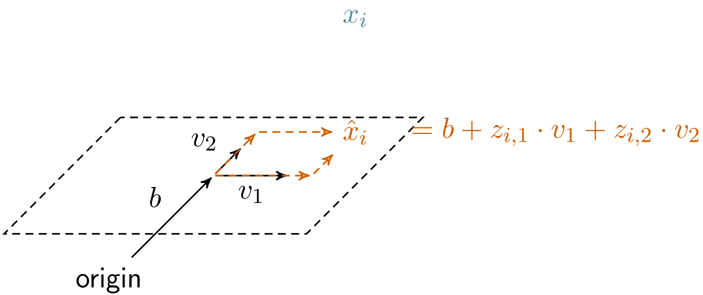

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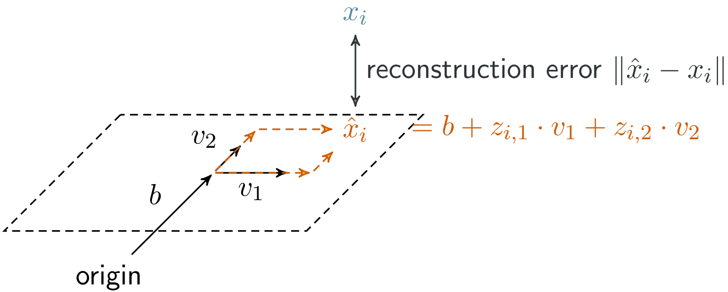

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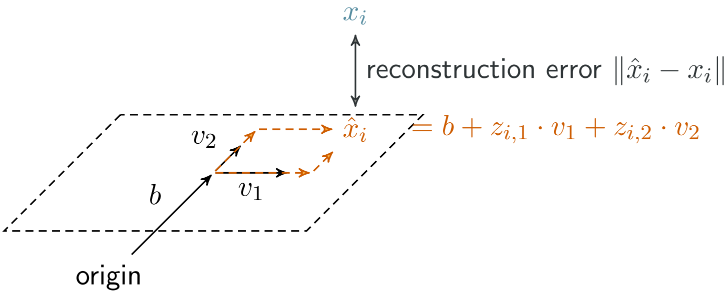

In summary:

- Columns of $\boldsymbol{V}$ span a hyperplane that contains all possible decoded points
- Without loss of generality, we can assume $\boldsymbol{V}$ to be (semi-)orthogonal
- … which means $\boldsymbol{V}^T\boldsymbol{V} = \boldsymbol{I}$ (but $\boldsymbol{V}\boldsymbol{V}^T \neq \boldsymbol{I}$!)

Deriving a

- Let's inspect the equation for $\hat{x}_i$:

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$\Rightarrow$ Without loss of generality, set $a = -\boldsymbol{U}\mu$, where μ is the mean: $\mu = \frac{1}{N}\sum_{i=1}^{N} x_i$

Deriving the optimal b

- Let's optimize reconstruction error w.r.t. b

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$$= \sum_{i=1}^{N} \|\boldsymbol{V}(\boldsymbol{U} x_i - \boldsymbol{U}\mu) + b - x_i\|^2$$

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$$\Rightarrow \nabla_b \ell(b) = 2\sum_{i=1}^{N} \boldsymbol{V}\boldsymbol{U}(x_i - \mu) + b - x_i$$

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$$= 2\boldsymbol{V}\boldsymbol{U}(\sum_{i=1}^{N} x_i - N\mu) + 2Nb - 2\sum_{i=1}^{N} x_i$$

Deriving the optimal b

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- Let's optimize reconstruction error w.r.t. b
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$$
\begin{aligned}
\ell(b) &= \sum_{i=1}^{N} \|\psi\big(\phi(x_i)\big) - x_i\|^2 = \sum_{i=1}^{N} \|\boldsymbol{V} z_i + b - x_i\|^2 \\
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\Rightarrow \nabla_b \ell(b) &= 2 \sum_{i=1}^{N} \boldsymbol{V}\boldsymbol{U}(x_i - \mu) + b - x_i \\
&= 2\boldsymbol{V}\boldsymbol{U}(\sum_{i=1}^{N} x_i - N\mu) + 2Nb - 2\sum_{i=1}^{N} x_i = 2Nb - 2\sum_{i=1}^{N} x_i
\end{aligned}
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\end{aligned}$$

Setting the gradient to zero yields $b = \mu$.

Deriving the optimal encoder

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Deriving the optimal encoder

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&= \sum_{i=1}^{N} \|\boldsymbol{V}\boldsymbol{U}(x_i - \mu) - (x_i - \mu)\|^2
\end{aligned}
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&= \sum_{i=1}^{N} (x_i - \mu)^T \boldsymbol{U}^T \boldsymbol{V}^T \boldsymbol{V}\boldsymbol{U}(x_i - \mu) - 2(x_i - \mu)^T \boldsymbol{U}^T \boldsymbol{V}^T (x_i - \mu) + (x_i - \mu)^T (x_i - \mu)
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\end{aligned}$$

Deriving the optimal encoder (continued)

Let's compute the gradient:

$$\nabla_{\boldsymbol{U}} \ell(\boldsymbol{U}) = \sum_{i=1}^{N} 2\boldsymbol{U}(x_i - \mu)(x_i - \mu)^T - 2\boldsymbol{V}^T(x_i - \mu)(x_i - \mu)^T$$

Deriving the optimal encoder (continued)

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\end{aligned}$$

$\Rightarrow$ Setting gradient to zero yields: $\boldsymbol{U} = \boldsymbol{V}^T$

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\nabla_{\boldsymbol{U}} \ell(\boldsymbol{U}) &= \sum_{i=1}^{N} 2\boldsymbol{U}(x_i - \mu)(x_i - \mu)^T - 2\boldsymbol{V}^T(x_i - \mu)(x_i - \mu)^T \\
&= 2\left(\boldsymbol{U} - \boldsymbol{V}^T\right) \sum_{i=1}^{N} (x_i - \mu)(x_i - \mu)^T \\
&= 2\left(\boldsymbol{U} - \boldsymbol{V}^T\right) \boldsymbol{C}
\end{aligned}$$

$\Rightarrow$ Setting gradient to zero yields: $\boldsymbol{U} = \boldsymbol{V}^T$

- **attention!** The last step is only valid because $\boldsymbol{C}$ is positive (semi-)definite and, hence, invertible

Summary thus far

- We set $a = -\boldsymbol{U}\mu$

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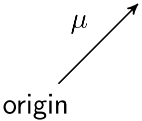
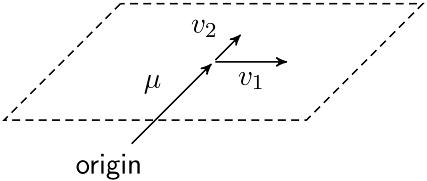
$\Rightarrow$ Only $\boldsymbol{V}$ remains to be optimized – for which we need some geometry, again

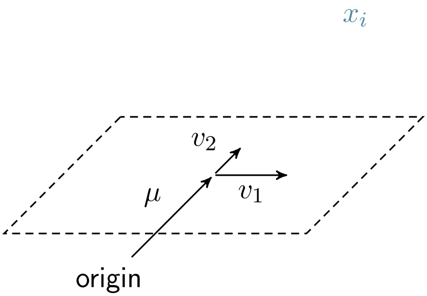
Geometric interpretation (continued)



Geometric interpretation (continued)



Geometric interpretation (continued)



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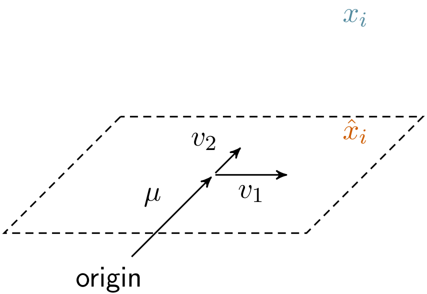

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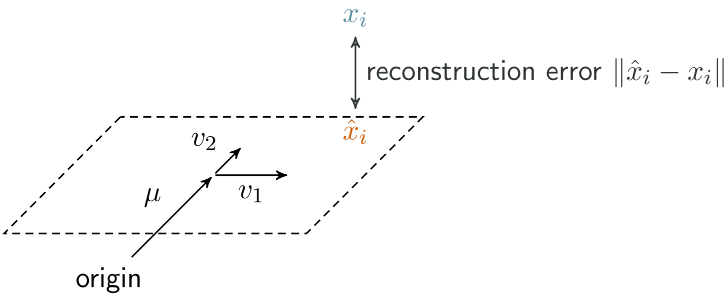

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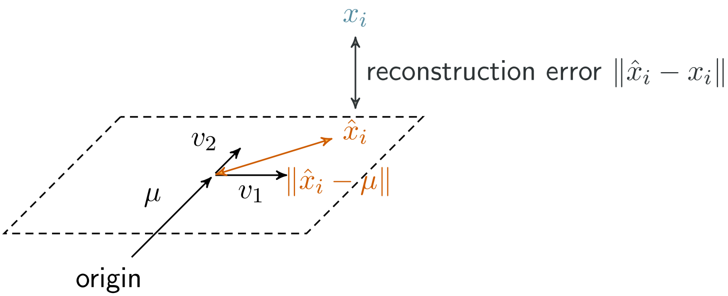

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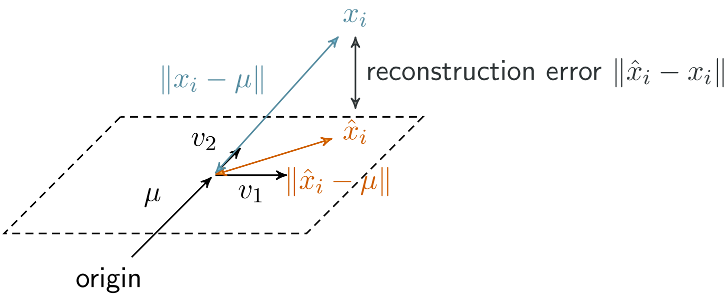
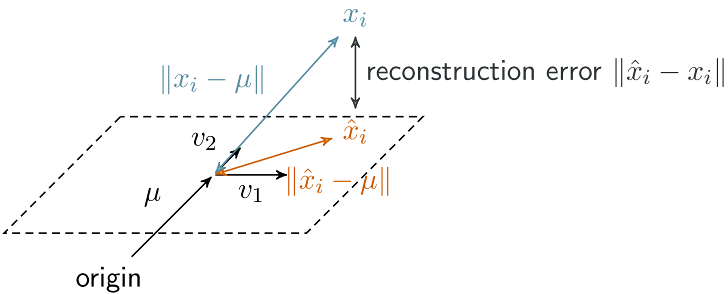
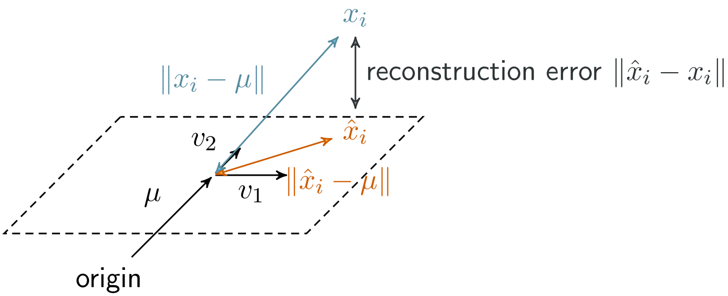


Geometric interpretation (continued)



- By construction: $\hat{x}_i$ is projection of x_i onto the hyperplane spanned by the columns of $\boldsymbol{V}$ (and anchored in μ)

Geometric interpretation (continued)



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$\Rightarrow$ The sides $\|\hat{x}_i - x_i\|$, $\|\hat{x}_i - \mu\|$, and $\|x_i - \mu\|$ form a right triangle

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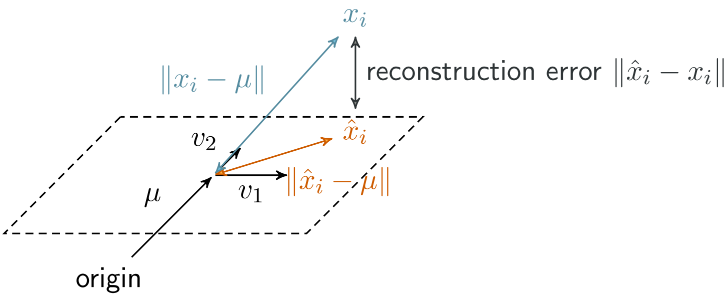

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$\Rightarrow$ Pythagoras: $\|\hat{x}_i - x_i\|^2 + \|\hat{x}_i - \mu\|^2 = \|x_i - \mu\|^2$

New optimization target

$$\min_{\boldsymbol{V}} \quad \sum_{i=1}^{N} \|\hat{x}_i - x_i\|^2$$

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$$\Leftrightarrow \min_{\boldsymbol{V}} - \sum_{i=1}^{N} \|\hat{x}_i - \mu\|^2$$

$$\Leftrightarrow \max_{\boldsymbol{V}} \sum_{i=1}^{N} \|\hat{x}_i - \mu\|^2$$

Deriving the optimal $\boldsymbol{V}$

$$\sum_{i=1}^{N} \|\hat{x}_i - \mu\|^2 = \sum_{i=1}^{N} \|\boldsymbol{V} z_i + \mu - \mu\|^2$$

Deriving the optimal $\boldsymbol{V}$

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\sum_{i=1}^{N} \|\hat{x}_i - \mu\|^2 &= \sum_{i=1}^{N} \|\boldsymbol{V} z_i + \mu - \mu\|^2 \\
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Deriving the optimal $\boldsymbol{V}$

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- Trick: To achieve orthogonal $\boldsymbol{V}$, optimize one column at a time; search for next column in orthogonal subspace, etc.

Deriving the first principal component

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Recall: We need to set v to maximize

$$\sum_{i=1}^{N} \|v^T(x_i - \mu)\|^2$$

Deriving the first principal component

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Deriving the first principal component

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$$= \sum_{i=1}^{N} v^T(x_i - \mu) \cdot (x_i - \mu)^T \cdot v$$

Deriving the first principal component

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&= \sum_{i=1}^{N} v^T(x_i - \mu) \cdot (x_i - \mu)^T \cdot v \\
&= v^T \Big(\sum_{i=1}^{N} (x_i - \mu) \cdot (x_i - \mu)^T \Big) \cdot v
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- Note: we also want $\|v\| = 1$ such that $\boldsymbol{V}$ is orthogonal

$\Rightarrow$ Lagrangian is given as $\ell(v, \lambda) = -v^T \boldsymbol{C} v - \lambda \cdot (1 - v^T v)$

Deriving the first principal component (continued)

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$$\nabla_v \ell(v, \lambda) = -2\boldsymbol{C}v + 2\lambda v$$

Deriving the first principal component (continued)

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Deriving the first principal component (continued)

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$\Rightarrow$ objective: $v^T \boldsymbol{C} v = v^T \lambda v = \lambda$

$\Rightarrow$ choose eigenvector v corresponding to largest eigenvalue

Summary: PCA procedure

function PCA(data matrix $\boldsymbol{X}$ with N rows and m columns, desired latent dimensionality $n \leq m$)

end function

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Keep only the columns of $\boldsymbol{V}$ corresponding to the n largest eigenvalues.

return $\phi(x) = \boldsymbol{V}^T \cdot (x - \mu)$ and $\psi(z) = \boldsymbol{V} \cdot z + \mu$.

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Summary: PCA procedure

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Implementation: sklearn.decomposition.PCA

How to choose n

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- Recall: Objective becomes variance of the data $\sum_{i=1}^{N} \|\hat{x}_i - \mu\|^2 = \lambda$

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- Recall: Objective becomes variance of the data $\sum_{i=1}^{N} \|\hat{x}_i - \mu\|^2 = \lambda$

$\Rightarrow$ Sum of eigenvalues after PCA quantifies the remaining variance

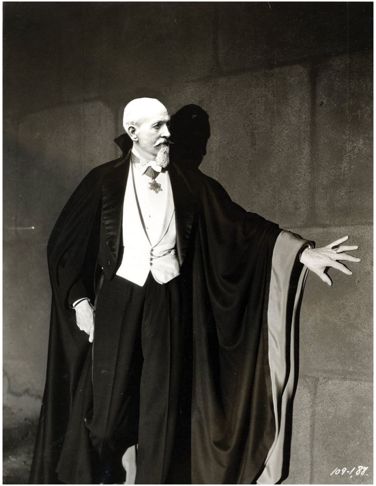
$\Rightarrow$ Quantify fraction of retained variance as $\sum_{j=1}^{n} \lambda_i / \sum_{j=1}^{m} \lambda_i$

$\Rightarrow$ Set n high enough to retain most of the variance (e.g. 95%)

Factor Analysis

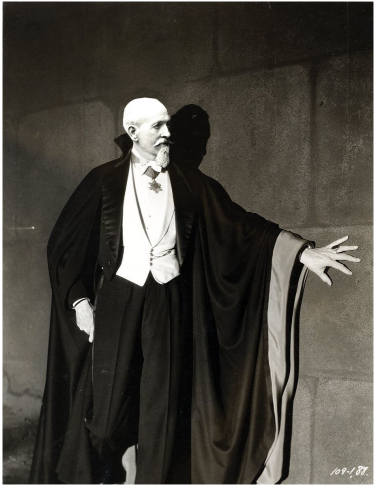
Intro

- IQ tests and Spearman $\rightarrow$ see first lecture



Intro

- IQ tests and Spearman → see first lecture
- "Modern" Factor Analysis: Probabilistic version of PCA



Intro

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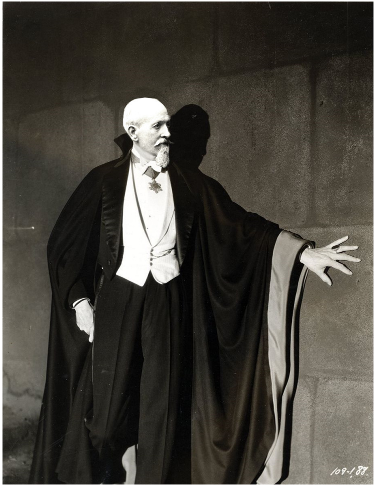
- IQ tests and Spearman → see first lecture
- "Modern" Factor Analysis: Probabilistic version of PCA
- Full derivation bit too complicated for this lecture ⇒ Refer to Barber (2012)



Probabilistic Model

- Assume data is generated as $x = \boldsymbol{V} z + b + \epsilon$

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$\Rightarrow$ $p_{X|Z}(x|z)$ is Gaussian with mean $\boldsymbol{V} z + b$ and covariance $\boldsymbol{\Psi}$

Probabilistic Model

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$\Rightarrow$ $p_X(x)$ is Gaussian with mean b and covariance $\boldsymbol{V}\boldsymbol{V}^T + \boldsymbol{\Psi}$

Probabilistic Model

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- Assume data is generated as $x = \boldsymbol{V}z + b + \epsilon$
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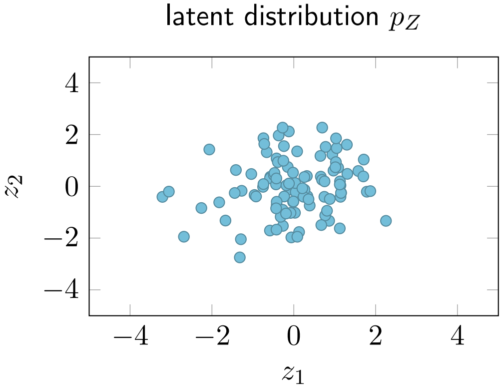
$\Rightarrow$ $p_{X|Z}(x|z)$ is Gaussian with mean $\boldsymbol{V}z + b$ and covariance $\boldsymbol{\Psi}$

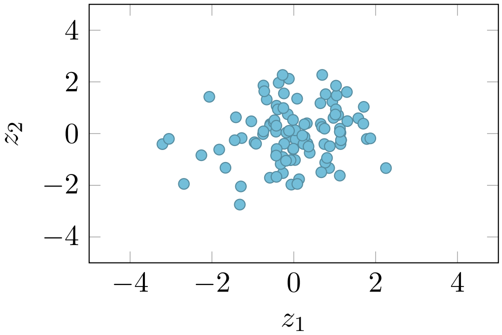
$\Rightarrow$ $p_X(x)$ is Gaussian with mean b and covariance $\boldsymbol{V}\boldsymbol{V}^T + \boldsymbol{\Psi}$ (this is not a trivial result! Follows from theory of Gaussians)

Visualization

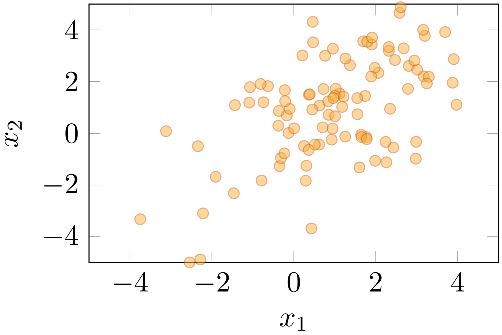


Visualization

latent distribution p_Z



data distribution p_X



Visualization

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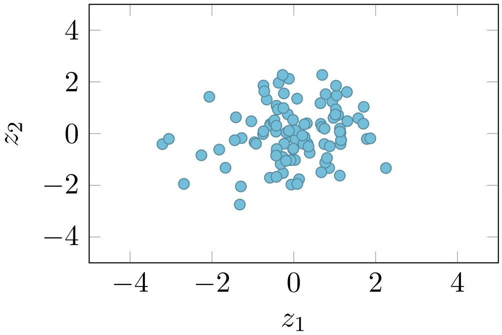

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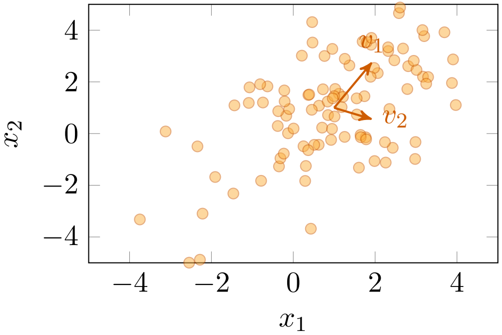
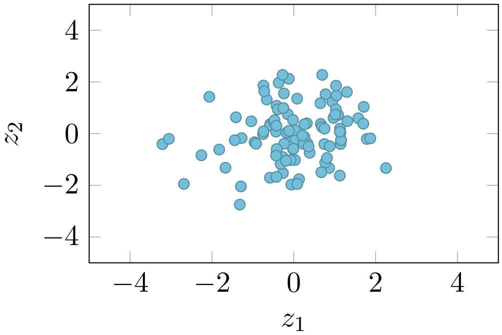


Visualization

latent distribution p_Z



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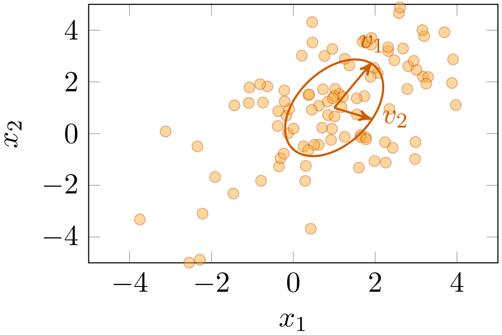
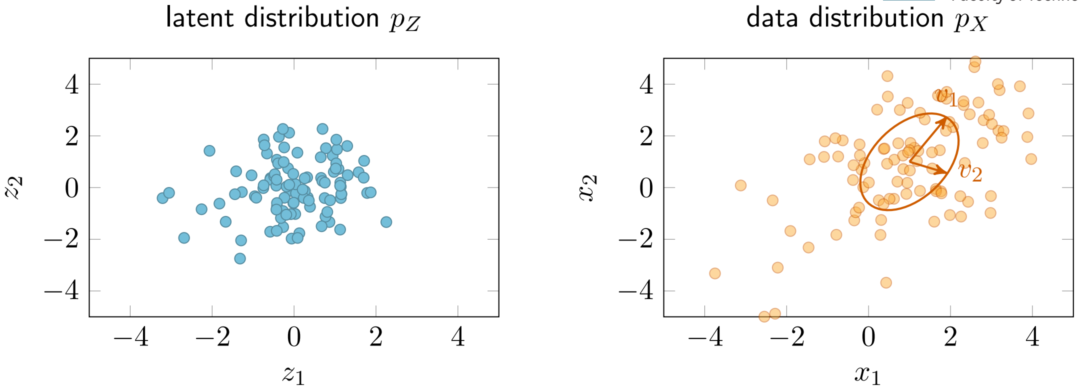
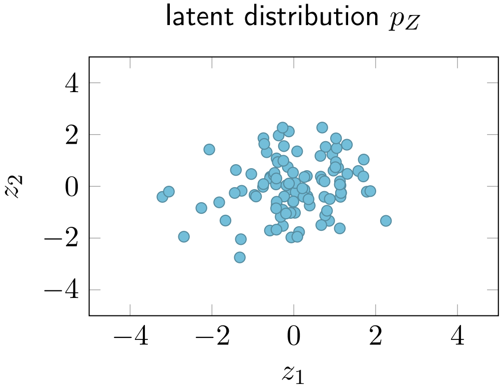


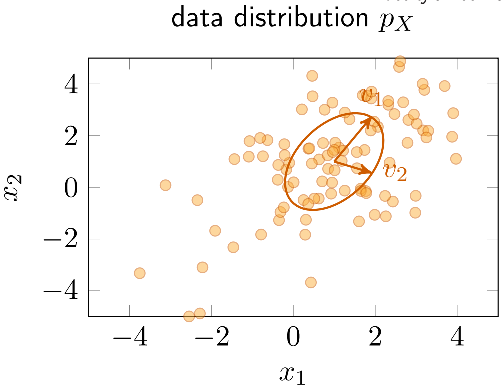
Visualization



- $\boldsymbol{V}$ rotates and stretches data distribution

Visualization





- $\boldsymbol{V}$ rotates and stretches data distribution
- columns of $\boldsymbol{V}$ can be interpreted as principal axes of the hyper-ellipse that forms the isoline of p_X (up to noise)

Maximum likelihood

- Let $\Sigma = \boldsymbol{V}\boldsymbol{V}^T + \boldsymbol{\Psi}$

Maximum likelihood

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- Optimal $\boldsymbol{V}$ is much harder to determine, requires a few tricks (Barber 2012)

Summary: FA procedure

function FA(data matrix $\boldsymbol{X}$ with N rows and m columns, desired latent dimensionality $n \leq m$)

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end for

return $\boldsymbol{V}$, μ, $\boldsymbol{\Psi}$.

end function

Notes on factor analysis

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- Implementation: sklearn.decomposition.FactorAnalysis

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- Implementation: sklearn.decomposition.FactorAnalysis
- For $\mathbf{\Psi} = \mathbf{0}$ (i.e.: no noise), model becomes equivalent to PCA
- But: $\boldsymbol{V}$ is not normalized
- Note: Encoding is **not** the focus of FA (it still works, though)

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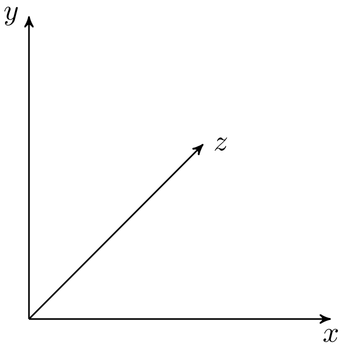
Factor Rotations

Factor Rotation Example



Factor Rotation Example

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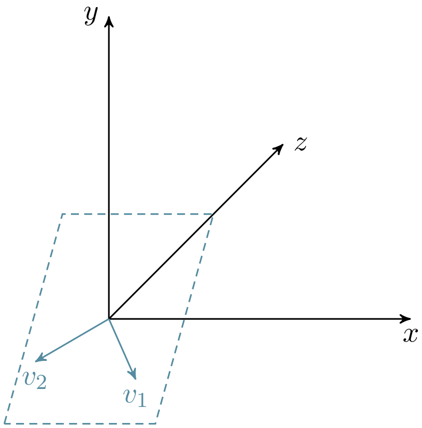

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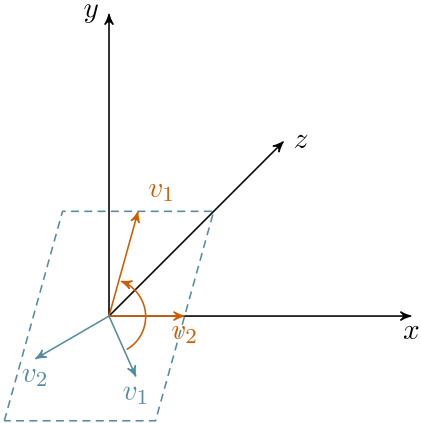

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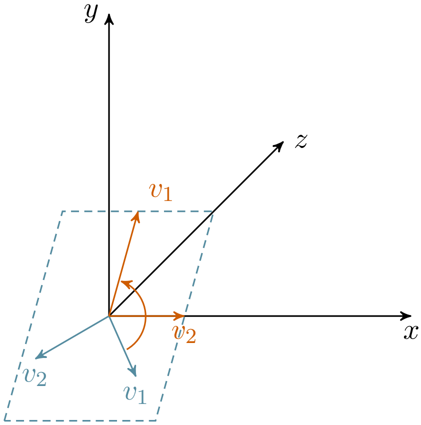

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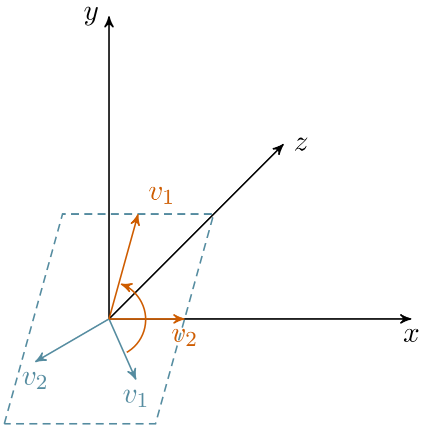

If $\boldsymbol{R}$ is a rotation matrix,
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because $\boldsymbol{V}\boldsymbol{R}(\boldsymbol{V}\boldsymbol{R})^T = \boldsymbol{V}\boldsymbol{R}\boldsymbol{R}^T\boldsymbol{V}^T = \boldsymbol{V}\boldsymbol{V}^T$

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- Nonlinear optmization, not discussed here, but implemented in Implementation: sklearn.decomposition.FactorAnalysis

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- PCA is essentially eigenvalue decomposition of covariance matrix
- highly useful for efficiently discovering underlying factors and dimensionality reduction
- Selection of n: percentage of variance covered
- factor analysis is more robust to noise but needs more iterations
- Interpretability can be enhanced with factor rotations

Literature I

Barber, David (2012). **Bayesian Reasoning and Machine Learning**. Cambridge, UK: Cambridge University Press. url: http://www.cs.ucl.ac.uk/staff/d.barber/brml/.

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