### The PCA

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### **Looking Back & Forth**



#### Last time:

- from changing bases to the SVD
- SVD facts and interpreting the SVD
- data matrices and the SVD
- rank-k approximation with the SVD

### **Today:**

- variance, covariance, and correlation
- eigenanalysis
- PCA (principal component analysis)

### Introduction



### **Principal Component Analysis (PCA)**:

- represents the data (also) in an alternative frame
   such that most data variance is aligned with the new "x-axis"
- PCA is based on an eigenanalysis of the covariance matrix and the corresponding eigenvalues indicate, how much variance is explained by each axis
- PCA can be used as a basis for dimension reduction:
   if only those k axes are used that correspond to the largest variance in the data, this leads to a k-dimensional approximation
- PCA can be useful, when dealing with noisy data:
   much of the signal can be concentrated into the first components, possibly raising the SNR (after dimension reduction)

### **Variance**

#### In 1D:

- 1st and 2nd order moments in descriptive statistics.
  - the mean  $\mu$  estimates the center of the data:
  - the standard deviation  $\sigma$  estimates  $\frac{1}{\mu-3\sigma}$   $\frac{1}{\mu-2\sigma}$   $\frac{1}{\mu-\sigma}$  the variation / dispersion of the data (68–95–99.7–rule):
  - the variance  $\sigma^2$  is the square of the standard deviation:

### **Rewriting variance:**

- shift the data by  $-\mu$  to center it
- computing the variance as  $\mathbf{x}^{\mathsf{T}}\mathbf{x}/(n-1)$  (col.  $\mathbf{x}$ )
- -x = [65; 58; 74; 54; 72; 62; 72]

$$mu = mean(x)$$

$$x_c = x-mu$$

x\_size = size(x); n = x\_size(1)
sigma\_2 = (x\_c.' \* x\_c) / (n-1)

$$\sigma = \sqrt{\frac{1}{n}} \sum_{i} (x_i - \mu)^2$$

$$\sigma^2 = \underbrace{\frac{1}{n}}_{i} \sum_{i} (x_i - \mu)$$

99.7% of the data are within 3 standard deviations of the mean

95% within
2 standard deviations
68% within
1 standard
deviation

for an unbiased estimator, divide by *n*-1

 $\mu + 3\sigma$ 

[MATLAB ex. 2d\_A]

### **Variance and Covariance**



#### In nD:

- the center is estimated per dimension (one may also rescale!)
- the variation is estimated (after centering):
  - within each dimension **x**:  $\sigma^2_{\mathbf{x}} = \mathbf{x}^{\mathsf{T}} \mathbf{x} / (n-1)$
  - between dims.  $\mathbf{x} \otimes \mathbf{y}$  (covariance):  $\sigma_{\mathbf{xy}}^2 = \mathbf{x}^T \mathbf{y} / (n-1)$

#### All variances / covariances in n**D**:

- variances and covariances show up in the covariance matrix:
  - given data matrix **D** (items in cols.):  $\Sigma^2_{\mathbf{D}} = \mathbf{D} \mathbf{D}^T / (n-1)$
  - transposed matrix **D** (items in rows):  $\Sigma_{\mathbf{D}}^2 = \mathbf{D}^{\mathsf{T}} \mathbf{D} / (n-1)$

### **Eigenanalysis**

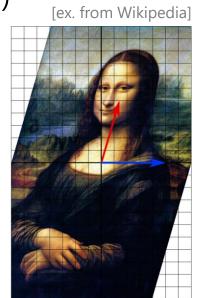


#### Assume a square matrix A in $\mathbb{R}^{n\times n}$ :

- then an eigenvalue problem is written as  $\mathbf{A} \mathbf{x} = \lambda \mathbf{x}$  with  $\lambda$  being a scalar value, i.e., an eigenvalue of  $\mathbf{A}$
- to solve an eigenvalue problem for both  $\mathbf{x}$  and  $\lambda$  means to find—in addition to all **eigenvalues**  $\lambda_i$ —all corresponding vectors  $\mathbf{x}_i$ , i.e., the **eigenvectors**  $\mathbf{x}_i$ , for which the left-multiplication with  $\mathbf{A}$  is the same as a scalar stretching/shrinking of  $\mathbf{x}$  (by  $\lambda$ )

(eigenvectors **x** do not change direction under **A**, only length, if at all)

the blue vector is an eigenvector of the depicted shear operation (but not so the red vector)



### **Eigenvalues**



### Given a square, real-valued matrix A, then:

- the eigenvalues can be positive, zero, or negative
- the eigenvalues can be complex (they appear in pairs for  $\mathbf{A} \in \mathbb{R}^{n \times n}$ )
- the eigenvalues can appear multiple times (algebraic multiplicity  $\mu$ )
- all eigenvalues add up to the trace of A
- all eigenvalues multiply to the determinant of A
- A is invertible, if and only if all eigenvalues of A are non-zero
- **A** is invertible ⇒ the eigenvalues of  $\mathbf{A}^{-1}$  are  $1/\lambda_i$
- if A is unitary, then the norm of all eigenvalues of A is 1
- if  $\mathbf{A} = \mathbf{A}^*$  ( $\mathbf{A}$  is self-adjoint), then all eigenvalues are real (in particular true for symmetric, real-valued matrices!)
- the eigenvalues of  $\mathbf{A}^k$  are  $\lambda_i^k$ , if k a positive integer
- if A is positive-/negative (semi-)definite,
   then all eigenvalues of A are positive/negative (incl. 0)

### **Eigenvectors**



### **Each eigenvalue** $\lambda_i$ (algebraic multiplicity $\mu_i \ge 1$ )

- corresponds to a subspace, i.e., the eigenspace spanned by the corresponding eigenvector(s)
- if A is symmetric,
   then the eigenvectors are orthogonal to each other
- any multiple of an eigenvector is also an eigenvector
- the eigenvectors can be complex (pairs of them)
- eigenspaces are  $\gamma_i$ -dimensional ( $\gamma_i \ge 1$ ) geometric multiplicity (the usual case is 1D)

```
in MATLAB: "[V, L]=eig(A)" gives the (normalized) eigenvectors (as columns of \mathbf{V}) and the eigenvalues (as major diagonal of \mathbf{L})
```



hyperbolic rotation

 $c = \cosh \varphi$ 

 $s = \sinh \varphi$ 

 $\lambda^2 - 2c\lambda + 1$ 

 $\lambda_1 = e^{\varphi}$ 

 $\lambda_2 = e^{-\varphi}$ 

 $\mu_1 = 1$ 

 $\mu_2 = 1$ 

 $\gamma_1 = 1$ 

 $\gamma_2 = 1$ 

 $(\lambda - 1)^2$ 

 $\lambda_1 = \lambda_2 = 1$ 

 $\mu_1 = 2$ 

 $\gamma_1 = 1$ 

 $u_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ 

<b>Eigenvalues and Eigenvectors in 2D</b>				
from Wikipedia]	scaling	unequal scaling	rotation	horizontal shear
illustration		L L L L L L L L L L L L L L L L L L L		P P y y x x x x x x x x x x x x x x x x
	[1. 0]	$\lceil k, 0 \rceil$	[c _s]	$\lceil 1  k \rceil$

 $|(\lambda-k_1)(\lambda-k_2)|$ 

 $\lambda_1 = k_1$ 

 $\lambda_2 = k_2$ 

 $\mu_1 = 1$ 

 $\mu_2 = 1$ 

 $\gamma_1 = 1$ 

 $\gamma_2 = 1$ 

 $\begin{bmatrix} s & c \end{bmatrix}$ 

 $c = \cos \theta$ 

 $s = \sin \theta$ 

 $\lambda^2 - 2c\lambda + 1$ 

 $\lambda_1 = e^{\mathbf{i}\theta} = c + s\mathbf{i}$ 

 $\lambda_2 = e^{-i\theta} = c - si$ 

 $\mu_1 = 1$ 

 $\mu_2 = 1$ 

 $\gamma_1 = 1$ 

 $\gamma_2 = 1$ 

 $\begin{bmatrix} n & 0 \\ 0 & k \end{bmatrix}$ 

 $(\lambda - k)^2$ 

 $\lambda_1 = \lambda_2 = k$ 

 $\mu_1 = 2$ 

 $\gamma_1 = 2$ 

All non-zero vectors

matrix

characteristic

polynomial

eigenvalues  $\lambda_i$ 

algebraic multipl.

 $\mu_i = \mu(\lambda_i)$ 

geometric multipl.

 $\gamma_i = \gamma(\lambda_i)$ 

eigenvectors

## Writing it all-in-one: a Decomposition!



### Assuming *n* solutions $\mathbf{x}_i \otimes \lambda_i$ to $\mathbf{A} \mathbf{x} = \lambda \mathbf{x}$ (multiplicity OK)

- then 
$$\mathbf{A}\,\mathbf{x}_1=\lambda_1\,\mathbf{x}_1$$
  $\mathbf{A}\,\mathbf{x}_2=\lambda_2\,\mathbf{x}_2$   $\Rightarrow$   $\mathbf{A}\,\mathbf{V}=\mathbf{V}\,\mathbf{\Lambda}$   $\vdots$   $\mathbf{A}\,\mathbf{x}_n=\lambda_n\,\mathbf{x}_n$ 

$$\Rightarrow$$
 **AV** = **V** $\Lambda$ 

with 
$$\mathbf{V} = (\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \mathbf{x}_n)$$
 and

$$\mathbf{\Lambda} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$$

$$\Rightarrow$$
  $\mathbf{A} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^{-1}$ 

### A better Frame



### Eigenanalysis...

- ... leads to the eigenvalue/eigenvector decomposition  $\mathbf{A} = \mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^{-1}$  with  $\mathbf{V}$  hosting all (normalized) eigenvectors and  $\boldsymbol{\Lambda}$  having all eigenvalues along the major diagonal
- ... if **A** is real-valued and symmetric, then **V** is unitary, i.e., an orthonormal basis of  $\mathbb{R}^n$  (important for PCA)

### This suggests...

... that we can consider our  $\mathbf{A}$  in terms of basis  $\mathbf{V}$ :  $\mathbf{X} = \mathbf{V}^* \mathbf{A}$  ( $\mathbf{X}$  is then  $\mathbf{A}$  in orthonormal  $\mathbf{V}$ -coordinates)

#### This leads to:

[see the MATLAB example 2d\_C]

- Given A in orthonormal V-coords. (by  $X = V^*A$ ),  $A = V \wedge V^*$  leads to  $X = V^*A = V^*V \wedge V^* = \Lambda V^*$
- in particular  $\mathbf{X} \mathbf{v} = [\mathbf{A} \mathbf{v}]_{\mathbf{V}} = \mathbf{\Lambda} \mathbf{V}^* \mathbf{v} = \mathbf{\Lambda} [\mathbf{v}]_{\mathbf{V}}$  (dim.-wise scaling!)

### **Eigenanalysis – Interpretation**

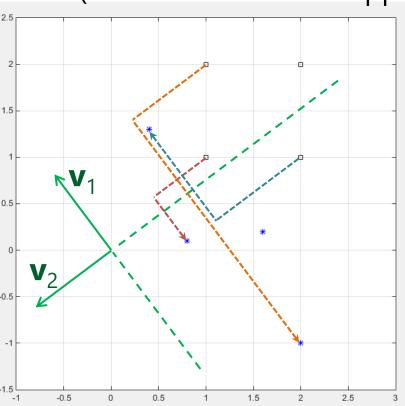


### Assuming a mapping A: $\mathbb{R}^2 \to \mathbb{R}^2$ (again),

- and also considering four vectors (1)
  - four vectors  $\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \begin{pmatrix} 2 \\ 2 \end{pmatrix}$

 $\mathbf{A} = \left( \begin{array}{cc} -0.4 & 1.2 \\ 1.2 & -1.1 \end{array} \right)$ 

('\*' below after the mapping)



### Then the eigenanalysis of A gives:

in MATLAB: "[V, L]=eig(A)"

- eigenvalues −2 and ½
- and eigenvectors  $\begin{pmatrix} -0.6 \\ 0.8 \end{pmatrix}^{\mathbf{V}_1} & \begin{pmatrix} -0.8 \\ -0.6 \end{pmatrix}^{\mathbf{V}_2}$

[see the MATLAB example 2d\_D]

### **SVD**–Eigenanalysis Comparison



### Both are decomposition/diagonalization approaches,

i.e., both lead to a factorization of A into PMQ
 with M (singular values or eigenvalues) being diagonal and P & Q representing two change of basis steps

#### **But**

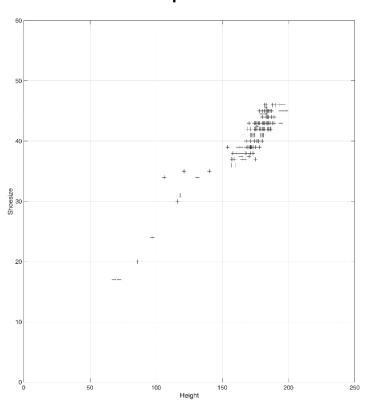
- the SVD exists always (+), even for rectangular matrices (+), while the eigendecomposition not necessarily exists (-) - the SVD exists always (+), even for rectangular matrices (+), while the eigendecomposition not necessarily exists (-) example: nilpotent matrix  $\begin{pmatrix} 0 \\ 0 \end{pmatrix}$
- the SVD results in a real-valued solution (+), while the eigenvalues/eigenvectors may be complex-valued (-)
- the SVD uses two bases  $\mathbf{U} \otimes \mathbf{V}$  (-), which always are unitary/orthonormal (+), the eigendecomp. uses one (+),  $\mathbf{V}$ , that may not be orthogonal (-)

### **PCA – Introduction**



#### Some data

- may be "intrinsically" r-dimensional, but represented d-dimensional with d>r
- example: if all data  $\mathbf{d}_i \in \mathbb{R}^3$  are of form  $\mathbf{d}_i = s_i \mathbf{v}$ ,  $\mathbf{v} \in \mathbb{R}^3$ , then their representation is 3D, while their intrinsic dimensionality is 1



### Let's look at some people's data:

- we consider Height vs. Shoesize now (they look correlated, right?!)
- the covariance matrix looks like

$$\Sigma_{\mathbf{D}}^2 = \begin{pmatrix} 388.7857 & 82.9229 \\ 82.9229 & 20.3942 \end{pmatrix}$$

with major off-diagonal values!

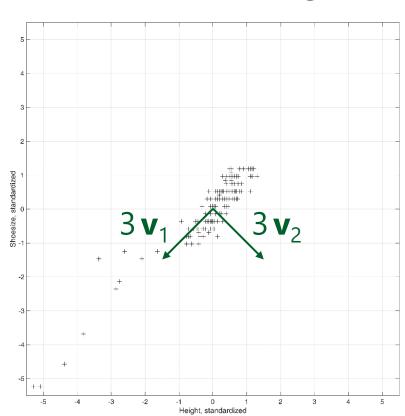
### **PCA** – Diagonalizing $\Sigma^2$



### **Next step** (after normalization/standardization):

- transform such that the covariance matrix becomes diagonal! (since  $\Sigma^2$  is real-valued and symmetric, we use the eigendecomp.)

### This leads to the eigenvalues & eigenvectors of $\Sigma^2$ :



eigenvalues ≈1.93 and ≈0.07
 with the corresponding eigenvectors

$$\mathbf{V} = \left( \begin{array}{ccc} -0.7071 & 0.7071 \\ -0.7071 & -0.7071 \end{array} \right)$$

called principal components (PC)

 the vast difference in eigenvalues tells that this dataset is mostly 1D!

### PCA – Look at the Scores

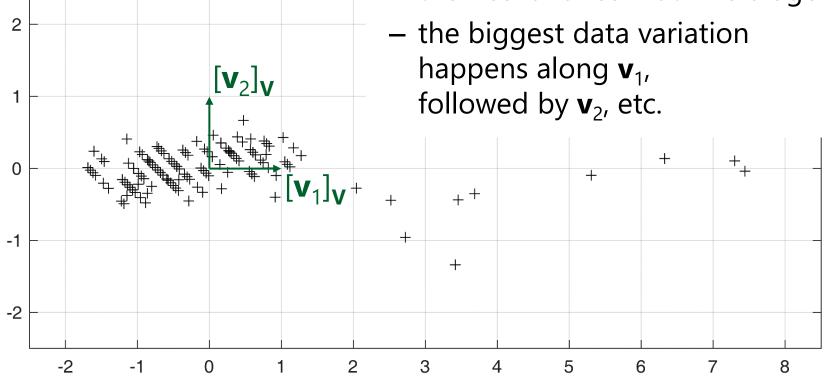


#### **Next step:**

– we can now look at the data in terms of  $\mathbf{V}$ , i.e., in the PC of  $\mathbf{D}$  (the  $[\mathbf{D}]_{\mathbf{V}}$  are called the *scores* in PCA)

#### The scores are then uncorrelated



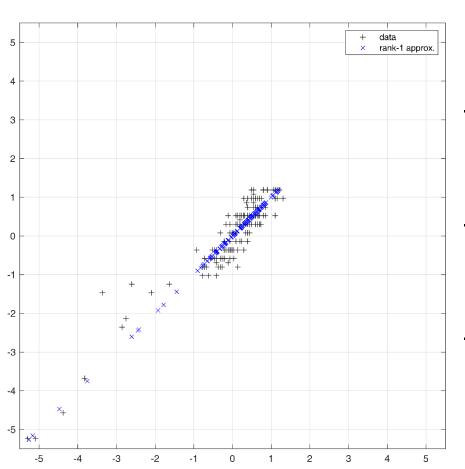


### **PCA – Low-rank Approximation**



#### Similar to the SVD,

– we can compute a lower-(k-)dimensional approximation of the (normalized) data **D** by "only" considering the largest eigenvalues



### Given scores [D]<sub>V</sub>,

- we keep only the data rows corresponding to the largest k eigenvalues
- assuming that we reordered V & Λ
   so that the eigenvalues in Λ
   became sorted in decreasing size
- we then compute  $\mathbf{D'}_k$  by  $\mathbf{D'}_k = (\mathbf{v}_1 \ \mathbf{v}_2 \ ... \ \mathbf{v}_k) \ (\mathbf{d}_{\mathbf{V}1}^{\mathsf{T}} \ \mathbf{d}_{\mathbf{V}2}^{\mathsf{T}} \ ... \ \mathbf{d}_{\mathbf{V}k}^{\mathsf{T}})^{\mathsf{T}}$

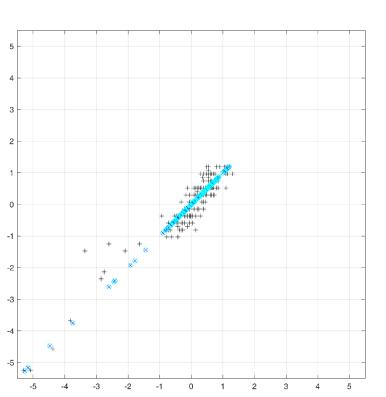
[see the MATLAB example 2d\_E]

### PCA vs. SVD



# The lower-dimensional approximation with PCA overlaps with the rank-k approximation with SVD:

- the eigenvalues from PCA,  $\lambda_i$ , are equal to  $\sigma_i^2/(n-1)$
- the left-singular vectors **U** are the PC from PCA (up to sign change), if data rows are given (otherwise it's **V**)



#### **Relation:**

- 1. data  $\mathbf{D}$ , d dims. x n items (in the cols.)
- 2.  $\Sigma^2 = \mathbf{D} \mathbf{D}^T / (n-1) / / \text{covariance-matrix}$
- 3.  $\Sigma^2 = V \Lambda V^* // eigendecomposition$
- 4.  $[D]_{V} = V * D // scores$
- 5. **D** = **U S W\*** // SVD
- 6.  $\Sigma^2 = U S W^* (W S^* U^*) / (n-1) // 2. \& 5.$ =  $U (S S^* / (n-1)) U^* = V \Lambda V^* // 3.$

### PCA – Investigate the Loadings (1)



#### With PCA

- we transform the data into a new Cartesian coordinate frame (the PCs are orthogonal to each other)
- so that the covariance between the scores is zero (we remove any redundancy from the data)

### **Challenging** (as with the SVD):

- considering the scores  $[\mathbf{D}]_{\mathbf{V}}$  of data  $\mathbf{D}$ , esp. after normalization, we usually lack a good interpretation of the new axes—they are linear combinations of the original data-axes, i.e., the "new data"  $[\mathbf{D}]_{\mathbf{V}}$  is a mix (linear combination) of  $\mathbf{D}$
- one way to interpret the principal components, is to look at their *loadings*: to which degree play the original data-axes into them?

### PCA – Investigate the Loadings (2)



### The loadings

- of PC i are given by the components of eigenvector  $\mathbf{v}_i$
- given data rows (items in cols.),
  - data item j is given by column j in **D**:  $(d_{...j})$
  - the scores of data item j are then  $(d_{\mathbf{v}_{...,j}}) = \mathbf{V}^*(d_{...,j})$ , i.e.,  $d_{\mathbf{v}_{1,j}} = \mathbf{v}_1^T(d_{...,j})$ ,  $d_{\mathbf{v}_{2,j}} = \mathbf{v}_2^T(d_{...,j})$ , aso.
- interpretation:
  - the "new" x-coordinate of some data item
    is a linear combination of all original attributes of this item,
    weighted by the entries of eigenvector #1,
    i.e.,
    - a large absolute component #k in eigenvector #g tells about a major influence of data attribute #k onto the principal component #g

### PCA – Investigate the Loadings (3)



#### **Back to our example:**

looking (again) at **V**, we see:

$$\mathbf{V} = \begin{pmatrix} -0.7071 & 0.7071 \\ -0.7071 & -0.7071 \end{pmatrix}$$

- the 1<sup>st</sup> principal component is a (negative) combination of Height and Shoesize, whereas
- the 2<sup>nd</sup> principal component expresses their disagreement (e.g., large feet, but short)
- taking also the vastly different eigenvalues (~1.93 vs. ~0.07)
   into account, we find that
  - mostly, it's about the overall size (height & feet)
  - minor differences exist (larger feet, while being a bit shorter)



### Considering all of the people's data, i.e.,

- the four data attributes Age, Height, Weight, and Shoesize

#### **Steps:** [see the MATLAB example 2d\_F]

- 1. load the data
- 2. set up the data  $\mathbf{D}$  (here data cols., again, i.e., items in the rows); compute also n, d, all per-dim. means  $\mathbf{mu}$  & std.-dev. values  $\mathbf{sigma}$
- 3. normalize the data: **Dz** becomes the z-score of **D**
- 4. visualize to check

[...]



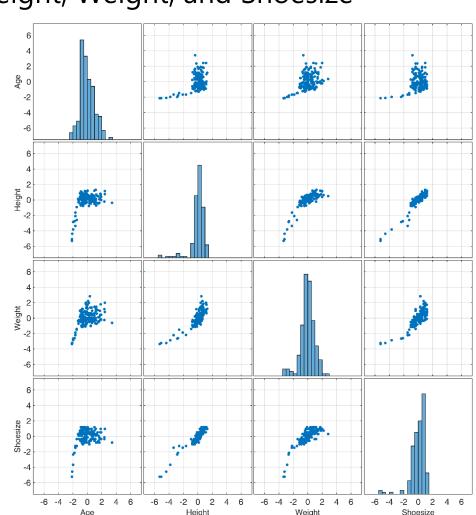
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[...]





### Considering all of the people's data, i.e.,

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#### **Steps:**

- [...]
- 5. compute the covariance matrix **S2z** and do the eigendecomposition into **Vz** and **Lz**
- 6. sort by the absolute eigenvalue value to get LzS and VzS
- 7. compute the scores **DzScores**
- 8. look at them
- [...]



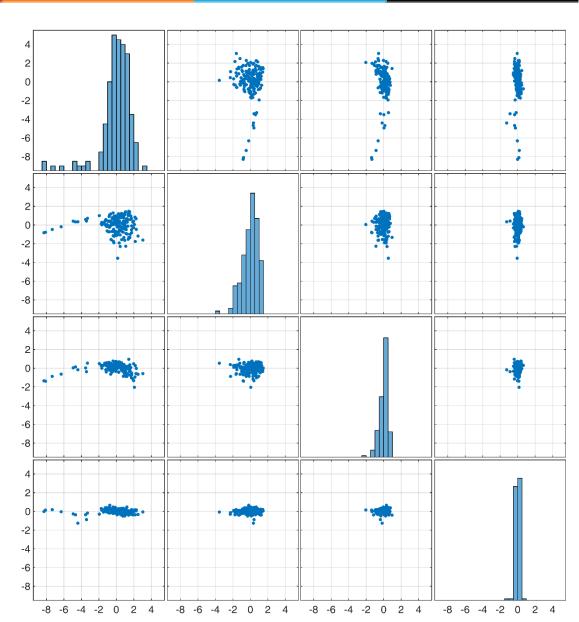
### **Considering all c**

the four data a

### **Steps:**

- [...]
- 5. compute the covand do the eiger
- 6. sort by the abso
- 7. compute the scc
- 8. look at them

[...]



[see the MATLAB example 2d\_F]



### Considering all of the people's data, i.e.,

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### **Steps:**

```
[...]
```

- 9. do a 2D-reconstruction **DzReco2**
- 10. do a comparative visualization
- 11. undo the normalization for the reconstruction, get **Dreco2**
- 12. visualize

```
[…]
```



Shoesize

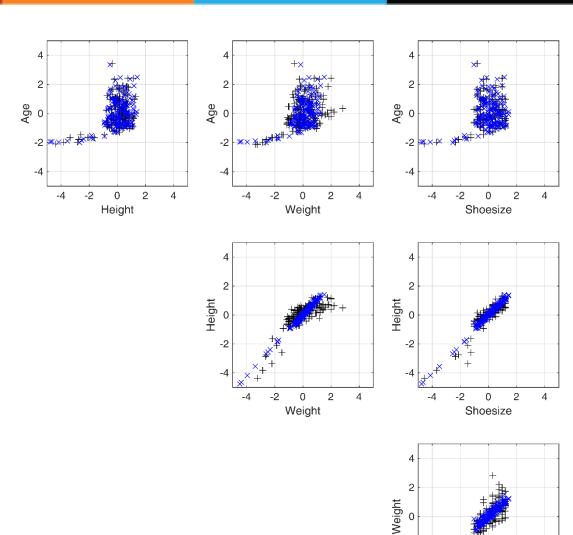
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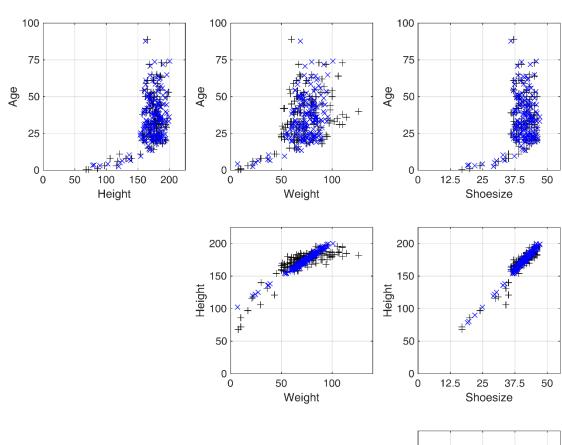


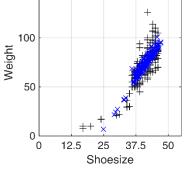
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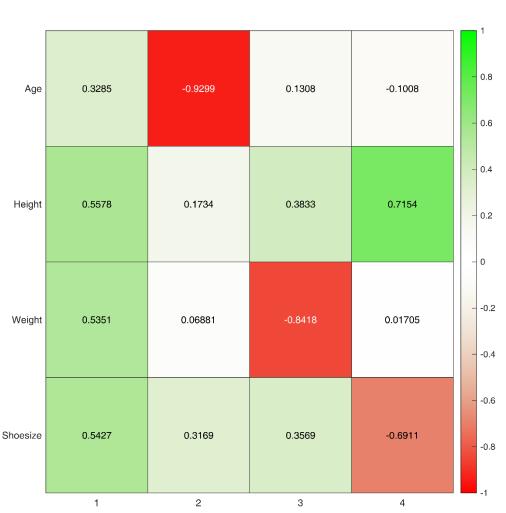
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#### **Steps:**

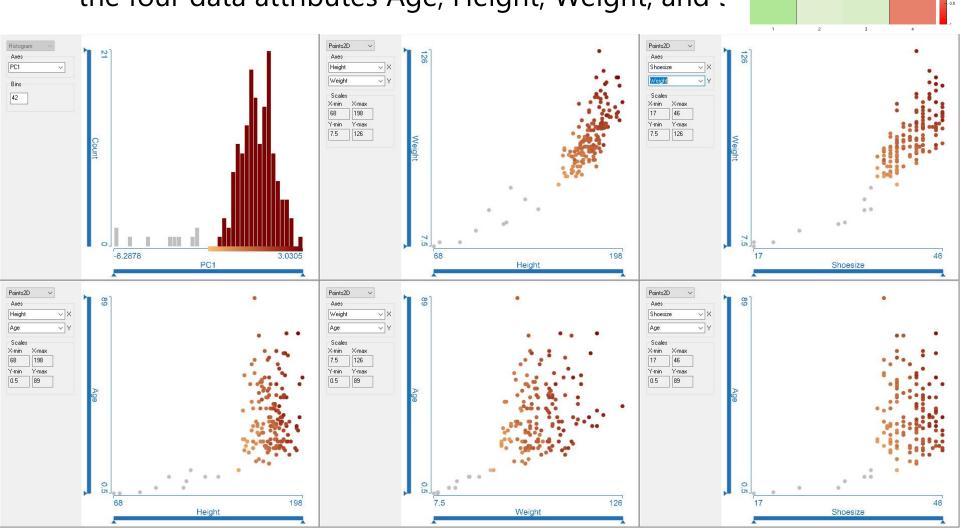
[...]

13. look at the loadings



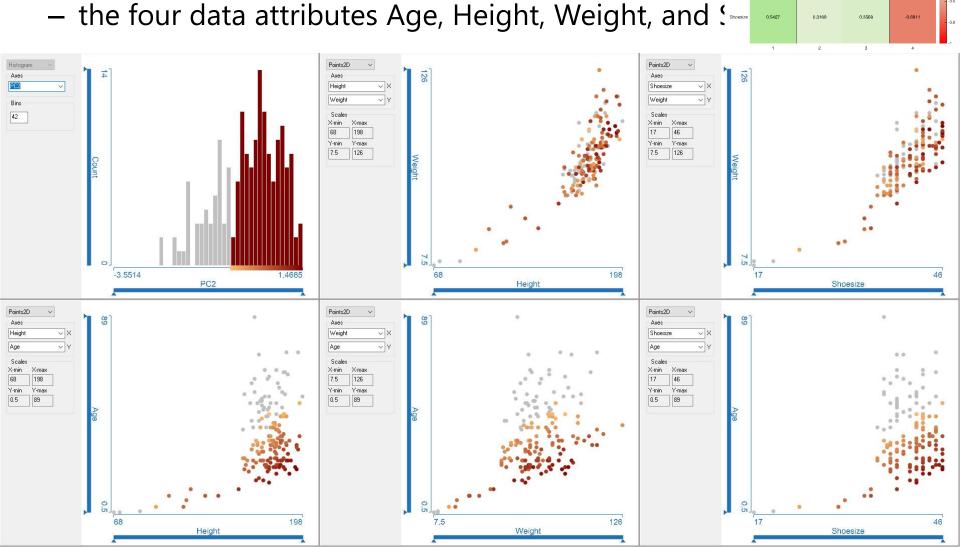
### Considering all of the people's data, i.e.,

the four data attributes Age, Height, Weight, and



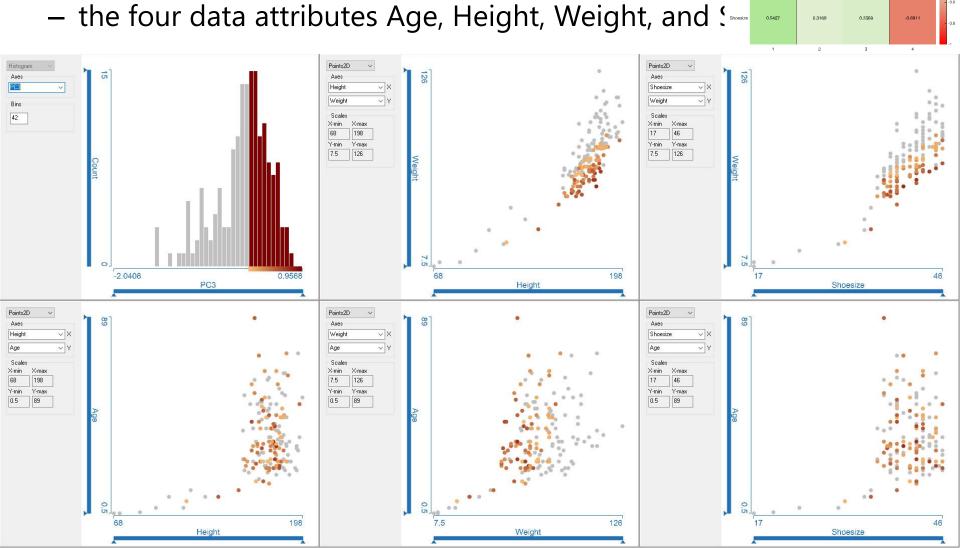
### Considering all of the people's data, i.e.,

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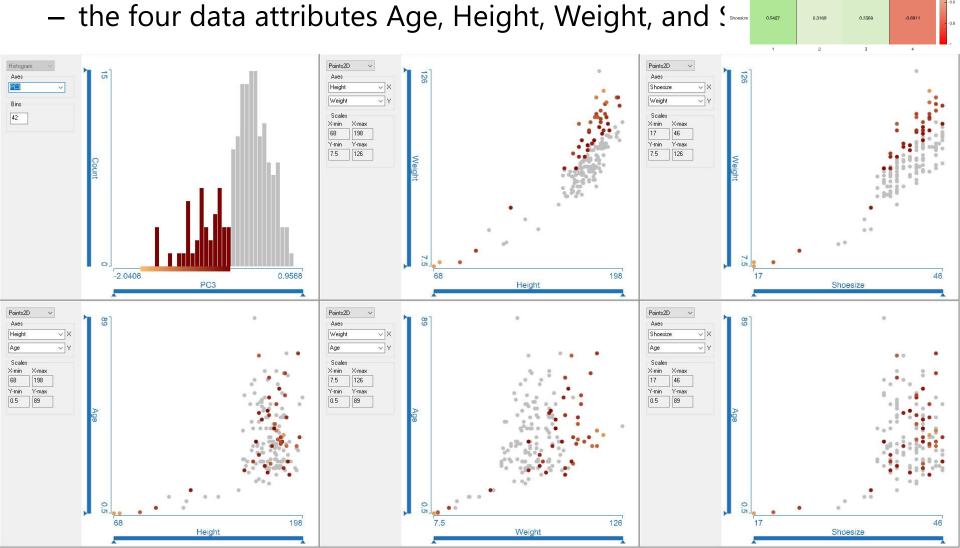
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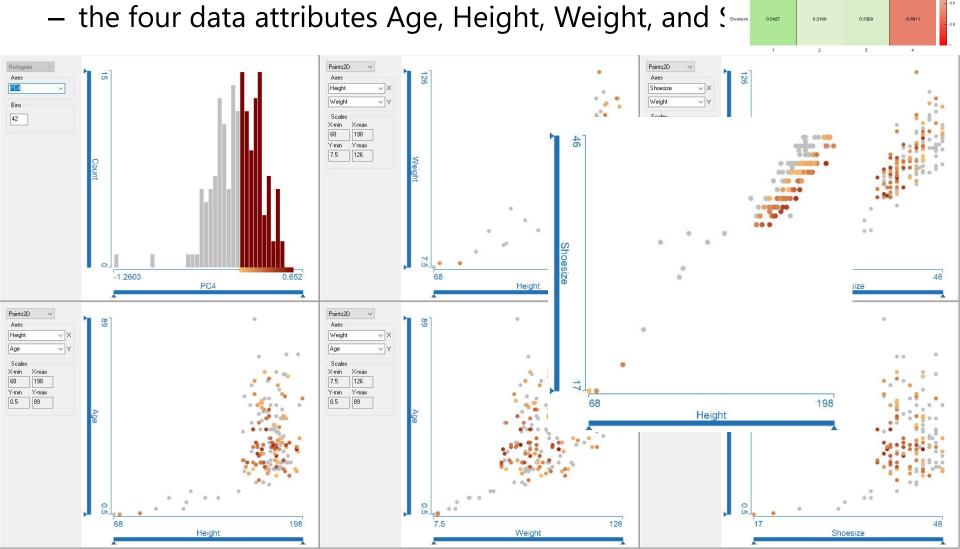
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### **PCA – Remarks**



### **Principal Component Analysis (PCA)**

- can be seen as a best-possible linear technique for dimension reduction (best in the least sum of squared distances sense)
- is sensitive to the scaling of individual dimensions
   (therefore, often normalization is done dimension-wise first)
- this issue (PCA sensitive to dim.-scaling) implies that PCA is to a certain degree "arbitrary", when dimensions of different units are studied (that cannot be mapped to each other, like temperatures and costs)
- PCA makes only sense, when the data is centered
- numerous extensions / alternative approaches exist,
   including non-linear techniques, sparse PCA, robust PCA, ...

### How to Solve an Eigenproblem



### Focus up to here:

how to use an eigenanalysis

#### **Not touched** (yet):

how to solve an eigenproblem

#### In short:

- given  $\mathbf{A} \mathbf{x} = \lambda \mathbf{x}$ ,
- we get to  $(\mathbf{A} \lambda \mathbf{I})\mathbf{x} = 0$ 
  - if  $(\mathbf{A} \lambda \mathbf{I})$  is non-singular, then only  $\mathbf{x} = \mathbf{0}$  is a solution
  - thus, and in order to find non-degenerated solutions, we need to require that  $(\mathbf{A} \lambda \mathbf{I})$  is singular, i.e.,  $\det(\mathbf{A} \lambda \mathbf{I}) = 0$
- $\det(\mathbf{A} \lambda \mathbf{I}) = 0$  is called the characteristic equation of  $\mathbf{A}$ , leading to the eigenvalues  $\lambda_i$
- having the  $\lambda_i$ , we can solve  $(\mathbf{A} \lambda \mathbf{I})\mathbf{x} = 0$  for the  $\mathbf{x}_i$

### Outlook



#### **Next**:

- a new part of INF250 with
  - data fitting (somehow a continuation of this part!)
  - splines
  - iterative methods

### Reading and Related Material



#### In the book:

- chapter 2 (on linear systems), mostly section 2.1, and related parts
- chapter 15 (on SVD, etc.)

#### **Course notes:**

section 4

#### An interactive online-book:

http://lmmersiveMath.com/,
 chapters (1–4 &) 5 (on Gaussian elimination)
 and 6 (on The Matrix)

#### On Wikipedia:

many good pages