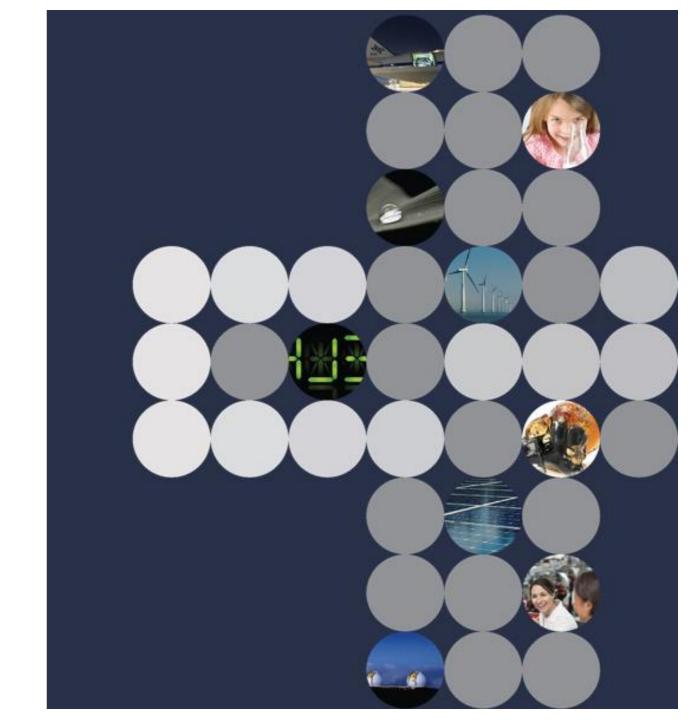
EE512 – Applied Biomedical Signal Processing

Principal Component Analysis (PCA)

Karen ADAM
CSEM Signal Processing and Al Group





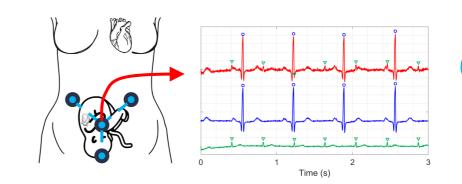
Introduction - Principal Component Analysis (PCA)

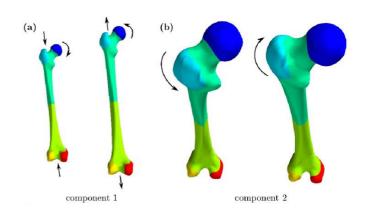
- Principal component analysis (PCA)
 - Also called Hotelling or Karhunen-Loève transform



- Motivation: use-cases
 - Dimensionality reduction
 - 2. Blind source separation
 - 3. Statistical shape analysis/modelling

SVD is useful to implement PCA

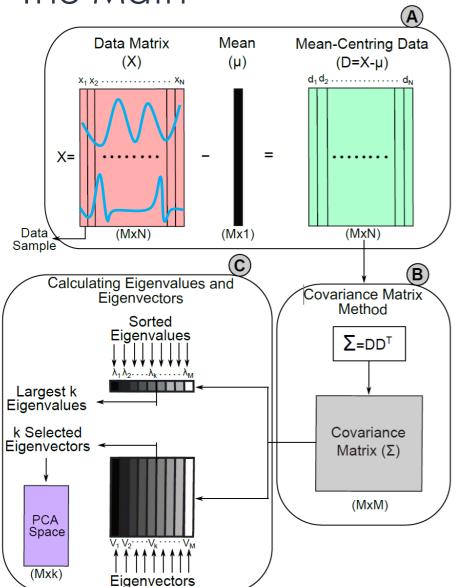








The Math



- Data matrix X of size $M \times N$
 - M: dimensions (e.g., # channels)
 - N: trials/experiments (e.g., # samples)
- 4-step approach:
 - A. Remove mean: $\mathbf{D} = \mathbf{X} \mu$
 - B. Covariance matrix: $\Sigma = DD^T$
 - C. Eigenvectors v_i and Eigenvalues λ_i :

$$W = \{v_1, v_2, \dots, v_M\} \\ \{\lambda_1, \lambda_2, \dots, \lambda_M\} \iff \text{eig}(\Sigma)$$

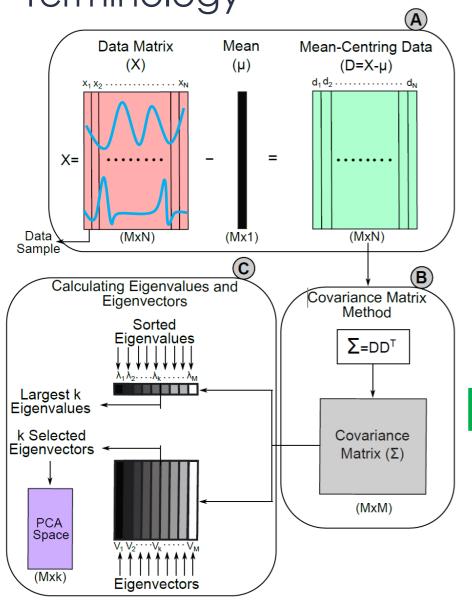
D. Principal components:

$$\mathbf{Y} = \mathbf{W}^T \mathbf{D} \in \mathbb{R}^{M \times N}$$





Terminology



- Data matrix X of size $M \times N$
 - M: dimensions (e.g., # channels)
 - N: trials/experiments (e.g., # samples)
- 4-step approach:
 - A. Remove mean: $\mathbf{D} = \mathbf{X} \mu$
 - B. Covariance matrix: $\Sigma = DD^T$
 - C. Eigenvectors v_i and Eigenvalues λ_i :
- Principal axes
- Principal directions
- Principal components (!)

$$W = \{v_1, v_2, ..., v_M\} \\ \{\lambda_1, \lambda_2, ..., \lambda_M\} \iff \text{eig}(\Sigma)$$

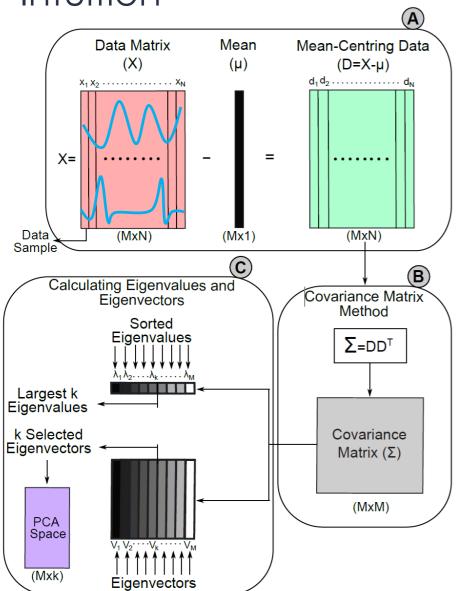
D. Principal components

$$\mathbf{Y} = \mathbf{W}^T \mathbf{D} \in \mathbb{R}^{M \times N}$$

Principal component scores







Data matrix X of size $M \times N$

What you'd like to reduce

- M: dimensions (e.g., # channels)
- N: trials/experiments (e.g., # samples)
- 4-step approach:
 - A. Remove mean: $\mathbf{D} = \mathbf{X} \mu$
 - B. Covariance matrix: $\Sigma = DD^T$
 - C. Eigenvectors v_i and Eigenvalues λ_i :

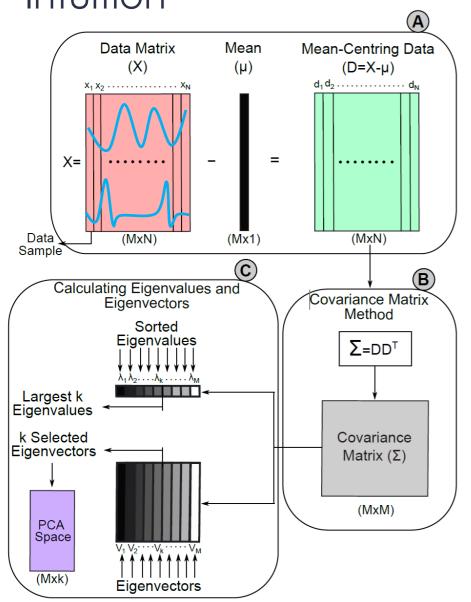
$$W = \{v_1, v_2, \dots, v_M\} \\ \{\lambda_1, \lambda_2, \dots, \lambda_M\} \iff \text{eig}(\Sigma)$$

D. Principal components:

$$\mathbf{Y} = \mathbf{W}^T \mathbf{D} \in \mathbb{R}^{M \times N}$$







Data matrix X of size $M \times N$

What you'd like to reduce

- M: dimensions (e.g., # channels)
- N: trials/experiments (e.g., # samples)
- 4-step approach:
 - A. Remove mean: $\mathbf{D} = \mathbf{X} \mu$
 - B. Covariance matrix: $\Sigma = DD^T$
 - C. Eigenvectors v_i and Eigenvalues λ_i :

MxM rotation matrix in decreasing λ order

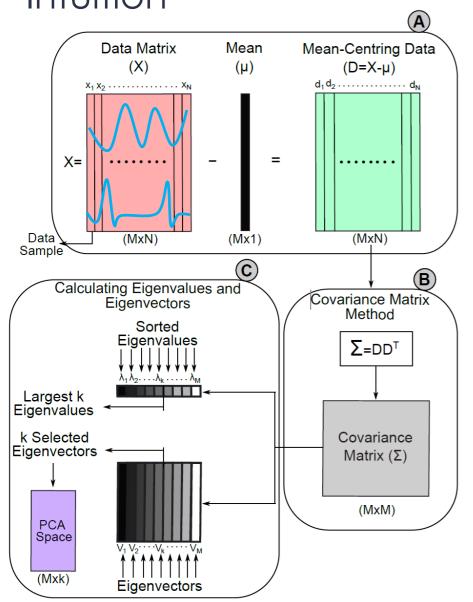
$$\frac{\boldsymbol{W} = \{v_1, v_2, \dots, v_M\}}{\{\lambda_1, \lambda_2, \dots, \lambda_M\}} \Leftarrow \operatorname{eig}(\boldsymbol{\Sigma})$$

D. Principal components:

$$\mathbf{Y} = \mathbf{W}^T \mathbf{D} \in \mathbb{R}^{M \times N}$$







Data matrix X of size $M \times N$

What you'd like to reduce

- M: dimensions (e.g., # channels)
- N: trials/experiments (e.g., # samples)
- 4-step approach:
 - A. Remove mean: $\mathbf{D} = \mathbf{X} \mu$
 - B. Covariance matrix: $\Sigma = DD^T$
 - C. Eigenvectors v_i and Eigenvalues λ_i :

MxM rotation matrix in decreasing λ order

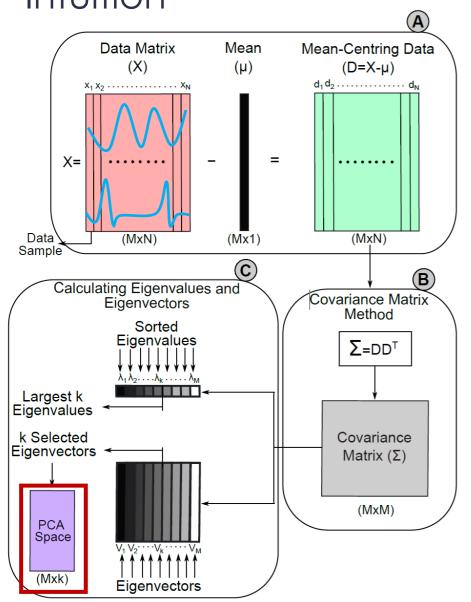
$$W = \{v_1, v_2, \dots, v_M\} \iff \text{eig } (\mathbf{\Sigma})$$

D. Principal components:

$$\mathbf{Y} = \mathbf{W}^T \mathbf{D} \in \mathbb{R}^{M \times N}$$

The rotated data matrix





Data matrix X of size $M \times N$

What you'd like to reduce

- M: dimensions (e.g., # channels)
- N: trials/experiments (e.g., # samples)
- 4-step approach:
 - A. Remove mean: $\mathbf{D} = \mathbf{X} \mu$
 - B. Covariance matrix: $\mathbf{\Sigma} = \mathbf{D}\mathbf{D}^T$
 - C. Eigenvectors v_i and Eigenvalues λ_i :

MxM rotation matrix in decreasing λ order

$$W = \{v_1, v_2, \dots, v_M\} \iff \text{eig } (\Sigma)$$

D. Principal components:

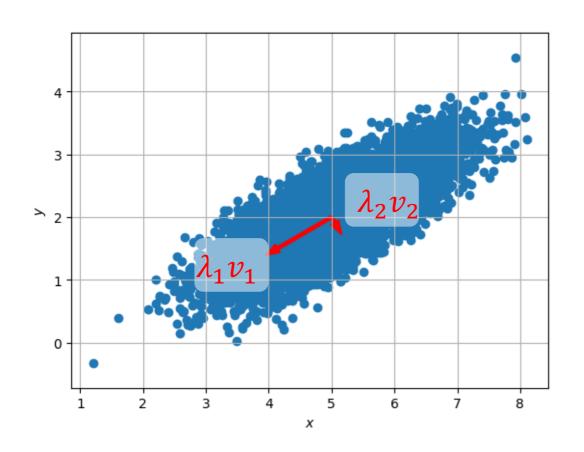
$$\mathbf{Y} = \mathbf{W}^T \mathbf{D} \in \mathbb{R}^{M \times N}$$

The rotated data matrix



Simple Examples

2D Gaussian distribution



$$\mathbf{X} = \begin{bmatrix} x_1 & x_2 & \cdots & x_N \\ y_1 & y_2 & \cdots & y_N \end{bmatrix} \quad \begin{array}{c} \mathbf{M} = 2 \\ \text{# dimensions} \\ \mathbf{N} = 10'000 \\ \text{# samples} \end{array}$$

Eigenvectors and Eigenvalues:

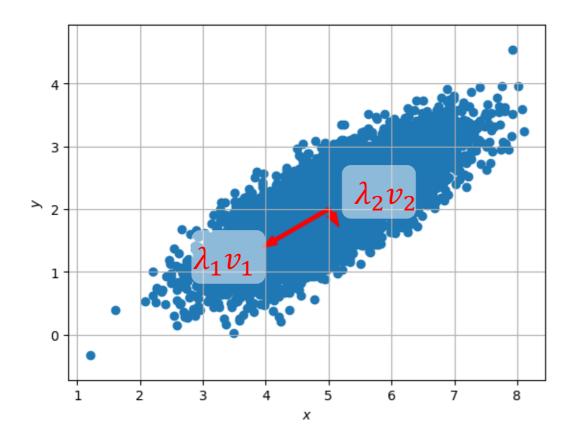
$$v_1 = \begin{bmatrix} -0.86 \\ 0.50 \end{bmatrix}$$
 with $\lambda_1 = 0.99$

$$v_2 = \begin{bmatrix} 0.50 \\ -0.86 \end{bmatrix}$$
 with $\lambda_2 = 0.10$

9

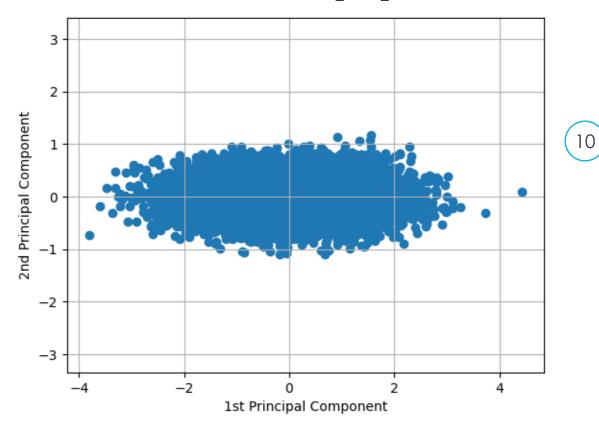
Simple Examples

$$\mathbf{X} = \begin{bmatrix} x_1 & x_2 & \cdots & x_N \\ y_1 & y_2 & \cdots & y_N \end{bmatrix}$$



PCA Space

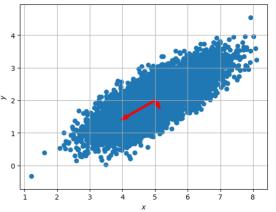
$$\mathbf{Y} = \mathbf{W}^{T}(\mathbf{X} - \overline{\mathbf{X}}) = \begin{bmatrix} v_{1}^{T} \\ v_{2}^{T} \end{bmatrix}^{T} (\mathbf{X} - \overline{\mathbf{X}})$$



Properties of PCA

Intuitive explanation [Wikipedia]:

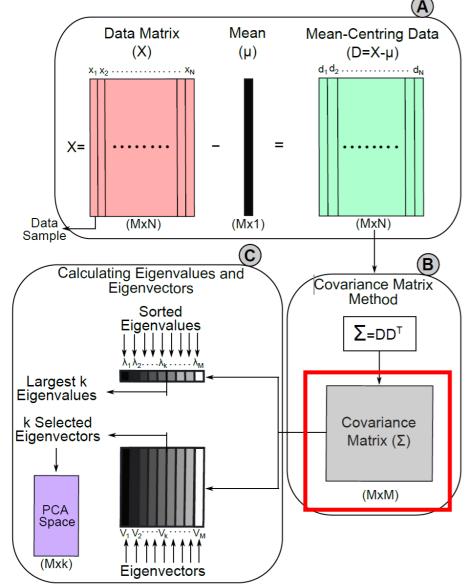
- Fitting an M-dimensional ellipsoid to the data (\mathbf{X}), where each axis of the ellipsoid represents a principal axis (v_i).
- If some axis of the ellipsoid is small, then the variance (λ_i) along that axis is also small.
- Linear transformation of data to new coordinate system (PCA space)
 - Orthogonal (lower-dimensional) system. i.e., the principal axes are perpendicular and normalized
 - The greatest variance of the data comes to lie on the first coordinate (1st PC),
 the second greatest variance on the second coordinate (2nd PC), etc.
- PCA assumes that the original data follows a Gaussian distribution.

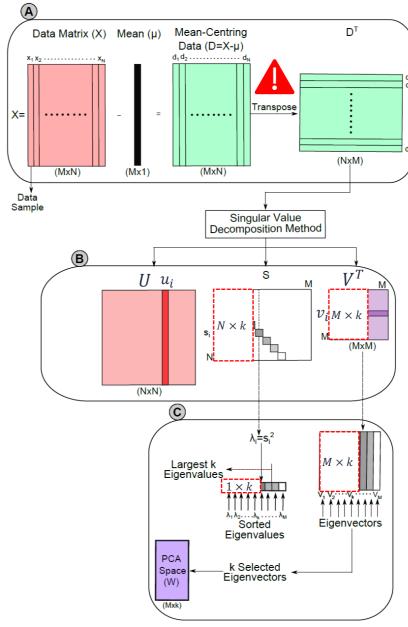






Practical Issues and SVD







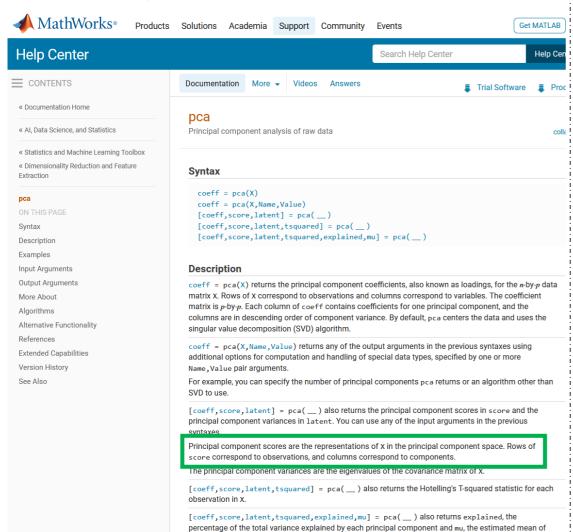


Code Examples



```
function [PC, PA, Lambda] = pca via covariance(X)
                                                             function [PC, PA, Lambda] = pca via svd(X)
%% PCA via covariance: Perform PCA using covariance.
                                                             %% PCA via SVD: Perform PCA using SVD.
        X - M x N matrix of input data
                                                                     X - M x N matrix of input data
            (M dimensions, N trials)
                                                                          (M dimensions, N trials)
       PC - M x N matrix of projected data
                                                                     PC - M x N matrix of projected data
             (e.g., the principal components)
                                                                          (e.g., the principal components)
       PA - each column is a principal axis
                                                                    PA - each column is a principal axis
% Lambdas - M x 1 matrix of variances
                                                             % Lambdas - M x 1 matrix of variances
    [M, N] = size(X);
                                                                  [M, N] = size(data);
    % subtract off the mean for each dimension
                                                                 % subtract off the mean for each dimension
    mn = mean(X, 2);
                                                                 mn = mean(X, 2);
    X = X - repmat(mn, 1, N);
                                                                 data = data - repmat(mn,1,N);
    % calculate the covariance matrix
                                                                 % construct the matrix Y
    covariance = 1 / (N-1) * X * X';
                                                                 Y = data' / sqrt(N-1);
    % find the eigenvectors and eigenvalues
                                                                 % SVD does it all
    [PA, Lambdas] = eig(covariance);
                                                                  [u, S, PA] = svd(Y);
    % extract diagonal of matrix as vector
                                                                 % calculate the variances
    Lambdas = diag(Lambdas);
                                                                 S = diag(S);
    % sort the variances in decreasing order
                                                                 Lambdas = S .* S;
    [~, rindices] = sort(-1*Lambdas);
    Lambdas = Lambdas(rindices);
    PA = PA(:, rindices);
    % project original data -> principal comps.
                                                                 % project original data -> principal comps.
    PC = PA' * X;
                                                                  PC = PA' * X;
end
                                                              end
```





Principal component scores \rightarrow principal components



scikit-learn 1.1.3

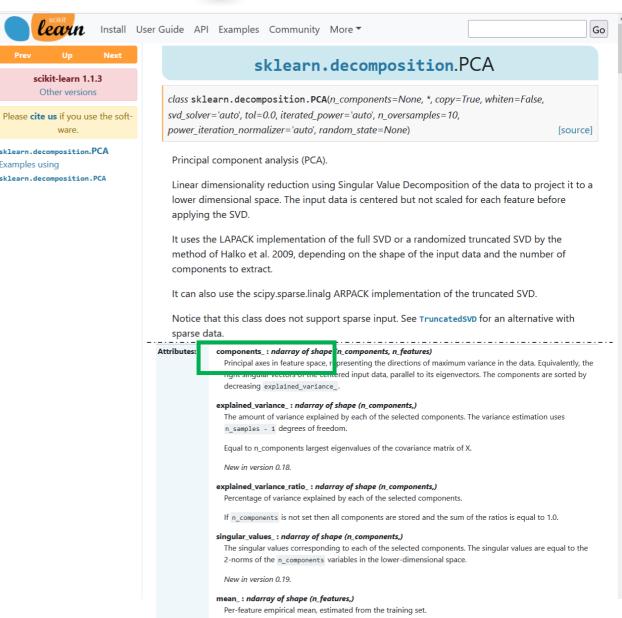
Other versions

ware.

sklearn.decomposition.PCA

sklearn.decomposition.PCA

Examples using



Equal to X.mean(axis=0)





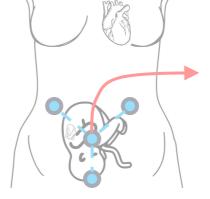
Usage Examples

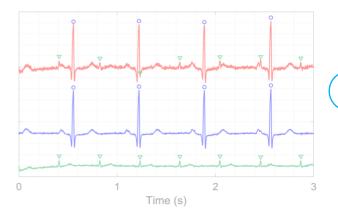
Dimensionality reduction



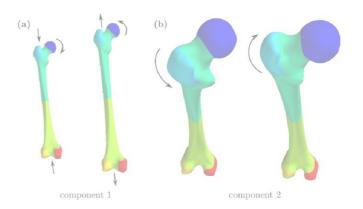
Blind source separation







Statistical shape modelling

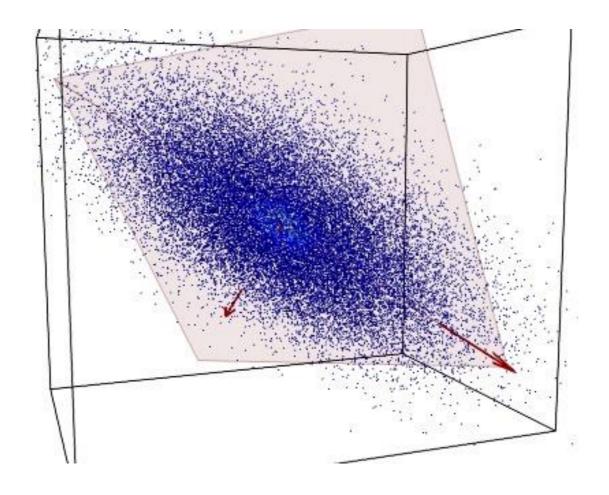






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Dimensionality Reduction





Dimensionality Reduction – Turtles

- Classical reference
- Jolicoeur and Mosimann studied statistically the size of turtle shells: length (L), width (W), height (H).

Growth, 1960, 24, 339-354.

SIZE AND SHAPE VARIATION IN THE PAINTED TURTLE.¹
A PRINCIPAL COMPONENT ANALYSIS

PIERRE JOLICOEUR AND JAMES E. MOSIMANN²

Walker Museum, University of Chicago and Institut de Biologie, Université de Montréal







TABLE 1

CARAPACE DIMENSIONS OF PAINTED TURTLES (Chrysemys picta marginata) IN MM

	24 Females			24 Males	
height	width	length	height	width	ength
38	81	98	37	74	93
38	84	103	35	78	94
42	86	103	35	80	96
40	86	105	39	84	101
44	88	109	38	85	102
50	92	123	37	81	103
46	95	123	39	83	104
51	99	133	39	83	106
51	102	133	38	82	107
51	102	133	40	89	112
48	100	134	40	$N \stackrel{\text{\tiny #}}{=} 2$	113
49	102	136	4. 40		114
51	98	137	43	90	116
51	99	138	C C 41	‡ türtl	117
53	105	141	C S41	† 10111	117 #
57	108	147	41	93	119
55	107	149	40	89	120
56	107	153	44	93	120
63	115	155	42	95	121
60	117	155	45	93	125
62	115	158	45	96	127
63	118	159	45	95	128
61	124	162	46	95	131
67	132	177	47	106	135

P. Jolicoeur and J. E. Mosimann, "Size and s

A principal component analysis," Growth, vol. 24, pp. 339–354, Dec. 196

M = 3: # features

EPFL

:: csem

Dimensionality Reduction – Turtles

TARLE 2

Mean Vectors $\overline{\mathbf{X}}$ and $\overline{\mathbf{C}}$ Covariance Matrices W

		24 Males			24 Females	
	length	width	height	length	width	height
\mathbf{x}	(113.38	88.29	40.71)	(136.00	102.58	51.96)
W	138.77 79.15 37.38	79.15 50.04 21.65	37.38 21.65 11.26	451.39 271.17 168.70	271.17 171.73 103.29	168.70 103.29 66.65

TABLE 4 Size and Shape Variation

		24 Males		24 Females		
Principal axes	1st (major)	2nd (inter- mediate)	3rd (minor)	1st (major)	2nd (inter- mediate)	3rd (minor)
Magnitude of variance	195.28	3.69	1.10	680.40	6.50	2.86
% of total	97.61	1.84	0.55	98.64	0.94	0.41

TABLE 3 COVARIANCE MATRICES Λ AND MATRICES OF DIRECTION COSINES U OF THE PRINCIPAL AXES

	24 Males			24 Females		
Λ	195.28	0.00	0.00	680.40	0.00	0.00
	0.00	3.69	0.00	0.00	6.50	0.00
	0.00	0.00	1.10	0.00	0.00	2.86
U	.84012	.49190	.22854	.81263	.49549	.30676
	48811	.86938	07696	54537	.83213	.10062
	23654	04690	.97049	20540	—.24907	.94645 _

P. Jolicoeur and J. E. Mosimann, "Size and shape variation in the painted turtle. A principal component analysis," *Growth*, vol. 24, pp. 339–354, Dec. 1960.





```
import pandas as pd
from sklearn.decomposition import PCA

# Load data
fn = r'1960Jolicoeur_TurtleData.xlsx'
```

```
# perform PCA
pca = PCA()
pca.fit_transform(data_females.values);
```

```
# mean vector X
pca.mean_
```

```
array([136. , 102.58333333, 51.95833333])
```

data = pd.read excel(fn)

 λ_i

data_males = data.iloc[1:, :3]
data_females = data.iloc[1:, 3:]

```
# covariance matrix W
pca.get_covariance()
```

```
array([[451.39130435, 271.17391304, 168.69565217],
[271.17391304, 171.73188406, 103.28623188],
[168.69565217, 103.28623188, 66.65036232]])
```

```
# explained variance (eigenvalues lambda)
pca.explained_variance_
```

```
array([680.41230604, 6.49962394, 2.86162075])
```

```
# percentage of total variance
pca.explained_variance_ratio_*100
```

```
array([98.64285247, 0.94228373, 0.4148638])
```

```
# principal axes in feature space, i.e., the eigenvectors
# NOTE: strictly speaking these are NOT the principal components(!)
pca.components_
```

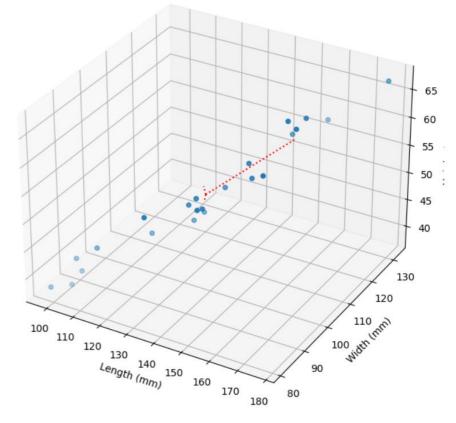
Dimensionality Reduction – Turtles

3 Eigenvectors and Eigenvalues:

First principal component:

$$Y = 0.813 L + 0.496 W + 0.307 H$$

- → explains 98.6% of total variance!
- For a turtle shell, it is not necessary to consider the three features length, width, and height. The abovementioned linear combination is sufficient.
- Other two components indicate marginal relations between:
 (2nd) L w.r.t W and H, (3rd) H w.r.t L and W.



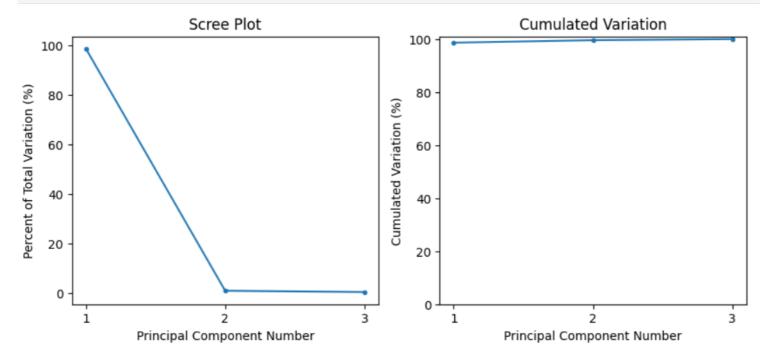


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Dimensionality Reduction – Turtles

```
# scree plot
plt.subplot(121)
plt.plot(np.arange(pca.n_components_) + 1, 100*pca.explained_variance_ratio_, '.-')
plt.xlabel('Principal Component Number');
plt.ylabel('Percent of Total Variation (%)')
plt.title('Scree Plot')

# cumulated variance
plt.subplot(122)
plt.plot(np.arange(pca.n_components_) + 1, np.cumsum(100*pca.explained_variance_ratio_), '.-')
plt.xlabel('Principal Component Number')
plt.ylabel('Cumulated Variation (%)')
plt.title('Cumulated Variation')
plt.show()
```





Dimensionality Reduction – Remarks

 It may be that the features have widely different amplitude ranges, which may lead to "numerically null" rows.

Use whitening/normalization:
$$X_N = \begin{bmatrix} \frac{1}{\sigma_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{1}{\sigma_M} \end{bmatrix} X$$

- The PCA works well only for linear relations between features.
 - If, for instance, there is a product-type relation, PCA will be a lot less useful.

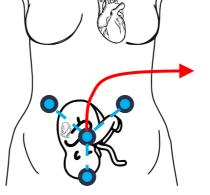
Usage Examples

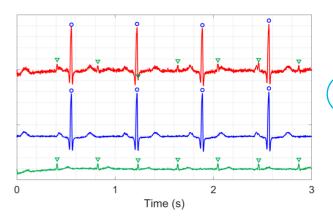
Dimensionality reduction



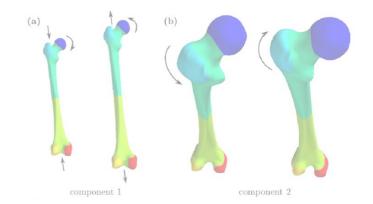
Blind source separation





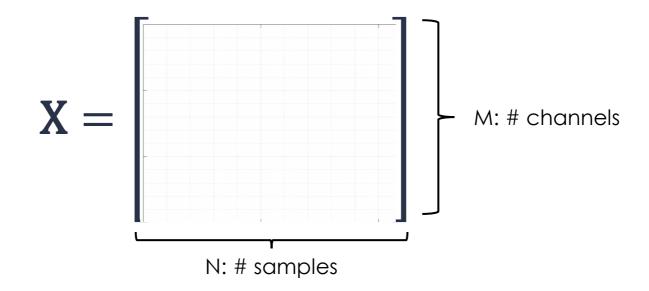


Statistical shape modelling

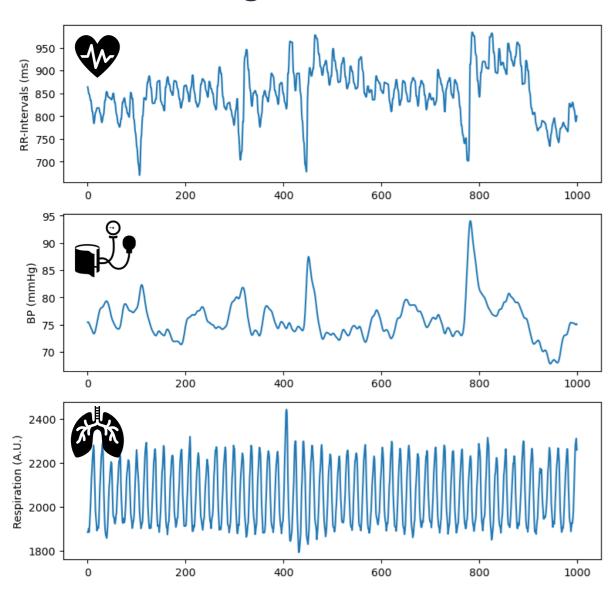












Example:



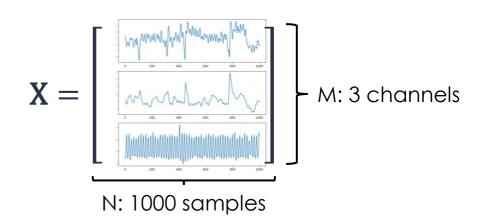
1. RR intervals



2. Blood pressure

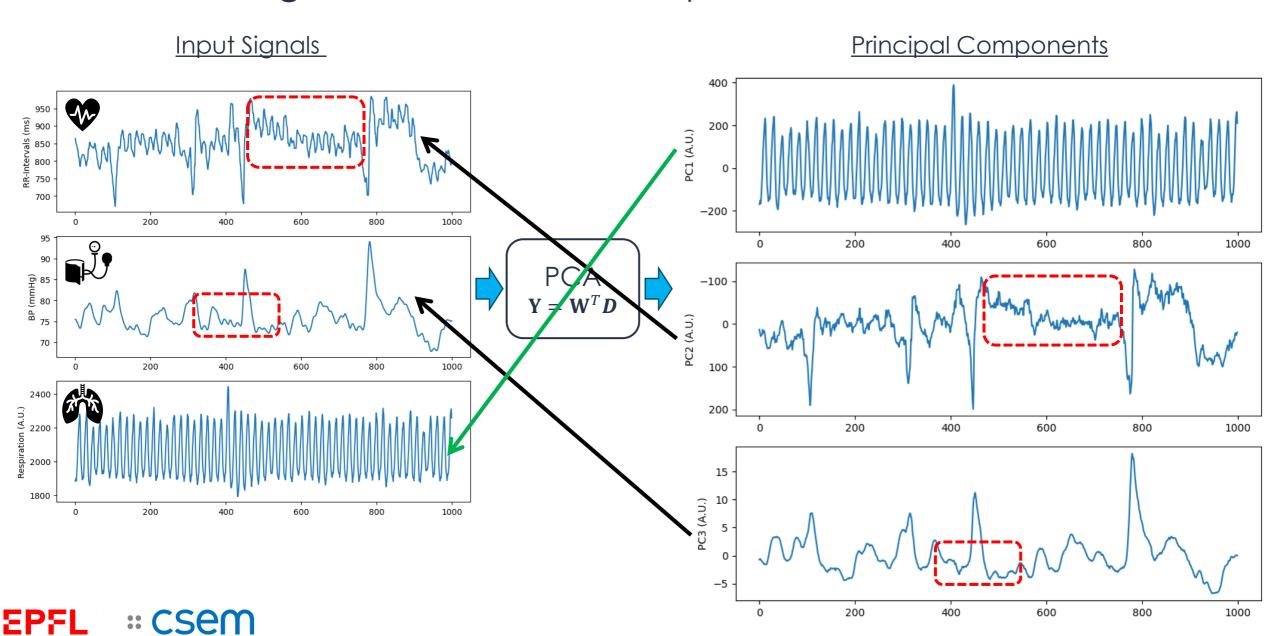


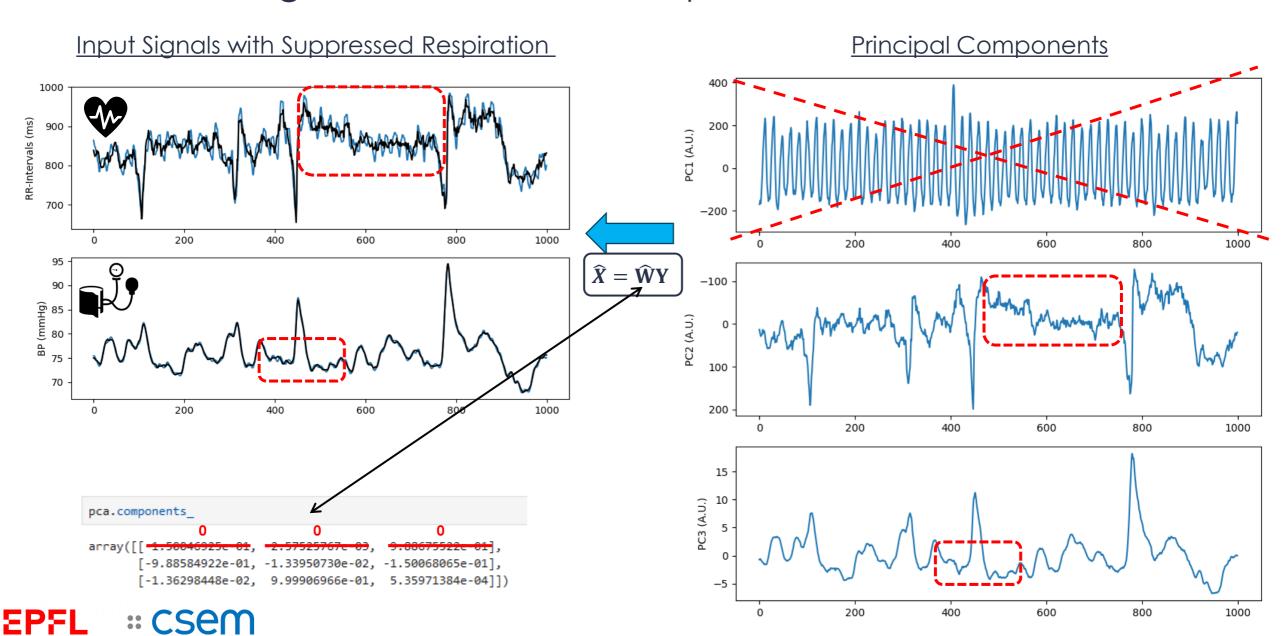
3. Respiration



EPFL :: CSem

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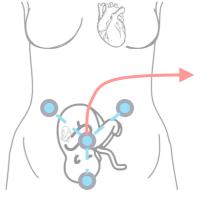
Usage Examples

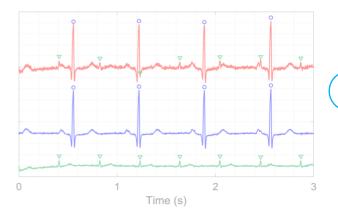
Dimensionality reduction



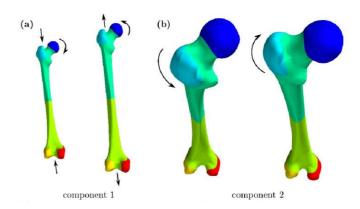
Blind source separation







Statistical shape modelling

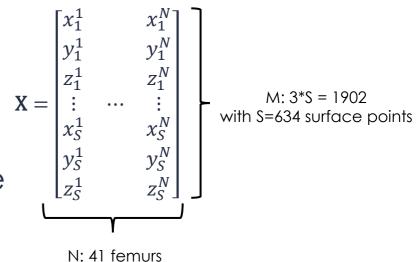


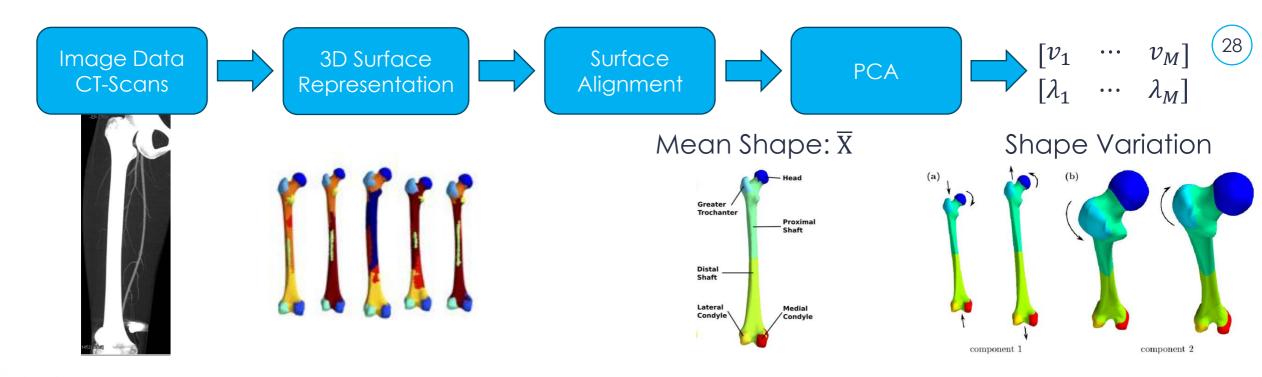




Statistical Shape Modelling – Motivation

- Mean Shape knowledge about general shape
- Describe natural anatomical variability (PCA)



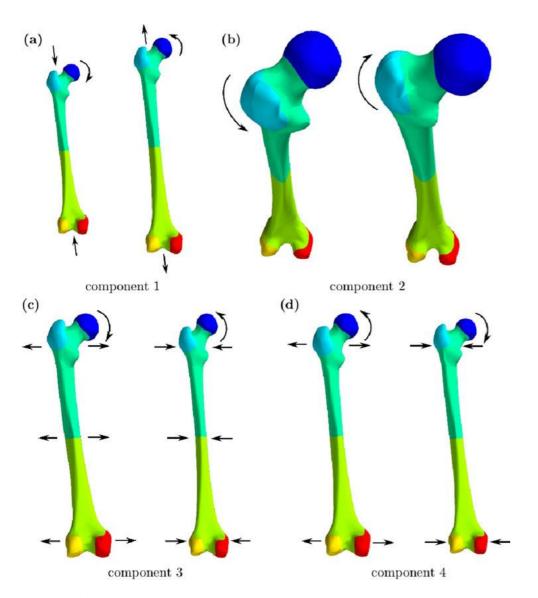


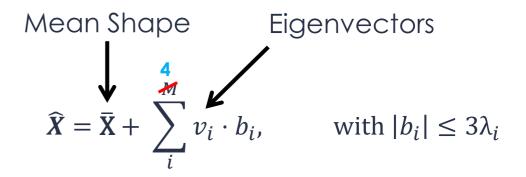


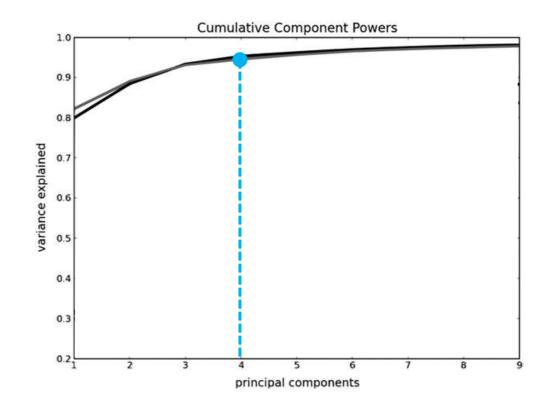


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Statistical Shape Modelling – Femurs

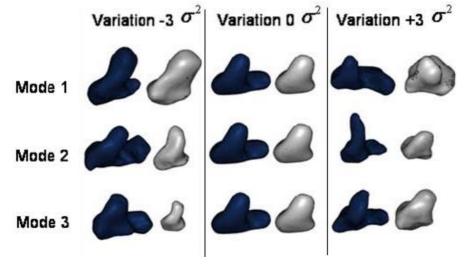








Statistical Shape Modelling – Hearing Aids



G. Unal, et al., "Customized Design of Hearing Aids Using Statistical Shape Learning," in Medical Image Computing and Computer-Assisted Intervention – MICCAI 2008, Berlin, Heidelberg, 2008, vol. 5241, pp. 518–526. doi: 10.1007/978-3-540-85988-8 62.

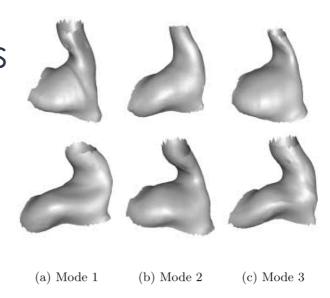
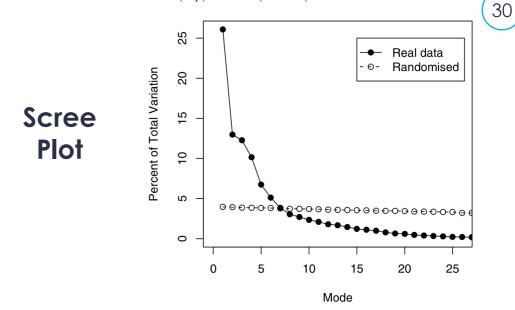


Fig. 2. Pure shape model. Each shape has been generated by varying the first three modes of variation between -3 (top) and +3 (bottom) standard deviations



R. Paulsen, et al., "Building and Testing a Statistical Shape Model of the Human Ear Canal," in Medical Image Computing and Computer-Assisted Intervention — MICCAI 2002, Berlin, Heidelberg, 2002, vol. 2489, pp. 373–380. doi: 10.1007/3-540-45787-9 47.



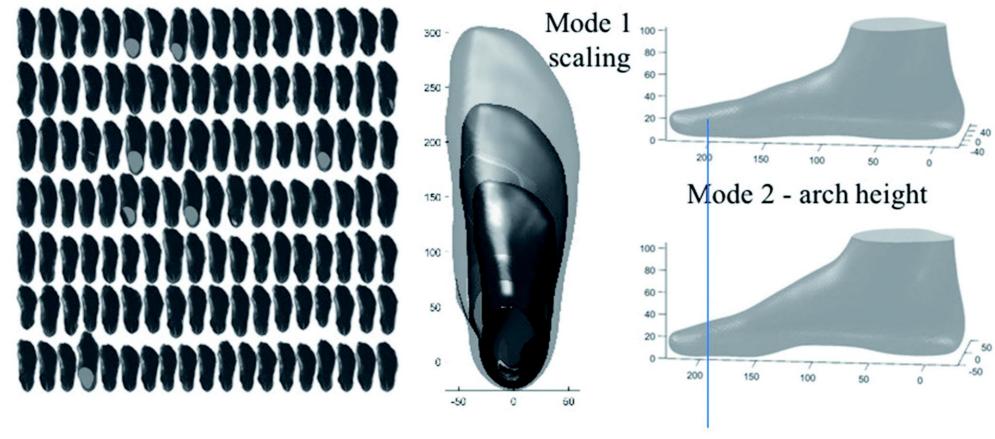


Statistical Shape Modelling – Feet

Statistical shape modelling describes anatomic variation in the foot

Bryan P. Conrad^{a*}, Michael Amos^b, Irene Sintini^c, Brian Robert Polasek^c and Peter Laz^c

^aNike Sport Research Lab, Portland, OR, USA; ^bNike Inc, Nike Sports Research Lab, Beaverton, OR, USA; ^cUniversity of Denver, Denver, CO, USA







- PCA works well only for linear relations between features.
 - If, for instance, there is a product-type relation, PCA will be a lot less useful.
- PCA is sensitive to outliers
 - Use robust PCA (RPCA)
- PCA assumes that the original data follows a Gaussian distribution

Try alternatives such as independent component analysis (ICA)

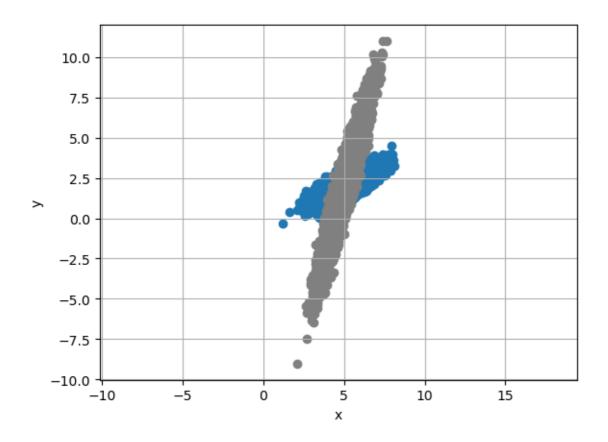


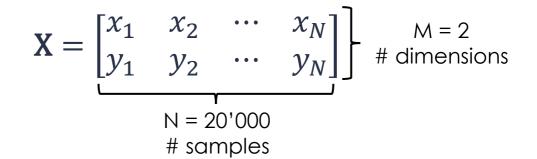




A First Limitation of PCA

Two <u>non</u>-orthogonal 2D Gaussians

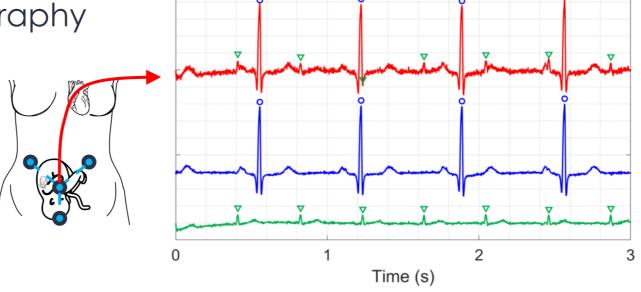




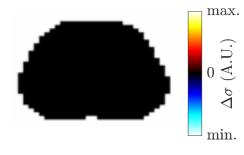
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Today's Lab – Blind Source Separation Using PCA

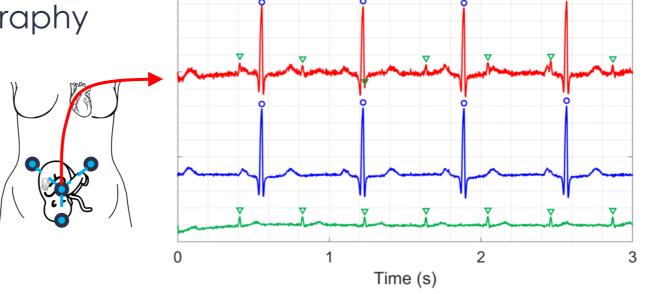
1. fECG: Fetal Electrocardiography



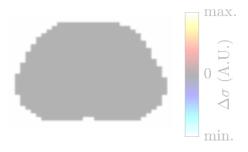
2. EIT: Electrical Impedance Tomography







2. EIT: Electrical Impedance Tomography



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Abdominal ECG for Fetal Heart Rate Estimation

CTG: Cardiotocography



Source: Philips CTG FM30

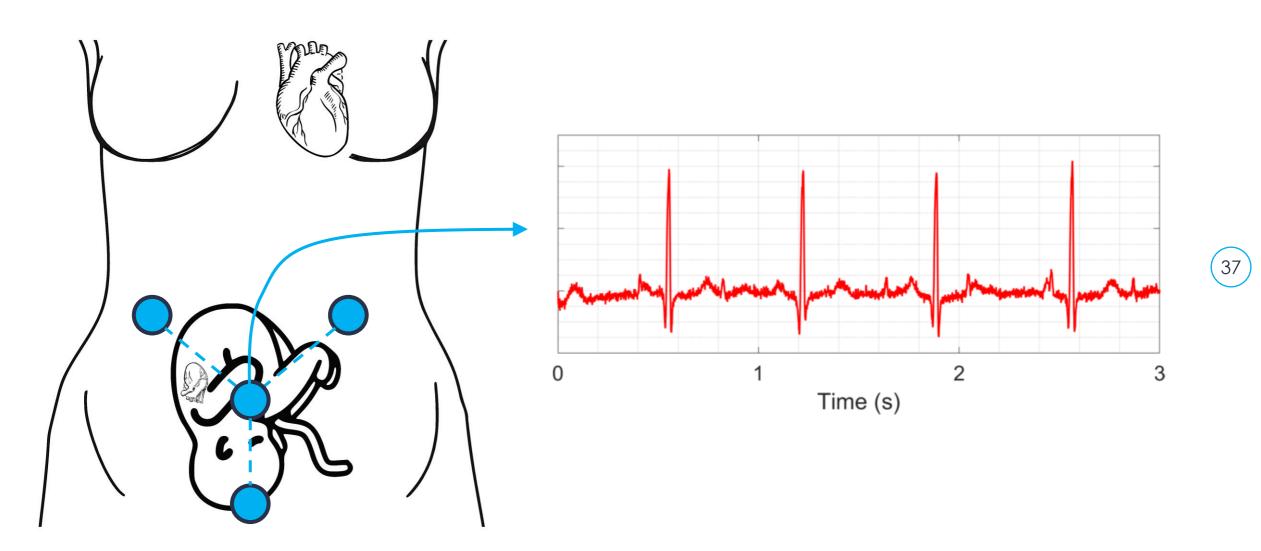
aECG: Abdominal ECG



Source: CSEM



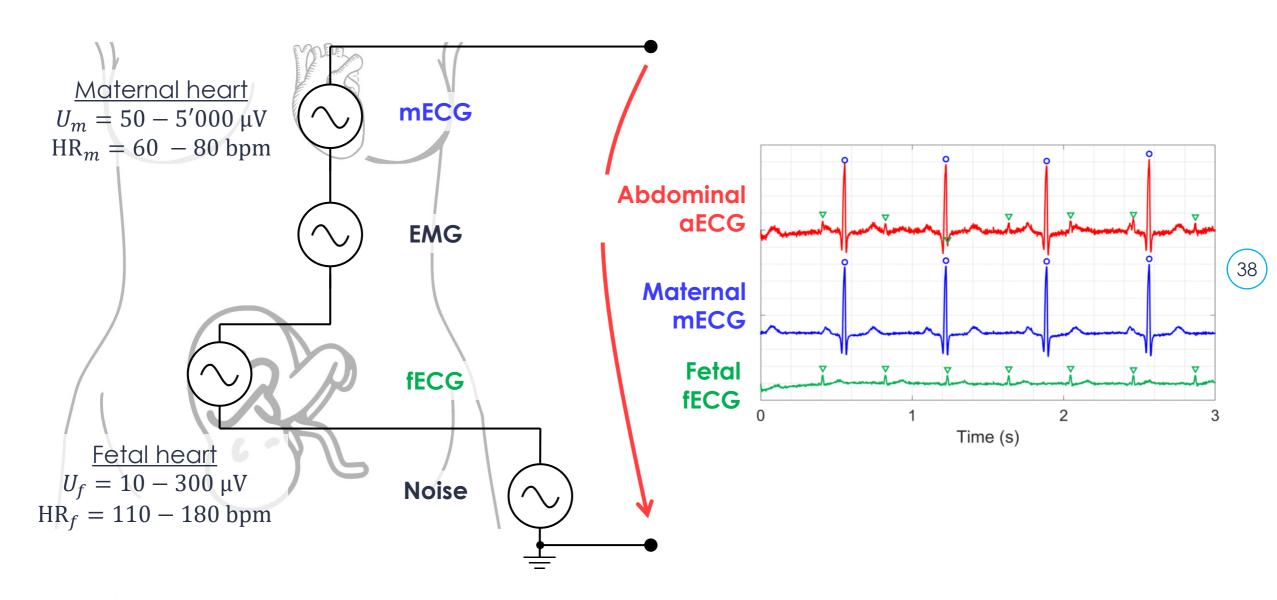
Fetal Physiology and Abdominal ECG





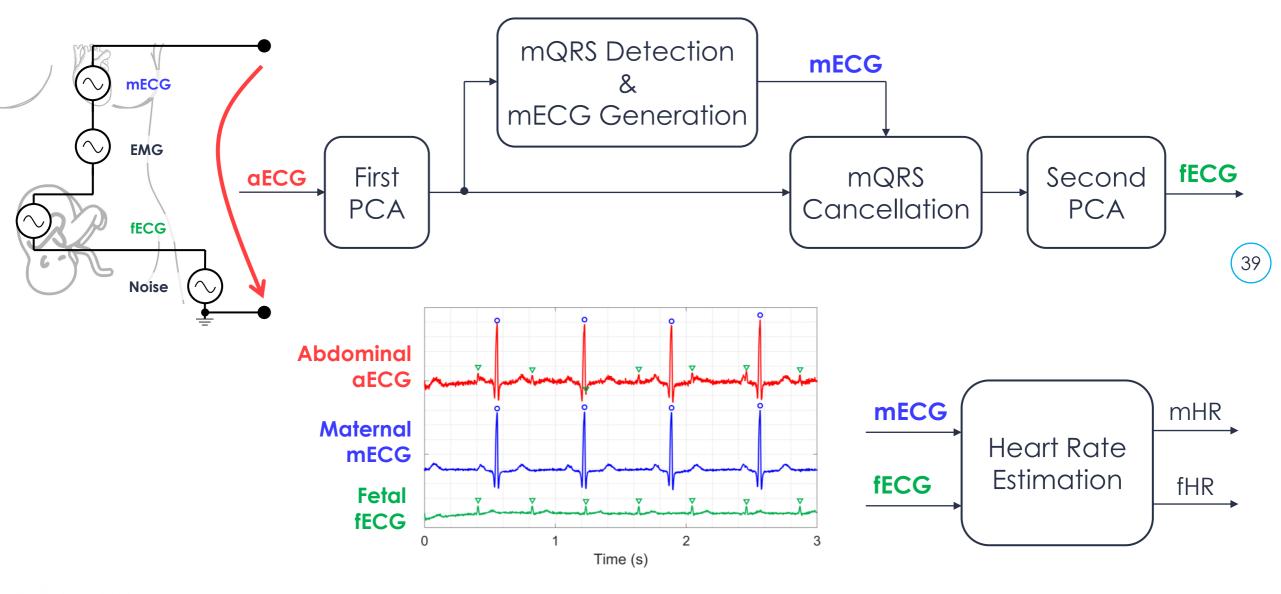


Challenges of Fetal ECG





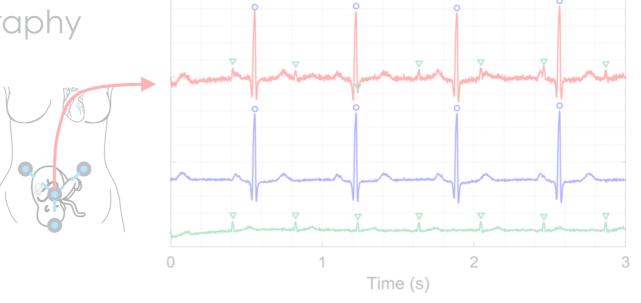
Blind Source Separation for Fetal ECG



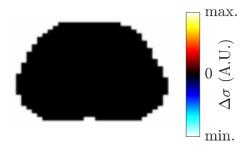


Lab #2

1. fECG: Fetal Electrocardiography



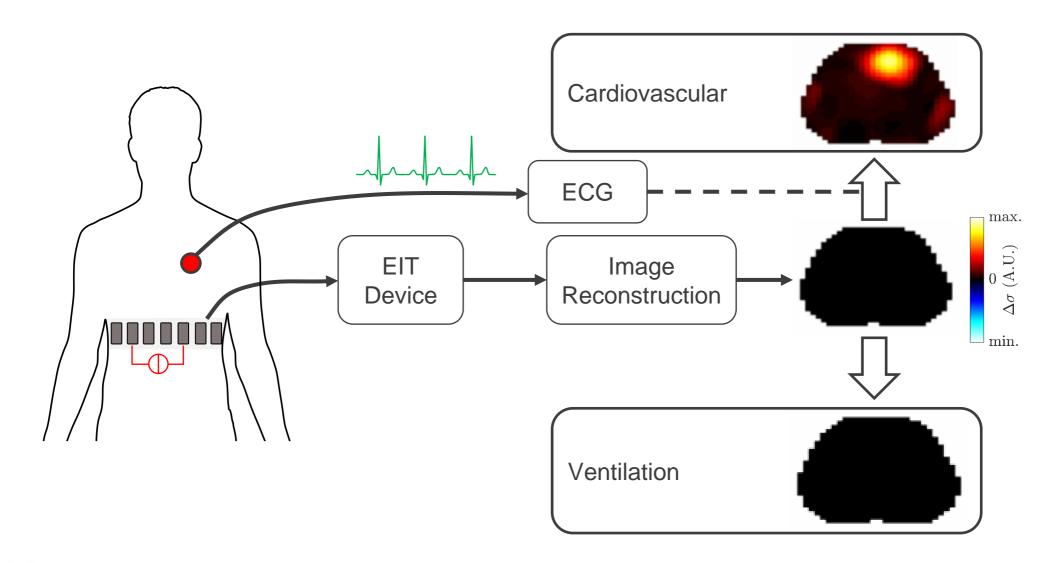
2. EIT: Electrical Impedance Tomography







EIT – Electrical Impedance Tomography









EIT – Electrical Impedance Tomography

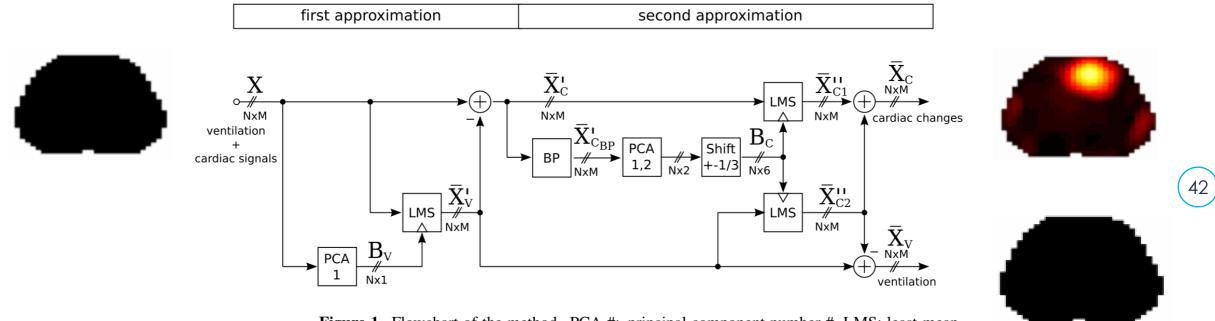


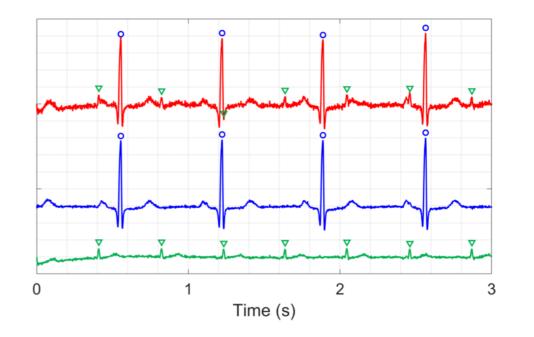
Figure 1. Flowchart of the method. PCA #: principal component number #, LMS: least-mean-squares fit, BP: bandpass, 'shift $\pm \frac{1}{3}$ ': input is phase shifted by [-1/3, 0, 1/3] heart cycle to account for phase shifts introduced by the blood flow. *N*: number of processed frames, *M*: number of pixels in one frame.

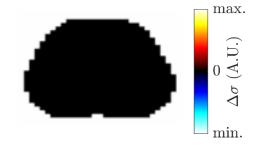




Today's Lab – Instructions

- Please submit your report as a single PDF file.
- We recommend working in groups of 3 students; the last group can be a group of 2 or 4.
- You can prepare one single report for the group (name1_name2_name3_lab_PCA.pdf), but every member needs to upload the same file individually.
- There are 2 experiments in this practical session. The Python code for each experiment is already coded and will be provided as Jupyter notebooks. These will only require minimal input from you. A major part of this practical session is thus focused on questions testing your understanding and correct interpretation of the signals and the analysis results that you see.







Karen Adam – kam@csem.ch

CSEM Signal Processing and Al Group







