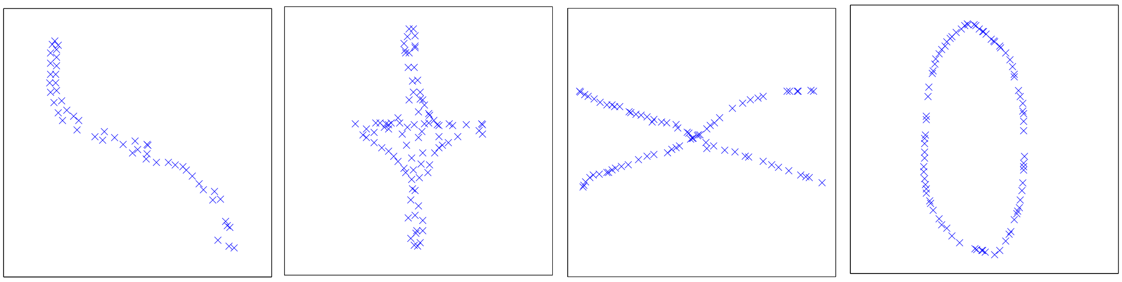
# Assignment 7

Machine Learning, Summer term 2014, Ulrike von Luxburg

To be discussed in exercise groups on June 2-4

**Exercise 1 (Direction of principal components, 1 point)** Below are a number of 2D-data sets. Plot the two principal components.



**Exercise 2 (Interpreting principal components, 2 points)** A carsharing service runs a survey among 1000 students, who provide information concerning their 1- income, 2- distance they cover by car per month, 3- distance they cover by bike per month, 4- distance they cover by public transport per month, 5- distance they cover by foot per month. Then they run a PCA on the data. Provide answers to the following questions:

- What would it mean if a single eigenvector covered 95% of the total data variance?
- How would you interpret the result if the eigenvector $v_1 = [0, 0, 1, -1, 0]$ covers 90% of the total data variance?
- Why might it be necessary to rescale the data before running PCA in order to obtain a sensible result?

**Exercise 3 (Generating samples from a Gaussian distribution, 0.5+0.5+0.5+1+0.5 points)** You are given the mean $\mu$ and the covariance matrix $\Sigma$ of a $d$-dimensional normal density $\mathcal{N}(\mu, \Sigma)$ and you want to sample $n$ points from this density. Assuming that $\Sigma$ is positive definite, the following MATLAB code will do this for you:

```
S1 = chol(Sigma); X = repmat(mu,n,1) + randn(n,d)*S1;
```

The command `S1 = chol(Sigma)` generates an upper triangular matrix `S1` which satisfies `Sigma=S1'*S1`. This decomposition is called the Cholesky decomposition. An alternative method, which also works when $\Sigma$ is only positive semi-definite, is to decompose $\Sigma$ to eigenvectors and eigenvalues by `[V,D] = eig(Sigma)` and then form `S2` by `S2=V*sqrt(D)`. However, the Cholesky decomposition is numerically more stable and computationally faster than eigen decomposition method.

(a) Show that in eigen decomposition, $\Sigma = S2 \cdot S2'$.

(b) Generate $n = 2000$ points in 3 dimensional space from a Gaussian distribution with mean `mu=[0,0,0]` and Covariance `Sigma=[2 0 0;0 1 0;0 0 4]`. Plot it with `plot3`.

(c) What are the eigenvalues and eigenvectors of the covariance matrix `Sigma`?

(d) Assume you know eigenvalues and eigenvectors of your covariance matrix:

$$\Lambda = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix}, V = \frac{\sqrt{2}}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}.$$

Generate $n = 400$ points in 2 dimensional space from a Gaussian distribution with mean zero and covariance matrix corresponding to these eigenvalues and eigenvectors ($\Sigma = V \Lambda V'$). Plot the points and guess the approximate direction of principal components in the figure.

(e) Add the eigenvectors in $V$ to your plot. Compare your guessed directions with these eigenvectors.

**Exercise 4 (PCA, 2+1 points)**

(a) Implement PCA in MATLAB. Do it in a three line MATLAB code: Subtract the mean of your data, calculate the covariance matrix $C$, and find its eigenvalues and eigenvectors using the MATLAB command `[V,D] = eig(C)`.

(b) To test your code (if you could not solve part (a), you can use the MATLAB command `pca`) generate 500 samples from a Gaussian distribution with mean $\mu = [1, 1]$ and covariance $\Sigma = [2, -1; -1, 2]$. For generating the points you can either use your code from Exercise 3, or use the MATLAB command `normrnd`. Apply your PCA code on this data and compare the result with the eigenvectors of the covariance matrix $\Sigma$.

**Exercise 5 (PCA on USPS data, 1+3 points)**

(a) Apply the PCA method on images of digits 5 from USPS dataset (use the training data of the complete dataset — available on the course webpage from Assignment 4). Plot the first and the second principal components as 16x16 grayscale images. You can either use your PCA implementation from Exercise 4 or the MATLAB command `pca`.

(b) Choose three images of digits 5 from USPS dataset at random and project them onto 1- the first principal component, 2- the first and the second principal component in $\mathbb{R}^{256}$ (i.e. as a result you should obtain vectors in the original space — this is View 1 in the notation of the lecture notes). Create a $3 \times 3$-subplot (use `help subplot` in case you do not know how this works) showing the original images in the first row, the results from 1 in the second row, and the results from 2 in the third row (using `imagesc`).

**Exercise 6 (Isomap on USPS data, 1+1+1 points)** In this exercise you will implement the Isomap method to embed digits 1,2,3,4 from USPS dataset into $\mathbb{R}^2$. The code for building kNN graph and the Isomap algorithm itself is provided on the course web page.

In preparation for the following, load the data from `usps_train_complete.mat` (available on the course webpage from Assignment 4). Select 300 examples from each of digits $\{1, 2, 3, 4\}$ and put them in variable `X`. Put the corresponding labels in `Y`.

(a) Set the connectivity parameter in the kNN graph to $k = 10$ and use the following code to plot the embedding in 2 dimensional space using Isomap. Read the manual of the command `scatter` to understand how it works.

```
A = buildKnnGraph(X,k);
D = graphallshortestpaths(A,'Directed', false);
xy = Isomap(D,2);
figure;
scatter(xy(:,1),xy(:,2),10,Y,'filled');
```

(b) Play with the parameter $k$. Describe the effect of the parameter on the embedding.

(c) Project the data onto the first two principal components of PCA in $\mathbb{R}^2$ (i.e. as a result you should obtain vectors in $\mathbb{R}^2$ — this is View 2 in the notation of the lecture notes). Plot the embedding, again using the command `scatter`. You can either use your PCA implementation from Exercise 4 or the MATLAB command `pca` to perform PCA.

## Table of Contents



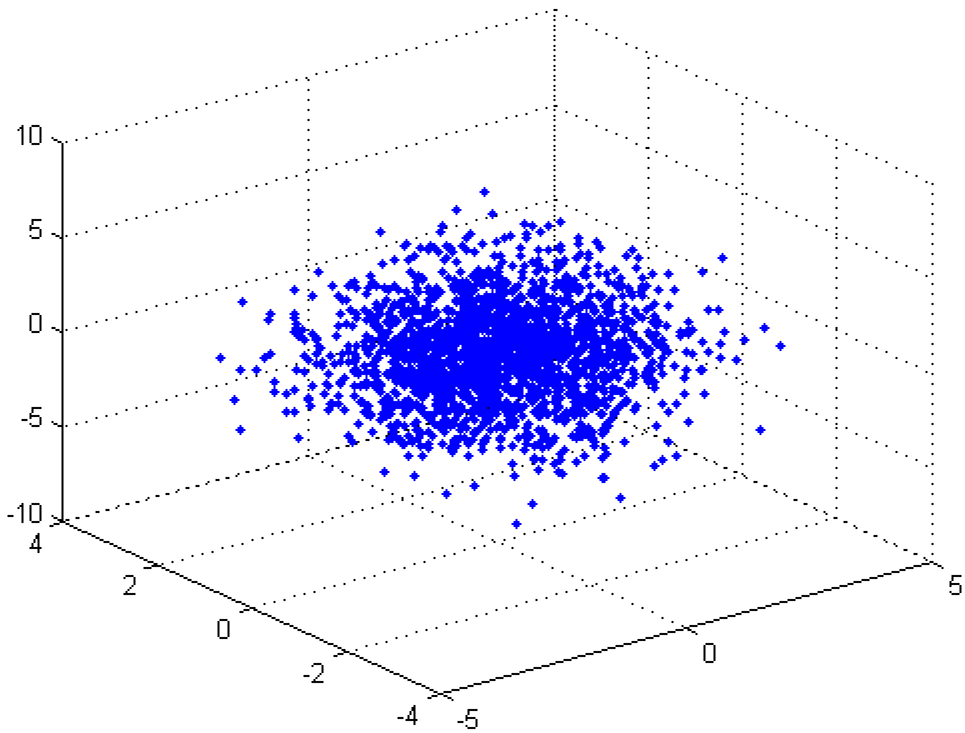
```
% Machine Learning Assignment 3

clear all; close all; clc;
```

# Part (a)

```
%[V,D] = eig(Sigma)
```

# Part (b)

```
% the Cholesky decomposition is a decomposition of a Hermitian,
% positive-definite matrix into the product of a lower triangular matrix
% and its conjugate transpose,

% R = chol(A) produces an upper triangular matrix R from
% the diagonal and upper triangle of matrix A, satisfying
% the equation R'*R=A.

% B = repmat(A,m,n) creates a large matrix B
% consisting of an m-by-n tiling of copies of A.
% each d dimensional point is a row
d = 3; n = 2000; mu = [0, 0 ,0]; Sigma=[2 0 0;0 1 0;0 0 4];
S1 = chol(Sigma); X = repmat(mu,n,1) + randn(n,d)*S1;

figure(1); plot3(X(:,1), X(:,2), X(:,3), '.'); grid on
```



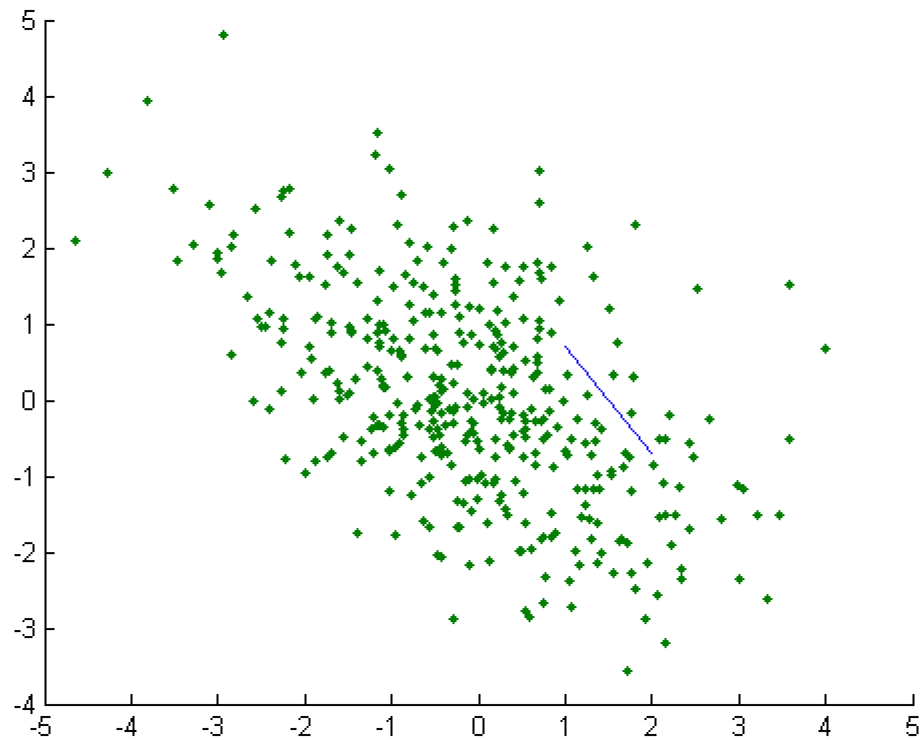

# Part (c)

```
[V D] = eig(Sigma)

V*D*V' % Is equal to Sigma
```

```
V =

     0     1     0
     1     0     0
     0     0     1


D =

     1     0     0
     0     2     0
     0     0     4


ans =

     2     0     0
     0     1     0
     0     0     4
```

# Part (d)

```
A =[3 0;0 1];%eigenvalues of cov matrix
V =(1/sqrt(2))*[1 1;-1 1];% eigen vectors cov matrix
d = 2; n = 400; mu = [ 0 0];
Sigma = V*A*V';
S1 = chol(Sigma); X = repmat(mu,n,1) + randn(n,d)*S1;

figure(2);hold all;
plot(V(:,1));% 1rst eigenvector
plot(X(:,1),X(:,2),'.');
```



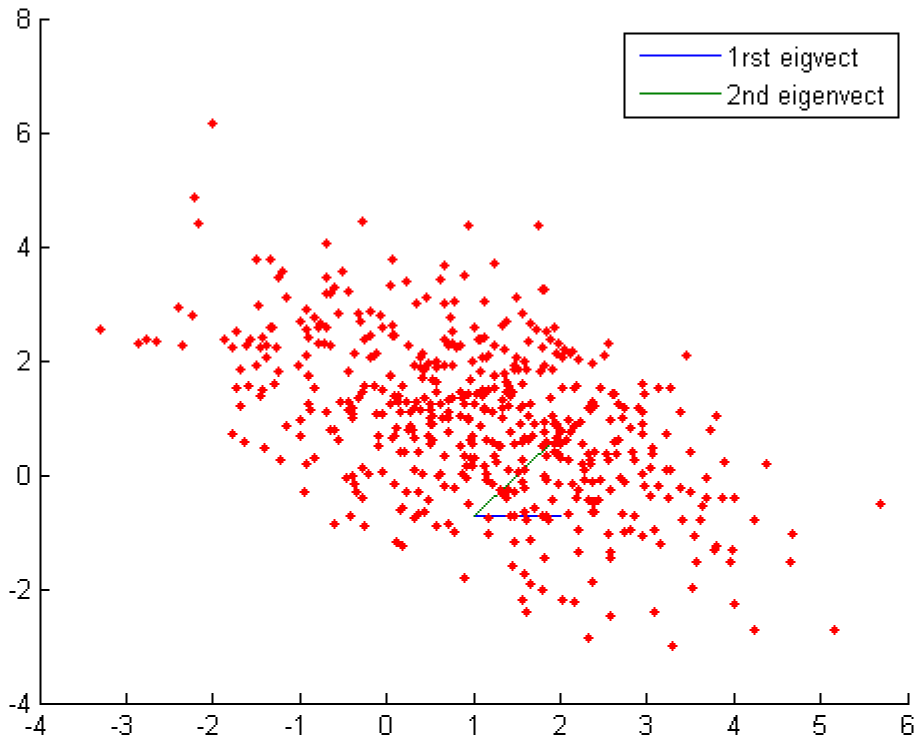

# Exercise 4

Each row represents a d dimensional point

```
d = 2; n = 500; mu = [1, 1]; Sigma=[2 -1 ;-1 2];
S1 = chol(Sigma); X = repmat(mu,n,1) + randn(n,d)*S1;

d= size(X,2);
x_mean = mean(X,2); % mean of columns of matrix X (horizontal)
Xc = X-x_mean*ones(1,d); % centered data matrix
C= (1/n)*Xc'*Xc; % covariance matrix
```

```
C= cov(Xc); % built-in command produces the same thing
[V,D] = eig(Sigma)

figure(3);hold all;
plot(V(:,1));% 1rst eigenvector
plot(V(:,2));% 2nd eigenvector
plot(X(:,1),X(:,2),'.');
legend ('1rst eigvect', '2nd eigenvect')
```

```
V =

   -0.7071   -0.7071
   -0.7071    0.7071


D =

     1     0
     0     3
```

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# MACHINE LEARNING- ASSIGNMENT 7

VICTOR BERNAL ARZOLA

## Exercise 1

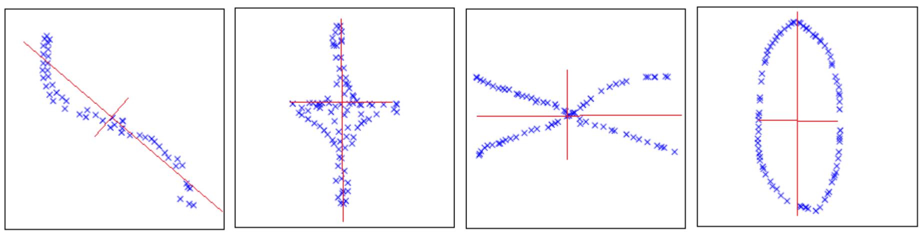

Figure 0.1. First 2 components

## Exercise 2

- Data is spread along this direction mostly.
- Negative correlated.
- Same scale (same units) allow us to compare and interpret properly.

## Exercise 3

In linear algebra, the Cholesky decomposition or Cholesky factorization is a decomposition of a Hermitian, positive-definite matrix into the product of a lower triangular matrix and its conjugate transpose.

**Solving a linear system.** The Cholesky decomposition is mainly used for the numerical solution of linear equations $Ax = b$. If $A$ is symmetric and positive definite, then we can solve $Ax = b$ by first computing the Cholesky decomposition $A = LL^T$, then solving $Ly = b$ for $y$ by forward substitution, and finally solving $L^T x = y$ for$x$ by back substitution. A closely related variant of the classical Cholesky decomposition is the $LDL$ decomposition.

**Generating correlated Gaussian numbers.** A general way to generate correlated (normal distributed) random numbers with a given correlation matrix $C$ is to generate uncorrelated numbers $R$ and then multiplying them with $L$ the Cholesky matrix of $C$ . Suppose $X$ is build of uncorrelated normal random vector with mean zero

$$cov\,(X,X) = E\left[XX^T\right] = \begin{pmatrix} 1 & 0 \\ : & : \\ 0 & 1 \end{pmatrix}$$

and that we want to generated correlated random vector with correlation matrix $C$, that using Cholesky decomposition is written as

$$C = LL^T$$

then $LX$ has the desired covariance given by

$$cov\,(Z,Z) = E\left[(LX)\,X^T L^T\right] = LE\left[XX^T\right]L^T = LL^T$$

**Covariance Matrix.** The covariance matrix (also called the variance-covariance matrix) of an $n \times 1$ random vector is an $n \times n$ matrix whose $i, j^{th}$ element is the covariance between the $i^{th}$ and the$j^{th}$ random variables. Lets define a matrix of observations where each row is a experiment (or individual) consisting of $d$ features (dimensions).

$$X = \begin{bmatrix} a_1 & .. & a_d \\ b_1 & : & b_d \\ n_1 & ... & n_d \end{bmatrix}$$

so the covariance

$$\Rightarrow cov\,(X, X) = \left(XX^T\right)_{nxn} \quad \text{interindividual}$$
$$\Rightarrow cov\,(X, X) = \left(X^T X\right)_{dxd} \quad \text{interdimensional}$$

As we are interested in the information of each of the d dimensions (features) we proceed with the second.

**Fact.** *When the matrix $X$ is a Hermitian matrix (resp. symmetric matrix), eigenvectors of $X$ can be chosen to form an orthonormal basis of $C^n$ (resp. $R^n$). Under such circumstance $P$ will be a unitary matrix (resp. orthogonal matrix) and $P^{-1}$ equals the conjugate transpose (resp. transpose) of $P$.*

| Orthogonal | Unitary |
|---|---|
| $OO* = I = O * O$ | $UU^+ = I = U^+U$ |
| $O$ is a real square matrix | $U$ is a complex square matrix |
| $O*$is the transpose | $U^+$ is the conjugate transpose |

Figure 0.2. Unitary vs Orthogonal Matrix

Lets consider the transformation change of basis of a matrix $X$

$$X = \begin{bmatrix} u & v \\ : & : \end{bmatrix} \begin{pmatrix} \lambda & 0 \\ 0 & \mu \end{pmatrix} \begin{bmatrix} u & v \\ : & : \end{bmatrix}^{-1}$$

where $u, v$ are eigenvectors. For every $n \times n$ real symmetric matrix (e.g. covariance matrix), the eigenvalues are real and the eigenvectors can be chosen such that they are orthogonal to each other. An Orthogonal matrix is a square matrix with real entries whose columns and rows are orthogonal unit vectors. So the matrix of eigenvectors $P$ is orthogonal then its inverse $P^{-1}$ is equal to its transpose $P^T$

$$V^T V = \begin{pmatrix} v_1 & ... \\ u_1 & ... \end{pmatrix} \begin{pmatrix} v_1 & u_1 \\ : & : \end{pmatrix}$$
$$= \begin{pmatrix} v^T v & v^T u \\ u^T v & u^T u \end{pmatrix} = \mathbb{1}$$

taking the transpose

$$\left(V^T V\right)^T = V V^T = \mathbb{1}^T$$
$$\Rightarrow V^T = V^{-1}$$

Thus a real symmetric matrix $X$ can be decomposed as

$$X = \begin{bmatrix} u & v \\ : & : \end{bmatrix} \begin{pmatrix} \lambda & 0 \\ 0 & \mu \end{pmatrix} \begin{bmatrix} u & v \\ : & : \end{bmatrix}^T$$

which resembles the Cholesky $LDL$ decomposition.