Methods 3: Multilevel Statistical Modeling and Machine Learning

Week 9: *Dimensionality Reduction, Principled Component Analysis (PCA)*
November 23, 2021

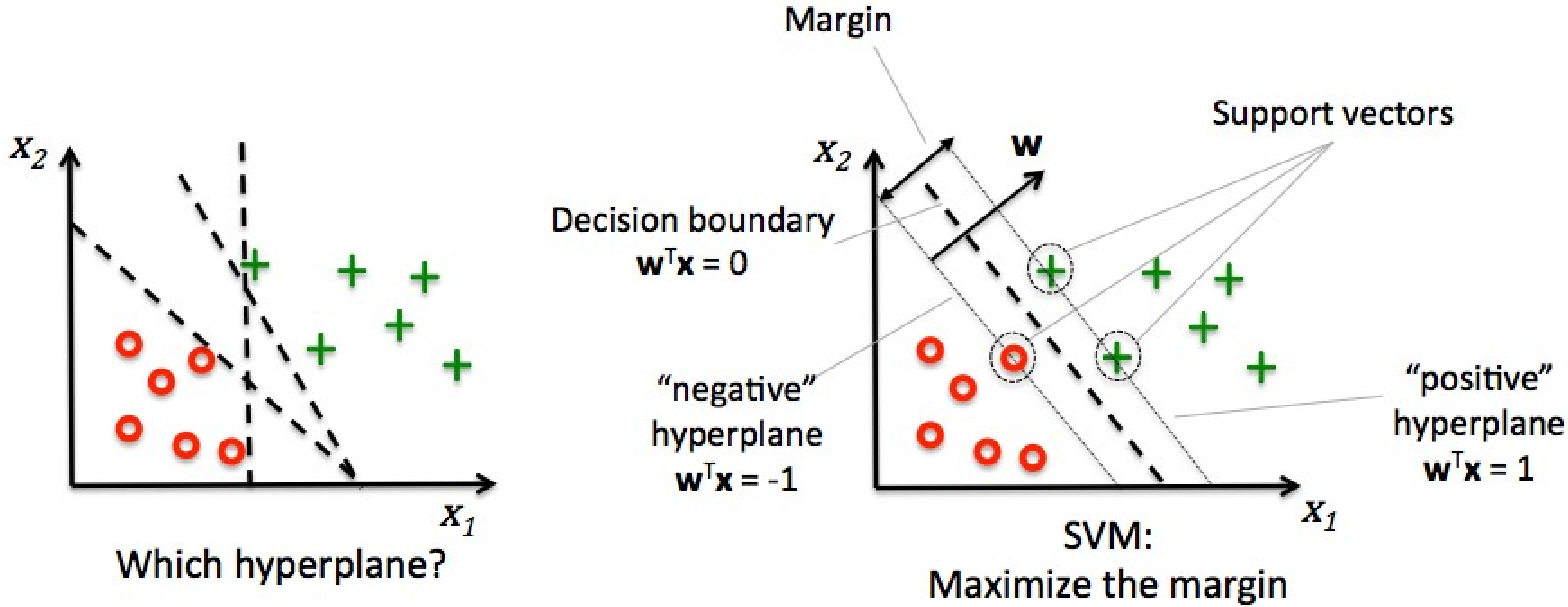
by: Lau Møller Andersen

Did you learn?

Logistic regression (machine learning)

1) Understanding of how logistic regression can be adapted to a classification framework
2) Understanding the idea of a Support Vector Machine
3) Getting acquainted with how Support Vector Machines can solve non-linear problems

SUPPORT VECTOR MACHINES
Recapitulation



(p. 69: Raschka, 2015)

$$\phi(x_1, x_2) = (z_1, z_2, z_3) = (x_1, x_2, \boxed{x_1^2 + x_2^2})$$

Creating the higher dimensions can be computationally expensive

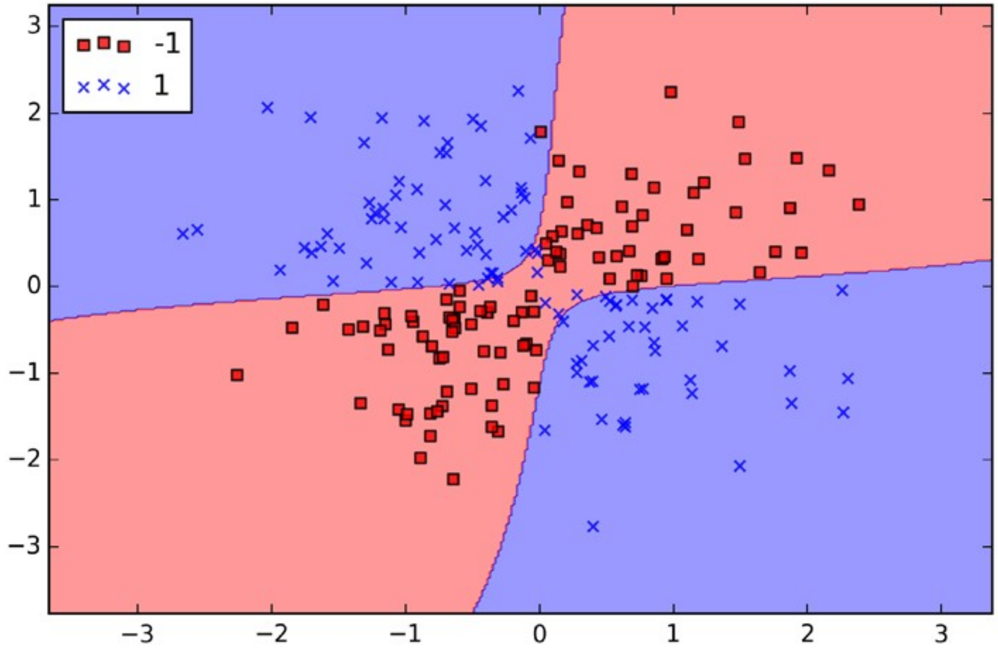
Kernel (*k*) function

$$k\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = \phi\left(\mathbf{x}^{(i)}\right)^T \phi\left(\mathbf{x}^{(j)}\right)$$

$$k\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = e^{\left(-\gamma \left\|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\right\|^2\right)}$$

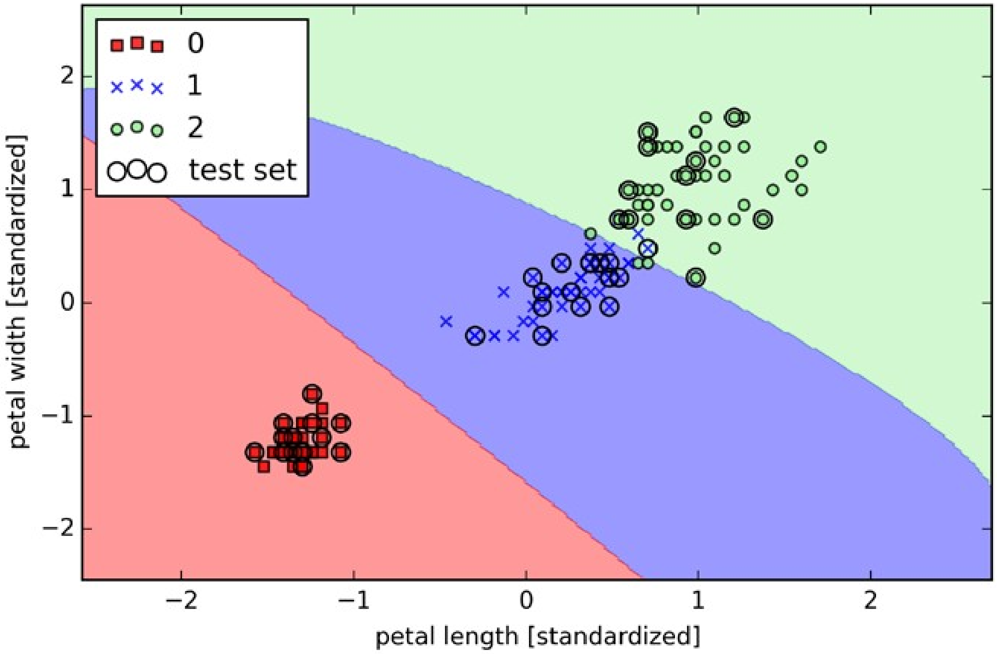
$$\left(\gamma = \frac{1}{2\sigma^2},\ \text{also called the precision}\right)$$

Non-linear decision boundaries



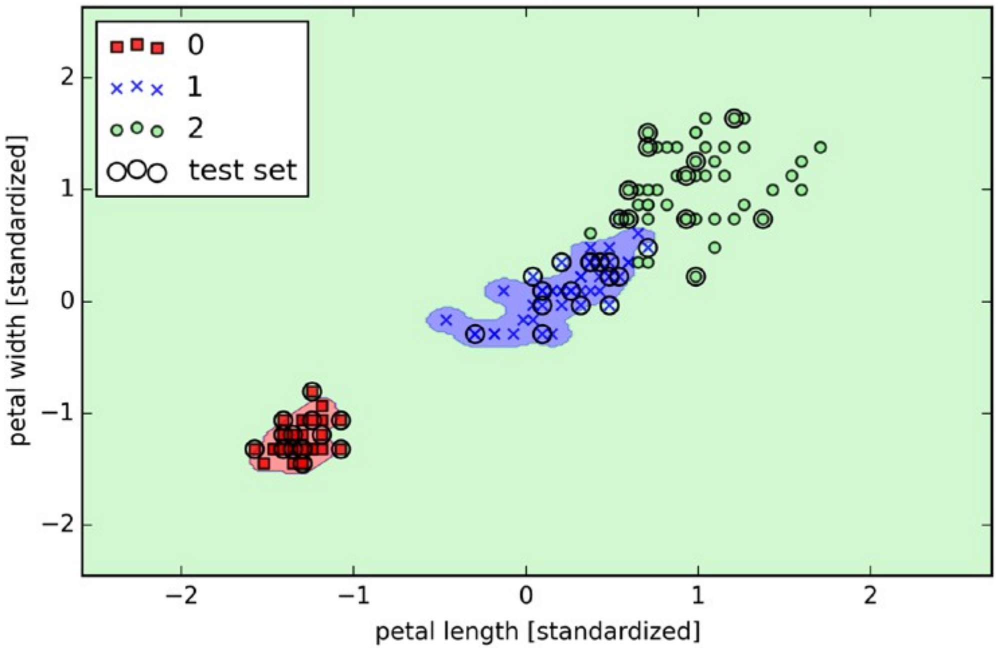
(p. 78: Raschka, 2015)

Low γ - soft boundary



(p. 79: Raschka, 2015)

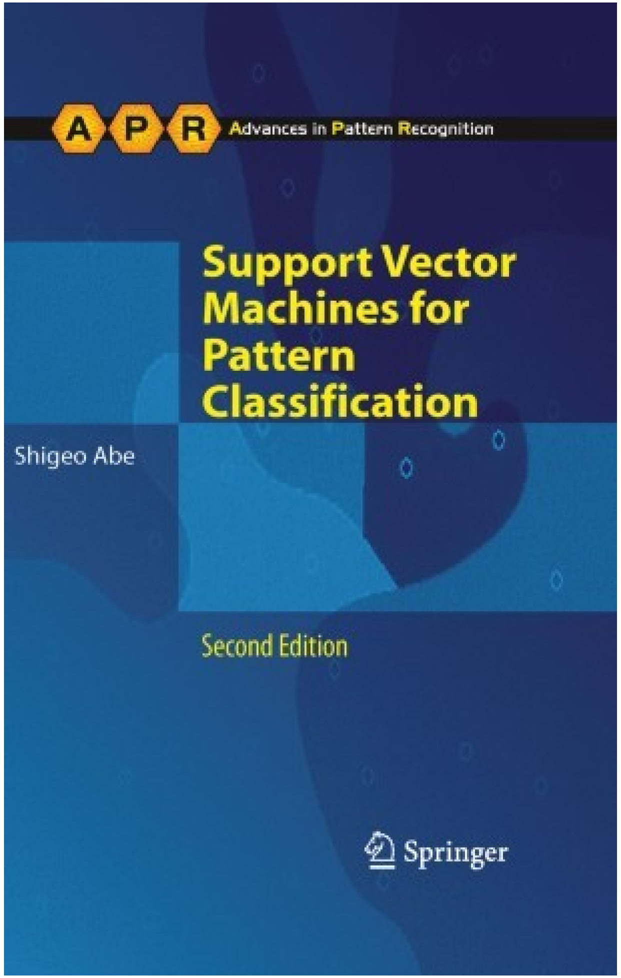
High γ - tight boundary



(p. 80: Raschka, 2015)

Live coding

RECAPITULATION_SUPPORT_VECTOR_MACHINE.ipynb



Available online on The Royal Library

Learning goals

Dimensionality reduction

1) Learning how we can extract the features that explain the most variance

2) Understanding how that can improve classification

3) Get acquainted with the concept of a eigenvector

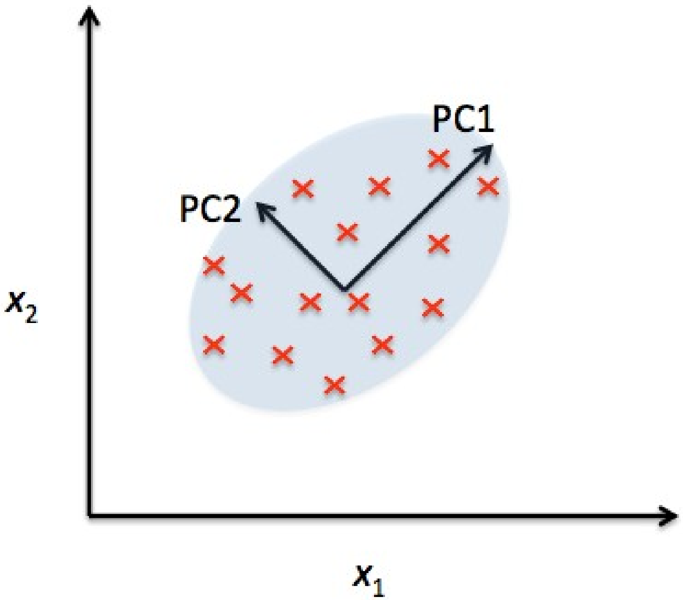
The curse of dimensionality

```
import numpy as np
import matplotlib.pyplot as plt
from os.path import join

path = '/home/lau/Skrivebord/class_subject'
data = np.load(join(path, 'megmag_data.npy'))

print('Shape: ' + str(data.shape))
print('n measurements: ' + str(np.prod(data.shape)))
print('n observations: ' + str(data.shape[0]))
print('n features: ' + str(np.prod(data.shape[1:])))
```

```
Shape: (682, 102, 251)
n measurements: 17460564
n observations: 682
n features: 25602
```

Principled components

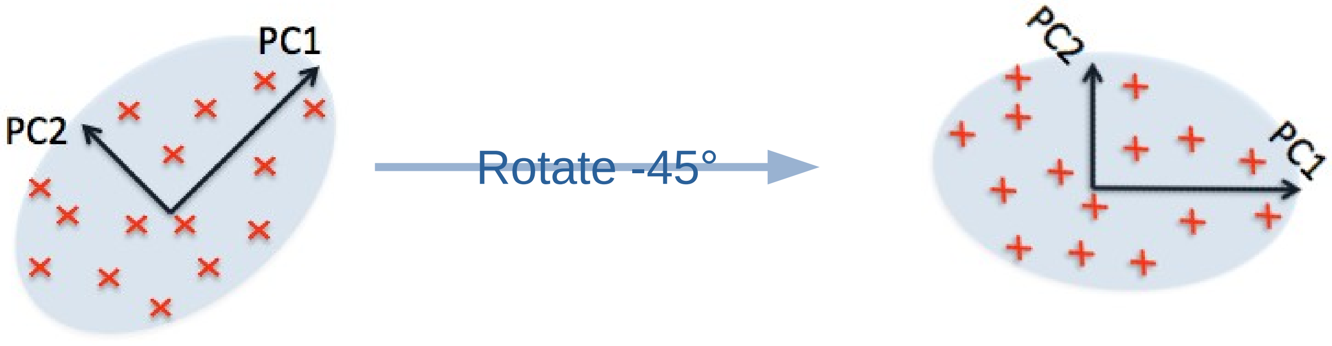
FINDING THE DIRECTIONS OF MOST VARIANCE



(p. 128: Raschka, 2015)

Principled components

FINDING THE DIRECTIONS OF MOST VARIANCE

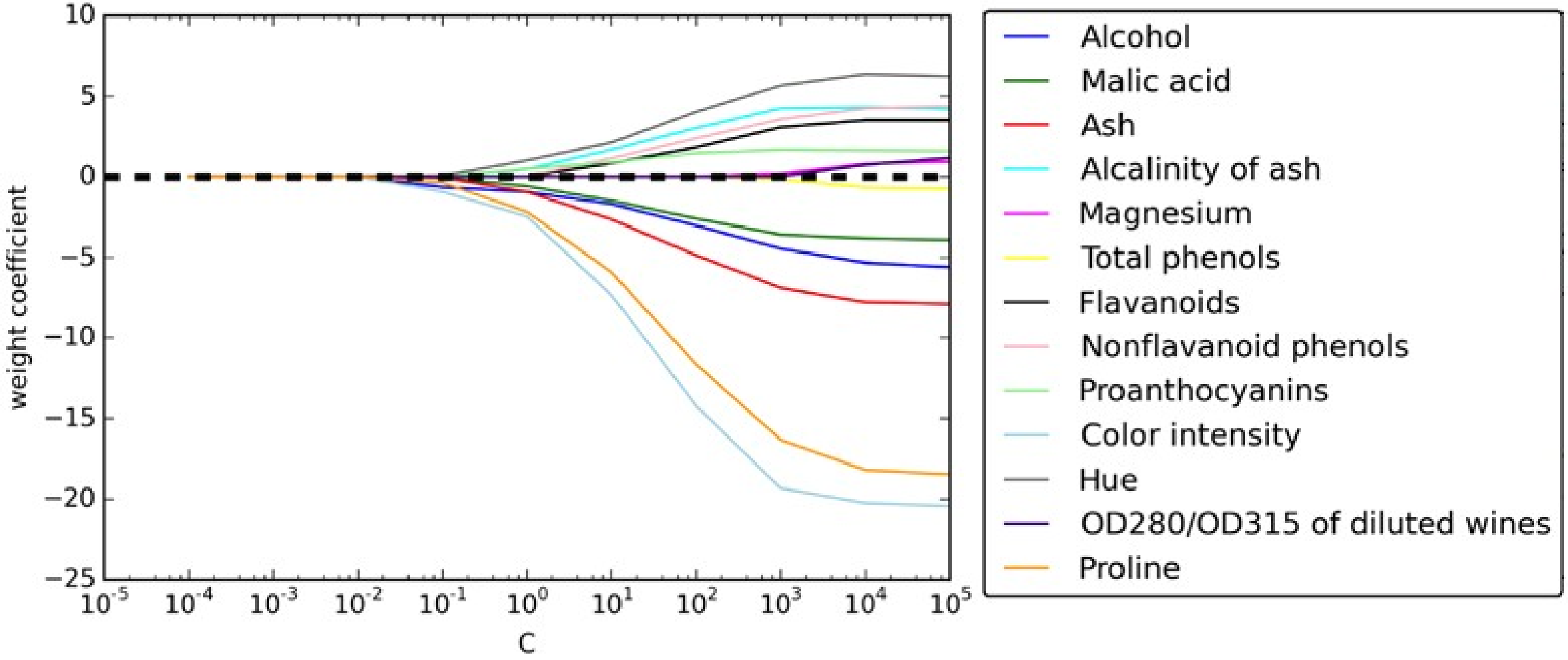


PC1 has the most variance

(p. 128: Raschka, 2015)

This can be **generalized** to as many dimensions as you like

A dataset (wine)



(p. 118: Raschka, 2015)

```python
## import wine data
import pandas as pd
url = 'https://archive.ics.uci.edu/ml/' + \
        'machine-learning-databases/wine/wine.data'
df_wine = pd.read_csv(url, header=None)
```

```python
X, y = df_wine.iloc[:, 1:].values, df_wine.iloc[:, 0].values
print(X.shape)
print(np.unique(y))
```

```
(178, 13)
[1 2 3]
```

AIM: for ***x***: find ***W*** such that:

$$\boldsymbol{x} = [x_1, x_2, \ldots, x_d], \boldsymbol{x} \in \mathbb{R}^{\boldsymbol{d}}$$

$$\downarrow \boldsymbol{xW}, \boldsymbol{W} \in \mathbb{R}^{d \times k}$$

$$\boldsymbol{z} = [z_1, z_2, \ldots, z_k], \boldsymbol{z} \in \mathbb{R}^{\boldsymbol{k}}$$

Approach

PRINCIPLED COMPONENT ANALYSIS

1) Standardize the *d*-dimensional dataset
2) Construct the covariance matrix
3) Decompose the covariance matrix into its eigenvectors and eigenvalues
4) Select *k* eigenvectors that correspond to the *k* largest eigenvalues where *k* is the dimensionality of the new feature subspace ($k \leq d$)
5) Construct a projection matrix ***W*** from the “top” *k* eigenvectors
6) Transform the *d*-dimensional input dataset ***X*** using the projection matrix ***W*** to obtain the new *k*-dimensional feature subspace

(p. 129: Raschka, 2015)

Standardize the dataset (1)

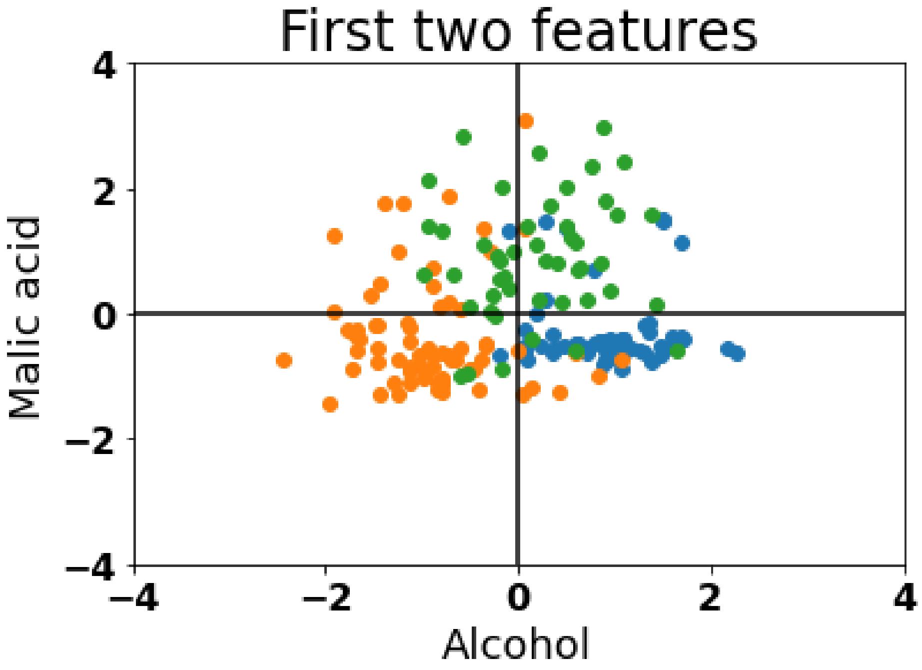
FINDING THE DIRECTIONS OF MOST VARIANCE

```
X_train, X_test, y_train, y_test = \
    train_test_split(X, y, test_size=0.3, random_state=0)

sc = StandardScaler()
X_train_std = sc.fit_transform(X_train)
X_test_std = sc.fit_transform(X_test)
X_std = sc.fit_transform(X)
```

Question: why do we need to standardize?

Compare the variance of a measurement made in millimetres to one made in kilometres!

Data



Construct the covariance matrix (2)

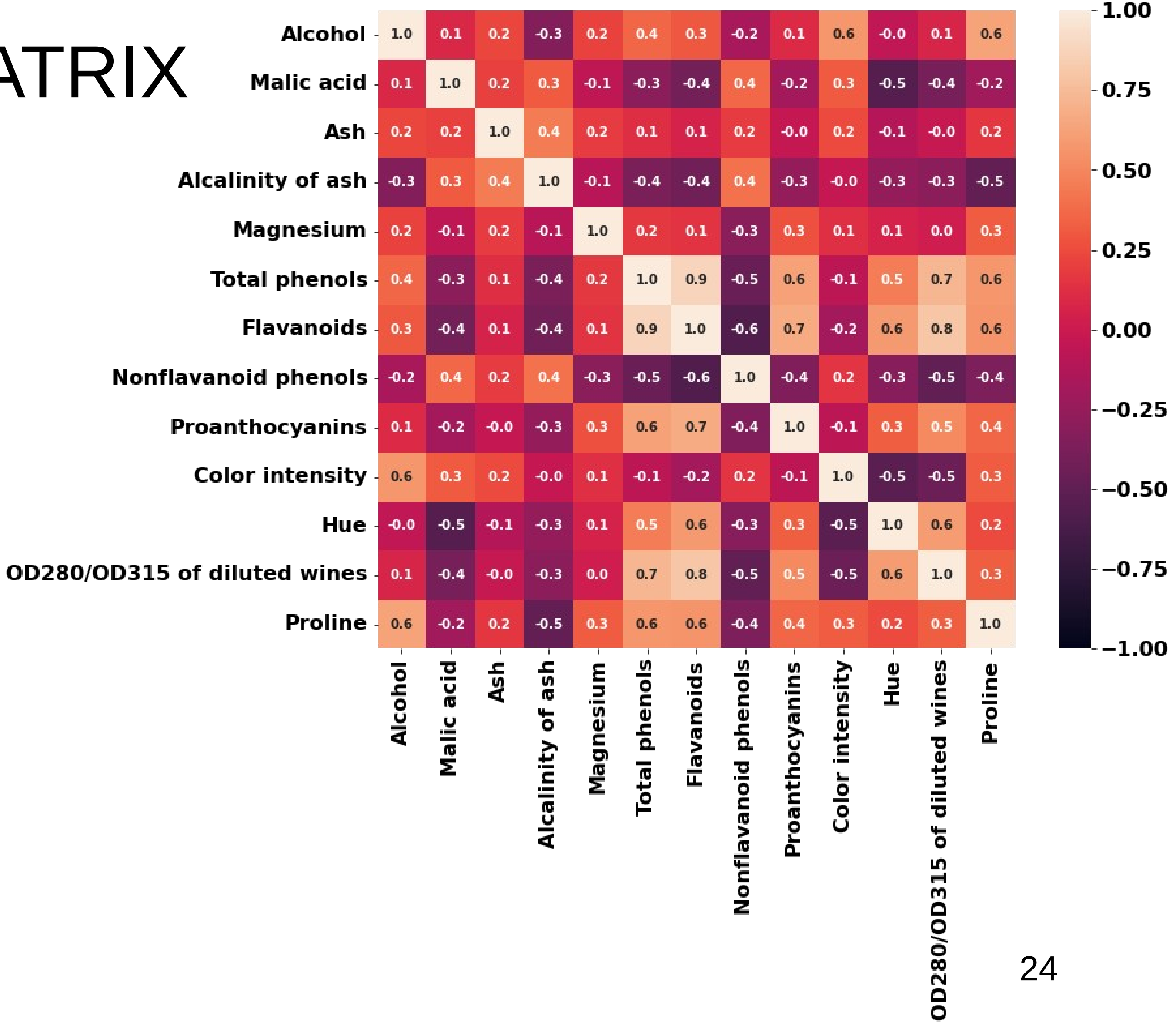
FINDING THE DIRECTIONS OF MOST VARIANCE

$$\sigma_{jk} = \frac{1}{n} \sum_{i=1}^{n} \left(x_j^{(i)} - \mu_j \right) \left(x_k^{(i)} - \mu_k \right)$$

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 \end{bmatrix}$$

Question: what will be the size of the covariance matrix in the *Wine* dataset?

COVARIANCE MATRIX



Find the eigenvectors and eigenvalues (3)

FINDING THE DIRECTIONS OF MOST VARIANCE

$$\Sigma \boldsymbol{v} = \lambda \boldsymbol{v}$$

$\boldsymbol{v}:$ eigenvector
$\lambda:$ eigenvalue
$\Sigma:$ covariance matrix

Link to Chris Mathys's lecture from Methods II

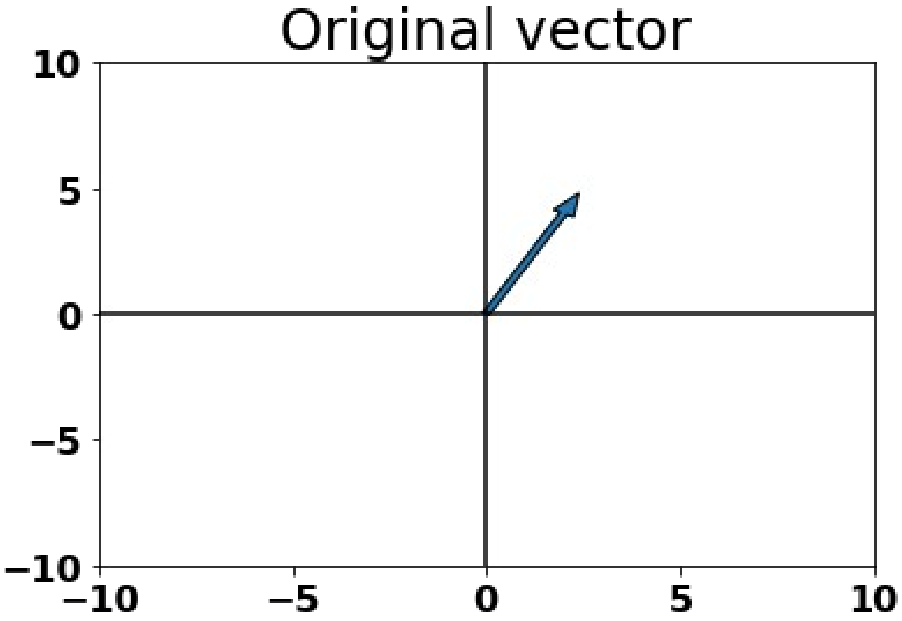
Link to 3blue1brown's video of the same matter

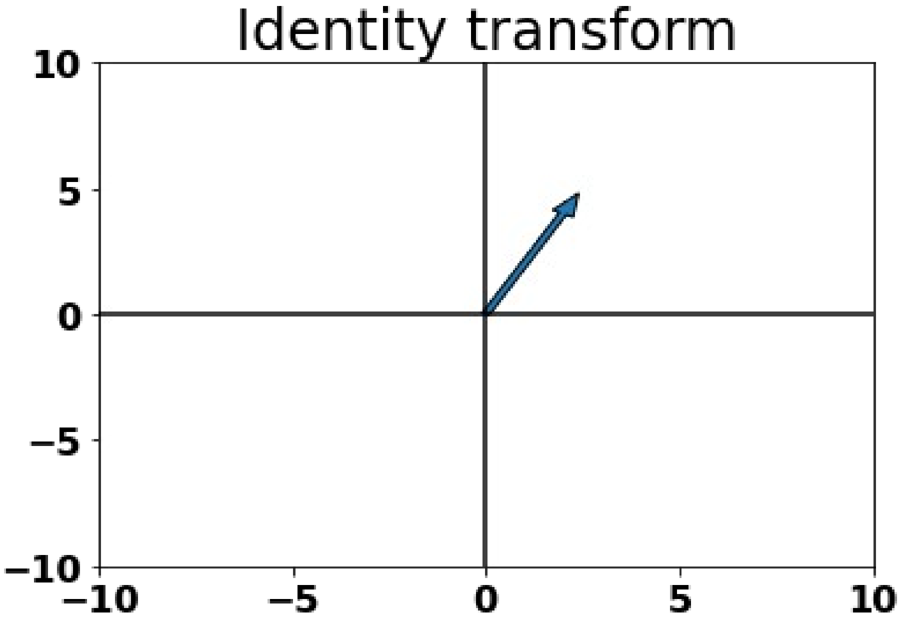
Remember: matrix multiplication of a vector can be seen as a **transformation** of the vector

$$T(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$$

$\boldsymbol{A}:$ transformation matrix
$\boldsymbol{x}:$ column vector
$\boldsymbol{T}:$ transformed column vector

Identity Transformation



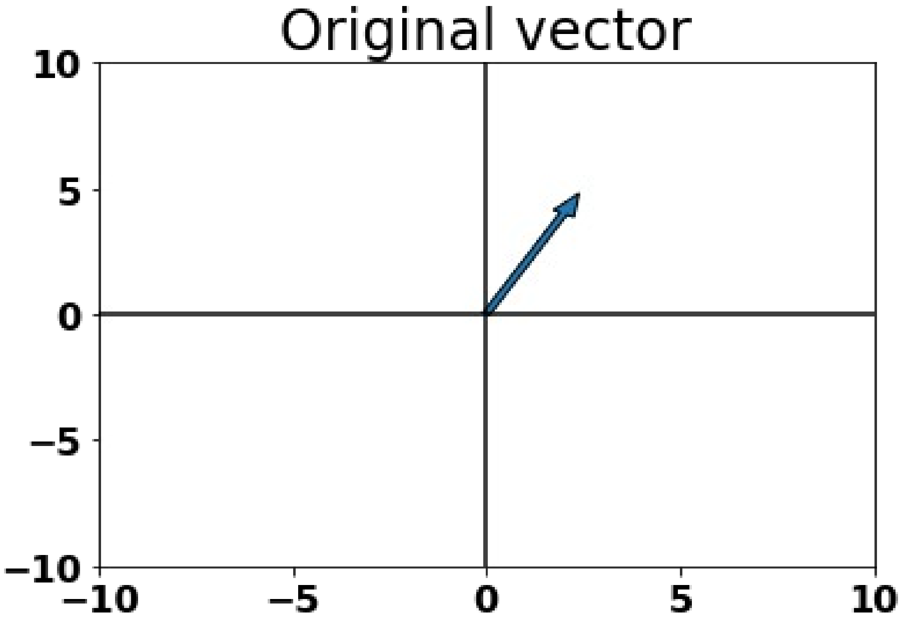


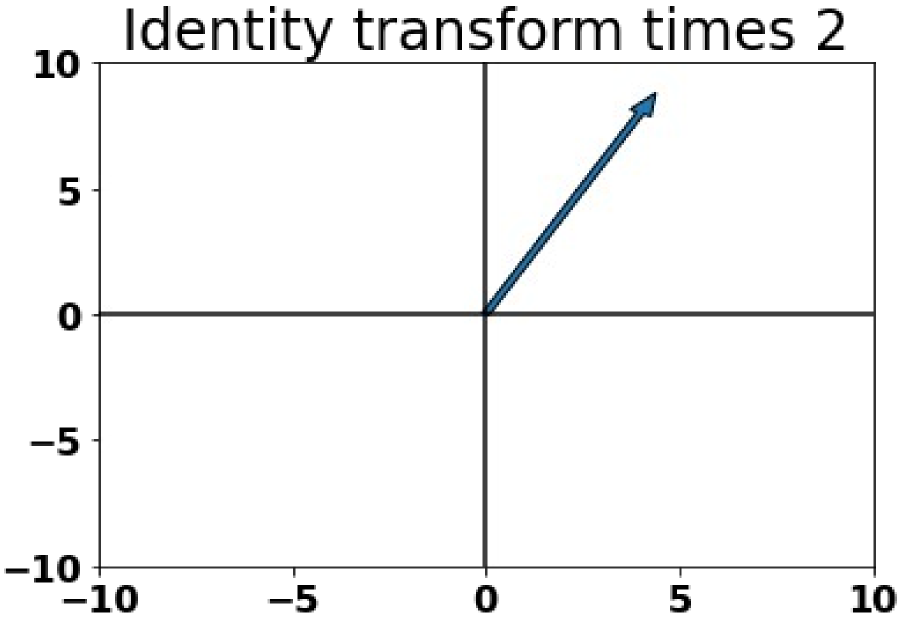

```python
## plot vector (2, 4)
v = (2, 4)
plot_vector(v, 'Original vector')
```

```python
A = np.identity(2)
print('A = \n' + str(A))
plot_vector(A @ v, 'Identity transform')
```

```
A =
[[1. 0.]
 [0. 1.]]
```

Scaling Transformation

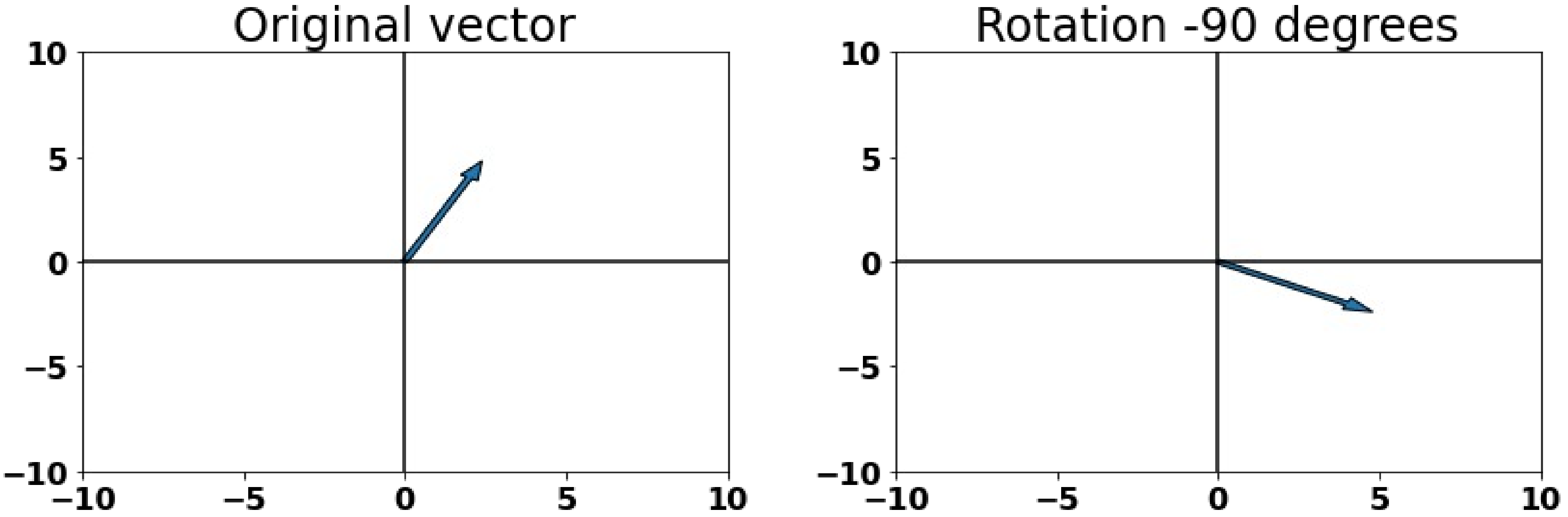





```python
## transform with identity matrix times 2
A = 2 * np.identity(2)
print('A = \n' + str(A))
plot_vector(A @ v, 'Identity transform times 2')
```

```
A =
[[2. 0.]
 [0. 2.]]
```

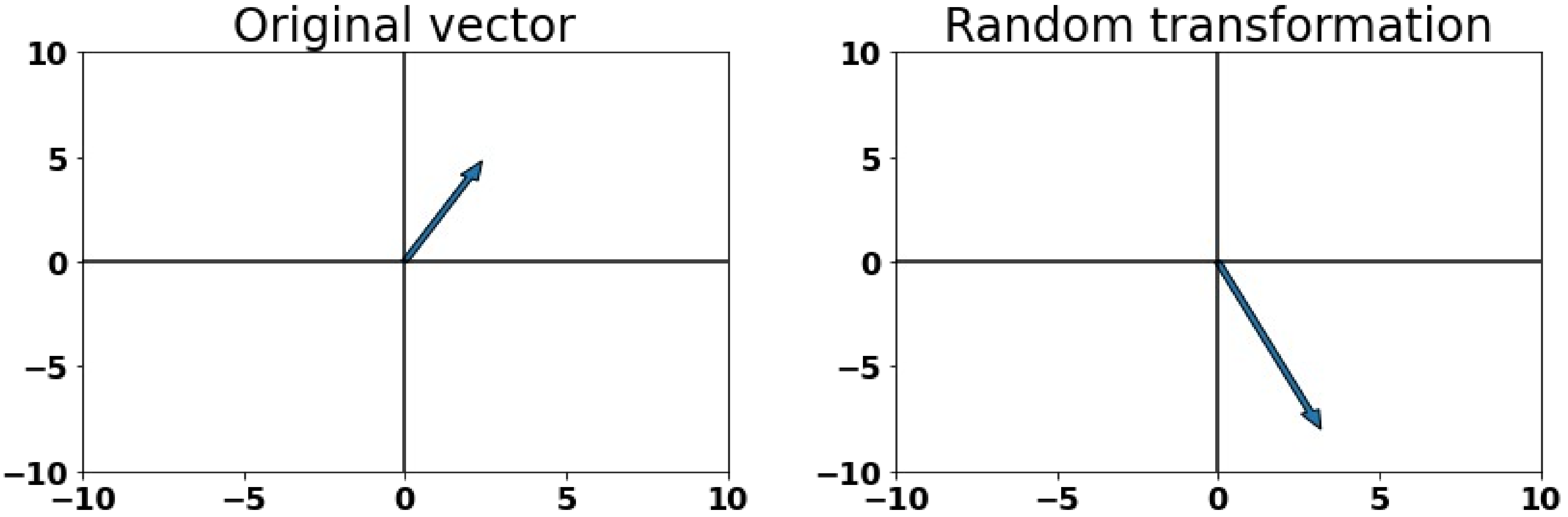
Rotation Transformation




```
A = np.array([[0, 1], [-1, 0]])
print('A = \n' + str(A))
plot_vector(A @ v, 'Rotation -90 degrees')
```

```
A =
[[ 0  1]
 [-1  0]]
```

Random Transformation




```
np.random.seed(1)
A = np.reshape(np.random.uniform(low=-2, high=2, size=4), newshape=(2, 2))
print('A = \n' + str(A))
plot_vector(A @ v, 'Random transformation')
```

```
A =
[[-0.33191198  0.88129797]
 [-1.9995425  -0.79066971]]
```

```
In [142]: ## eigenvalues and eigenvectors
eigen_vals, eigen_vecs = np.linalg.eig(cov_mat)
print(eigen_vals.shape)
print(eigen_vecs.shape)
```

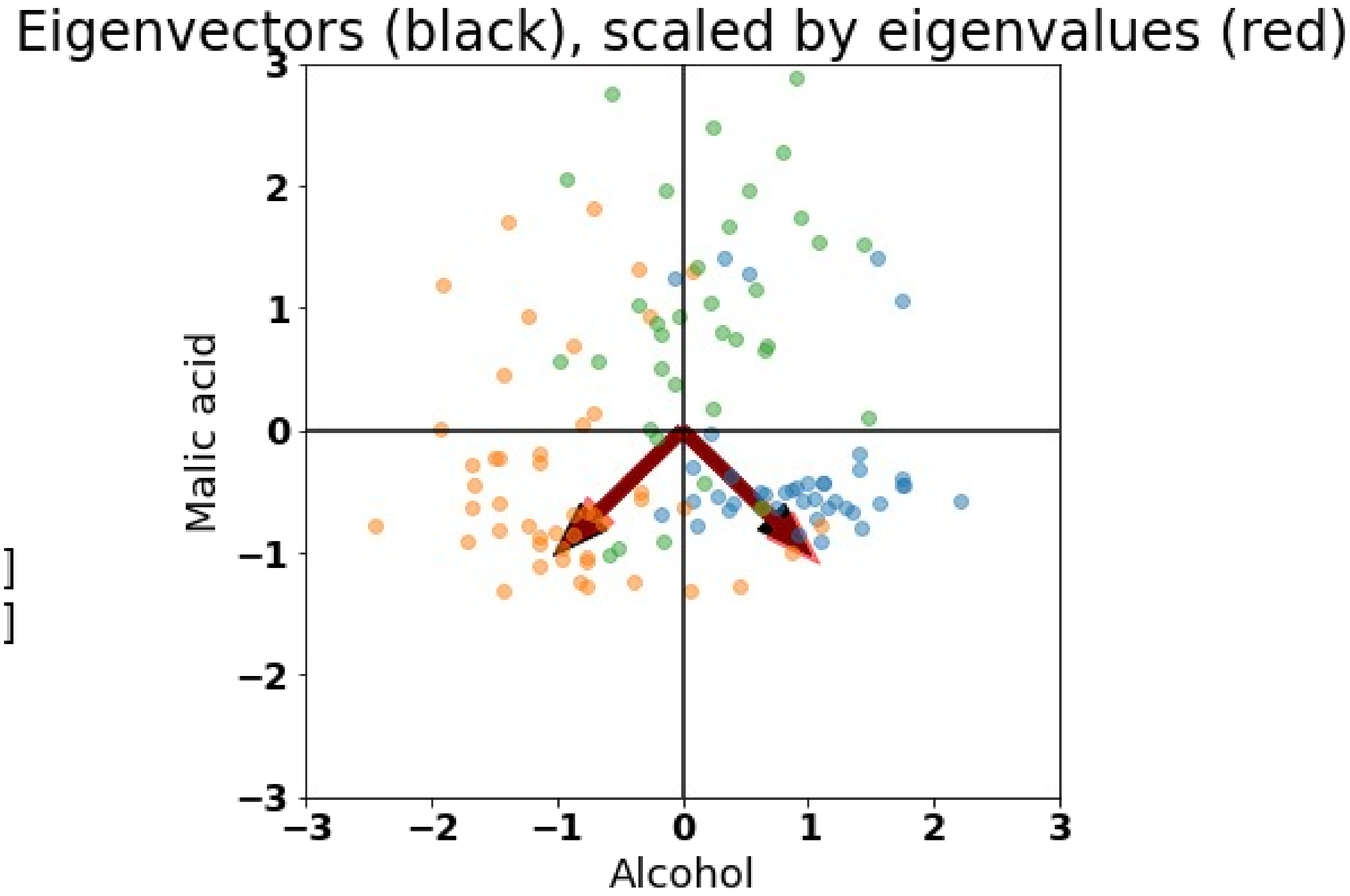
```
(13,)
(13, 13)
```

```
In [17]: # checking whether the equation holds
evec_0 = eigen_vecs[:, 0]
eval_0 = eigen_vals[0]

mat_trans = cov_mat @ evec_0 ## A times x
scalar_trans = eval_0 * evec_0 # lambda times x
print(mat_trans)
print(scalar_trans)

print(np.isclose(mat_trans, scalar_trans)) ## instead of using "==", due to rounding error
```

```
[ 0.7176924  -1.18513985 -0.14644842 -1.24846827  0.5909797   1.90479358
  2.07074217 -1.49875647  1.49568723 -0.48283127  1.46928422  1.80140436
  1.43147537]
[ 0.7176924  -1.18513985 -0.14644842 -1.24846827  0.5909797   1.90479358
  2.07074217 -1.49875647  1.49568723 -0.48283127  1.46928422  1.80140436
  1.43147537]
[ True  True  True  True  True  True  True  True  True  True  True  True
  True]
```

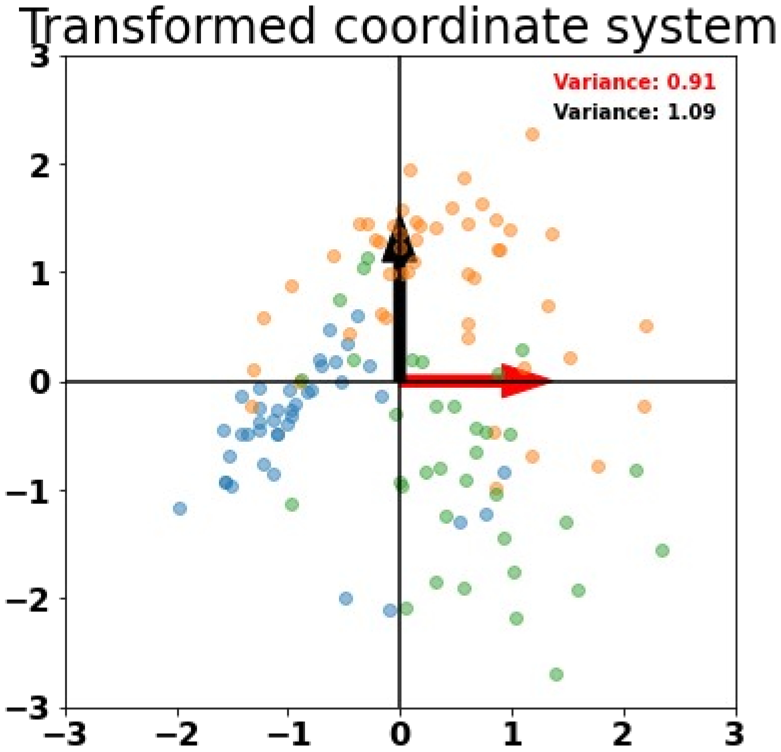
$$\Sigma \boldsymbol{v} = \lambda \boldsymbol{v}$$

```
Eigenvalues:
[0.92015307 1.09610709]

Eigenvectors:
 [[-0.70710678 -0.70710678]
 [ 0.70710678 -0.70710678]]

Covariance matrix:
[[1.00813008 0.08797701]
 [0.08797701 1.00813008]]
```



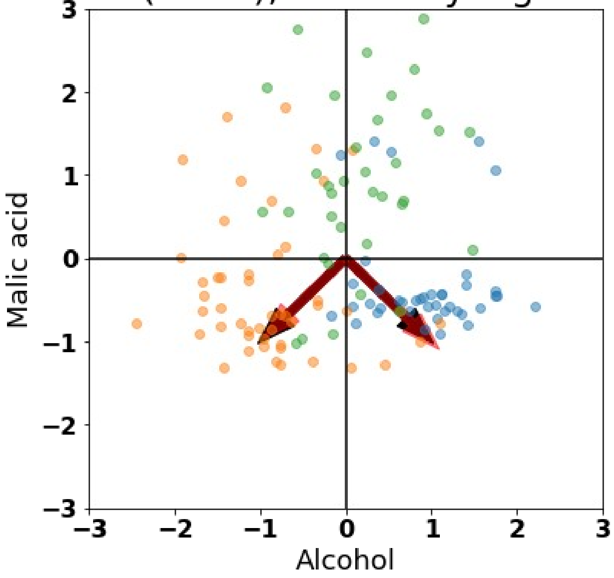
Applying a transformation

```python
radian = np.arctan(reduced_eigen_vecs[1, 1] / reduced_eigen_vecs[1, 0])


A = np.array([
                [np.cos(radian), np.sin(radian)],
                [-np.sin(radian), np.cos(radian)]
            ])
```

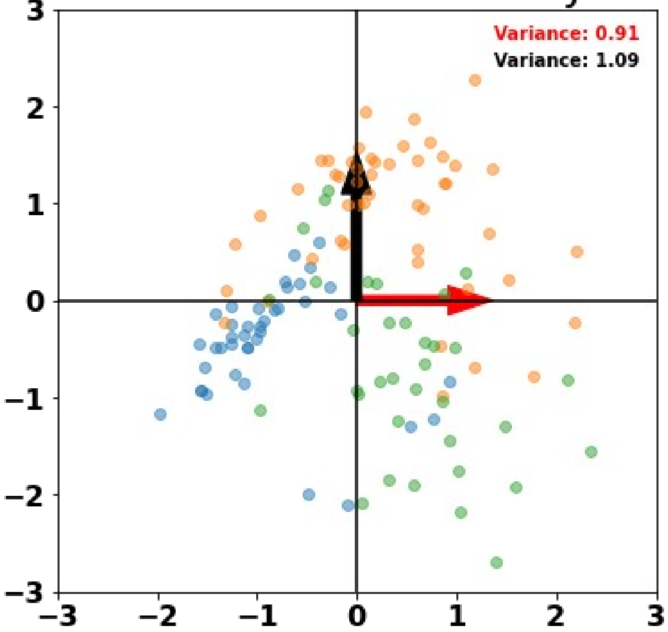


For comparison

Eigenvectors (black), scaled by eigenvalues (red)



Transformed coordinate system



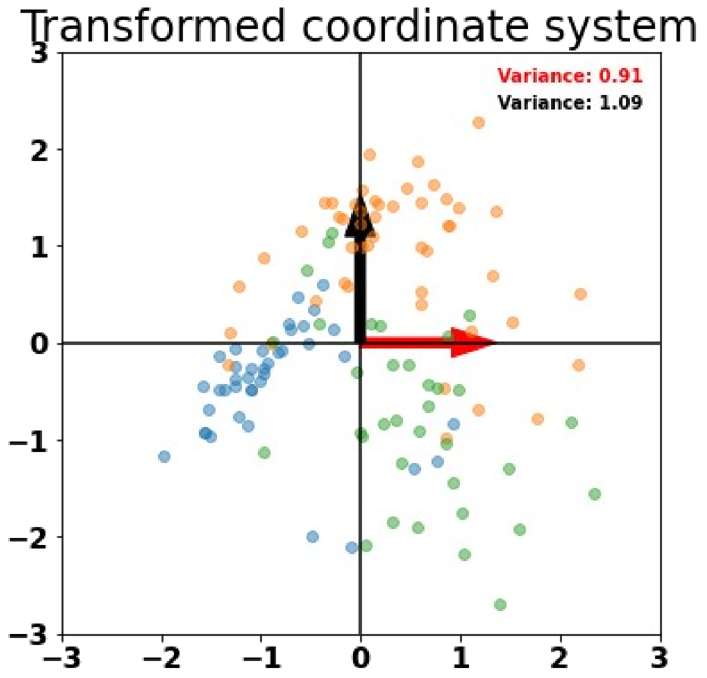
In the case where k=d...

4) Select k eigenvectors that correspond to the k largest eigenvalues where k is the dimensionality of the new feature subspace ($k \leq d$)

5) Construct a projection matrix $\boldsymbol{W}$ from the “top” k eigenvectors

6) Transform the d-dimensional input dataset $\boldsymbol{x}$ using the projection matrix $\boldsymbol{W}$ to obtain the new k-dimensional feature subspace

... applying steps 4, 5 & 6 result in:



this is **not** feature reduction, however...

“reducing” to a new subspace (k=d) (4)

Eigenvalues for the **full** covariance matrix

```
## going back to the full feature matrix
print(eigen_vals)
```

```
[4.8923083  2.46635032 1.42809973 1.01233462 0.84906459 0.60181514
 0.52251546 0.08414846 0.33051429 0.29595018 0.16831254 0.21432212
 0.2399553 ]
```

Variance explained ratio

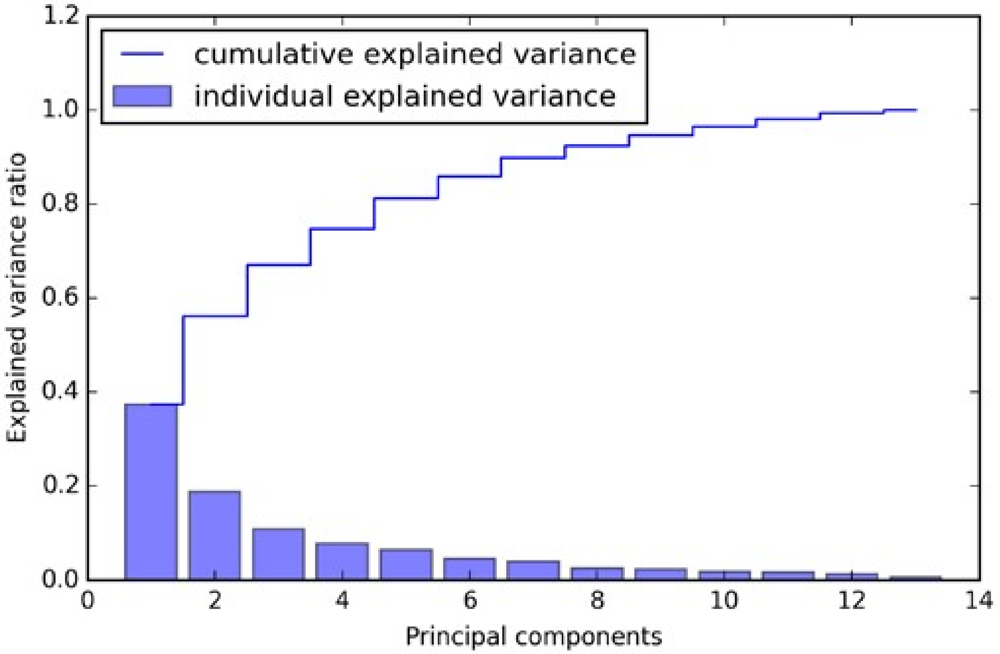
$$\frac{\lambda_j}{\sum_{j=1}^{d} \lambda_j}$$

$$\frac{\lambda_1}{\sum_{j=1}^{d} \lambda_j} = 37\,\%$$

$$\lambda_1 = max(\lambda_j)$$
$$\lambda_7 = min(\lambda_j)$$

$$\frac{\lambda_7}{\sum_{j=1}^{d} \lambda_j} = 0.64\,\%$$

Sorted explained variance



(p. 132: Raschka, 2015)

Setting $k = 2$

Construct a projection matrix ***W*** from the “top” *k* eigenvectors (5)

```
print('Weight matrix:\n', W)
```

```
Weight matrix:
 [[ 0.14669811  0.50417079]
 [-0.24224554  0.24216889]
 [-0.02993442  0.28698484]
 [-0.25519002 -0.06468718]
 [ 0.12079772  0.22995385]
 [ 0.38934455  0.09363991]
 [ 0.42326486  0.01088622]
 [-0.30634956  0.01870216]
 [ 0.30572219  0.03040352]
 [-0.09869191  0.54527081]
 [ 0.30032535 -0.27924322]
 [ 0.36821154 -0.174365  ]
 [ 0.29259713  0.36315461]]
```

Transform the *d*-dimensional input dataset ***X*** using the projection matrix ***W*** to obtain the new *k*-dimensional feature subspace (6)

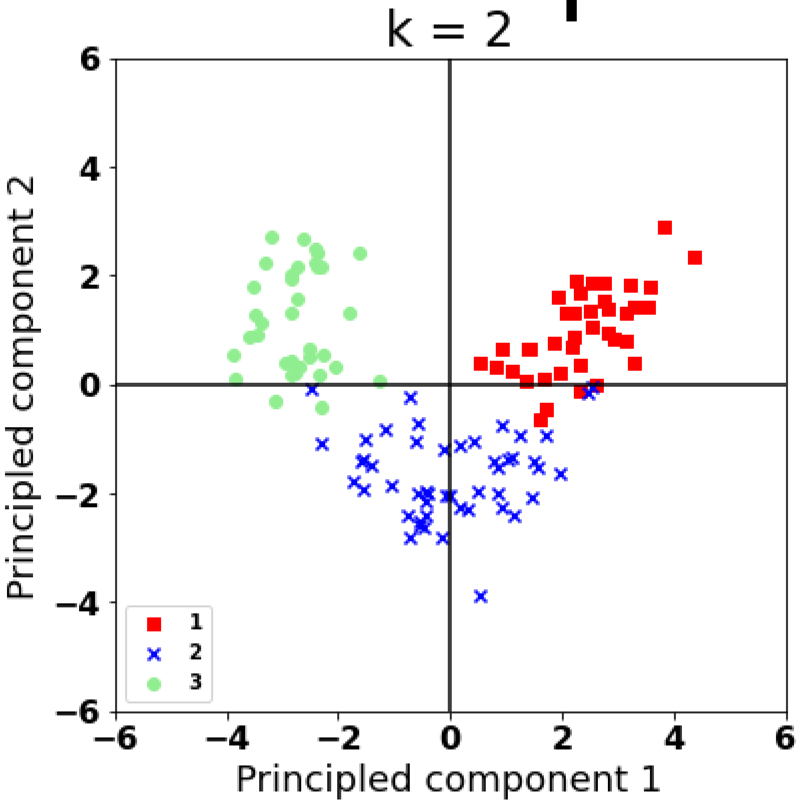
$$\boldsymbol{x} = [x_1, x_2, \ldots, x_d], \boldsymbol{x} \in \mathbb{R}^{\boldsymbol{d}}$$

$$\downarrow \boldsymbol{x}\boldsymbol{W}, \boldsymbol{W} \in \mathbb{R}^{d \times k}$$

$$\boldsymbol{z} = [z_1, z_2, \ldots, z_k], \boldsymbol{z} \in \mathbb{R}^{\boldsymbol{k}}$$

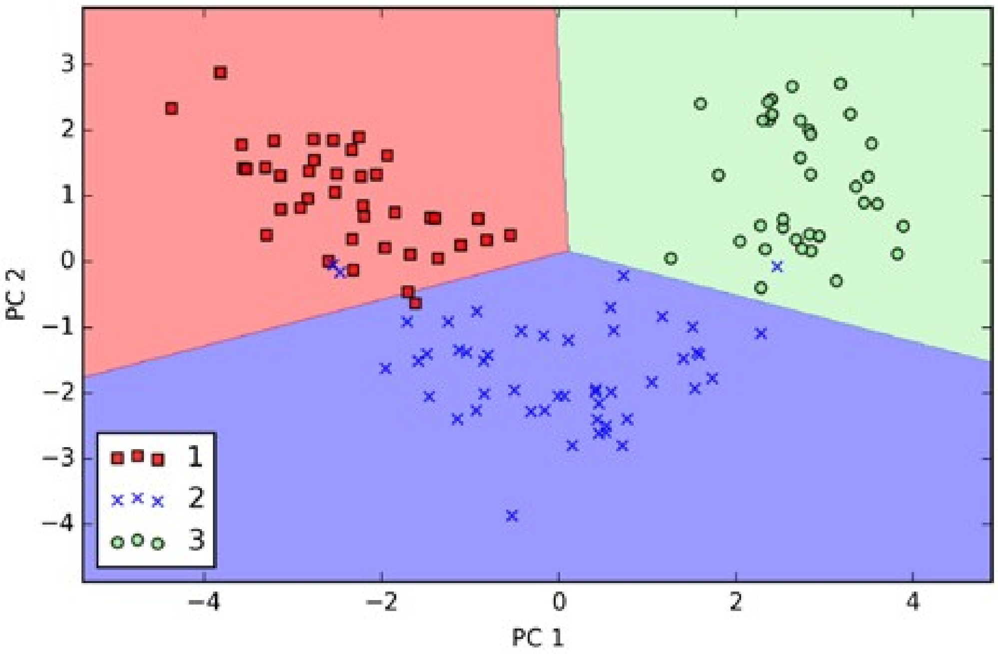
$$\mathbf{Z} = \boldsymbol{X}\boldsymbol{W}$$

Reduced space

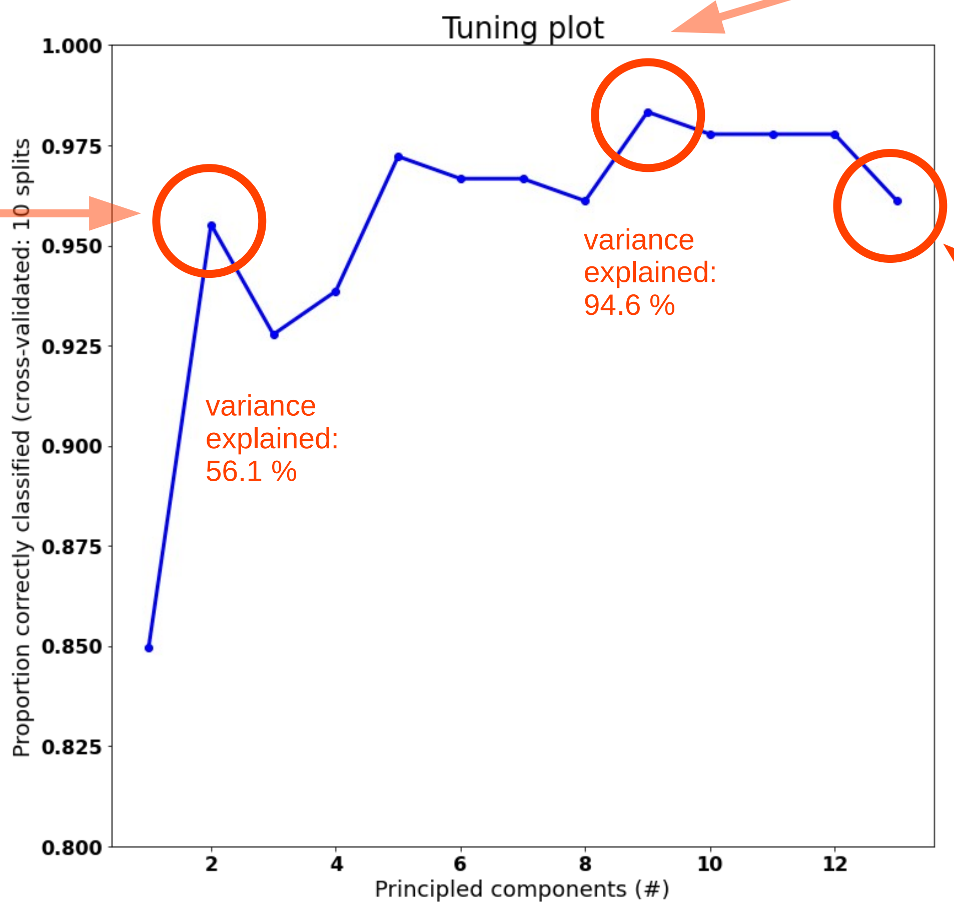


We can now do logistic regression in this space

Logistic regression on reduced space (k = 2)



(p. 136: Raschka, 2015)



peak
k = 9

k = 2

What does this analysis correspond to?

Did you learn?

Dimensionality reduction

1) Learning how we can extract the features that explain the most variance

2) Understanding how that can improve classification

3) Get acquainted with the concept of a eigenvector

(OPTIONAL)

Live coding

WEEK_09.ipynb

(OPTIONAL)

Live coding

NUMPY.ipynb

References

- Abe, S., 2010. Support Vector Machines for Pattern Classification. Springer, London.
- Raschka, S., 2015. Python Machine Learning. Packt Publishing Ltd.