# Introduction to Machine Learning CentraleSupélec Paris — Fall 2017

# 3. Dimensionality Reduction

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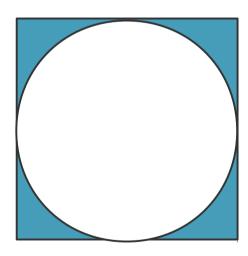




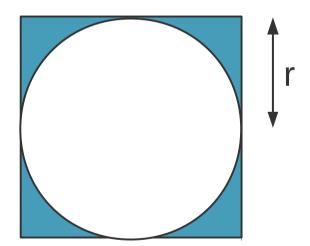
### Learning objectives

- Give reasons why one would wish to reduce the dimensionality of a data set.
- Explain the difference between feature selection and feature extraction.
- Implement some filter strategies.
- Implement some wrapper strategies.
- Derive the computation of principal components from a "max variance" definition
- Implement PCA.

- Methods / intuitions that work in low dimension may not apply to high dimensions.
- p=2: Fraction of the points within a square that fall outside of the circle inscribed in it:

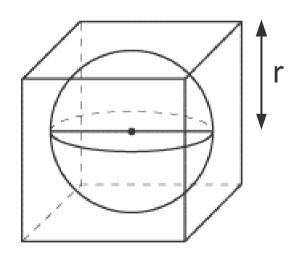


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- p=2: Fraction of the points within a square that fall outside of the circle inscribed in it:



$$1 - \frac{\pi r^2}{4r^2} = 1 - \frac{\pi}{4}$$

- Methods / intuitions that work in low dimension may not apply to high dimensions.
- p=3: Fraction of the points within a cube that fall outside of the sphere inscribed in it:



$$1 - \frac{4/3\pi r^3}{8r^3} = 1 - \frac{\pi}{6}$$

• Volume of a p-sphere:  $\frac{2r^p\pi^{p/2}}{p\Gamma(p/2)}$ 

The Gamma function  $\Gamma$  generalizes the factorial.  $\Gamma(n) = (n-1)!$ 

When p 

 ¬ the proportion of a hypercube outside of its inscribed hypersphere approaches 1.

- What this means:
  - hyperspace is very big
  - all points are far apart
    - ⇒ dimensionality reduction.

# More reasons to reduce dimensionality

- Computational complexity (time and space)
- Interpretability
- Simpler models are more robust (less variance)
- Data visualization
- Cost of data acquisition
- Eliminate non-relevant attributes that can make it harder for an algorithm to learn.

#### Feature selection

Choose m < p features, ignore the remaining (p-m)

Filtering approaches

Apply a statistical measure to assign a score to each feature (correlation,  $\chi^2$ -test).

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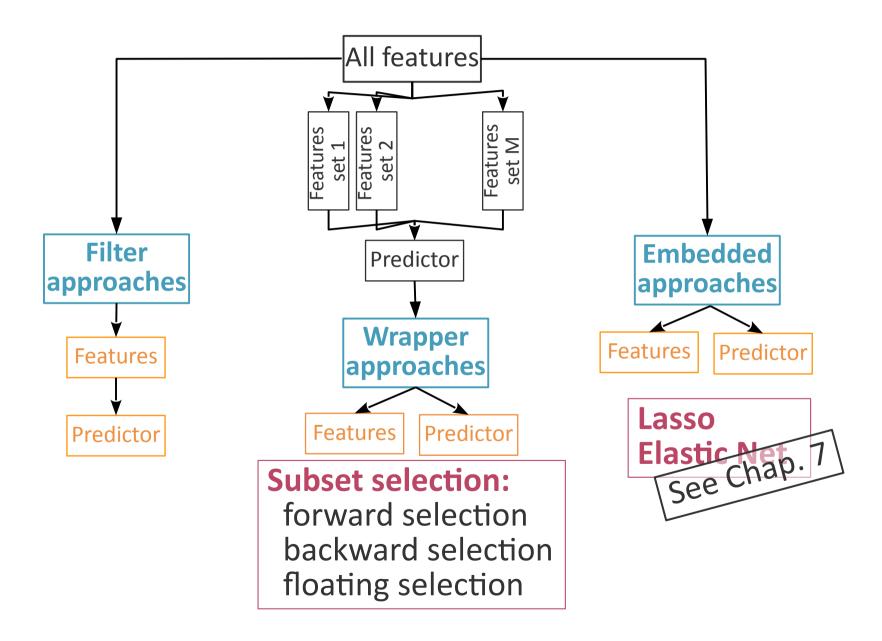
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Are those approaches supervised or unsupervised?

### Feature selection: Overview



# Feature selection: Subset selection

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Wrapper approaches

Search problem: Find the best set of features for a given predictive model.

Embedded approaches

Simultaneously fit a model and learn which features should be included.

All these feature selection approaches are supervised.

- Goal: Find the subset of features that leads to the best-performing algorithm.
- How many subsets of p features are there?

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- Issue:  $2^p$  such sets.

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- Greedy approach: forward search
   Add the "best" feature at each step

 $E(\mathcal{F})$ : Error of a predictor trained only using the features in  $\mathcal{F}$ 

- Initially:  $\mathcal{F} = \emptyset$
- New best feature:  $j* = \arg\min_{j \in \{1,...,p\}} E(\mathcal{F} \cup \{j\})$
- stop if  $E(\mathcal{F}) < E(\mathcal{F} \cup \{j\})$
- else:  $\mathcal{F} \leftarrow \mathcal{F} \cup \{j\}$

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What is the complexity of this algorithm?

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Complexity: O(p<sup>2</sup> x C) where C=complexity of training and evaluating the model (might depend on p also).

Much better than O(2<sup>p</sup>)!

Greedy approach: forward search

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Complexity: O(p<sup>2</sup>)

- Alternative strategies:
  - Backward search: start from {1, ..., p}, eliminate features.
  - Floating search: alternatively add q features and remove r features.

#### Feature extraction

Project the p features on m < p new dimensions

<ul> <li>Principal Components Analysis (PCA)</li> </ul>	
<ul> <li>Factor Analysis (FA)</li> </ul>	
<ul> <li>Non-negative Matrix Factorization (NMF)</li> </ul>	Linear
<ul> <li>Linear Discriminant Analysis (LDA)</li> </ul>	Supervised
Multidimensional scaling (MDS)	
<ul> <li>Isometric feature mapping (Isomap)</li> </ul>	Non linear
<ul> <li>Locally Linear Embedding (LLE)</li> </ul>	Non inteat
Autoencoders	

Most of these approaches are unsupervised.

# Feature extraction: Principal Component Analysis

• Goal: Find a low-dimensional space such that information loss is minimized when the data is projected on that space.

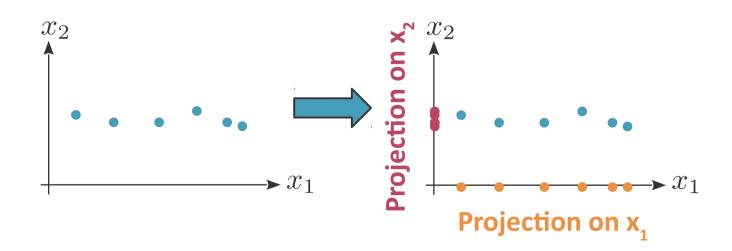
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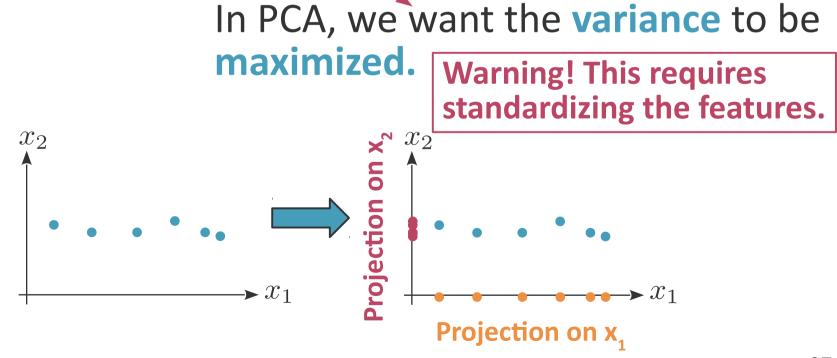
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• Variance of feature j in data set  $\mathcal{D}$ :  $\mathcal{D} = \{ m{x}^1, m{x}^2, \dots, m{x}^n \}$   $m{x} \in \mathbb{R}^p$ 

$$oldsymbol{\mathcal{D}} = \{oldsymbol{x}^1, oldsymbol{x}^2, \dots, oldsymbol{x}^n\} \hspace{0.5cm} oldsymbol{x} \in \mathbb{R}^n$$

• Variance of feature j in data set  $\mathcal{D}$ :

$$\sigma_j^2 = \frac{1}{n} \sum_{i=1}^n (x_j^i - \mu_j)^2 \qquad \mu_j = \frac{1}{n} \sum_{i=1}^n x_j^i$$

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Features that take large values will have large variance

Compare [10, 20, 30, 40, 50] with [0.1, 0.2, 0.3, 0.4, 0.5].

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Features that take large values will have large variance

Compare [10, 20, 30, 40, 50] with [0.1, 0.2, 0.3, 0.4, 0.5].

- Standardization:
  - mean centering: give each feature a mean of 0
  - variance scaling: give each feature a variance of 1

$$x_j^i \leftarrow \frac{x_j^i - \mu_j}{\sigma_j}$$

- Goal: Find a low-dimensional space such that variance is maximized when the data is projected on that space.
- Assumption: the data is centered i.e. it has mean 0.

If not: subtract the mean:  $X \leftarrow X - \mu$ 

 What formula gives us the projection of x on the direction of w (assuming w to be a unit vector)?



- Goal: Find a low-dimensional space such that variance is maximized when the data is projected on that space.
- Projection of X on the direction of  $\mathbf{w}$ :  $\mathbf{z} = X\mathbf{w}$
- Compute Var(z) as a function of wand X.

$$oldsymbol{z} = X oldsymbol{w}$$
 ions: (n, 1) (n, p) x (p, 1) unit vector:  $||oldsymbol{w}|| = 1$ 

dimensions: (n, 1) (n, p) x (p, 1) n samples p features

- Goal: Find a low-dimensional space such that variance is maximized when the data is projected on that space.
- Projection of X on the direction of  $\mathbf{w}$ :  $\mathbf{z} = X\mathbf{w}$
- Var(z) can be computed as:

$$\begin{aligned} \operatorname{Var}(\boldsymbol{z}) &= \operatorname{Var}(X\boldsymbol{w}) = \operatorname{Var}(\boldsymbol{w}^{\top}X^{\top}) \\ &= \mathbb{E}[((\boldsymbol{w}^{\top}X^{\top}) - \mathbb{E}[\boldsymbol{w}^{\top}X^{\top}])^{2}] \\ &= \mathbb{E}[(\boldsymbol{w}^{\top}X^{\top} - \boldsymbol{w}^{\top}\mathbb{E}[X])^{2}] - 0 \text{ (data centered)} \\ &= \mathbb{E}[\boldsymbol{w}^{\top}X^{\top}X\boldsymbol{w}] \\ &= \boldsymbol{w}^{\top}\mathbb{E}[X^{\top}X]\boldsymbol{w} - \underset{\Sigma = X^{\top}X}{\operatorname{Estimated from data:}} \end{aligned}$$
 dimensions: (1, p) x (p, n) x (n, p) x (p, 1)

## First principal component (PC1)

• Goal: find  $m{w}_1 = rg \max_{m{w} \in \mathbb{R}^p} \mathrm{Var}(X m{w})$  subject to  $||m{w}_1|| = 1$ .



What kind of optimization problem do we have?

# First principal component (PC1)

- Goal: find  $m{w}_1 = \arg\max_{m{w} \in \mathbb{R}^p} \mathrm{Var}(Xm{w})$  subject to  $||m{w}_1|| = 1$ .
- Optimization problem: Maximize f(w) s.t. g(w)=Cte/

$$f(\boldsymbol{w}) = \boldsymbol{w}^{\top} \Sigma \boldsymbol{w}$$

$$g(\boldsymbol{w}) = ||\boldsymbol{w}|| - 1$$

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$$f(oldsymbol{w}) = oldsymbol{w}^{ op} \Sigma oldsymbol{w}$$
  $g(oldsymbol{w}) = ||oldsymbol{w}|| - 1$  iso-contours of f  $\{w: g(w) = 0\}$ 

$$\nabla f({m w}^*) = \alpha \nabla g({m w}^*)$$
 Lagrangian:  $L(\alpha, {m w}) = f({m w}) - \alpha g({m w})$ 

Maximize f(w) s.t. g(w)=0

$$L(\alpha, \boldsymbol{w}) = f(\boldsymbol{w}) - \alpha g(\boldsymbol{w})$$

- If  $(\alpha^*, \boldsymbol{w}^*)$  maximize the Lagrangian, then
  - $\nabla_{\alpha}L(\alpha^*, \boldsymbol{w}^*) = 0$  (stationarity point) hence  $g(\boldsymbol{w}^*) = 0$
  - For any admissible  $\boldsymbol{w}, f(\boldsymbol{w}) \alpha^* g(\boldsymbol{w}) \leq f(\boldsymbol{w}^*) \alpha g(\boldsymbol{w}^*)$  (by definition of the maximum of L), hence  $f(\boldsymbol{w}) \leq f(\boldsymbol{w}^*)$  (because of admissibility).
- That is to say, any maximizer of the Lagrangian gives us a maximizer of f under the constraint that g=0.

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$$\nabla f(\boldsymbol{w}^*) = \alpha \nabla g(\boldsymbol{w}^*) \quad \text{Lagrangian: } L(\alpha, \boldsymbol{w}) = f(\boldsymbol{w}) - \alpha g(\boldsymbol{w})$$
 
$$L(\alpha, \boldsymbol{w}) = \nabla x (\boldsymbol{x} \boldsymbol{w}) - \alpha (\boldsymbol{w}^\top \boldsymbol{w} - 1)$$
 
$$\boldsymbol{w}^\top \Sigma \boldsymbol{w}$$
 Hence: 
$$\boldsymbol{w}_1 = \arg\max_{\boldsymbol{w} \in \mathbb{R}^p} \left(\boldsymbol{w}^\top \Sigma \boldsymbol{w} - \alpha (\boldsymbol{w}^\top \boldsymbol{w} - 1)\right)$$
?

$$\boldsymbol{w}_1 = \arg\max_{\boldsymbol{w} \in \mathbb{R}^p} \left( \boldsymbol{w}^{\top} \Sigma \boldsymbol{w} - \alpha (\boldsymbol{w}^{\top} \boldsymbol{w} - 1) \right)$$

 The maximum is an extremum point, hence necessarily the gradient is zero.

$$\nabla_{\boldsymbol{w}} L(\boldsymbol{w}_1) = 0$$
$$2\Sigma \boldsymbol{w}_1 - 2\alpha \boldsymbol{w}_1 = 0$$

• Hence  $\Sigma \boldsymbol{w}_1 = \alpha \boldsymbol{w}_1$ 

What does it tell us about  $\alpha$ ,  $\mathbf{w}_1$  w.r.t the matrix  $\Sigma$ ?

$$\boldsymbol{w}_1 = \arg\max_{\boldsymbol{w} \in \mathbb{R}^p} \left( \boldsymbol{w}^{\top} \Sigma \boldsymbol{w} - \alpha (\boldsymbol{w}^{\top} \boldsymbol{w} - 1) \right)$$

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 $(lpha, oldsymbol{w}_1)$  are an (eigenvalue, eigenvector) of  $\Sigma$ 

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- $(\alpha, \boldsymbol{w}_1)$  are an (eigenvalue, eigenvector) of  $\Sigma$
- Now we want to find the maximum of all possible extremum points

$$m{w}_1 = rg \max_{(\alpha, \, m{w}) \text{ (eigenvalue, eigenvector) of } \Sigma} (m{w}_1 = rg \max_{(\alpha, \, m{w}) \text{ (eigenvalue, eigenvector) of } \Sigma} m{w}_1 = rg \max_{(\alpha, \, m{w}) \text{ (eigenvalue, eigenvector) of } \Sigma}$$

• Hence  $w_1$  is the eigenvector of  $\Sigma$  corresponding to its largest eigenvalue.

- Goal: find w<sub>2</sub>
  - of unit length
  - orthogonal to w<sub>1</sub>
  - such that the projection of x on w<sub>2</sub> has maximal variance.

Write out each of these requirements.

- Goal: find w<sub>2</sub>
  - of unit length  $||oldsymbol{w}_2||=1$
  - orthogonal to  $\mathbf{w_1} \quad \mathbf{w}_2^{\top} \mathbf{w}_1 = 0$
  - such that the projection of x on  $\mathbf{w_2}$  has maximal variance.  $\mathbf{w}_2 = \arg\max_{\mathbf{w} \in \mathbb{R}^n} \mathrm{Var}(X\mathbf{w})$
- Hence the following optimization problem (Lagrangian):

(Lagrangian): 
$$w_2 = \arg\max_{\boldsymbol{w} \in \mathbb{R}^p} \left( \boldsymbol{w}^{\top} \boldsymbol{\Sigma} \boldsymbol{w} - \alpha (\boldsymbol{w}^{\top} \boldsymbol{w} - 1) - \beta (\boldsymbol{w}^{\top} \boldsymbol{w}_1) \right).$$

$$w_2 = \arg \max_{\boldsymbol{w} \in \mathbb{R}^p} \left( \boldsymbol{w}^{\top} \Sigma \boldsymbol{w} - \alpha (\boldsymbol{w}^{\top} \boldsymbol{w} - 1) - \beta (\boldsymbol{w}^{\top} \boldsymbol{w}_1) \right).$$

Take the derivative, set it to 0

$$2\Sigma \boldsymbol{w}_2 - 2\alpha \boldsymbol{w}_2 - \beta \boldsymbol{w}_1 = 0$$

$$2\boldsymbol{w}_1^{\top} \Sigma \boldsymbol{w}_2 - 2\alpha \boldsymbol{w}_1^{\top} \boldsymbol{w}_2 - \boldsymbol{w}_1^{\top} \beta \boldsymbol{w}_1 = 0$$

$$= \boldsymbol{w}_2^{\top} \Sigma \boldsymbol{w}_1$$

$$= \lambda_1 \boldsymbol{w}_2^{\top} \boldsymbol{w}_1$$

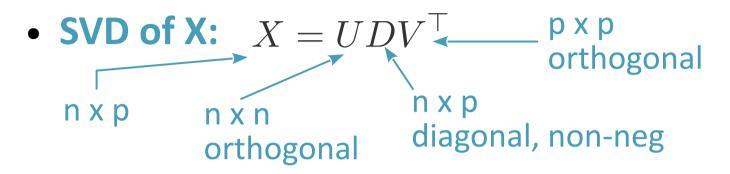
$$= 0$$
Hence  $\beta = 0$ 

$$2\Sigma \boldsymbol{w}_2 - 2\alpha \boldsymbol{w}_2 = 0$$

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- The second principal component is given by the eigenvector of  $\Sigma$  with the second largest eigenvalue.
- And so on and so forth for all other PCs.

# Singular value decomposition



• Cov(X): 
$$X^{\top}X = VD^{\top}U^{\top}UDV^{\top}$$
  
=  $V(D^{\top}D)V^{\top}$ 

• Eigendecomposition of Σ:

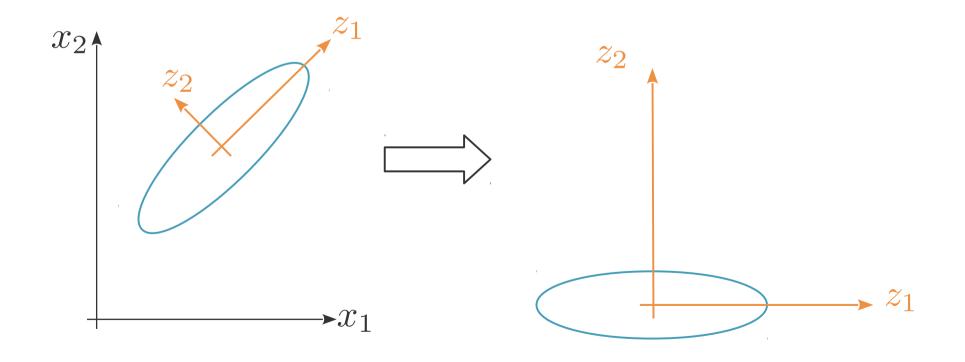
diagonal, eigenvalues 
$$\Sigma = Q \Lambda Q^{-1}$$
 
$$\rho \times \rho$$
 
$$\rho \times \rho$$

pxp

- The singular values of X are the square root of the eigenvalues of  $\Sigma$ .
- The left-singular vectors of X (the columns of U) are the eigenvectors of  $\Sigma$ .

#### What PCA does

- W: p x m matrix of the m leading eigenvectors of  $\Sigma$ .
- m first PCs:  $Z=(X-\mu)W$  dimensions: (n, m) (n, p) x (p, m)  $\Sigma=(X-\mu)^{\top}(X-\mu)$

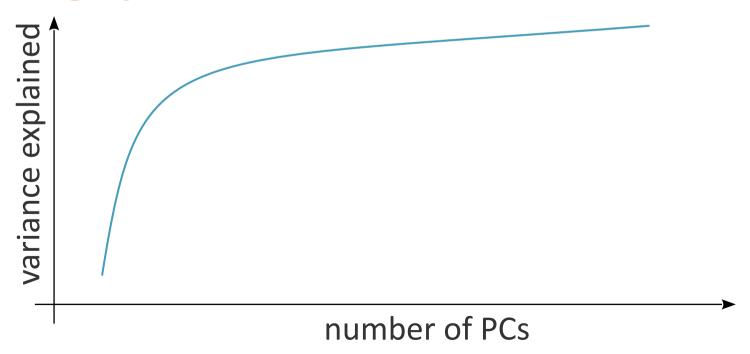


#### How to choose m

#### Percentage of variance explained:

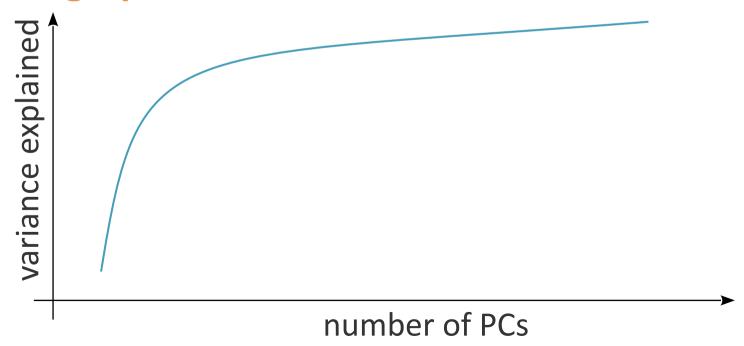
- Total variance in the data = Tr( $\Sigma$ ) =  $\lambda_1 + \lambda_2 + ... + \lambda_p$
- The first m PCs account for  $\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_m}{\lambda_1 + \lambda_2 + \cdots + \lambda_p}$  of the total variance.

#### Scree graph:

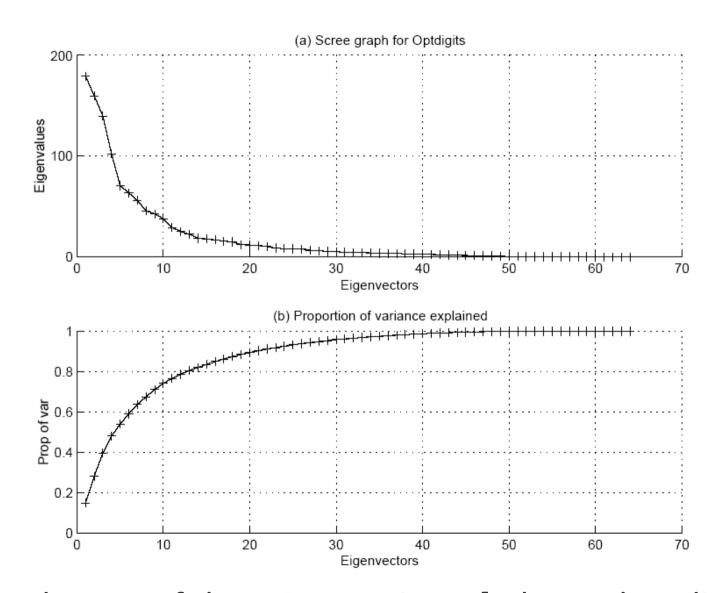


#### How to choose m

- Pick enough components to explain a fixed percentage of the variance.
- Find the "elbow" (where adding more components doesn't really help much).
- Scree graph:

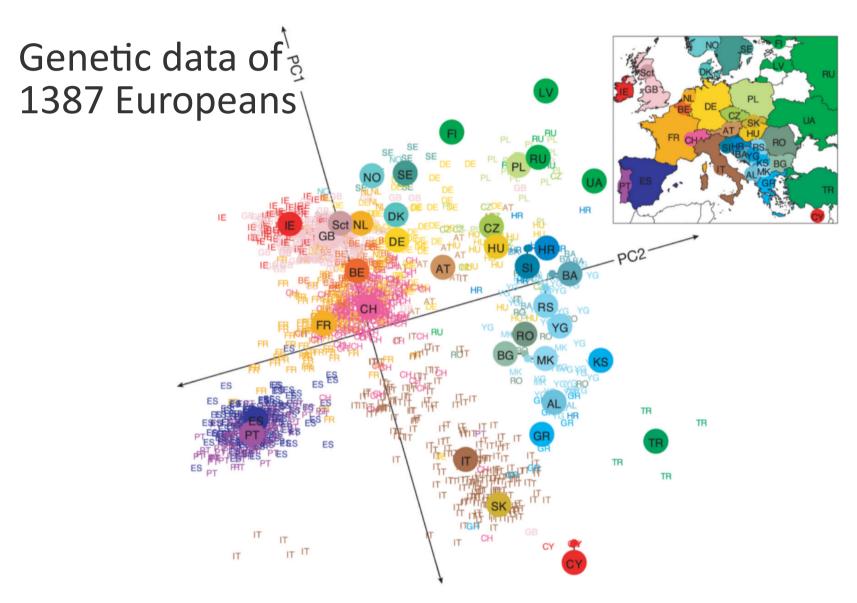


# Scree graph (example)



Optdigits dataset of the UCI repository [Ethem Alpaydin]

#### PCA example: Population genetics



Novembre et al, 2008

#### Non-linear feature extraction

$$\arg \min_{Z \in \mathbb{R}^{n \times m}} \sum_{t=1}^{n} \sum_{u=t+1}^{n} (||z^{t} - z^{u}|| - d_{tu})^{2}$$

• Find a mapping that preserves the **dissimilarities** between the data points.

$$\arg \min_{Z \in \mathbb{R}^{n \times m}} \sum_{t=1}^{n} \sum_{u=t+1}^{n} (||z^{t} - z^{u}|| - d_{tu})^{2}$$

- In Euclidean space:  $d_{tu} = || \boldsymbol{x}^t - \boldsymbol{x}^u ||$  Equivalent to PCA!

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$$d: \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$$

$$d(\boldsymbol{x}, \boldsymbol{v}) = 0 \Leftrightarrow \boldsymbol{x} = \boldsymbol{v} \text{ (identity of indiscernables)}$$

$$d(\boldsymbol{x}, \boldsymbol{v}) = d(\boldsymbol{v}, \boldsymbol{x}) \text{ (symmetry)}$$

$$d(\boldsymbol{x}, \boldsymbol{v}) \leq d(\boldsymbol{x}, \boldsymbol{w}) + d(\boldsymbol{w}, \boldsymbol{v}) \text{ (triangular inequality)}$$

$$\arg \min_{Z \in \mathbb{R}^{n \times m}} \sum_{t=1}^{n} \sum_{u=t+1}^{n} (||z^{t} - z^{u}|| - d_{tu})^{2}$$

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- ... or be non-metric.

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Application: place cities on a map so as to respect their pairwise distances.

Works up to translation / rotation.

#### Reconstructing a map of the Netherlands

http://www.wouterspekkink.org/?p=299

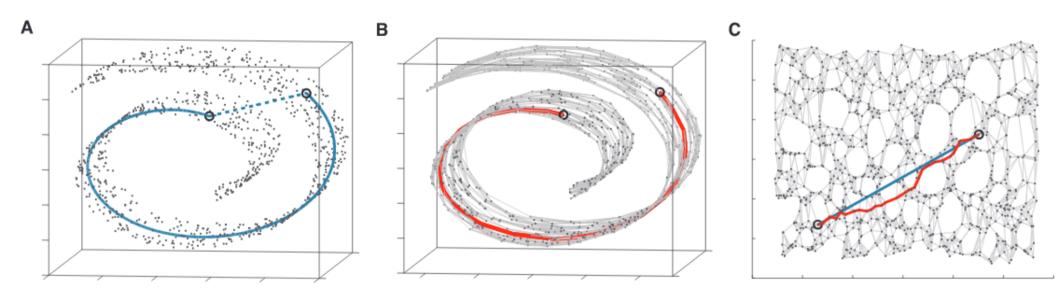




#### IsoMap

- Incorporate local structure in MDS
- Create a neighborhood graph
  - connect each point to its K nearest neighbors (or all neighbors within a distance  $\varepsilon$ )
  - weight by distance
- Compute geodesic distances on the neighborhood graph
  - length of the shortest (weighted) path e.g. Djikstra
- Apply MDS to the resulting dissimilarity matrix.

# IsoMap on "Swiss roll" data



**Fig. 3.** The "Swiss roll" data set, illustrating how Isomap exploits geodesic paths for nonlinear dimensionality reduction. (A) For two arbitrary points (circled) on a nonlinear manifold, their Euclidean distance in the high-dimensional input space (length of dashed line) may not accurately reflect their intrinsic similarity, as measured by geodesic distance along the low-dimensional manifold (length of solid curve). (B) The neighborhood graph G constructed in step one of Isomap (with K=7 and N=1

1000 data points) allows an approximation (red segments) to the true geodesic path to be computed efficiently in step two, as the shortest path in G. (C) The two-dimensional embedding recovered by Isomap in step three, which best preserves the shortest path distances in the neighborhood graph (overlaid). Straight lines in the embedding (blue) now represent simpler and cleaner approximations to the true geodesic paths than do the corresponding graph paths (red).

Tennenbaum et al. (2000) A Global Geometric Framework for Nonlinear Dimensionality Reduction. Science. http://web.mit.edu/cocosci/Papers/sci\_reprint.pdf

# t-Stochastic Neighbor Embedding (tSNE)

- Very popular at the moment
- Approximate the distribution of pairwise distances in the data by a t-distribution (Student's)

$$\underset{Q}{\operatorname{arg\,min}} \sum_{i=1}^{n} KL(P_i \parallel Q_i)$$

follows a t-distribution

- distribution of the conditional probability that x<sup>i</sup> picks x<sup>j</sup> as a neighbor
- neighbors are picked in proportion to their probability density under a Gaussian centered in  $\mathbf{x}^i$ .

centered in  $\mathbf{x}^{\mathbf{i}}$ .  $P_i(\mathbf{x}^j) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{||\mathbf{x}^j - \mathbf{x}^i||^2}{2\sigma^2}\right)$ 

Kullback-Leibler divergence (measures how much P diverges from Q).

https://distill.pub/2016/misread-tsne/

#### Summary

- Goal: Use m < p features.
- Feature selection:
  - Filter approaches
  - Wrapper approaches: Subset selection
     Greedy search of the best set of features.
  - Embedded approaches: Lasso, Elastic Net
- Feature extraction: unsupervised
  - Linear: Principal Components Analysis
     Center the data and align it with axes of largest variance.
  - Non-linear: MDS, IsoMap, tSNE
     Preserve local distances/structure.

#### References

• An Introduction to Feature Selection. In: Applied Predictive Modeling. (2013) Kuhn and Johnson

https://link.springer.com/chapter/10.1007/978-1-4614-6849-3\_19

This book chapter should be available to you from within CentraleSupelec. If you cannot access it, please let me know.

- Feature Selection: Chapter 19.1 19.3
- A Course in Machine Learning. http://ciml.info/dl/v0\_99/ciml-v0\_99-all.pdf
  - PCA: Chapter 15.2
- The Elements of Statistical Learning.
   http://web.stanford.edu/~hastie/ElemStatLearn/
  - **PCA:** Chapter 14.5.1
  - MDS: Chapter 14.8
- To go further
  - An Introduction to Variable and Feature Selection (2003), Guyon and Elisseeff.
     http://www.jmlr.org/papers/v3/guyon03a.html

#### Lab 1: some pointers

- If pandas.plotting does not work
  - Update your version of pandas
    - Pip: pip install pandas --upgrade
    - Anaconda: conda update pandas
  - Or try using pandas.tools.plotting instead.

#### **Standardization**

```
import numpy as np
# transform data from to numpy array
X = data.values
# TODO: standardise the data
X mean = np.mean(X, axis=0)
X \text{ std} = \text{np.std}(X, axis=0)
print "X mean", X mean
print "X std", X std
X centered = (X - X mean) / X std
print "X centered mean", np.mean(X centered, axis=0)
print "X centered std", np.std(X centered, axis=0)
X mean [ 10.99804878 7.26 14.47707317 1.97682927 49.61634146
  14.60585366 44.32560976 4.76243902 58.31658537 279.02487805
                   0.31251927 0.81431175
                                           0.08785906
X std [ 0.2597956
  0.46599998 3.33639725 0.27458865 4.76759315 11.530011771
X centered mean [ -1.94965995e-16 -2.29085044e-15 -1.47036854e-15 4.92559922e-15
  -1.07231297e-15 -2.77826542e-15 -7.31122480e-16 -8.44852643e-16
 -8.41806299e-16 -2.89741131e-151
```

#### Finding the first 2 components

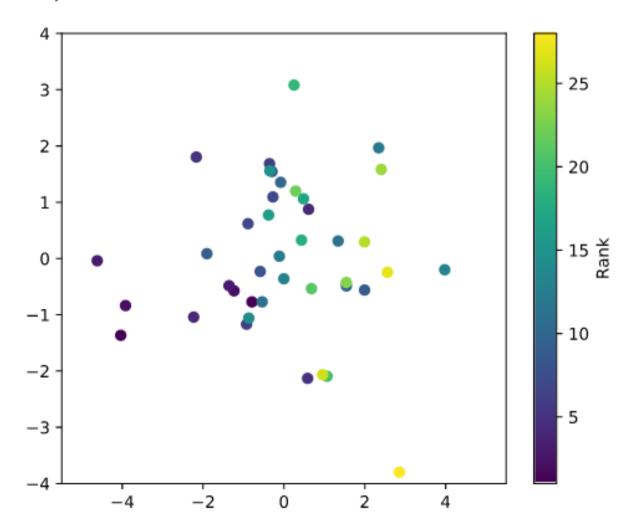
```
from numpy import linalg

# TODO: calculate the the covariance matrix with numpy
N = X_centered.shape[0]
X_cov = X_centered.T.dot(X_centered) / N

# TODO: find its two first principal components
w, v = linalg.eig(X_cov)
w, v = w[:2], v[:,:2]

# TODO: project X onto the principal components
X_projected = X_centered.dot(v)
```

<matplotlib.colorbar.Colorbar at 0x7f05bb1a2310>



#### Computing the percentage of variance explained (sklearn)

```
# TODO: project X on principal components
X_projected = pca.transform(X_scaled)
```

pca.explained variance ratio gives the percentage of variance explained by each of the components.

```
print pca.explained_variance_ratio_
[ 0.32719055   0.1737131 ]
```

Question: How is pca.explained\_variance\_ratio\_computed? Check this is the case by computing it yourself.

```
tot_var = np.var(X_scaled, axis=0).sum()
print (1 / tot_var) * np.var(X_projected, axis=0)
```

[ 0.32719055 0.1737131 ]