Lecture 3

Dimensionality Reduction

Ioanna Miliou, PhD

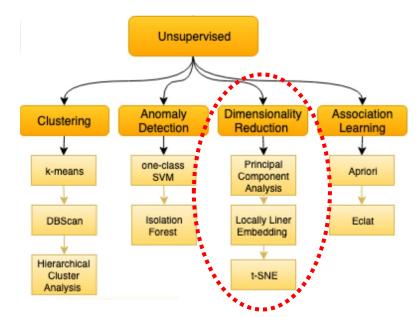
Senior Lecturer, Stockholm University



Unsupervised learning

Experience: objects for which **no class labels** have been given

<u>Performance:</u> typically concerns the ability to output useful **characterizations**(or groupings) of objects



Dimensions

Features (attributes)

Class label

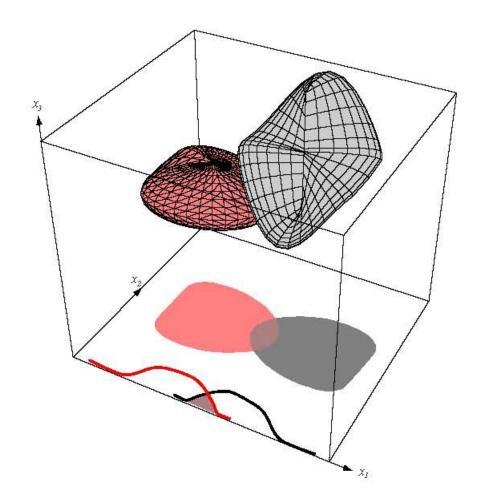
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	e1	yes	0	no	3	0	yes
	e2	yes	3	no	0	0.2	yes
	e3	no	0	no	0	1	no
	e4	no	4	yes	4	0.5	yes
	e5	yes	0	yes	2	0	no
	e6	no	0	no	0	0	no



Data Dimensionality

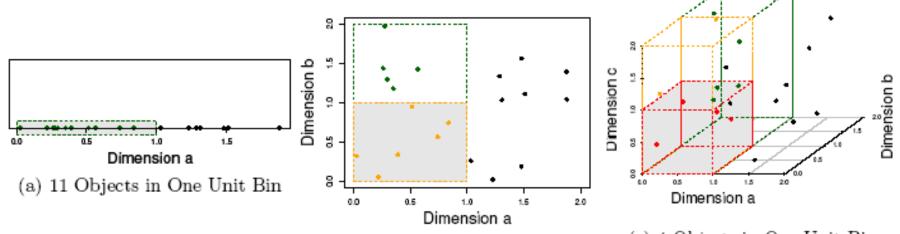
- From a theoretical point of view, increasing the number of features should lead to better performance
- In practice, the inclusion of more features leads to worse performance (i.e., the curse of dimensionality)
- Need an exponential number of training examples as dimensionality increases
- Index structures fail as the dimensionality of the data increases





The Curse of Dimensionality

- Data in only one dimension is relatively packed
- Adding a dimension "stretches" the points across that dimension, making them further apart
- Adding more dimensions will make the points further apart—high dimensional data is extremely sparse
- Distance measures become meaningless



(b) 6 Objects in One Unit Bin



Data Dimensionality

 Significant improvements can be achieved by first mapping the data into a lowerdimensional space:

$$x = \begin{bmatrix} a_1 \\ a_2 \\ \dots \\ a_N \end{bmatrix} --> reduce \ dimensionality --> y = \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_K \end{bmatrix} \ (K << N)$$

- Dimensionality can be reduced by:
 - Combining features (linearly or non-linearly)
 - Selecting a subset of features (i.e., feature selection)
- We will focus on <u>combining features</u>

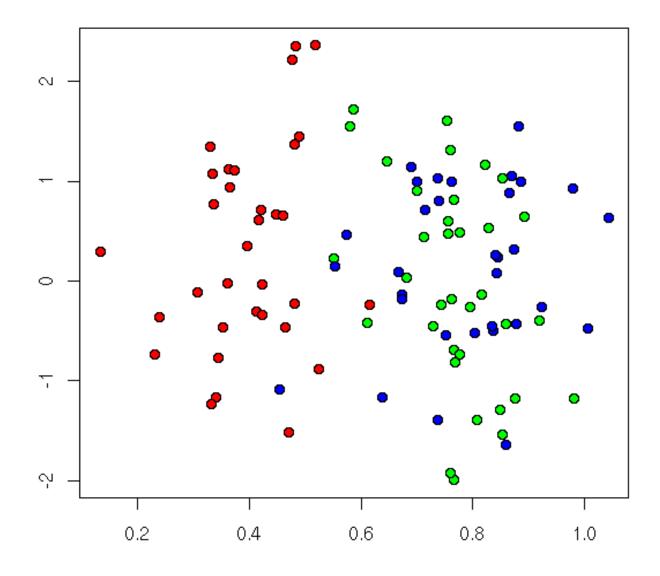


Data Understanding

Name	Solubility	No. C atoms	Fraction of rotatable bonds	Topol. diam.	Geom. diam.	LogP	No. heavy bonds	
methylpentane	good	6	0.40	4	3.46	2.44	5	
methylcyclohexene	good	7	0	4	3.00	2.51	7	
nonene	med.	9	0.75	8	6.93	3.53	8	
hexadiene	good	6	0.60	5	4.36	2.14	5	
butadiene	good	4	0.33	3	2.65	1.36	3	
naphthalene	good	10	0	5	3.61	2.84	11	
acenaphthylene	good	12	0	5	3.58	3.32	14	
pyrene	poor	16	0	7	5.00	4.58	19	
dimethylanthracene	poor	16	0	7	5.29	4.61	18	
hexahydropyrene	med.	16	0	7	5.00	3.82	19	
triphenylene	poor	18	0	7	5.00	5.15	21	
benzo(e)pyrene	poor	20	0	7	5.29	5.64	24	



Plot the Data: two variables





Dimensionality Reduction

- Statistical methods that provide information about point scatters in multivariate space
- Simplify complex relationships between cases and/or variables
- Make it easier to identify patterns
- Remove correlation between features



Why reduce the dimensionality?

- Better presentation than ordinal axes
- Do we need a 100-dimensional space to view the data?
- Question: How to find the "best" low dimensional space that conveys maximum useful information?
- One answer: Find "Principal Components"



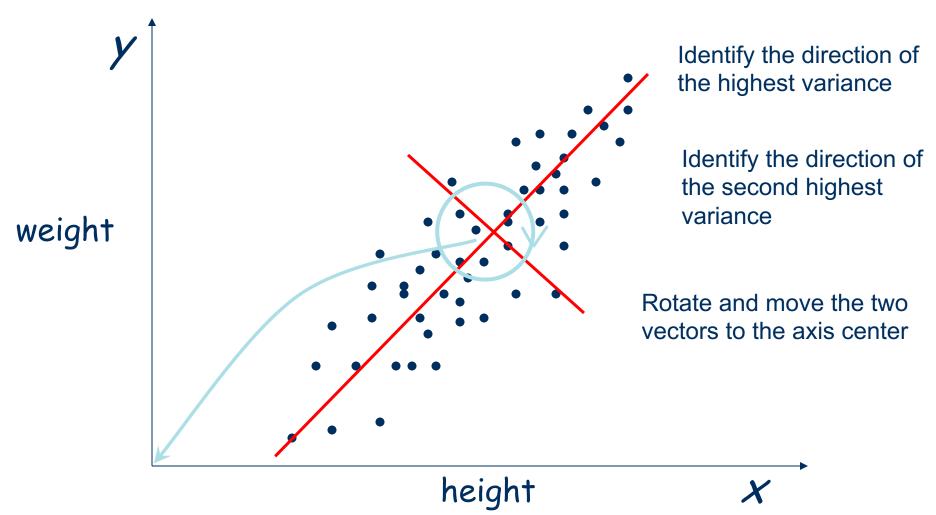
The goal

 We wish to explain/summarize the underlying variance-covariance structure of a large set of variables

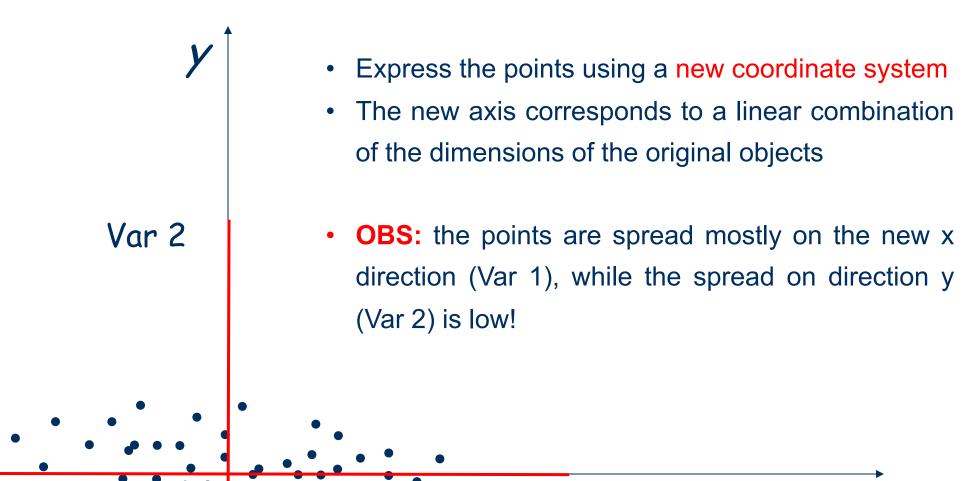
• Use a few linear combinations of these variables



Imagine a two-dimensional scatter of points that show a high degree of correlation ...



Imagine a two-dimensional scatter of points that show a high degree of correlation ...





What does this mean?

- More "efficient" description
 - 1st Var captures max. variance
 - 2nd Var captures the max. amount of residual variance,
 at right angles (orthogonal) to the first

• The 1st Var may capture so much of the information content in the original data set that we can ignore the remaining axis



Principal Components Analysis (PCA)

• Why:

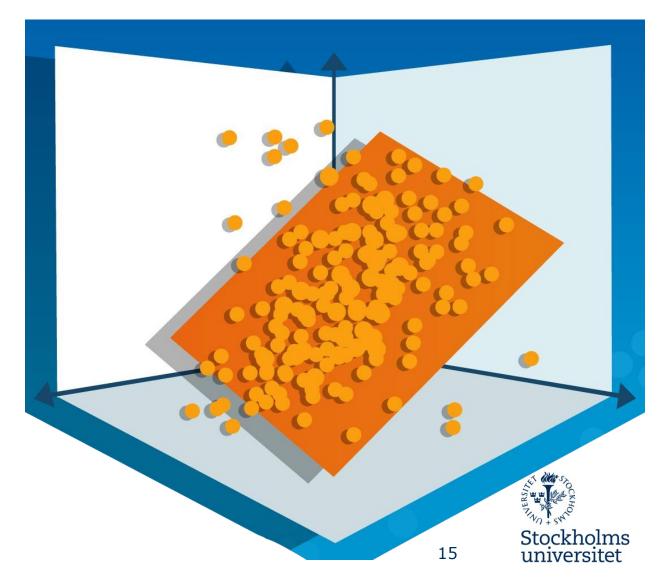
- clarify relationships among variables
- clarify relationships among objects

• When:

significant correlations exist among variables

How:

- define new axes (components)
- examine correlation between axes and variables
- find scores of objects on new axes



Philosophy of PCA

• We typically have a data matrix of *M* observations on *N* correlated variables

$$x = x_1, x_2, ..., x_N$$

- PCA looks for a transformation of x_i into N new variables $y = b_1, b_2, ..., b_N$ that are uncorrelated
- Dimensionality reduction implies information loss
- PCA preserves as much information as possible, that is, it minimizes the error
 ||x-y||

PCA: output

• New variables b_i that are linear combination of the original variables (x_i) :

$$b_i = u_{i1}x_1 + u_{i2}x_2 + ... u_{iN}x_N$$
, $i=1...N$

- The new variables b_i are derived in decreasing order of importance
- They are called "Principal Components"



PCA: more formally

```
From N original variables: x_1, x_2, ..., x_N:

Produce N new variables: b_1, b_2, ..., b_N:

b_1 = u_{11}x_1 + u_{12}x_2 + ... + u_{1N}x_N
b_2 = u_{21}x_1 + u_{22}x_2 + ... + u_{2N}x_N
```

$$b_{\rm N} = u_{\rm N1} x_1 + u_{\rm N2} x_2 + ... + u_{\rm NN} x_{\rm N}$$

such that:

 u_N 's are uncorrelated (orthogonal)

 u_1 explains as much as possible of the original variance in the data set u_2 explains as much as possible of the remaining variance

• • •



PCA: Covariance Matrix

Question: How should we determine the "best" lower dimensional space?

Answer:

The "best" low-dimensional space can be determined by the "best" eigenvectors of the covariance matrix of the data (i.e., the eigenvectors corresponding to the "largest" eigenvalues – also called "Principal components")



PCA: Covariance Matrix

$$\mathbf{X} = \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix}$$

$$cov(X_i, X_j) = E[(X_i - \mu_i)(X_j - \mu_j)]$$

$$\Sigma = \begin{bmatrix} E[(X_1 - \mu_1)(X_1 - \mu_1)] & E[(X_1 - \mu_1)(X_2 - \mu_2)] & \cdots & E[(X_1 - \mu_1)(X_n - \mu_n)] \\ E[(X_2 - \mu_2)(X_1 - \mu_1)] & E[(X_2 - \mu_2)(X_2 - \mu_2)] & \cdots & E[(X_2 - \mu_2)(X_n - \mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ E[(X_n - \mu_n)(X_1 - \mu_1)] & E[(X_n - \mu_n)(X_2 - \mu_2)] & \cdots & E[(X_n - \mu_n)(X_n - \mu_n)] \end{bmatrix}.$$

$$cov(X,Y) = \frac{1}{n} \sum_{i=1}^{n} (x_i - E(X))(y_i - E(Y))$$



Eigenvectors

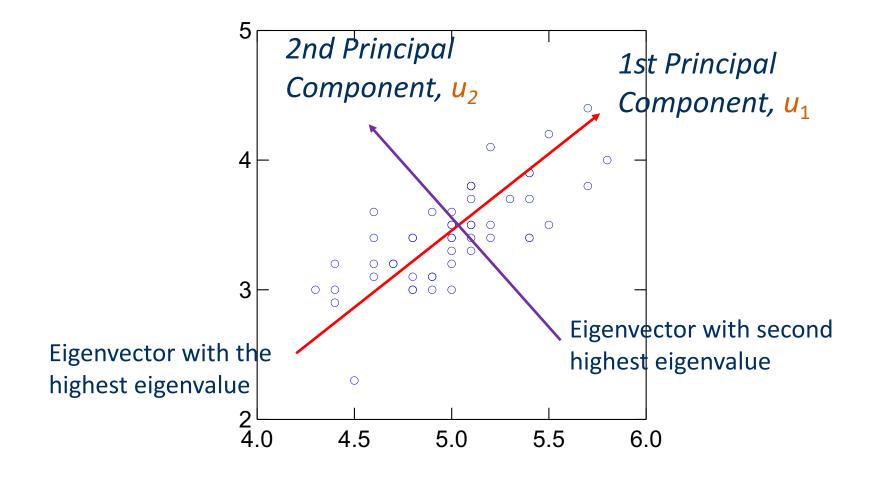
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\{u_{11}, u_{12}, ..., u_{1N}\}: 1<sup>st</sup> eigenvector of the covariance matrix, and coefficients of the 1<sup>st</sup> principal component
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 $\{u_{21}, u_{22}, ..., u_{2N}\}$: 2nd eigenvector of the covariance matrix, and coefficients of the 2nd principal component

. . .

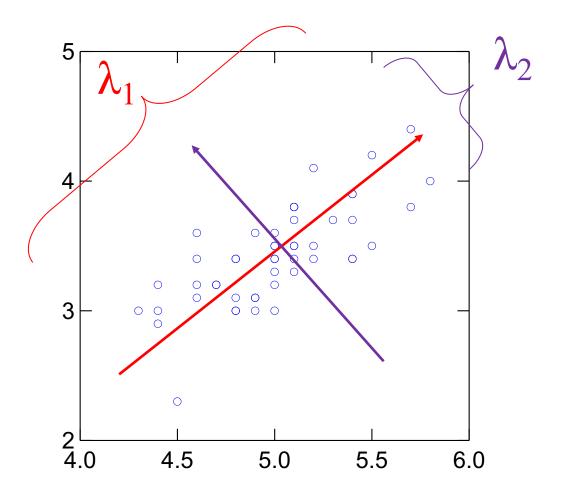
 $\{u_{N1}, u_{N2}, ..., u_{NN}\}$: N^{th} eigenvector of the covariance matrix, and coefficients of the N^{th} principal component

Singular Value Decomposition (SVD)



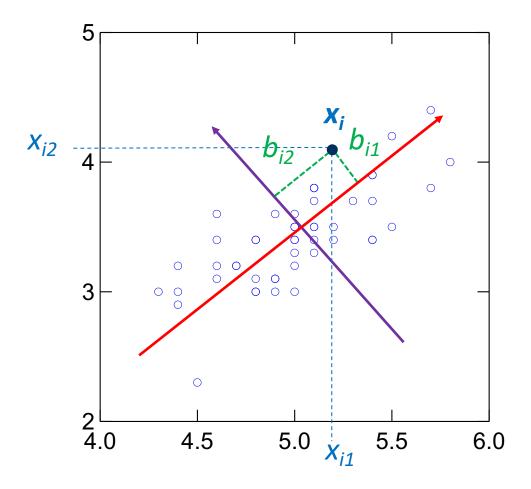


PCA Eigenvalues





PCA Scores



PCA Steps

Step 1:
$$\bar{x} = \frac{1}{M} \sum_{i=1}^{M} x_i$$

Step 2: subtract the mean: $\Phi_i = x_i - \bar{x}$ (i.e., center at zero)

Step 3: form the matrix $A = [\Phi_1 \ \Phi_2 \cdots \Phi_M]$ (NxM matrix), then compute:

$$C = \frac{1}{M} \sum_{n=1}^{M} \Phi_n \Phi_n^T = AA^T$$

(sample covariance matrix, NxN, characterizes the scatter of the data)

Step 4: compute the eigenvalues of $C: \lambda_1 > \lambda_2 > \cdots > \lambda_N$

Step 5: compute the eigenvectors of $C: u_1, u_2, \ldots, u_N$



PCA Steps (cont'd)

Since C is symmetric, u₁, u₂, ..., u_N form a basis, (i.e., any vector x or actually (x − x̄), can be written as a linear combination of the eigenvectors):

$$x - \bar{x} = b_1 u_1 + b_2 u_2 + \dots + b_N u_N = \sum_{i=1}^N b_i u_i$$
, where $b_i = \frac{(x - \bar{x}) \cdot u_i}{(u_i \cdot u_i)}$

Step 6: (dimensionality reduction step) keep only the terms corresponding to the K largest eigenvalues:

$$\hat{x} - \overline{x} = \sum_{i=1}^{K} b_i u_i$$
 where $K << N$

- The representation of $\hat{x} - \bar{x}$ into the basis $u_1, u_2, ..., u_K$ is thus

$$\begin{bmatrix} b_1 \\ b_2 \\ ... \\ b_K \end{bmatrix}$$



PCA: Linear Transformation

• Every object x in the original space is mapped as follows:

$$\begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_K \end{bmatrix} = \begin{bmatrix} u_1^T \\ u_2^T \\ \dots \\ u_K^T \end{bmatrix} (x - \bar{x}) = U^T (x - \bar{x})$$

Step 4: Singular Value Decomposition (SVD)*

$$\mathbf{A} = \mathbf{U} \quad \mathbf{S} \quad \mathbf{V}^{\mathrm{T}} = \begin{bmatrix} \mathbf{u}_{1} & \mathbf{u}_{2} & \cdots & \mathbf{u}_{r} \end{bmatrix} \begin{bmatrix} \lambda_{1} & & & \\ & \lambda_{2} & & \\ & & \ddots & \\ & & & \lambda_{r} \end{bmatrix} \begin{bmatrix} \mathbf{v}_{1} & \\ & \mathbf{v}_{2} & \\ \vdots & \\ & & \mathbf{v}_{r} \end{bmatrix}$$

- r: rank of matrix A
- $\lambda_1 \ge \lambda_2 \ge ... \ge \lambda_r$: singular values (square roots of eig-values AA^T , A^TA)
- $\vec{u}_1, \vec{u}_2, \dots, \vec{u}_r$: left singular vectors (eig-vectors of AA^T)
- $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_r$: right singular vectors (eig-vectors of A^TA)

$$A = \lambda_1 \vec{\mathbf{u}}_1 \vec{\mathbf{v}}_1^{\mathrm{T}} + \lambda_2 \vec{\mathbf{u}}_2 \vec{\mathbf{v}}_2^{\mathrm{T}} + \dots + \lambda_r \vec{\mathbf{u}}_r \vec{\mathbf{v}}_r^{\mathrm{T}}$$



• Initial matrix:

$$A = \left[\begin{array}{rrr} 3 & 1 & 1 \\ -1 & 3 & 1 \end{array} \right]$$

Transpose:

$$A^T = \begin{bmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix}$$

• Then compute:

$$AA^{T} = \begin{bmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{bmatrix} \begin{bmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 11 & 1 \\ 1 & 11 \end{bmatrix}$$

Find the eigenvectors and eigenvalues!

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• Matrix:

$$AA^{T} = \begin{bmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{bmatrix} \begin{bmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 11 & 1 \\ 1 & 11 \end{bmatrix}$$

• Finding eigenvectors and eigenvalues:

$$\left[\begin{array}{cc} 11 & 1 \\ 1 & 11 \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \end{array}\right] = \lambda \left[\begin{array}{c} x_1 \\ x_2 \end{array}\right]$$

• Solve the above system of equations!

System of equations:

$$\left[\begin{array}{cc} 11 & 1 \\ 1 & 11 \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \end{array}\right] = \lambda \left[\begin{array}{c} x_1 \\ x_2 \end{array}\right]$$

• After solving it, we get:

$$\left[\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array}\right]$$

• After normalizing:

$$U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$$



In a similar way we get V:

$$V^{T} = \begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} & \frac{-5}{\sqrt{30}} \end{bmatrix}$$

We have also recorded the eigenvalues of U and V (they are the same!)

$$S = \left[\begin{array}{ccc} \sqrt{12} & 0 & 0 \\ 0 & \sqrt{10} & 0 \end{array} \right]$$

So finally, we have:

$$A_{mn} = U_{mm} S_{mn} V_{nn}^{T} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \sqrt{12} & 0 & 0 \\ 0 & \sqrt{10} & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} & \frac{-5}{\sqrt{30}} \end{bmatrix} = \begin{bmatrix} \frac{\sqrt{12}}{\sqrt{2}} & \frac{\sqrt{10}}{\sqrt{2}} & 0 \\ \frac{\sqrt{12}}{\sqrt{2}} & \frac{-\sqrt{10}}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{20}} & \frac{2}{\sqrt{20}} & \frac{-5}{\sqrt{20}} \end{bmatrix} = \begin{bmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{bmatrix}$$

More about SVD:

https://datajobs.com/data-science-repo/SVD-Tutorial-%5BKirk-Baker%5D.pdf



How to choose K?

• Choose **K** using the following criterion:

$$\frac{\sum_{i=1}^{K} \lambda_i}{\sum_{i=1}^{N} \lambda_i} > Threshold \text{ (e.g., 0.9 or 0.95)}$$

• In this case, we say that we "preserve" 90% or 95% of the information in the data

• If K=N, then we "preserve" 100% of the information in the data

Normalization

- The principal components are dependent on the units used to measure the original variables as well as on the range of values they assume
- Data should always be normalized prior to using PCA
- A common normalization method is to transform all the data to have zero mean and unit standard deviation:

$$\frac{x_i - \mu}{\sigma}$$

(μ and σ are the mean and standard deviation of x_i 's)



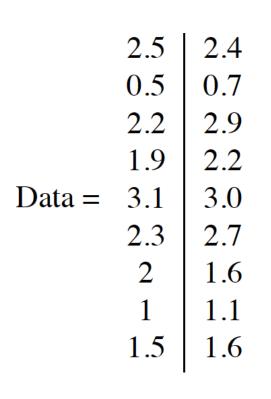
PCA Summary

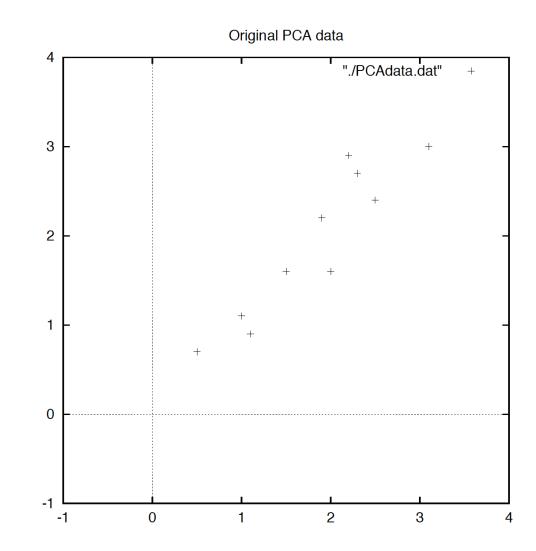
Rotates a multivariate dataset into a new configuration which is easier to interpret

• Purpose:

- simplify data
- look at relationships between variables
- identify patterns in the correlated variables









• Subtract the mean (can also divide by standard deviation)

_	$\boldsymbol{\mathcal{X}}$	У		\mathcal{X}	У
-	2.5	2.4		.69	.49
	0.5	0.7		-1.31	-1.21
	2.2	2.9		.39	.99
	1.9	2.2		.09	.29
Data =	3.1	3.0	DataAdjust =	1.29	1.09
	2.3	2.7		.49	.79
	2	1.6		.19	31
	1	1.1		81	81
	1.5	1.6		31	31
	1.1	0.9		71	-1.01



• Compute the covariance matrix:

$$cov = \begin{pmatrix} .616555556 & .615444444 \\ .615444444 & .716555556 \end{pmatrix}$$

Compute the eigenvalues and eigenvectors:

$$eigenvalues = \begin{pmatrix} .0490833989 \\ 1.28402771 \end{pmatrix}$$

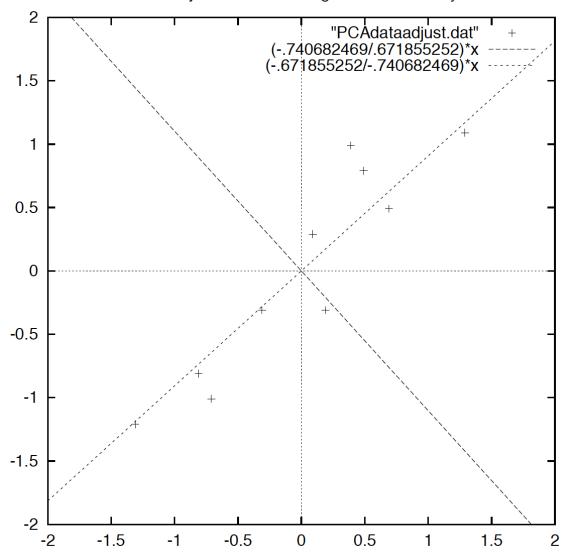
$$eigenvectors = \begin{pmatrix} -.735178656 & -.677873399 \\ .677873399 & -.735178656 \end{pmatrix}$$



Plot

$$\begin{pmatrix} -.735178656 & -.677873399 \ .677873399 & -.735178656 \end{pmatrix}$$

Mean adjusted data with eigenvectors overlayed





Choose eigenvectors from:

$$FeatureVector = (eig_1 \ eig_2 \ eig_3 \ \ eig_n)$$

Choose both eigenvectors:

$$\begin{pmatrix} -.677873399 & -.735178656 \\ -.735178656 & .677873399 \end{pmatrix}$$

• Or just the first:

$$\begin{pmatrix} -.677873399 \\ -.735178656 \end{pmatrix}$$

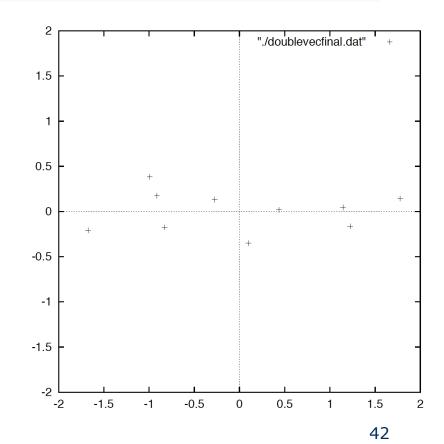


Derive the final data:

 $FinalData = RowFeatureVector \times RowDataAdjust$

Hence, using both eigenvectors:

_	x	y
	827970186	175115307
	1.77758033	.142857227
	992197494	.384374989
	274210416	.130417207
Transformed Data=	-1.67580142	209498461
	912949103	.175282444
	.0991094375	349824698
	1.14457216	.0464172582
	.438046137	.0177646297
	1.22382056	162675287





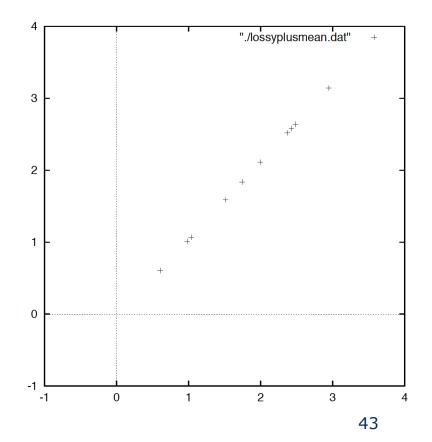
Derive the final data:

 $FinalData = RowFeatureVector \times RowDataAdjust$

And using one eigenvector:

Transformed Data (Single eigenvector)

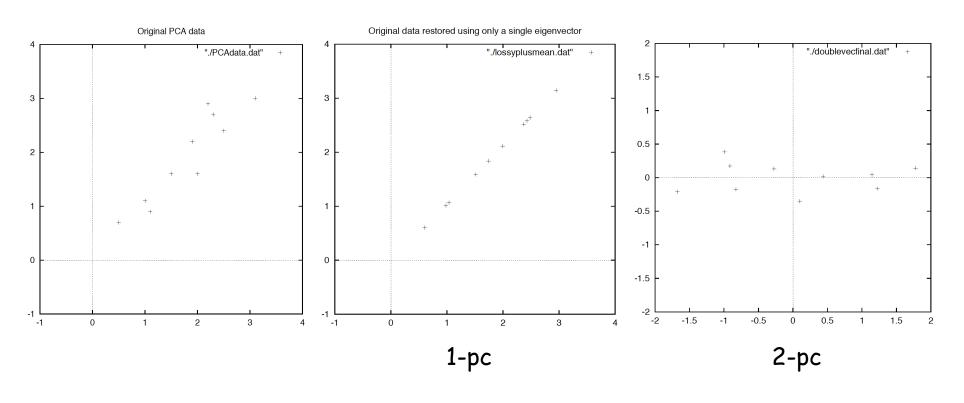
x
827970186
1.77758033
992197494
274210416
-1.67580142
912949103
.0991094375
1.14457216
.438046137
1.22382056





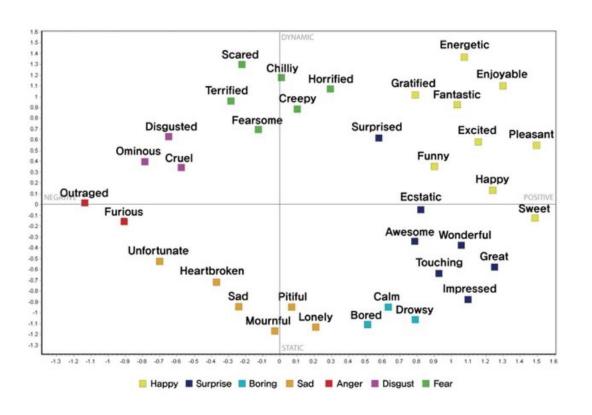
Getting back the original data:

 $RowOriginalData = (RowFeatureVector^T \times FinalData) + OriginalMean$





Multi-Dimensional Scaling (MDS)



- So far, we assumed that we know both data points X and distance matrix D between these points
- What if the original points X are not known but only distance matrix D is known?
- Can we reconstruct X or some approximation of X?

Problem

- Given distance matrix D between n points
- Find a k-dimensional representation of every x_i point i
- So that d(x_i,x_i) is as close as possible to D(i,j)

Why do we want to do that?

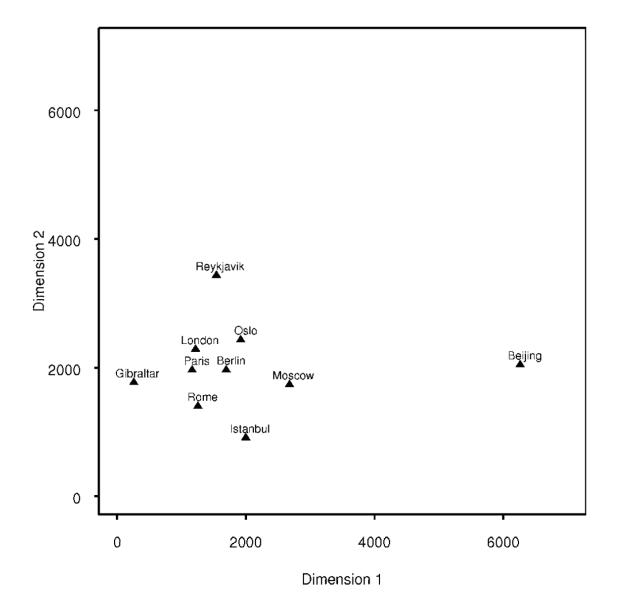


Distances between 10 cities

	London	Berlin	Oslo	Moscow	Paris	Rome	Beijing	Istanbul	Gibraltar	Reykjavik
London	_									
Berlin	570	_								
Oslo	710	520	_							
Moscow	1550	1000	1020	_						
Paris	210	540	830	1540	_					
Rome	890	730	1240	1470	680	_				
Beijing	5050	4570	4360	3600	5100	5050	_			
Istanbul	1550	1080	1520	1090	1040	850	4380	_		
Gibraltar	1090	1450	1790	2410	960	1030	6010	1870	_	
Reykjavik	1170	1480	1080	2060	1380	2040	4900	2560	2050	_



Distances between 10 cities





Financial Indicators of Countries

Country	Increase	Life	IMR	TFR	GDP
Albania	1.2	69.2	30	2.9	659.91
Argentina	1.2	68.6	24	2.8	4343.04
Australia	1.1	74.7	7	1.9	17529.98
Austria	1.0	73.0	7	1.5	20561.88
Benin	3.2	45.9	86	7.1	398.21
Bolivia	2.4	57.7	75	4.8	812.19
Brazil	1.5	64.0	58	2.9	3219.22
Cambodia	2.8	50.1	116	5.3	97.39
China	1.1	66.7	44	2.0	341.31
Colombia	1.7	66.4	37	2.7	1246.87
Croatia	-1.5	67.1	9	1.7	5400.66
El Salvador	2.2	63.9	46	4.0	988.58
France	0.4	73.0	7	1.7	21076.77
Greece	0.6	75.0	10	1.4	6501.23
Guatemala	2.9	62.4	48	5.4	831.81
Iran	2.3	67.0	36	5.0	9129.34
Italy	-0.2	74.2	8	1.3	19204.92
Malawi	3.3	45.0	143	7.2	229.01
Netherlands	0.7	74.4	7	1.6	18961.90
Pakistan	3.1	60.6	91	6.2	385.59
Papua New Guinea	1.9	55.2	68	5.1	839.03
Peru	1.7	64.1	64	3.4	1674.15
Romania	-0.5	66.6	23	1.5	1647.97
USA	1.1	72.5	9	2.1	21965.08
Zimbabwe	4.4	52.4	67	5.0	686.75



Financial Indicators of Countries: First coordinate

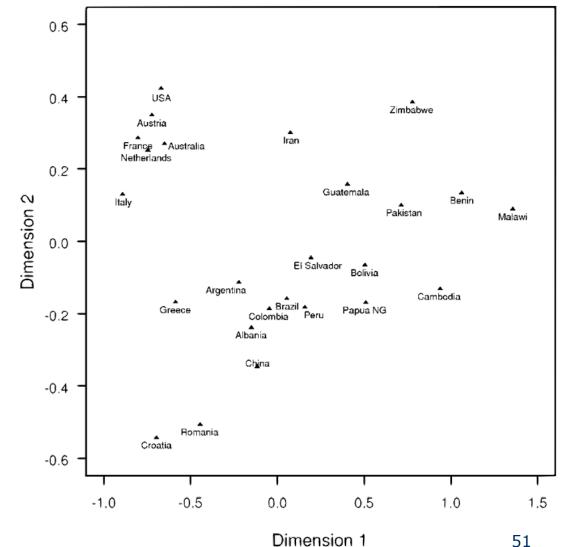
Dim1: Measure of overall development

Malawi	-2.027
Benin	-1.616
Cambodia	-1.414
Zimbabwe	-1.302
Pakistan	-1.133
Bolivia	-0.798
Papua New Guinea	-0.783
Guatemala	-0.706
El Salvador	-0.344
Peru	-0.277
Iran	-0.167
Brazil	-0.112
Colombia	0.036
China	0.188
Albania	0.220
Argentina	0.327
Romania	0.786
Greece	0.921
Australia	1.049
USA	1.105
Netherlands	1.158
Austria	1.164
Croatia	1.167
France	1.230



Financial Indicators of Countries: Two coordinates







How can we do that? (Algorithm)

```
Irror_mod.use_z = False
        od.use_y = False
_operation == "MIRROR_Y"
Irror_mod.use_x = False
lrror_mod.use_y = True
lrror_mod.use_z = False
 operation == "MIRROR Z"
 _rror_mod.use_x = False
lrror_mod.use_y = False
 lrror_mod.use_z = True
 selection at the end -add
  ob.select= 1
  er ob.select=1
  ntext.scene.objects.action
 "Selected" + str(modified
  irror ob.select = 0
 bpy.context.selected_obj
 ata.objects[one.name].sel
int("please select exaction
OPERATOR CLASSES ----
```

High-level view of the MDS algorithm

- Randomly initialize the positions of n points in a k-dimensional space
- Compute pairwise distances D' for this placement
- Compare D' to D
- Move points to adjust their pairwise distances better (make D' closer to D)
- Repeat until D' is close to D



The MDS algorithm

- Input: nxn distance matrix D
- Random n points in the k-dimensional space $(x_1,...,x_n)$
- stop = false
- while not stop
 - totalerror = 0.0
 - For every pair of points i,j compute
 - $D'(i,j)=d(x_i,x_i)$
 - error = (D(i,j) D'(i,j)) / D(i,j)
 - totalerror +=error
 - $x_i = ((x_i x_i) / D'(i,j)) * error$
 - If totalerror small enough, stop = true



Questions about MDS

- Running time of the MDS algorithm
 - O(n²I), where I is the number of iterations of the algorithm
- MDS does not guarantee that the metric property is maintained in D'
- Faster? Guarantee of metric property?



Today...

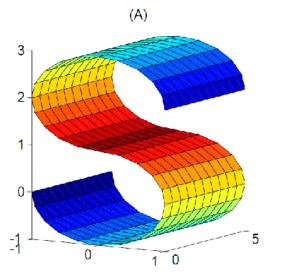
What is the Curse of Dimensionality?

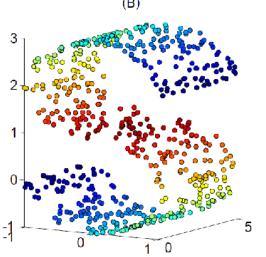
The importance of efficient **Data Representation**

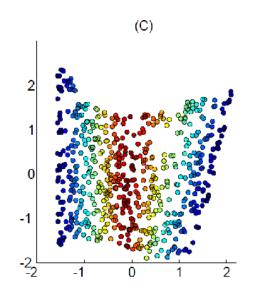
How do we reduce Data Dimensionality?

What is the **PCA** algorithm?

What is the MDS algorithm?









TODOs



Reading:

Main course book: Chapter 6

(Sec. 6.1, 6.3, 6.5)



Lab 1

Recommended to complete the lab before the end of the week



Quiz 1



Coming up next

