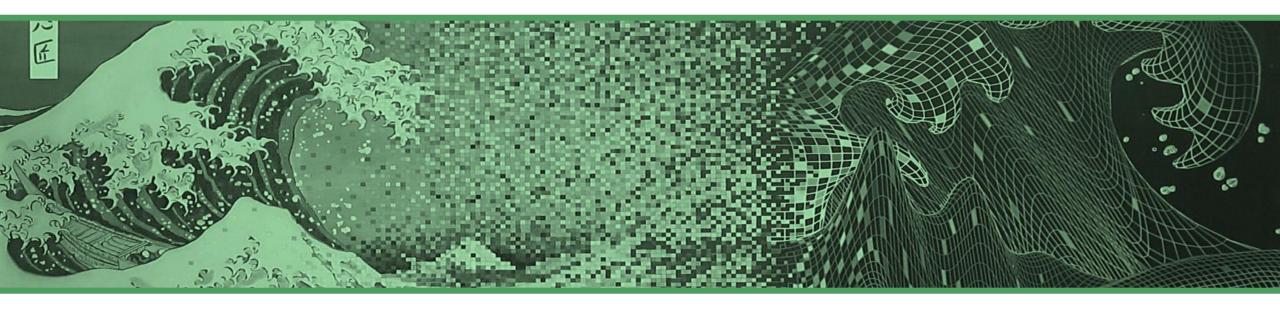


Dimensionality reduction

Feature selection and PCA transformations



Outline



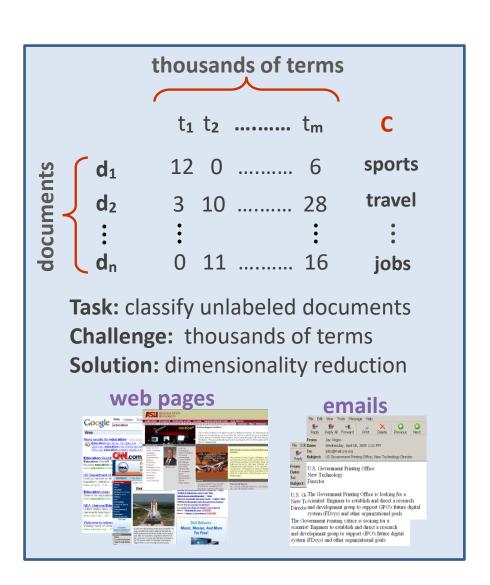
- High-dimensional data
- Feature selection
- Feature extraction
 - algebra essentials: eigenvalues and eigenvectors
 - KL transform
 - principal component analysis
 - additional notes
 - linear discriminant analysis
 - pseudoinverse
 - alternative approaches to dim reduction

Motivation

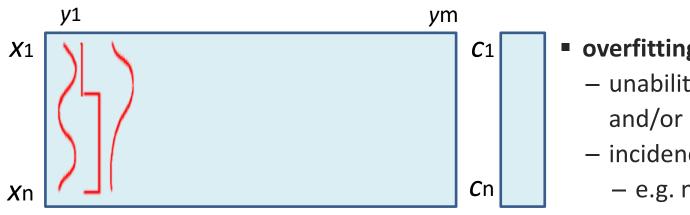
- At a first glimpse, increasing the number of variables should lead to better performance...
- In practice, the inclusion of more features can degrade performance (curse of dimensionality)
 - challenges: learning complexity and generalization difficulty (over/underfitting)
 - common definition of **high-dimensionality**: $|Y| \gg |X|$ (i.e. $m \gg n$)
- The number of training observations required increases **exponentially** with dimensionality
- How then can we learn in high-dimensional data spaces with a limited number of observations?
 - revise the learning approach
 - example: adequate distances in high-dimensional data spaces for lazy learning and clustering
 - − dimensionality reduction ←

Data domains with high-dimensionality

- biological data
 - gene expression (>20k genes)
 - molecular concentrations (metabolites, proteins...)
- text and web content data
- social behavioral data
- healthcare data (clinical records)
- consumer data
- signal, audio, image and video data

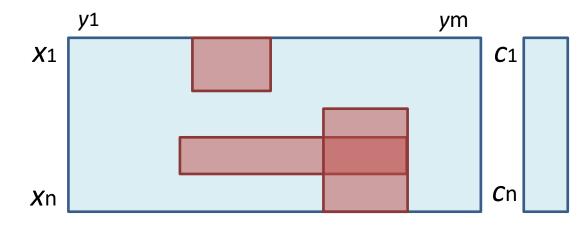


Generalization: overfitting and underfitting risks



overfitting

- unability to discard non-informative and/or non-discriminative regions
- incidence: global learning
 - e.g. naïve Bayes, neural networks, SVMs...



underfitting

- exclusion of informative or discriminative regions from the learning
- incidence: local learning
 - e.g. decision trees, kNN, pattern mining...

Goals of dimensionality reduction

- Guide supervised learning (focus on discriminative regions)
- Guide unsupervised learning (focus on informative regions)
- Visualization (project high-dim data into interpretable low-dim data)
- Data compression (efficient storage and retrieval)
- Noise removal (denoising data)
- Speed-up learning
- Guarantee simplicity and comprehensibility of mined results
- Map multimedia data (image and signal data) into feature-based data

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Dimensionality reduction

- Project the m-dimensional points into a k-dimensional space ($k \ll m$)
 - preserve most of relevant information or structure from data
- Solve the learning problem in low dimensions
- Two common approaches
 - feature selection ←
 - choosing a subset of all features

$$[y_1, y_2, ..., y_m] \longrightarrow [y_{i1}, y_{i2}, ..., y_{ik}]$$

- feature extraction
 - creating new features by combining existing ones

$$[y_1, y_2, ..., y_m] \longrightarrow [c_1, c_2, ..., c_k] = f([y_{i1}, y_{i2}, ..., y_{im}])$$

Feature selection

- as a *filter*: measure feature importance and select top-k features or above importance threshold
 - unsupervised settings
 - categorical features with high entropy
 - numeric features with high variability
 - supervised setting
 - classification, e.g. features with high information gain
 - regression, e.g. features with high correlation
 - check our former class on univariate data stances!
- as a wrapper: assess learning performance with varying subsets of features
 - simplest way: to measure feature importance and test models on top-k features with varying k

Feature selection

Example

- entropy of a variable
- variable-conditional entropy
- information gain

$$H(y_j) = -\sum_{v \in y_j} P(v) \log_2 P(v)$$

$$H(z|y_j) = \sum_{v \in y_j} P(v)E(z|v)$$

$$IG(z|y_j) = H(z) - H(z|y_j)$$

	Hair	Height	Weight	Lotion	Result
i_1	1	2	1	0	1
i_2	1	3	2	1	0
i_3	2	1	2	1	0
i_4	1	1	2	0	1
i_5	3	2	3	0	1
i_6	2	3	3	0	0
i_7	2	2	3	0	0
i_8	1	1	1	1	0

$$rank(hair) = IG(result|hair) = 0.45$$

$$rank(height) = IG(result|height) = 0.26$$

hair variable has higher IG than height, hence is more important and less susceptible to removal

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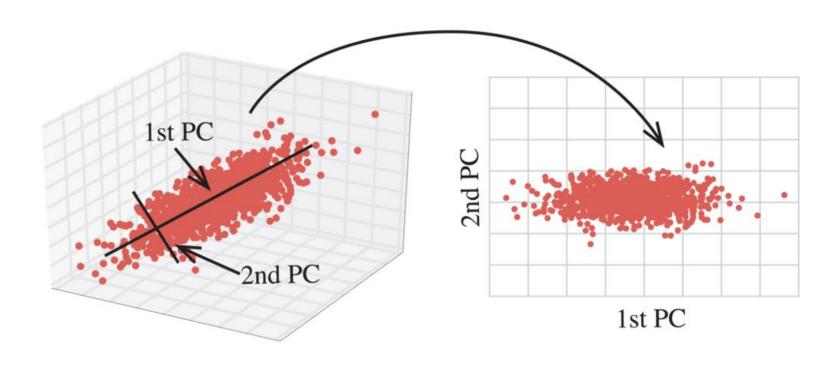
- feature extraction ←
 - creating new features by combining existing ones

$$[y_1, y_2, ..., y_m] \longrightarrow [c_1, c_2, ..., ck] = f([y_{i1}, y_{i2}, ..., y_{im}])$$

Feature extraction

- Find combinations of features that explain data
 - simple to compute and analytically tractable
- Classical approaches aim at finding a linear transformation
 - Goal: reduction that preserves as much information in data as possible (in a least-squares sense)
 - Principal Component Analysis (PCA)
- Simple extensions available to:
 - handle **non-linearity** (*kernel* trick)
 - sensitivity to targets (ensure new features yield discriminative power)
 - Goal: reduction that best separates the data (in a least-squares sense)
 - Linear Discriminant Analysis (LDA)

Space transformation



Axes of greater variance given by eigenvectors of covariance matrix

Covariance

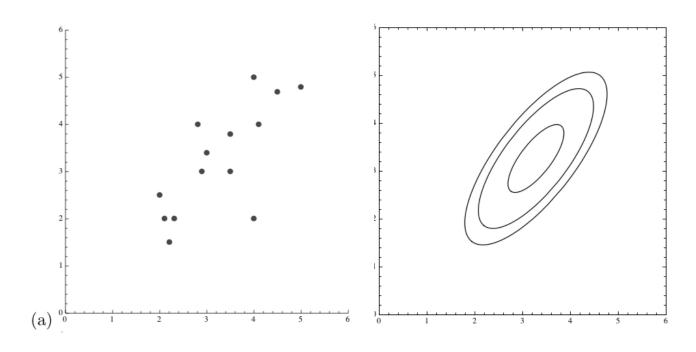
- The covariance matrix measures the tendency of two features, y_i and y_i , to vary in the same direction
 - covariance matrix C is symmetric and positive-definite
 - when normalizing covariance by their variances we obtain a correlation in [-1,1]
- Remember
 - sample covariance: n-1 in the denominator (Bessel's correction)

$$cov(y_1, y_2) = \frac{\sum_{i=1}^{n} (x_{1i} - \overline{y_1}) \cdot (x_{2i} - \overline{y_2})}{n-1}$$

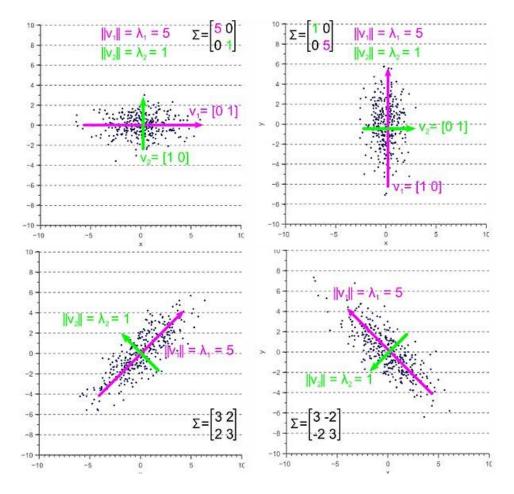
- whole population: n is the denominator

$$cov(y_1, y_2) = \frac{\sum_{i=1}^{n} (x_{1i} - \overline{y_1}) \cdot (x_{2i} - \overline{y_2})}{n}$$

Covariance



the covariance matrix of the data points defines the ellipses of equiprobability (defined by eigenvectors \mathbf{v} and eigenvalues λ)



Eigenvalues and eigenvectors

- Let C be a $m \times m$ covariance matrix
- Vectors v having same direction as Cv are called <u>eigenvectors</u>
 - eigenvectors define the linear composition of variables
- In the equation $C\mathbf{v} = \lambda \mathbf{v}$, λ is called an <u>eigenvalue</u> of A
- Example:

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 12 \\ 8 \end{pmatrix} = 4 \begin{pmatrix} 3 \\ 2 \end{pmatrix}$$

$$\mathbf{v}=[3\ 2]^T$$
 and $\lambda=4$ meaning that data is described by $y_{new}=3y_1+2y_2$

Eigenvalues and eigenvectors

- $C\mathbf{v} = \lambda \mathbf{v} \Leftrightarrow (C \lambda I)\mathbf{v} = 0$
- Given A, how to calculate \mathbf{v} and λ :
 - determine roots to $det(C \lambda I) = 0$, roots are eigenvalues λ
 - solve $(C \lambda I)\mathbf{v} = 0$ for each λ to obtain eigenvectors \mathbf{v}

	y_1	y_2	(0 0 0)	c_1
-	-5.1	9.25	$C = \begin{pmatrix} 2 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}$	-0.8
1	14.9	20.25	(0.8 0.6)	21.9
	5.9	33.25	Eigenvectors and eigenvalues:	19
	5.9	-30.75	\mathbf{v}_1 =[0.91, 0.41], λ_1 =2.36	-7.2
			\mathbf{v}_2 =[-0.41, 0.91], λ_2 =0.23	
-	-9.1	-10.75		-12.7
-	-9.1	-21.75	(x_{i1})	-17.2
	5.9	19.25	$\mathbf{x}_i = (0.91 0.41) \begin{pmatrix} x_{i1} \\ x_{i2} \end{pmatrix}$	13.3

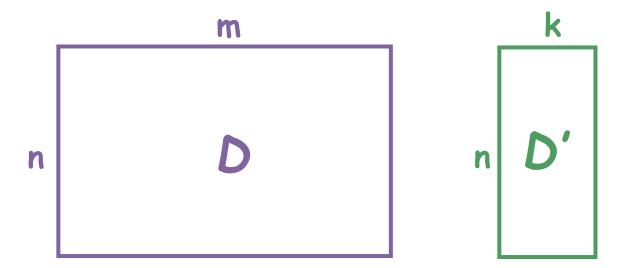
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Dimensionality reduction

■ Map data with *m* variables into *k* variables without significant loss



- *Residual variation*: information in *D* not retained in *D*'
- Trade-off: *k*-dimensionality and interpretability *versus* information loss
 - the semantics of the variables are degraded in the reduced dataset D'

The Karhunen-Loève transform

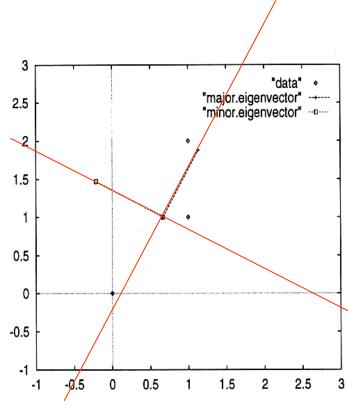
- Intuition: find the axis that shows the greatest variation and rotate that into this axis
- The Karhunen-Loève (KL) transform is a linear transform that maps possibly correlated variables into a set of values of linearly uncorrelated variables
 - centering data and computing covariance matrix
 - eigenvectors that minimize sum of square differences

$$D = \begin{bmatrix} 1 & 2 \\ 1 & 1 \\ 0 & 0 \end{bmatrix}$$

$$D_{centered} = \begin{bmatrix} 1/3 & 1 \\ 1/3 & 0 \\ -2/3 & -1 \end{bmatrix} \text{ and } C = \begin{bmatrix} 2/3 & 1 \\ 1 & 2 \end{bmatrix}$$

$$\lambda_1 = 2.53 \quad \mathbf{v}_1 = \begin{bmatrix} 0.47 \\ 0.88 \end{bmatrix}$$

$$\lambda_2 = 0.13 \quad \mathbf{v}_2 = \begin{bmatrix} -0.88 \\ 0.47 \end{bmatrix}$$

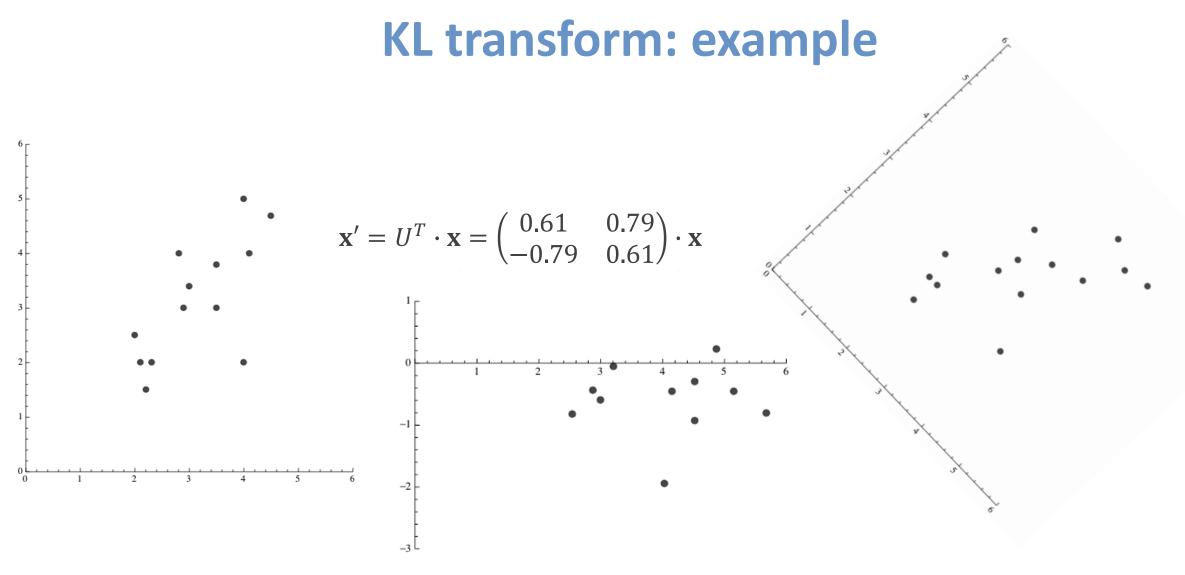


The Karhunen-Loève transform

- Transform defined by U matrix, orthonormal matrix of $m \times m$ dimension, i.e. $U^T \cdot U = I$
 - symmetric and positive definite that can be diagonalized

$$U^{-1}CU = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \dots & 0 \\ 0 & 0 & \lambda_m \end{pmatrix}$$

- there are m eigenvalues and eigenvectors, $C\mathbf{v}_i = \lambda_i \mathbf{v}_i$
- lacktriangle The normalized eigenvectors define the orthonormal matrix U of dimension m imes m
 - each normalized eigenvector is a column
 - U defines the KL transform
 - KL transform rotates the coordinate system $\mathbf{x}' = U^T \cdot \mathbf{x}$



It rotates the system (the points) in such a way hat the new covariance matrix will be diagonal

KL transform: example

• Considering
$$D = \{(1,1), (2,2), (3,3), (4,4), (5,5), (6,6)\}$$

- the covariance matrix is
$$C = \begin{pmatrix} 3.5 & 3.5 \\ 3.5 & 3.5 \end{pmatrix}$$

– the two eigenvalues are
$$\lambda_1 = 7$$
, $\lambda_2 = 0$

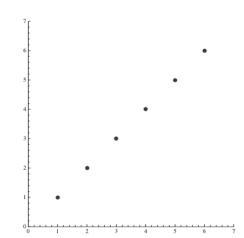
- the two eigenvectors are
$$\mathbf{u}_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$
, $\mathbf{u}_2 = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$

the matrix that describes the KL transform

The equation
$$\lambda_1 = 7$$
, $\lambda_2 = 0$ and $\lambda_1 = 7$, $\lambda_2 = 0$ and $\lambda_2 = 0$ and $\lambda_3 = 0$ and $\lambda_4 = 0$ and $\lambda_$

- let us transform the first observation
$$\begin{pmatrix} \sqrt{2} \\ 0 \end{pmatrix} = \begin{pmatrix} \sqrt{2} \cdot \frac{1+1}{2} \\ \sqrt{2} \cdot \frac{1-1}{2} \end{pmatrix} = \sqrt{2} \cdot \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

1.0 transformed data space 0.5-0.5

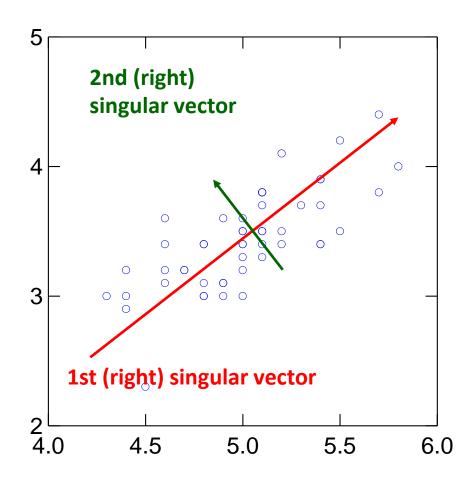


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Singular value decomposition



1st singular vector:

direction of maximal variance λ_1 : how much of the data variance is explained by 1st vector

2nd singular vector:

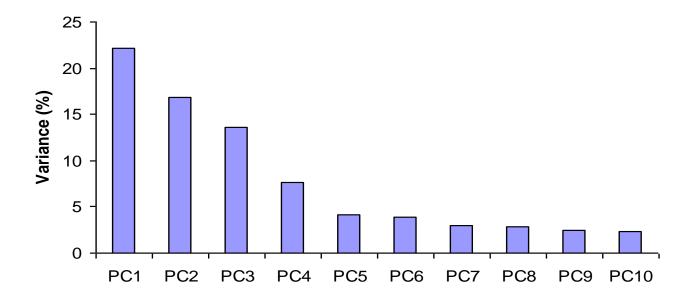
direction of maximal variance, after removing projection of 1^{st} vector λ_2 : how much of the data variance is explained by the 2^{nd} vector

•••

mth singular vector ...
(until variance below threshold)

Principal components

- PCA is SVD done on centered data (singular vector/value = eigenvector/value)
- First component (PC1): highest eigenvalue (direction with greatest variation)
- Second component (PC2): direction with max variation orthogonal to PC1
- In general: only few directions needed to capture most data variability



Principal component analysis

- PCA projects data along the directions where the data varies most
- These directions are determined by the eigenvectors corresponding to the largest eigenvalues (magnitude defines the direction's variance)
 - reduction can imply information loss
 - SVD/PCA preserve as much information as possible by minimizing the reconstruction error
- Components (summary variables)
 - linear combinations of the original variables
 - uncorrelated with each other
 - the largest eigenvalues are called *principal components*
 - the squares of the eigenvalues represent the variances along the eigenvectors

Principal component analysis

- The variance in the direction of the k^{th} singular vector (or principal component) is given by the singular value $\lambda_{\mathbf{k}}$
 - singular values can be used to estimate how many components to keep
 - rule of thumb: keep enough to explain 85% of the variation

$$\frac{\sum_{j=1}^{k} \lambda_j}{\sum_{j=1}^{n} \lambda_j} \approx 0.85$$

if k = m, we preserve 100% of the original variation

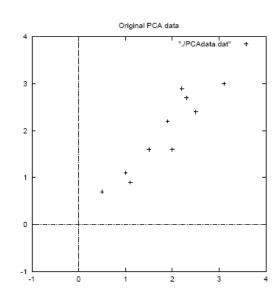
- Eigenvector v weights input variables to compose a new component c
 - these absolute weights provide a view on the relevance of each input variable for component ${f c}$

Principal component analysis

Revising how

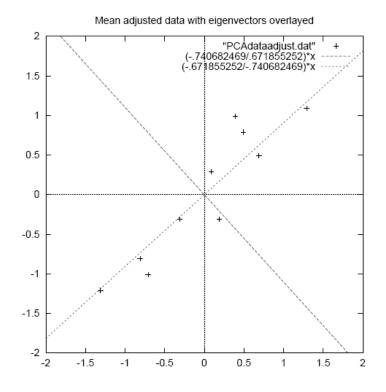
- 1. Compute the covariance matrix $m \times m$ (scatter of data)
- 2. Compute eigenvalues, $\lambda_1 \ge \lambda_2 \ge ... \ge \lambda_m$, and eigenvectors, $v_1, v_2, ... v_m$
- 3. Keep the large k eigenvalues ($k \le m$) and construct the transformed space
- 4. Transform the dataset $D \rightarrow D'$

Exercise: apply PCA on the following dataset



Optionally center data (removing mean)

Dataset D		Centere	d dataset D
$\mathbf{y_1}$	\mathbf{y}_2	y_1	$\mathbf{y_2}$
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
3.1	3.0	1.29	1.09
2.3	2.7	.49	.79
2	1.6	.19	-0.31
1	1.1	-0.81	-0.81
1.5	1.6	-0.31	-0.31
1.1	0.9	-0.71	-1.01
mean 1.81	1.91	mean 0	0



1. Calculate the **covariance matrix**:

$$cov = \begin{pmatrix} y_1 & y_2 \\ .616555556 & .615444444 \\ .615444444 & .716555556 \end{pmatrix} y_2$$

2. Calculate its (unit) eigenvectors and eigenvalues

$$eigenvalues = \begin{pmatrix} 0.049 \\ 1.284 \end{pmatrix}, \qquad eigenvectors = \begin{pmatrix} -0.735 & -0.678 \\ 0.678 & -0.735 \end{pmatrix}$$

3. Order eigenvectors by eigenvalue, highest to lowest and select top p

$$\mathbf{v}_1 = \begin{pmatrix} -0.6779 \\ -0.7352 \end{pmatrix}$$
 $\lambda_1 = 1.284$ $\mathbf{v}_2 = \begin{pmatrix} -0.7352 \\ 0.6779 \end{pmatrix}$ $\lambda_2 = .0491$

... and construct the transformed feature vector

$$FeatureVector(k = 2) = \begin{pmatrix} -0.6779 & -0.7352 \\ -0.7352 & 0.6779 \end{pmatrix} FeatureVector(k = 1) = \begin{pmatrix} -0.6779 \\ -0.7352 \end{pmatrix}$$

4. Derive the new data set

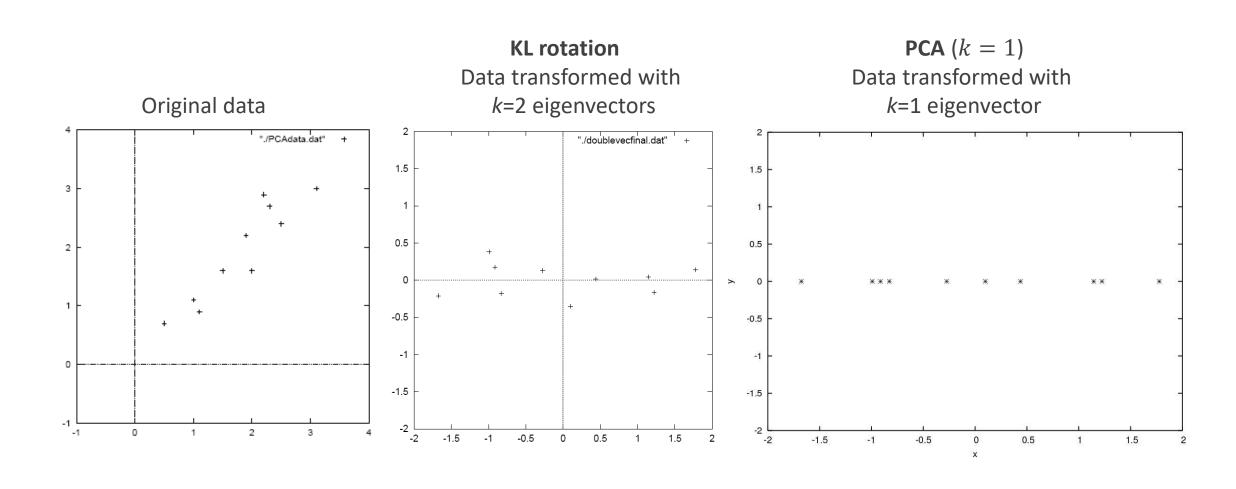
 $TransformedData = RowFeatureVector \times RowDataAdjust$

$$DataAdjusted = \begin{pmatrix} .69 & -1.31 & .39 & .09 & 1.29 & .49 & .19 & -.81 & -.31 & -.71 \\ .49 & -1.21 & .99 & .29 & 1.09 & 79 & -.31 & -.81 & -.31 & -1.01 \end{pmatrix}$$

FeatureVector
$$(p = 2)^T = \begin{pmatrix} -.6779 & -.7352 \\ -.7352 & .6779 \end{pmatrix}$$

FeatureVector
$$(p = 1)^T = (-.6779 -.7352)$$

	c_1	c_2		c_2
•	827970186	175115307	•	827970186
	1.77758033	.142857227		1.77758033
	992197494	.384374989		992197494
	274210416	.130417207		274210416
Transformed Data=	-1.67580142	209498461	Transformed Data=	-1.67580142
p = 2	912949103	.175282444	p = 1	912949103
	.0991094375	349824698	P	.0991094375
	1.14457216	16 .0464172582	1.14457216	
	.438046137	.0177646297		.438046137
	1.22382056	162675287		1.22382056



(uncovered) Reconstruction error

- There is no information loss incurred in KL rotation (k = m)
- PCA minimizes the reconstruction error: $\|\mathbf{x} \hat{\mathbf{x}}\|$
- It can be shown that the reconstruction error is: $error = 1/2 \sum_{i=k+1}^{\infty} \lambda_i$
- Example from previous slide:
 - using 2 components: recovery error = 0 (from previous slide)
 - using 1 component

DataRecovered = (FeatureVector(p=1) x TransformedData) + OriginalMean

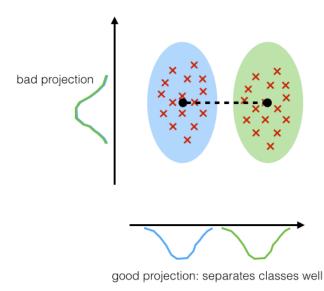
Outline



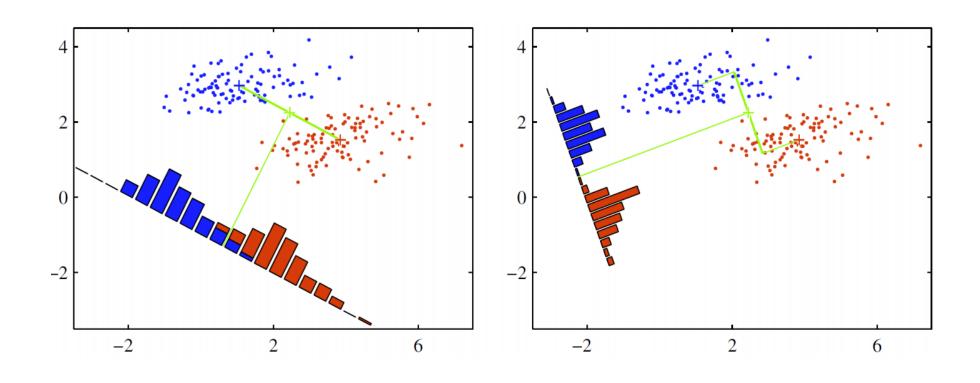
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Linear discriminant analysis (LDA)

- Challenges of PCA in supervised settings?
 - Reduction does not consider impact on the ability to discriminate output variables
- Goal: data transformation guaranteeing class separation
- Principle: pick a new dimension that
 - maximize separation between means of projected classes
 - minimize variance for the observations within each class
- Solution: LDA
 - eigenvectors based on between-class and within-class covariance matrices



Linear discriminant analysis (LDA)



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(uncovered) Pseudoinverse

- At different moments of our journey we detect the need to invert matrices
 - e.g. linear regression closed-form solution
- *Problem*: not every matrix is invertible
- Solution: compute the pseudoinverse of D, i.e. D^{\dagger} , using SVD principles
 - so that D^{\dagger} is a right inverse, i.e. $D^{\dagger}D = I$

$$D^{\dagger} = U \cdot S' \cdot V^{T}$$

$$D^{\dagger} \qquad \qquad U \qquad \qquad S \qquad \qquad V^{T}$$

$$\begin{pmatrix} x_{11} & x_{12} & x_{1n} \\ & \ddots & \\ x_{m1} & & x_{mn} \end{pmatrix} = \begin{pmatrix} u_{11} & u_{m1} \\ & \ddots \\ u_{1m} & & u_{mm} \end{pmatrix} \begin{pmatrix} \sigma_{1} & & 0 \\ & \ddots & \\ & & \ddots \\ & & & 0 \end{pmatrix} \begin{pmatrix} v_{11} & v_{1n} \\ & \ddots & \\ & v_{n1} & & v_{nn} \end{pmatrix}$$

$$m \times m \qquad m \times m \qquad m \times n \qquad n \times n$$

where U and V are orthogonal projections from D^TD and DD^T and S' are the reciprocal non-zero elements from S

(uncovered) Pseudoinverse: example

$$D = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$$

$$DD^T = \begin{pmatrix} 17 & 8 \\ 8 & 17 \end{pmatrix}$$

$$\lambda_1 = 25, \lambda_2 = 9$$

$$\mathbf{u}_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$
, $\mathbf{u}_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$

$$D^T D = \begin{pmatrix} 13 & 12 & 2 \\ 12 & 13 & -2 \\ 2 & -2 & 8 \end{pmatrix}$$

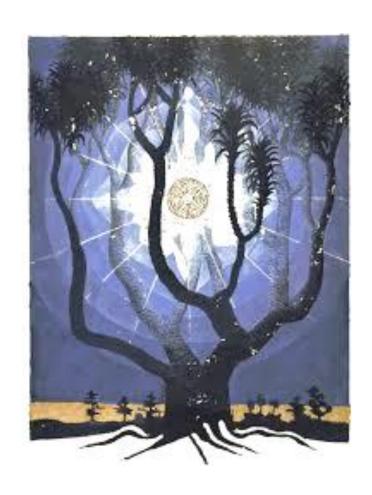
$$\lambda_1 = 25, \lambda_2 = 9, \lambda_3 = 0$$

$$\mathbf{u}_{1} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \mathbf{u}_{2} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\mathbf{v}_{1} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}, \mathbf{v}_{2} = \begin{pmatrix} \frac{1}{\sqrt{18}} \\ -\frac{1}{\sqrt{18}} \\ 4/\sqrt{18} \end{pmatrix}, \mathbf{v}_{3} = \begin{pmatrix} \frac{2}{3} \\ -\frac{2}{3} \\ -\frac{1}{3} \end{pmatrix}$$

$$D^{\dagger} = USV^{T} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{18}} & -\frac{1}{\sqrt{18}} & \frac{4}{\sqrt{18}} \\ \frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} \end{pmatrix}$$

Outline



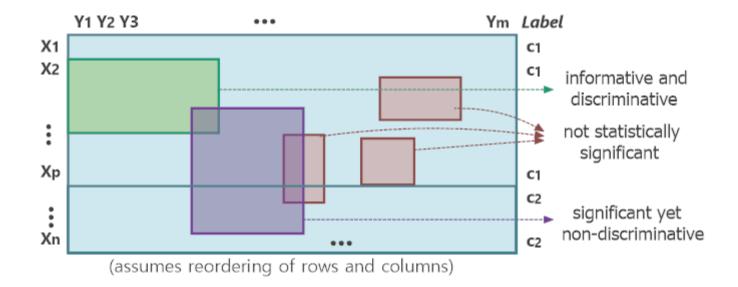
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How? Dimensionality reduction

- 1. Feature selection
- 2. Feature extraction/transformation
 - KL transformation and principal component analysis
 - linear discriminant analysis
- 3. Sparse kernels and regularization applied in parametric models to exclude non-relevant parameters
 - neural networks (excluding interactions)
 - regression approaches (sparse hyperplanes)
 - support vector machines
- 4. Subspace selection to jointly select variables and observations
 - pattern mining, decision trees and random forests
 - associative classifiers and decision tables

Alternative dimensionality reduction: subspace selection

- Addresses limitations of feature selection: single space → multiple compact spaces
- While...
 - minimizes overfitting: remove uninformative regions (focus on informative/discriminative subspaces)
 - minimizes underfitting: mine all relevant subspaces



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Summary

- High-dimensional data analysis susceptible to under- and overfitting risks
- Correlation and information theoretic measures for (un)supervised feature selection
- Feature transformation tackles limitations of feature selection
- **Eigenvalue analysis** algorithms (KL, PCA, SVD) project data into orthogonal axes where data varies the most
- Principal components: linear combination of original features
- Dimensionality can be fixed in accordance with error-tolerance (explained variability)
- Kernels can be placed to handle non-linear data
- Transformations ca be evaluated by assessing models before-and-after reduction,
 and by plotting learning curves of reconstruction error

Literature



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Thank You



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