#### **Data Analysis**

**Dimensionality Reduction** 

#### **Announcements**

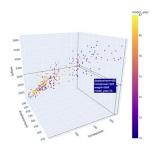
- We are almost there!
- Master Open Day tomorrow at PHS (with vlaai)
- Clinic 1 grading is half-way
- Clinic 3 is due next week Friday (remaining wildcards to be used)
- Clinics 4 and 5 are not graded but count as "bootcamps"
- Mid-course survey, fill it please 
   https://forms.gle/nUAP8Lb4WmkQ62k36
- Last lecture on Monday, March 10th, pick the content 
   https://app.wooclap.com/UMDA
- Anything else?

#### Learning goals

- Discuss and justify the need for DR
- Interpret the rationale of SVD and PCA
- Analyze the result of SVD (singular values, U and V matrices)
- Analyze the result of PCA (PCs) in context
- Select the proper dimensionality reduction (rank, dimension)
- Derive the linear transformation process of PCA
- Assess the contributions of original variables to the PCs (loadings)
- Explain the outcome of PCA in terms of variance/axis transformation
- Apply PCA to datasets for DR and/or visualization
- Design & assess matrix factorizations from an optimization perspective

#### Visualization motivation

NOTEBOOK DEMO



#### Why dimensionality reduction?

Visualization:

Understand structure of the data

Statistical:

Computational:
 Compress data → time/space efficiency

Remove redundancies

Fewer dimensions 

better generalization

(Anomaly detection, Noise removal):
 Better detection of outliers/noise

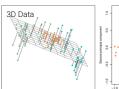
#### **High-Level Objective of Dimensionality Reduction**

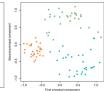
High-dimensional data might actually have a smaller **intrinsic dimension** 

<u>Dimensionality reduction</u>: take high-dimensional data (many columns) and find a smaller set of new features (columns) that approximately capture the information in the original data.

Useful for **data visualization**, **EDA** and some **modeling tasks**.

Can be framed as a matrix factorization problem.





#### Dimensionality of Data?

Consider the dataset below.
We can think of the variables (columns)
of a dataset as its dimensionality.



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No unter word

What would you call the columns space of this dataset?

A. 1-dimensional

B. 2-dimensional



#### Dimensionality of Data?

Consider the datasets shown.

Weight (Ibs)	Weight (kg)
113.0	51.3
136.5	61.9
153.0	69.4

1-dimensional

ĺ	Height (in)	eight (in) Weight (kg)		Age
I	65.8	51.3	113.0	17
I	71.5	61.9	136.5	21
ĺ	69.4	69.4	153.0	18

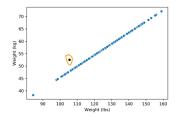


- 3-dimensional, because two weight columns are redundant.
- 😵 notice: matrix of dataset has (column) rank 3, while the dataset on the left has rank 1

#### Dimensionality - what does it mean ...?

Note that in the dataset below, I've added one outlier point to the 1d-dataset

- Just this one outlier is enough to change the rank of the matrix to 2.
- But the data is still approximately 1 dimensional!



Intrinsic Dimension of a dataset is the minimal set of dimensions needed to approximately represent the data.

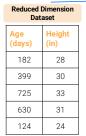
**Dimensionality reduction** is generally an **approximation of the original data**. This is often achieved through matrix factorization.

#### **Dimensionality Reduction as Matrix Factorization**

of the

(≈)

Original Dataset						
Age (days)	Height (in)	Height (ft)				
182	28	2.33				
399	30	2.5				
725	33	2.75				
630	31	2.58				
124	24	2				





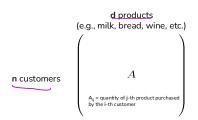
630 31

124 24

We are Keep are

One linear technique to dimensionality reduction is via matrix decomposition, which is closely tied to matrix multiplication.

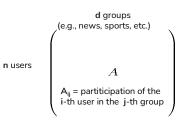
#### Market basket matrices



Find a subset of the products that characterize customer behavior

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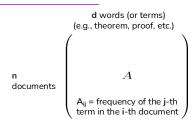
# **Social-network matrices**



Find a subset of the groups that accurately clusters social-network users

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#### **Document matrices**



Find a subset of the terms that accurately clusters the documents

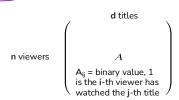
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#### **Digital images**

**d** pixels (if I order them, e.g. if image is 12x12, then |p|=144 An images pixel value of j-th pixel for image

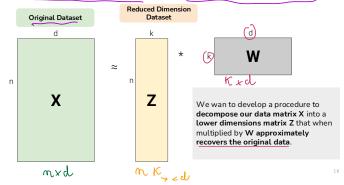
Find which pixels are more important across all images Maastricht University

#### **Netflix data**



Find a subset of the movies that accurately describe the behavior or the viewers Maastricht University

Dimensionality Reduction as Matrix Factorization

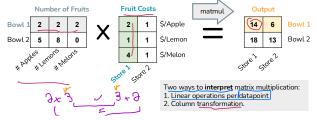


#### Interpreting Matrix multiplication

Consider the matrix multiplication example below.

- Each row of the fruits matrix represents one bowl of fruit.
  - First bowl: 2 apples, 2 lemons, 2 melons.
- Each column of the dollars matrix represents the cost of fruit at a store.

   First store: 2 dollars for an apple, 1 dollar for a lemon, 4 dollars for a melon.
- Output is the cost of each bowl at each store.



#### Matrix Decomposition (Matrix Factorization)

Transformation

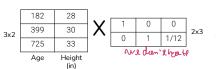
Matrix decomposition (a.k.a. Matrix

Factorization) is the opposite of matrix • multiplication, i.e. taking a matrix and decomposing it into two separate matrices.

Just like with real numbers, there are infinitely many such decompositions. 9.9 = 1.1 \* 9 = 3.3 \* 3.3 = 1 \* 9.9 = ...

Matrix sizes aren't even unique.. gethere

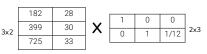
Some example factorizations:

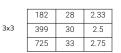


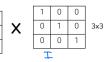
182 28 2.33 399 30 2.5 2.75

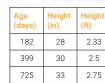
#### Matrix Decomposition: Infinite ways?

Some example factorizations:

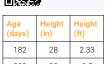




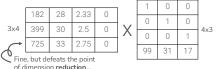




What are **possible** matrix factorizations? Select all that apply. **A.** (3x2) x (2x3) **C.** (3x1) x (1x3) **E.** (3x x) x (2x3) **D.** (3x4) x (4x3)



## Matrix Decomposition: Limited by Rank



Age (days)	Height (in)	Height (ft)
182	28	2.33
399	30	2.5
725	33	2.75

Impossible, because rank of original > 1! ax/bx = a/b = 182/399 ay/by = a/b = 28/30Contradiction!

Х b 3x1 С

In practice we usually construct decompositions < rank of the original matrix!

They provide approximate reconstructions of the original

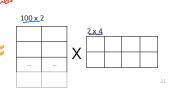
#### Automatic and Approximate factorization

A rank R matrix can be decomposed into an R dimensional representation x (times) some transformation matrix.

But what if we wanted a lower-dimensionality?

In the example below, the rank of the 4D matrix is 3, so we can no longer exactly reconstruct the 4-D matrix. Still, some 2D matrices yield better a ns than others. How well can we do?





#### Principal Component Analysis (PCA)

Goal: Transform observations from high-dimensional data down

to low dimensions (e.g. 2) through linear transformations.

Related Goal: Low-dimension representation should capture (as much as

possible) of the variance of the original data.

100 x 4				Principal Components (cols)	Latent Factors (cols)
width	length	area	perimeter	4x2	100 × 2
20	20	400	80		
16	12	192	56	V 0 0 0	
10	10	100	40	X First S	
				0	
24	12	288	72	Transformation Matrix	

# Two Equivalent Framings of PCA

There are two equivalent ways to frame PCA:

- 1. Finding the directions of maximum variance in the data in the low dun
- Finding the low dimensional (rank) matrix factorization that best approximates the data

We will focus on the first one, aka variance maximization framing (more common) and then return to the best approximation framing (more general).

The second framing allows the problem to be done like a (normal) optimization problem

#### **Capturing Total Variance**

We define the total variance of a data matrix as the sum of variances of attributes. of my O avalles

-				
	width	length	area	perimeter
	20	20	400	80
	16	12	192	56
	24	12	288	72

Total Variance: 402.56 = 7.69

Depends on the Unt



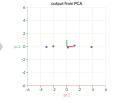
Goal of PCA, restated:

Find a linear transformation that creates a low-dimension representation which captures as much of the original data's total variance as possible.

### Let's derive PCA, in all gory math 🔢 🌢 💀



NOTEBOOK

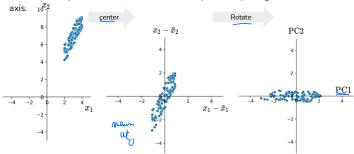


DCA "Uncorrelates the Doth https://setosa.io/ev/principal-component-analysis/



#### How PCA Transforms Data, Visually

PCA first centers the data matrix, then rotates it such that the direction with the most variance (i.e. the direction that's the most spread-out) is aligned with the x-



#### Important Note on Centering and Standardizing the Data

When running PCA it is important to center the data (ensure data is centered at 0):

$$X = X - np.mean(X, axis = 0)$$

The scikit-Learn PCA code does this automatically

You should also consider standardizing your data (ensure unit variance on each dimension)

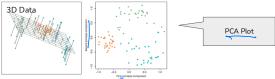
$$X = (X - np.mean(X, axis = 0)) / np.std(X, axis = 0)$$

- The scikit-Learn PCA code does not do this
- You should standardize your data if features have vastly different ranges
- You should not standardize your data if the units are all the same and the differences in variability across dimensions is meaningful (e.g., everything is in the same units)

#### **PCA Plot**

We often construct a scatter plot of the data projected onto the first two principal components. This is often called a PCA plot.

PCA plots allow us to visually assess similarities between our data points and if there are any clusters in our dataset.

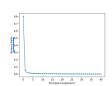


If the first two singular values are large and all others are small, then two dimensions are enough to describe most of what distinguishes one **observation from another.** If not, then a PCA plot is omitting lots of information.

#### Scree Plot

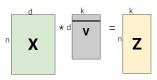
If the first two singular values are large and all others are small, then  $two\ dimensions\ are\ enough\ to\ describe\ most$ of what distinguishes one observation from another. If not, then a PCA scatter plot is omitting lots of information.

A scree plot shows the variance ratio captured by each principal component, largest first.





#### **Biplot**

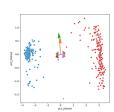


The i-th row of Vindicates how feature i contributes to each PC.

Biplots superimpose the directions onto the plot of PC1 vs. PC2. Row i of V corresponds to the direction for feature i, e.g.,  $(v_{i1}, v_{i2})$ .

• There are several ways to scale biplots vectors

Through biplots, we can interpret how features correlate with the principal components shown: positively, negatively, or not much

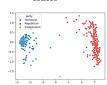


#### Summary of PCA plots

#### **PCA Plot**

Scatter plot of PC1 against PC2

Helps us assess similarities between our data points and if there are any clusters in our dataset.



#### Scree Plot

Line plot showing the variance ratio captured by each principal

- omponent, largest first.

  If first two is large enough, we know PCA plot is good representation of data

  "Elbow" method to assess
- how many PCs to use

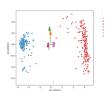


#### **Biplot**

PCA plot + directions of feature → Prot + airections of feat importance for PC1 and PC2

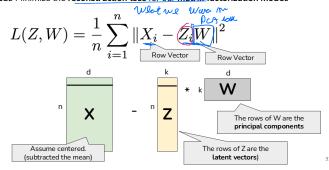
 All benefits from PC4

- All benefits from PCA plot, and
- Shows how much some features contribute to PC1/2



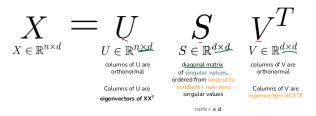
#### **Derive PCA using Loss Minimization**

Goal: Minimize the reconstruction loss for our matrix factorization model:



Singular Value Decomposition

We can use 500 to do fto fto fto singular value decomposition (SVD) describes a matrix decomposition into 3 matrices:



\*note 1: assume d < n.

There are infinite possible factorizations! SVD chooses a special (but non-unique) one with these properties.

#### SVD one-by-one



- Columns of U are orthonormal:  $\vec{u}_i^{ op} \vec{u}_j = 0$  for all i, j and all vectors
- Columns of U are orthonormal:  $u_i \ u_j = 0$  for all are unit vectors Columns of U are called the left singular vectors (aka are the eigenvectors of  $XX^T$ )  $UU^T = I_n$  and  $U^TU = I_d$
- Can think of  ${m U}$  as a rotation

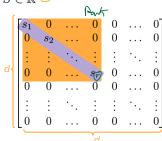
Eigenvectors of XXT:

$$XX^{T} = USV^{T} (USV^{T})^{T} = USV^{T}VS^{T}U^{T}$$
$$= USS^{T}U^{T}$$

#### SVD one-by-one



- Diagonal values (singular values), are ordered from greatest to least
- r non-zero singular values



- r is the rank of X
- The majority of the matrix is zero
- The singular values s<sub>1</sub>, s<sub>2</sub>, ..., s<sub>r</sub> are non**negative** and **sorted**  $s_1 \ge s_2 \ge ... \ge s_r$
- ullet Can think of ullet as a scaling operation

#### SVD one-by-one

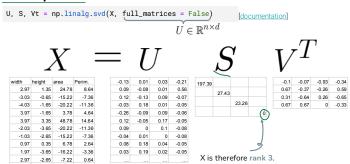


- Columns of  $\boldsymbol{V}$  are orthonormal  $\rightarrow$  rows of  $\boldsymbol{V^T}$  are orthonormal
- Columns of  $oldsymbol{V}$  are called the  $oldsymbol{\mathsf{right}}$  singular vectors
- (aka are the eigenvectors of  $X^TX$ )  $VV^T = V^TV = I_d$
- ullet Can think of  $oldsymbol{V}$  as a rotation

Eigenvectors of XTX:

$$X^TX = (USV^T)^T USV^T = VS^TU^TUSV^T$$
$$X^TX = VS^TSV^T$$

#### NumPy SVD



#### Principal Components are the Eigenvectors of the Covariance Matrix!

Assume we have constructed the Singular Value Decomposition (SVD) of X:

$$X = USV^T$$

Because **X** is centered the covariance matrix of **X** is: 
$$\Sigma = \underbrace{X^TX}_{} = \underbrace{\left(USV^T\right)^T}_{} USV^T = VS^T\underbrace{U^TU}_{} SV^T$$
 
$$= VS^2\underbrace{V^T}_{}$$

Right multiplying both sides by V we get:

The columns of V are the eigenvectors of the covariance matrix ∑ and therefore the Principal Components

$$\Sigma V = V S^2 V^T V = V S^2$$

#### Variance and Singular Values

We define the total variance of a data matrix as the sum of variances of attributes.

width	length	area	perimeter	
20	20	400	80	
16	12	192	56	
24	12	288	72	
7.69	5.35	338.73	50.79	

Total Variance: 402.56 =

Formally, the ith singular value tells us the component score, i.e., how much of the variance is captured by the ith principal component. N is # of datapoints.

i-th component	_ (i-th singular value)2
score	N

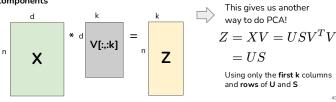
→ 197.39 <sup>2</sup> /100=389.63	0	0	0	197.4
→ 27.43 <sup>2</sup> /100 = 7.52	0	0	27.43	0
→ 23.26 <sup>2</sup> / 100= 5.41	0	23.26	0	0
Sum = <b>402.56</b> .	0	0	0	0

#### From SVD to PCA

We have now shown that if we construct the singular value decomposition of X:

$$X = USV^T$$

The first k columns of V are the first k principal components and we can construct the  $latent\ vector\ representation\ of\ X$  by projecting X onto the principalcomponents



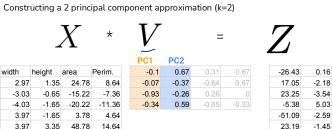
#### Computing Latent Vectors Using X \* V

-20.22

-3.65

-2.03

-11.36



#### Computing Latent Vectors Using U \* S

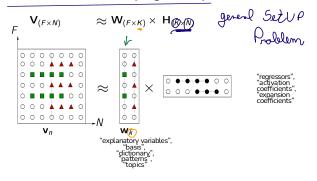
Constructing a 2 principal component approximation (k=2)



0.16 17.05 -2.18 23.25 -3.54 -5.38 5.03 -51.09 -2.59 23.19 -1.45

Some Roll

#### Matrix factorization (in general)



#### A popular variant: Non-Negative MF

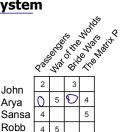
- Some entries in our matrices are non-negative
  - Think about ratings (or even our rectangle data)
  - Factorization is an algebraic operation meaning that getting non-negative entries does not help us understand what is going on in the data
  - We would like to encode prior knowledge that latent dimensions are non-
- Also: We would like the effect of factors to be accumulative (i.e. no cancellations due to negative contributions)
- Also: Standard SVD assumes missing entries to be zero

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#### NMF example - Recommender system

- Given a NXM matrix R with some entries unknown
  - N columns represent items
  - M rows represents users
  - Entry R<sub>ii</sub> represents the i-th user's rating of j-th
- We are interested in the unknown entries' possible values & the hidden dimensions
- Here I will attempt:

Maastricht Uni $R_{\rm WSM} \approx W_{N \times 2} \times H_{2 \times M}$ 

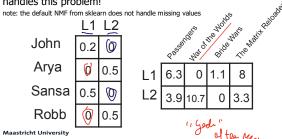


John

Arya

#### NMF example - Recommender system

• Problem is that there are many missing entries but NMF handles this problem!

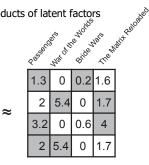


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# NMF example – Recommender system

- Estimate unknown ratings as inner products of latent factors
  - Rating of Arya for Passengers: 6.3\*0 + 3.9\*0.5 = 1.95

John	2		3	
Arya		5		4
Sansa	4			5
Robb	4	5		
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# NMF as an optimization problem

Minimize:

Nodret Depote  $\|V - WH\|^2$ subject to the constraints W>0, H>0

- Possible numerical methods exist:
  - Coordinate descent: Fix W and optimize H, fix H and optimize W until the tolerance threshold is met
  - Multiplicative Update using the following steps (Lee & Seung), 2001) so as to guarantee non-negative entries:

$$H_{a\mu} \leftarrow H_{a\mu} \frac{\sum_i W_{ia} V_{i\mu} / (WH)_{i\mu}}{\sum_k W_{ka}} \qquad W_{ia} \leftarrow W_{ia} \frac{\sum_{\mu} H_{a\mu} V_{i\mu} / (WH)_{i\mu}}{\sum_{\nu} H_{a\nu}}$$

#### Cool applications of MF

# PCA used for denoising images



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# Denoised image using 15 PCA components



- I compute the PCA of the image I "reconstruct" the
- I "reconstruct" the image using only 15 PCs

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#### **PCA: Eigenfaces**

Eigenfaces are

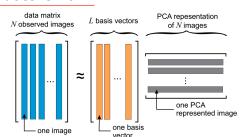
the eigenvectors of the covariance matrix of the probability distribution of the vector space of human faces

- human faces

  Eigenfaces are the 'standardized face ingredients' derived from the statistical analysis of many pictures of human faces
- A human face may be considered to be a combination of these standard faces

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#### How does it work?



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#### **Eigenfaces (cont.)**

 the principal eigenface looks like a bland androgynous average human face



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http://en.wikipedia.org/wiki/Image:Eigenfaces.png

#### Eigenfaces - Steps 1,2

#### Input:

- Dataset of N face images
- Assume each image is KxK
- Represent this as a K^2 x N matrix





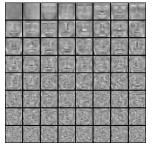


#### **Eigenfaces – Step 3**

- Apply PCA and keep only the m significant dimensions
- Fold back into KxK images







#### **Eigenfaces - Step 4**

- Represent faces onto this basis
  - Using the best K eigenvectors



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### **Eigenfaces – Face Recognition**

- When properly weighted, eigenfaces can be summed together to create an approximate gray-scale rendering of a human face.
- Remarkably few eigenvector terms are needed to give a fair likeness of most people's faces
- Hence, eigenfaces provide a means of applying <u>data compression</u> to faces for identification purposes.

Mostly Insensitive to lighting expression, orientation

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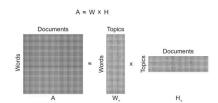
#### **Eigenfaces – Face Recognition**

 What happens when I project a new face?



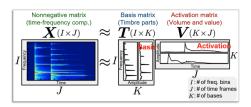
 Remember the the eigenfaces is the "new representation basis", hence everything has to be represented based on these

#### NMF for text topic modeling



# NMF for audio source separation

#### http://d-kitamura.net/demo-defNMF\_en.html



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