Principal Component Analysis (PCA)

TOP: Data Clustering 076/091

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Portland State University

Outline

2024 GDP Prediction of U.S.

- U.S. GDP for the first quarter of 2024
- U.S. GDP for the entirety of 2023, 2022, and so on.
- Unemployment rate
- Inflation rate
- Number of people work in each industry
- Number of members of the House and Senate belong to each political party
- Stock price data
- Number of CEOs seem to be mounting a bid for public office

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That is a lot of parameters/features!

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- k-means/median: $(1 + \epsilon)$-approximation in n^d time
- For large d, distance computation is expensive: for $d = logn$, takes $O(\log n)$ time

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Dependent vs Independent features/variables

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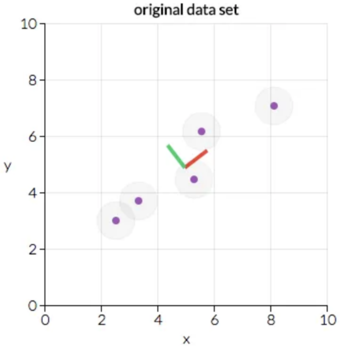
- Feature extraction
  - New features are created that are independent
  - Old features are combined to create new features
  - Number of new features is small
  - New features are not interpretable
  - Information loss is controlled

Outline

Feature Extraction using PCA

Finds main directions of the data (that have higher variance)



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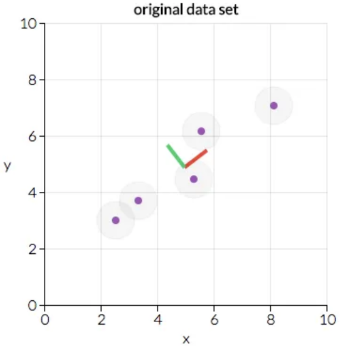
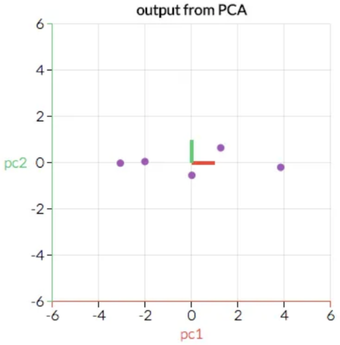


What line can be fit into this data?

Output of PCA

Transformed data by independent directions/vectors



We can drop the y direction without losing a lot of information (dimensionality reduction)

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Eigenvectors and Eigenvalues

- Consider a square matrix A ($d \times d$)
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- $A\vec{v} = \begin{pmatrix} -2 \\ 2 \end{pmatrix} = 2\begin{pmatrix} -1 \\ 1 \end{pmatrix} = \lambda\vec{v}$

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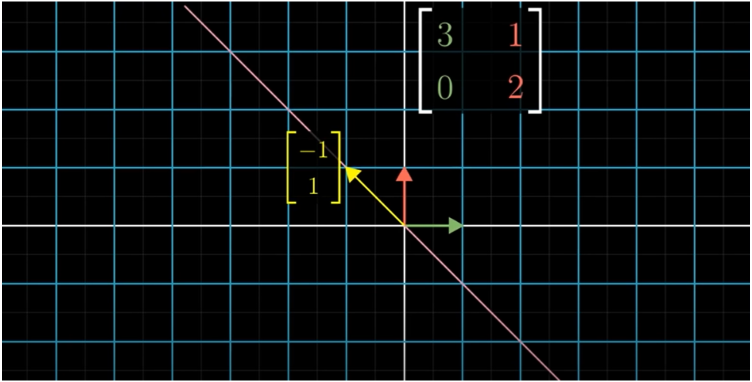
Link to youtube video

An Example



Before transformation

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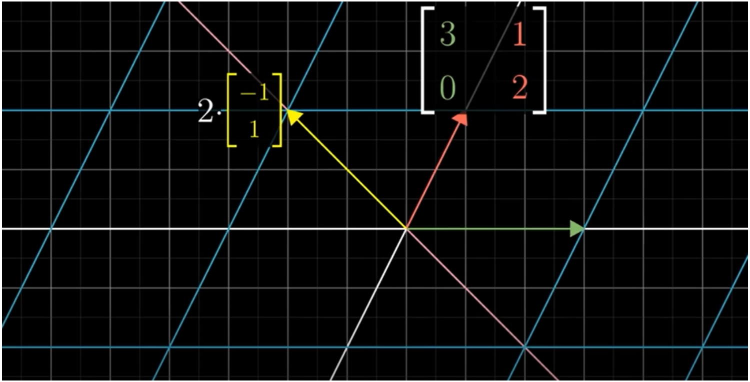

After transformation

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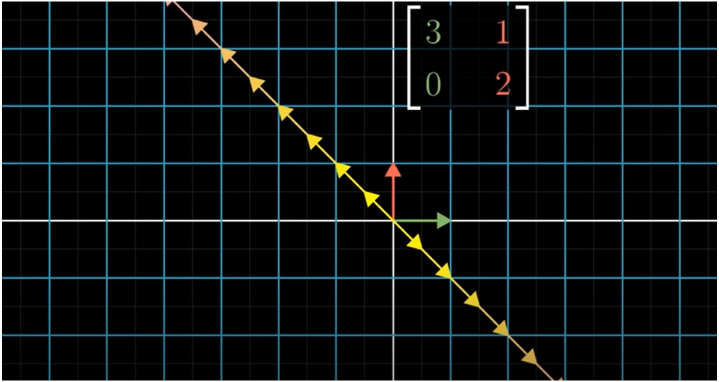
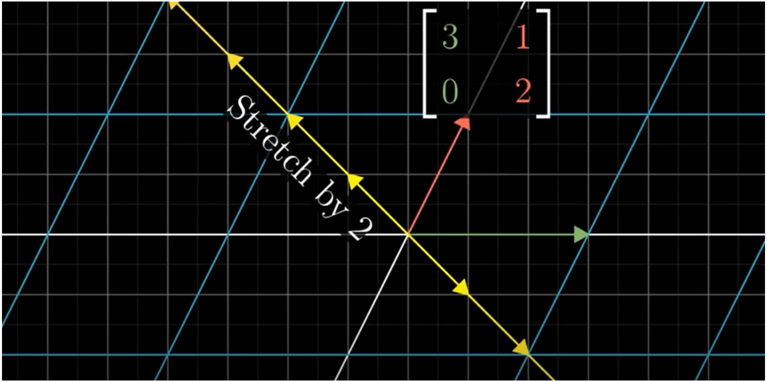


Span of $\begin{pmatrix} -1 \\ 1 \end{pmatrix}$ before

An Example



The span remains the same afterwards

Outline

PCA - Step 1 - Centering

Given the dataset $\{x_1, \ldots, x_n\}$ in $\mathbb{R}^d$

- Create an $n \times d$ matrix X using the dataset: rows :: points, columns :: features

$$\begin{array}{c c} & \begin{array}{cccc} f_1 & f_2 & \cdots & f_d \end{array} \\ \begin{array}{c} x_1 \\ x_2 \\ \vdots \\ x_n \end{array} & \left[\begin{array}{cccc} \; & \; & \; & \; \\ \; & \; & \; & \; \\ \; & \; & \; & \; \\ \; & \; & \; & \; \end{array} \right] \end{array}$$

$$X_{n \times d}$$

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x_n
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- Each column has a mean of zero

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\end{array}}_{X^T_{d\times n}}
\times
\underbrace{\begin{array}{c|c}
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\underbrace{\left[\begin{array}{ccc}
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f_2^T f_1 & & f_2^T f_d \\
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- So, C is basically the covariance matrix of X
- Shows how every variable in X relates to every other variable in X

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- Eigenvectors represent directions - principal components
- Eigenvalues represent magnitude, or importance
- Bigger eigenvalues correlate with more important directions

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- Dimension is still d
- No information loss so far

Summary of PCA

1. Create the matrix X whose each column has a mean of zero
2. Compute the covariance matrix $C = X^T X$
3. Calculate the eigenvectors and their corresponding eigenvalues of C
4. Compute the sorted matrix of eigenvectors P^* from P, where $C = PDP^{-1}$
5. Calculate $X^* = XP^*$

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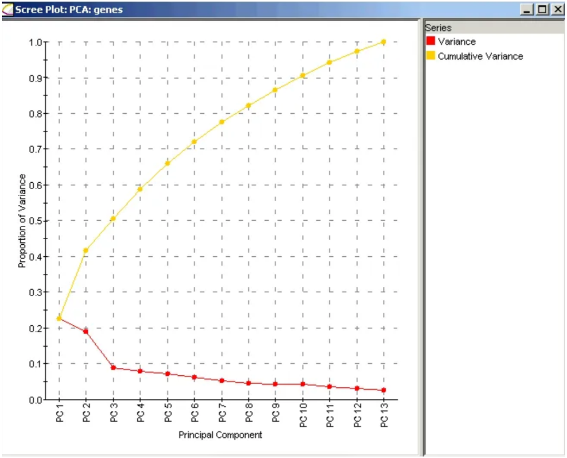
3. Add features until a significant drop in the eigenvalue - Elbow method

An Example


Scree Plot: PCA: genes
Series
Variance
Cumulative Variance
Proportion of Variance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
PC 1
PC 2
PC 3
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Principal Component

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- $k = O(\log n/\epsilon^2)$
- k cannot be arbitrarily small

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- The proof uses properties of $N(0, 1)$ – Random projections work

Proof: Chapter 2.7

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For k-means/median, the dimension can be improved from $O(\log n)$ to $O(\log k)$ to preserve the cost of all clustering