Exploratory Data Analysis

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Outline

1. Principal Component Analysis (PCA)
2. Introduction to Document Modeling
3. Term-Frequency Inverse Document Frequency (TF-IDF)
4. Latent Semantic Analysis (LSA)

Principal Component Analysis: Goal

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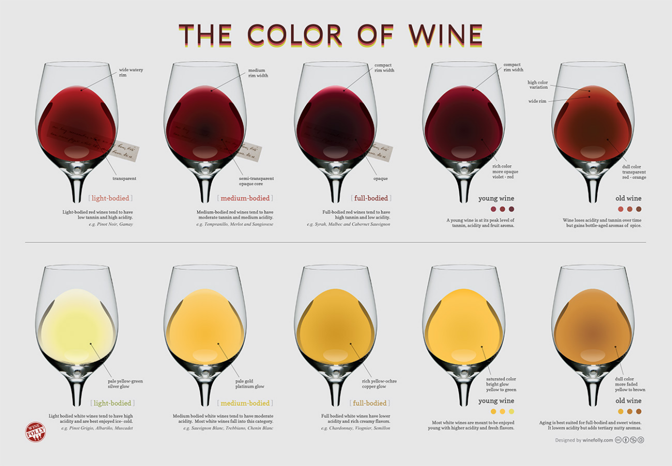

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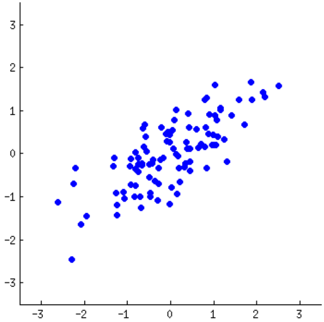

A synthetic wine data: x-axis - color intensity, y-axis - alcohol content

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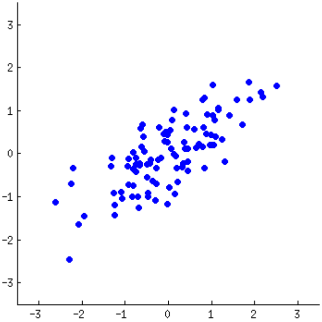

We are interested in some properties

- that strongly differ across data points
- that would allow you to “reconstruct” well the original data points

Eigenvectors and Eigenvalues: Overview

Let C be an $n \times n$ matrix and $\mathbf{u}$ is an $n \times 1$ vector.— $C\mathbf{u}$ is well-defined.

Typically, multiplication by a matrix changes the direction of a *non-zero* vector $\mathbf{u}$

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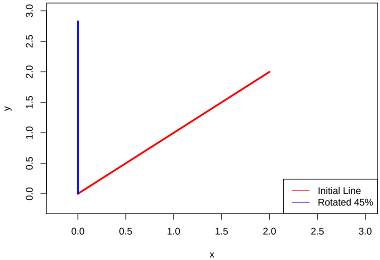

$$(x_1, y_1) = (0, 0)$$
$$(x_2, y_2) = (2, 2)$$

$$C = \begin{bmatrix} \cos(\frac{\pi}{4}) & \sin(\frac{\pi}{4}) \\ -\sin(\frac{\pi}{4}) & \cos(\frac{\pi}{4}) \end{bmatrix}$$

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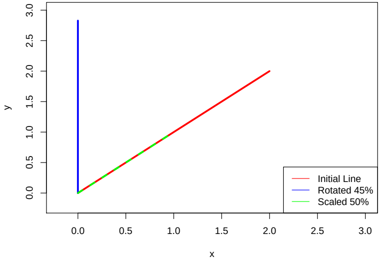

$$C = \begin{bmatrix} .5 & .0 \\ .0 & .5 \end{bmatrix}$$

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The $n \times n$ matrix C can have upto n distinct eigenvalues.

Eigenvectors and Eigenvalues: Facts

Let U be an $n \times n$ matrix with n eigenvectors of C and Λ is the $n \times n$ diagonal matrix with the eigenvalues of C along its diagonal.

The column vectors of U are linearly independent, which gives

$$CU = U\Lambda \rightarrow C = U\Lambda U^{-1}.$$

This **diagonalizes** the matrix C.

If C is symmetric ($C = C^{\mathsf{T}}$), then its eigenvectors are perpendicular and we can have $U^{-1} = U^{\mathsf{T}}$ and

$$C = U\Lambda U^{\mathsf{T}}$$

Principle Component Analysis: Approach

Let X be a centered $m \times n$ data matrix.

We can write the $n \times n$ covariance matrix C as:

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where U is the matrix of eigenvectors $\mathbf{u}_i$ (each column is an eigenvector) and Λ is the diagonal matrix with eigenvalues λ_i on the diagonal.

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PCA transformation: projections of the data X on the **principal components**, i.e. XU. One only needs to keep the most informative principal components.

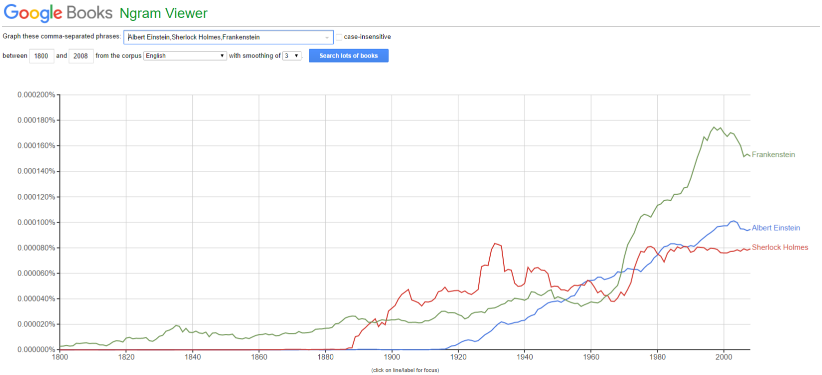
Text Corpus Exploration

We have a big pile of text documents (corpus).—What's going on inside?[1]

[1] PC: Olivia Harris, Reuters

Text Corpus Exploration

- Comparing document covariates—How do individual words correlate?



- Clustering and topic modeling
- Organizing and searching documents—information retrieval

An Information Retrieval Problem

Keyword-based search:

- searching for documents of interest
- e.g., keywords: computers, laptop, etc.

Implementing Keyword-based Search

An approach is via **Vector Space Modeling**

- Convert a corpus m documents and n vocabulary terms into a **term-document** $(n \times m)$ matrix
- Translate both documents and user keywords into vectors in vector space
- Define similarity between these vectors, e.g., via cosine similarity—small angle $\equiv$ large cosine $\equiv$ similar

TF-IDF

Term frequency inverse document frequency matrix (TF-IDF)[2]—a popular scheme

For each term t in document d, we compute

$$\text{tf-idf}_{dt} = \text{tf}_{dt} \times \log\left(\frac{n}{\text{df}_t}\right)$$

- tf_{dt} is the frequency of term t in document d
- df_t is the number of documents where term t appears

[2] Salton et al. (1975)

Hands-on Python: keyword-based document retrieval via TF-IDF

Information Retrieval: Challenges

If we search for the keyword *computers*, we may miss documents that do not have *computers* and contain *PC*, *laptop*, *desktop*, etc.

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- Problem #2: Polysemy—words with multiple meanings

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One solution: search and explore documents based on the themes or **topics** that run through them.

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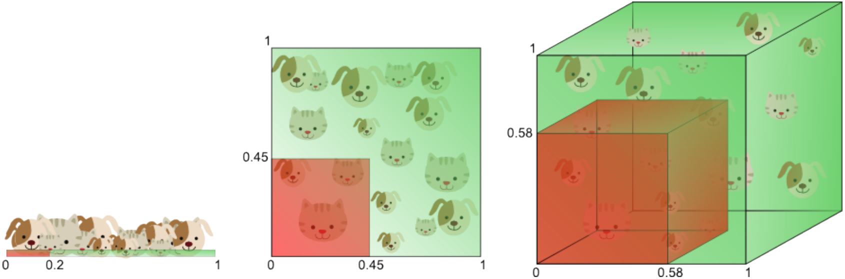
Problem #3: Working in the vocabulary space can cause computational challenges for large corpora.

[3] Salton et al. (1975)

The Curse of Dimensionality[5]



Suppose the available data (documents) are fixed and we keep adding dimensions (words).[4]

The more features we use, the more sparse the data becomes

[4] Image source: `www.visiondummy.com`
[5] Bellman (1961)

Latent Semantic Analysis (LSA)

LSA (Deerwester et al. 1990) aims to explore the "semantics" underlying documents.

By factorizing the TF-IDF ($n \times m$) matrix—Singular Value Decomposition

Singular Value Decomposition (SVD)

Let A be an $m \times n$ matrix with real values and $m > n$. Let $B = A^{\mathsf{T}}A$ be an $n \times n$ matrix.—it's symmetric.

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The corresponding eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$ are perpendicular. We normalize them to have length 1. Let

$$U = [\mathbf{u}_1, \ldots, \mathbf{u}_n] \text{ and } V = [\mathbf{v}_1, \ldots, \mathbf{v}_n]$$

where we define $\mathbf{v}_i = \frac{1}{\sigma_i} A \mathbf{u}_i$.

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We can easily show that $\mathbf{v}_i$'s are perpendicular m-dimensional vectors of length 1 (orthonormal vectors).

Singular Value Decomposition (SVD)

By construction, we have

$$\mathbf{v}_j^\mathsf{T} A \mathbf{u}_i = \mathbf{v}_j^\mathsf{T} (\sigma_i \mathbf{v}_i) = \sigma_i \mathbf{v}_j^\mathsf{T} \mathbf{v}_i = \begin{cases} \sigma_i, & \text{if } i = j \\ 0, & \text{otherwise} \end{cases}$$

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$$V^\mathsf{T} A U = \Sigma$$

where Σ is the diagonal $n \times n$ matrix with $\sigma_1, \ldots, \sigma_n$ along the diagonal.—singular values.

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Since U and V have orthonormal columns, we can have $A = V\Sigma U^\mathsf{T}$

Singular Value Decomposition (SVD): Summary

SVD factorizes an $m \times n$ data matrix A into:

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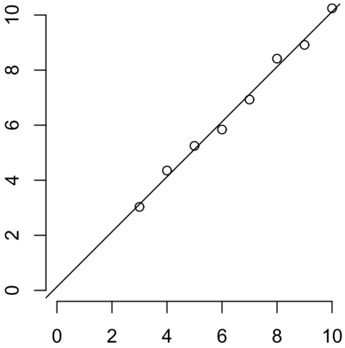
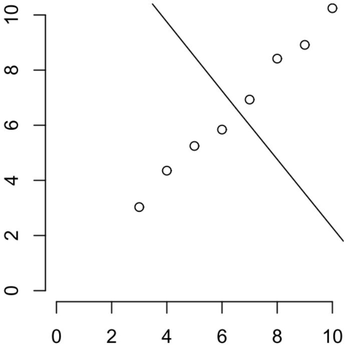
One can identify **similarities** between documents in this **semantic space**.

SVD: Geometric Interpretation



Regression line along 1st dimension



Regression line along 2nd dimension

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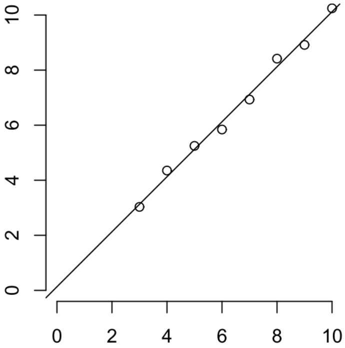

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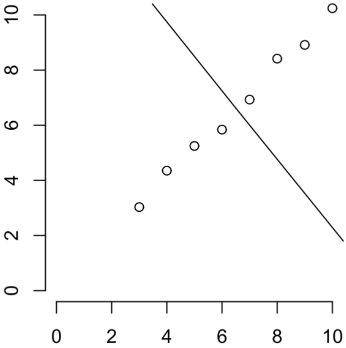

Regression line along 2nd dimension

The regression line on the 1st dimension (left) is the best approximation for the data—it is the line that minimizes the distance between each point and the line.

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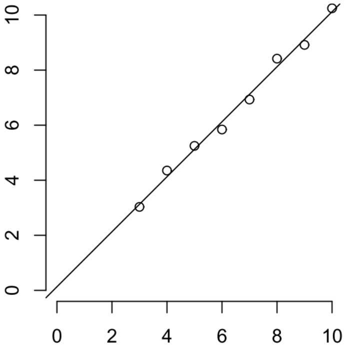

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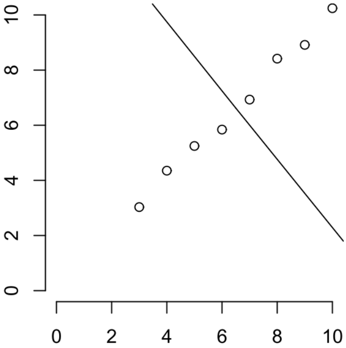

Regression line along 2nd dimension

The regression line on the 2nd dimension (right) does a poorer job of approximating the data, because it corresponds to a dimension exhibiting less variation

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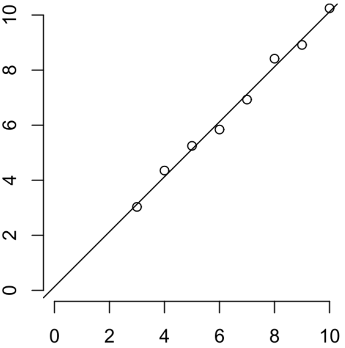

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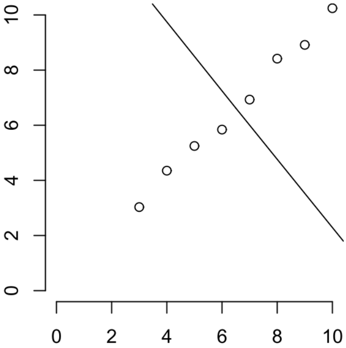
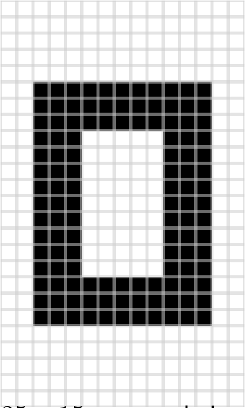


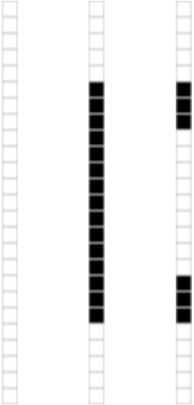
Regression line along 2nd dimension

SVD aims to find the dimensions along which data points exhibit the most variation.

Application of SVD: Data Compression



25×15 gray-scale image (375 cells)



Three types of columns/features

SVD on the matrix, A, gives three non-zero singular values.[6]

[6]Example from: http://www.ams.org/samplings/feature-column/fcarc-svd

Hands-on Python: Latent Semantic Analysis

PCA vs LSA

We assume a *centered* data matrix X. We write its covariance matrix C as[7]

$$\begin{aligned} C &= \frac{X^\mathsf{T} X}{n-1} && (1) \\ &= \frac{USV^\mathsf{T} VSU^\mathsf{T}}{n-1} \text{ (using SVD)} && (2) \\ &= U\frac{S^2}{n-1}U^\mathsf{T} && (3) \end{aligned}$$

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$$

Note: The right singular vectors U are principal axes, and singular values are related to the eigenvalues of the covariance matrix C via $\lambda_i = s_i^2/(n-1)$.

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Questions?