Dimensionality reduction

Outline

- Dimensionality Reductions or data projections
- Random projections
- Singular Value Decomposition and Principal Component Analysis (PCA)

The curse of dimensionality

- The efficiency of many algorithms depends on the number of dimensions **d**
  - Distance/similarity computations are at least linear to the number of dimensions
  - Index structures fail as the dimensionality of the data increases

Goals

- Reduce dimensionality of the data
- Maintain the meaningfulness of the data

Dimensionality reduction

- Dataset **X** consisting of **n** points in a **d**–dimensional space
- Data point $\mathbf{x_i} \in \mathbf{R^d}$ (**d**–dimensional real vector):

  $\mathbf{x_i = [x_{i1}, x_{i2}, \ldots, x_{id}]}$
- Dimensionality reduction methods:
  - **Feature selection:** choose a subset of the features
  - **Feature extraction:** create new features by combining new ones

Dimensionality reduction

- Dimensionality reduction methods:
  - **Feature selection:** choose a subset of the features
  - **Feature extraction:** create new features by combining new ones
- Both methods map vector $x_i \epsilon R^d$, to vector $y_i \epsilon R^k$, $(k<<d)$

- $F : R^d \rightarrow R^k$

Linear dimensionality reduction

- Function F is a **linear** projection
- $y_i = x_i A$
- $Y = X A$
- **Goal:** Y is as **close** to X as possible

Closeness: Pairwise distances

- **Johnson–Lindenstrauss lemma:** Given $\varepsilon > 0$, and an integer n, let k be a positive integer such that $k \geq k_0 = O(\varepsilon^{-2} \log n)$. For every set X of n points in R^d there exists $F: R^d \rightarrow R^k$ such that for all $x_i, x_j \in X$

$$(1-\varepsilon)||x_i - x_j||^2 \leq ||F(x_i) - F(x_j)||^2 \leq (1+\varepsilon)||x_i - x_j||^2$$

What is the intuitive interpretation of this statement?

JL Lemma: Intuition

- Vectors $x_i \epsilon R^d$, are projected onto a k–dimensional space ($k<<d$): $y_i = x_i A$
- If $||x_i||=1$ for all i, then,

  $||x_i-x_j||^2$ is approximated by $(d/k)||y_i-y_j||^2$
- **Intuition:**
  – The expected squared norm of a projection of a unit vector onto a random subspace through the origin is k/d
  – The probability that it deviates from expectation is very small

Finding random projections

- Vectors $x_i \epsilon R^d$, are projected onto a k–dimensional space ($k<<d$)
- Random projections can be represented by linear transformation matrix A
- $y_i = x_i A$

- What is the matrix A?

Finding random projections

- Vectors $x_i \epsilon R^d$, are projected onto a k-dimensional space ($k<<d$)
- Random projections can be represented by linear transformation matrix A
- $y_i = x_i A$

- What is the matrix A?

Finding matrix A

- Elements A(i,j) can be Gaussian distributed
- Achlioptas* has shown that the Gaussian distribution can be replaced by

$$A(i,j) = \begin{cases} +1 \text{ with prob } \frac{1}{6} \\ 0 \text{ with prob } \frac{2}{3} \\ -1 \text{ with prob } \frac{1}{6} \end{cases}$$

- All zero mean, unit variance distributions for A(i,j) would give a mapping that satisfies the **JL** lemma

- **Why is Achlioptas result useful?**

Datasets in the form of

We are given **n** objects and **d** features describing the objects.
(Each object has **d** numeric values describing it.)

Dataset
An **n-by-d** matrix **A**, A_{ij} shows the "**importance**" of feature **j** for object **i**.
Every row of **A** represents an object.

Goal

1. **Understand** the structure of the data, e.g., the underlying process generating the data.
2. **Reduce the number of features** representing the

Market basket matrices

$$
\begin{array}{cc}
 & \textbf{d} \text{ products (e.g., milk, bread, wine, etc.)} \\
\textbf{n} \text{ customers} & \left(\begin{array}{c} \\ \\ A \\ \\ \end{array} \right)
\end{array}
$$

A_{ij} = quantity of j-th product purchased by the i-th customer

Find a subset of the products that characterize customer behavior

Social-network matrices

d groups
(e.g., BU group, opera, etc.)

n users

$$\left(\begin{array}{c} \\ A \\ \\ \end{array}\right)$$

A_{ij} = partiticipation of the **i**-th user in the **j**-th group

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

Document matrices

d terms
(e.g., theorem, proof, etc.)

$$
\begin{array}{cc}
 & \textbf{d} \text{ terms} \\
\textbf{n} \text{ documents} & \begin{pmatrix} \\ A \\ \\ \end{pmatrix}
\end{array}
$$

A_{ij} = frequency of the **j**-th term in the **i**-th document

Find a subset of the terms that accurately clusters the documents

Recommendation systems

$$\begin{array}{cc} & \textbf{d}\text{ products} \\ \textbf{n}\text{ customers} & \left(\begin{array}{c} \\ \\ A \\ \\ \end{array}\right) \end{array}$$

A_{ij} = frequency of the j-th product is bought by the i-th customer

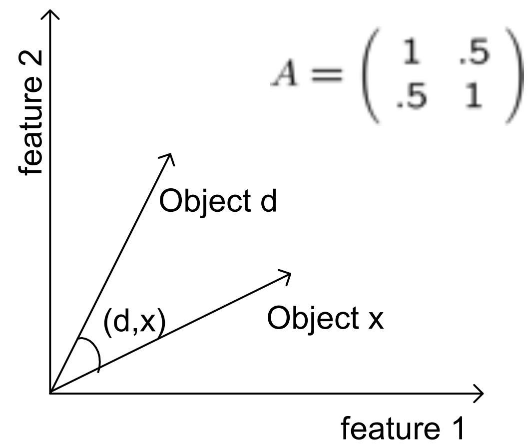
Find a subset of the products that accurately describe the behavior or the customers

The Singular Value Decomposition (SVD)

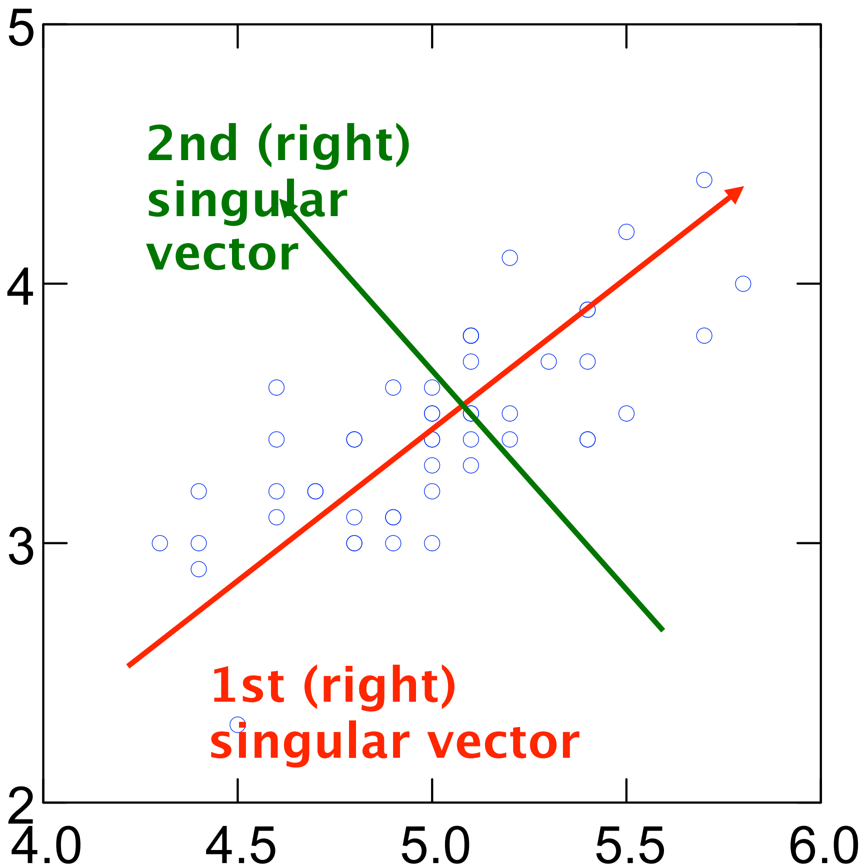
Data matrices have **n** rows (one for each object) and **d** columns (one for each feature).

Rows: vectors in a Euclidean space,

Two objects are "**close**" if the angle between their corresponding vectors is small.



SVD: Example



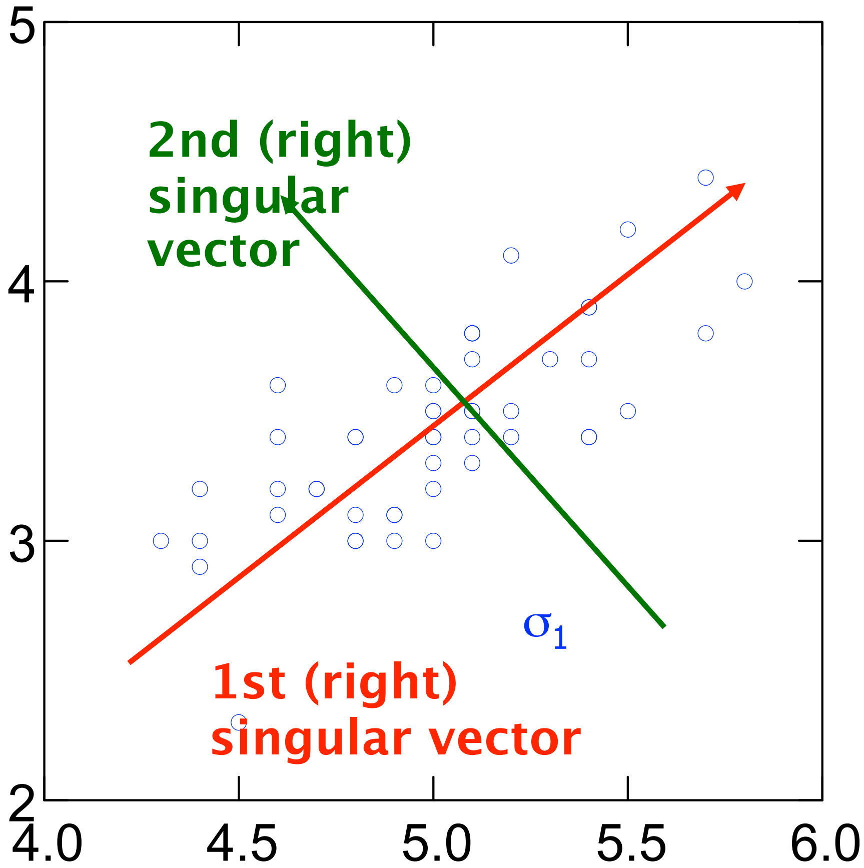
Input: **2-d** dimensional points

Output:

1st (right) singular vector: direction of maximal variance,

2nd (right) singular vector: direction of maximal variance, after removing the projection of the data along the first singular vector.

Singular values



σ_1: measures how much of the data variance is explained by the first singular vector.

σ_2: measures how much of the data variance is explained by the second singular vector.

SVD decomposition

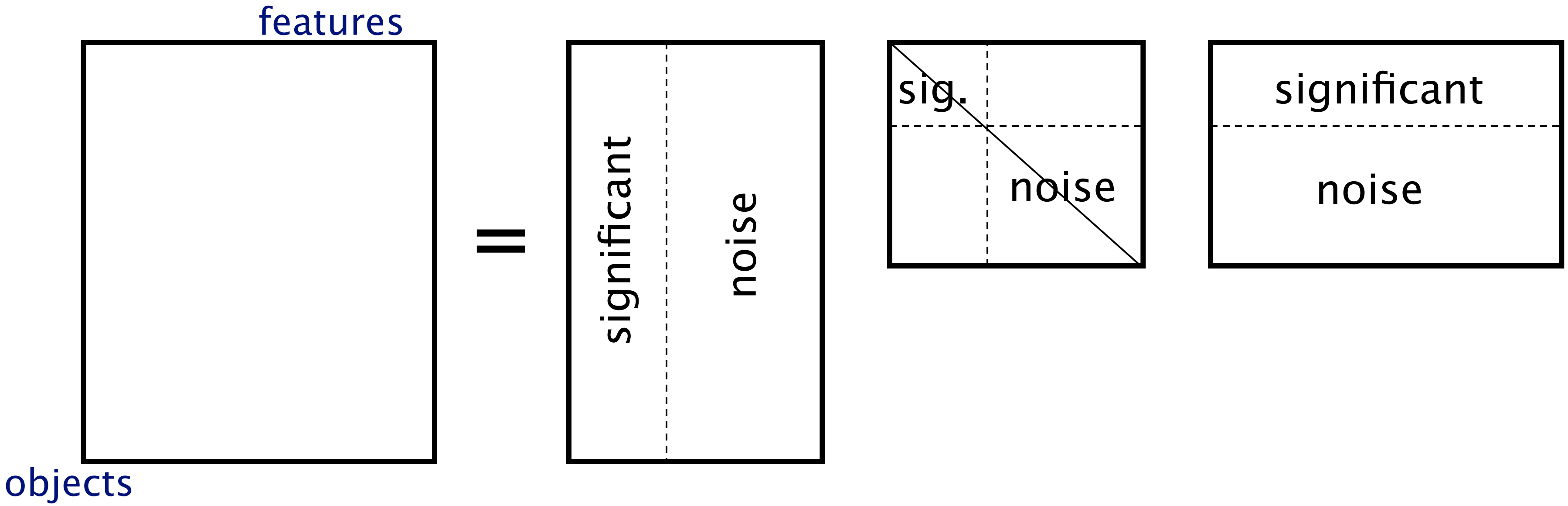
$$\underset{n \times d}{\begin{pmatrix} \\ A \\ \\ \end{pmatrix}} = \underset{n \times \ell}{\begin{pmatrix} \\ U \\ \\ \end{pmatrix}} \cdot \underset{\ell \times \ell}{\begin{pmatrix} \Sigma \\ 0 \end{pmatrix}} \cdot \underset{\ell \times d}{\begin{pmatrix} V \end{pmatrix}^T}$$

U (V): orthogonal matrix containing the left (right) singular vectors of **A**.
Σ: diagonal matrix containing the **singular values** of **A:**
$(\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_\ell)$

Exact computation of the SVD takes **O(min{mn², m²n})** time.
The top k left/right singular vectors/values can be **computed faster** using Lanczos/Arnoldi methods.

SVD and Rank-k

$$\mathbf{A} = \mathbf{U} \quad \Sigma \quad \mathbf{V}^T$$



Rank-k approximations (A_k)

$$A_k = U_k \cdot \Sigma_k \cdot V_k^T$$

n x d   n x k   k x d

U_k (V_k): orth
(right) singu
Σ_k: diagonal
values of A

A_k is the **best** approximation of A

A_k is an approximation of A

SVD as an optimization problem

Find C to minimize:

$$\min_{C} \left\| \underset{n\times d}{A} - \underset{n\times k}{C}\ \underset{k\times d}{X} \right\|_F^2$$

Frobenius norm:

$$\|A\|_F^2 = \sum_{i,j} A_{ij}^2$$

Given C it is easy to find X from standard least squares.

However, the fact that we can find the optimal C is fascinating!

PCA and SVD

- PCA is SVD done on **centered** data
- PCA looks for such a direction that the data projected to it has the maximal variance
- PCA/SVD continues by seeking the next direction that is orthogonal to all previously found directions
- All directions are orthogonal

How to compute the PCA

- Data matrix A, **rows = data points**, **columns = variables** (attributes, features, parameters)

1. Center the data by subtracting the mean of each column
2. Compute the SVD of the centered matrix A' (i.e., find the first k singular values/vectors)
   $A' = U\Sigma V^T$
3. The principal components are the columns of V, the coordinates of the data in the basis defined by the principal components are $U\Sigma$

Singular values tell us something about the variance

- The variance in the direction of the **k**–th principal component is given by the corresponding singular value σ_k^2

- Singular values can be used to estimate how many components to keep

- **Rule of thumb:** keep enough to explain **85%** of the variation:

$$\frac{\sum_{j=1}^{k} \sigma_j^2}{\sum_{j=1}^{n} \sigma_j^2} \approx 0.85$$

SVD is “**the Rolls-Royce and the Swiss Army Knife of Numerical Linear Algebra.**”*

*Dianne O’Leary, MMDS ’06

SVD as an optimization problem

Find C to minimize:

$$\min_C \left\| \underset{n\times d}{A} - \underset{n\times k}{C}\ \underset{k\times d}{X} \right\|_F^2$$

Frobenius norm:

$$\|A\|_F^2 = \sum_{i,j} A_{ij}^2$$

Given C it is easy to find X from standard least squares.
However, the fact that we can find the optimal C is fascinating!