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 $x_i \epsilon R^d$ (**d**–dimensional real vector):

  $x_i = [x_{i1}, x_{i2}, \ldots, x_{id}]$
- 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 $\mathbf{x_i \epsilon R^d}$, to vector $\mathbf{y_i \ \epsilon\ R^k, (k<<d)}$

- $\mathbf{F : R^d \rightarrow R^k}$

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

d products
(e.g., milk, bread, wine, etc.)

n customers

$$\begin{pmatrix} \\ & A & \\ \\ \end{pmatrix}$$

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

$$
\begin{array}{cc}
 & \textbf{d} \text{ groups (e.g., BU group, opera, etc.)} \\
\textbf{n} \text{ users} & \left(\begin{array}{c} A \end{array} \right)
\end{array}
$$

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.)

n
documents

$$A$$

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

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

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

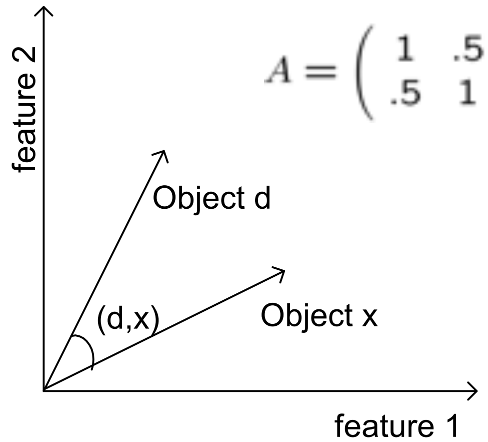
The Singular Value Decomposition (SVD)

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

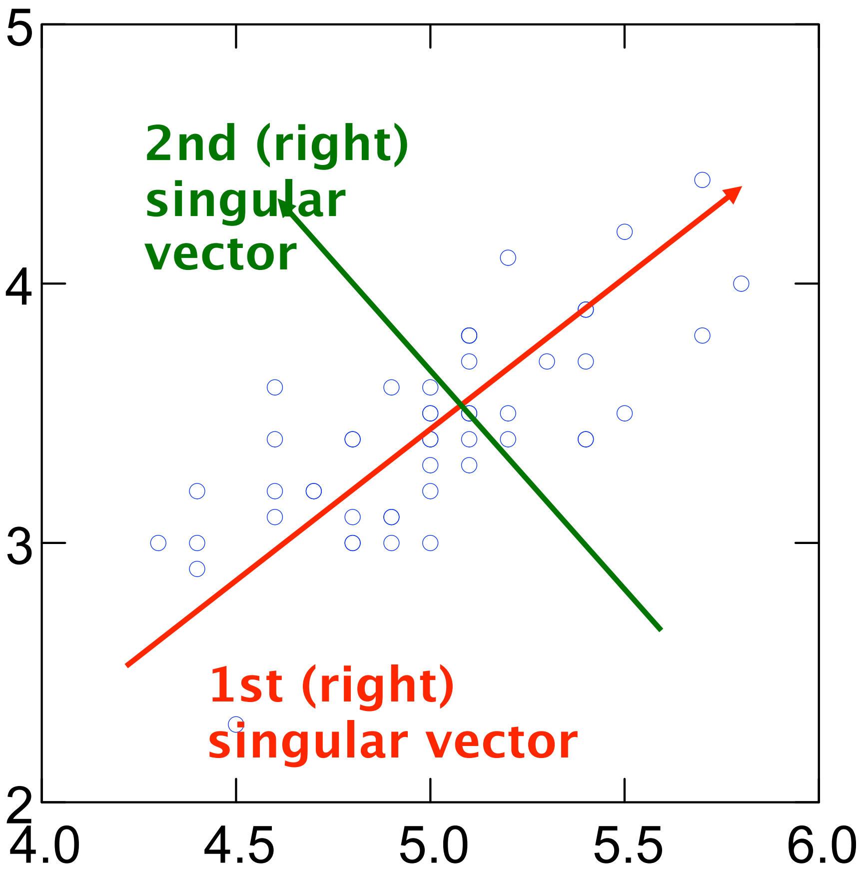
Rows: vectors in a Euclidean space,

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

$$A = \begin{pmatrix} 1 & .5 \\ .5 & 1 \end{pmatrix}$$



SVD: Example



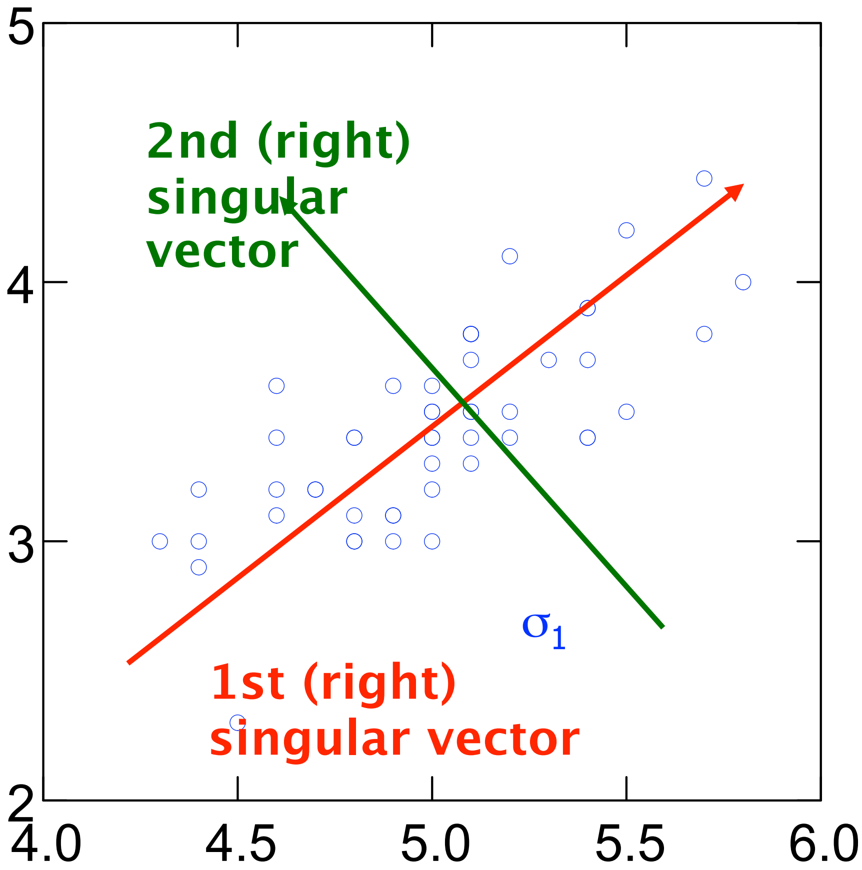
Input: 2-d dimensional points

Output:

<u>1st (right) singular vector:</u> direction of maximal variance,

<u>2nd (right) singular vector:</u> 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

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

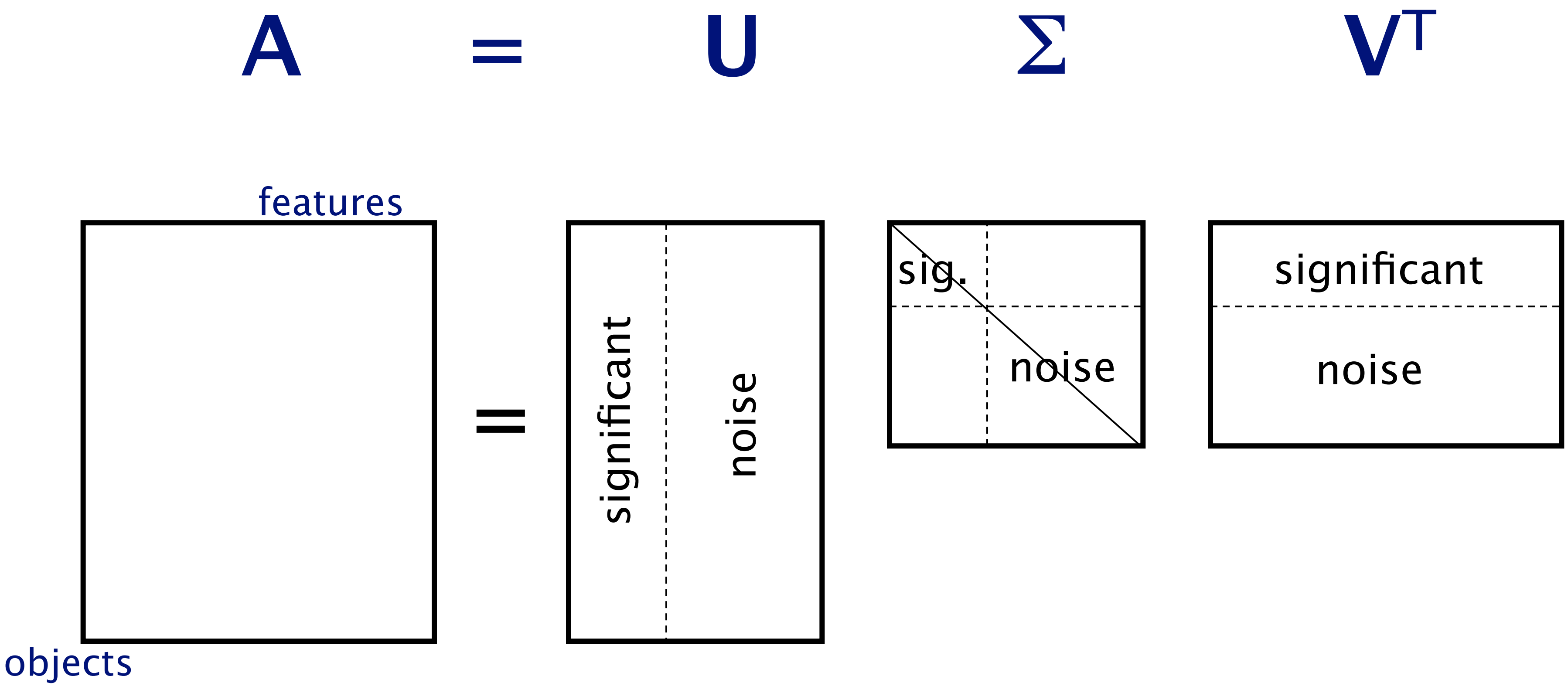
U (V): orthogonal matrix containing the left (right) singular vectors of **A.**

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 **$O(\min\{mn^2, m^2n\})$** time.

The top k left/right singular vectors/values can be **computed faster** using Lanczos/Arnoldi methods.

SVD and Rank-k



Rank-**k** approximations (A_k)

$$\begin{pmatrix} \\ \\ A_k \\ \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \\ U_k \\ \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \Sigma_k \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ V_k^T \\ \\ \end{pmatrix}$$

n x d   **n x k**   **k x k**   **k x d**

U_k (V_k): orthogonal matrix containing the top **k** left (right) singular vectors of **A**.
Σ_k: diagonal matrix containing the top **k** singular values of **A**

A_k is an approximation of **A**

Rank-k approximations (A_k)

$$\left(A_k \right) = \left(U_k \right) \cdot \left(\Sigma_k \right) \cdot \left(V_k^T \right)$$

n x d n x k k x k k x d

A_k is the best approximation of A

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

Find C to minimize:

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

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