Lecture 1: Introduction to Data Analytics and Linear Algebra in Big Data Analytics

Haesun Park

School of Computational Science and Engineering
Georgia Institute of Technology
Atlanta GA, U.S.A.

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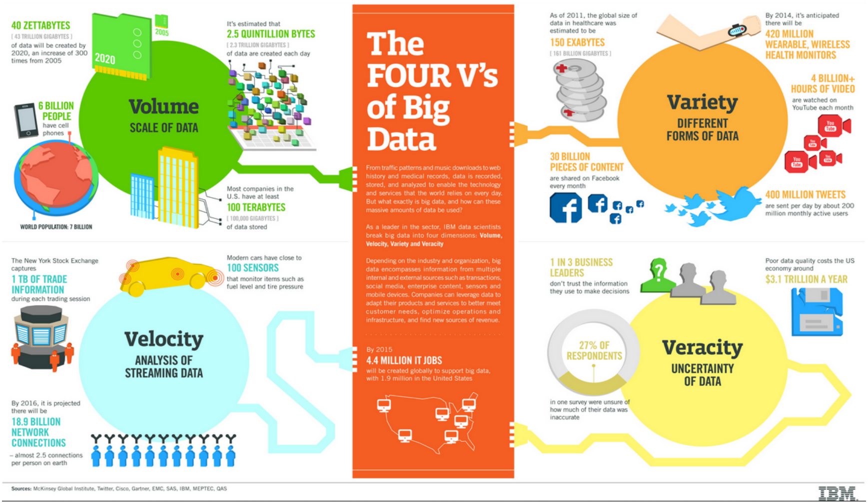
Overview of Lectures, June 18-19

- Introduction to Data Analytics. Linear Algebra in Data Analytics (focus: Low Rank Approximation)
- Constrained Low Rank Approximation (CLRA) and Data Analytic Tasks (focus: Dimension Reduction and Clustering)
- Constrained Low Rank Approximation:
  - Nonnegative Matrix Factorization (NMF) for dimension reduction, clustering, and topic modeling
  - Symmetric NMF for graph clustering and community detection
  - JointNMF for clustering utilizing content/attributes and connection information
- Applications in text and social network analyses

Overview of Lecture 1

- Introduction to Data Analytics : Challenges
- Role of Linear Algebra in Data Analytics, specifically, Low Rank Approximation (LRA) : SVD and Rank



- Volume: Large number of data items, High-dimensional, Complex relationships
- Variety: Of heterogeneous formats, sources, reliability
- Velocity: Time varying, dynamic,...
- Veracity: Noisy, varying quality, errors and missing values are inevitable in real data set
  ... Vast majority of data is unstructured: Text

(Reproduction from a slide courtesy of IBM)

The Challenge

- Transform the data into knowledge (understanding, insight), making it useful to people
- Ways to get to Knowledge: Automated algorithms and Visualization
  - Faster methods to solutions
  - Accurate solutions/less errors
  - Better understanding/interpretation

DATA

- Data is taken from some phenomena from the world
- Data refers to qualitative or quantitative attributes of a variable or set of variables
- Data is the lowest level of abstraction from which information and then knowledge are derived
- Examples: Text data from news articles, image data from satellites, video data from surveillance cameras, connection data from social network
- How to provide data to vector-space based algorithms:
    - Data Representation in matrices or tensors
    - Feature (attribute)-data relationship or data-data relationship
    - *Dimension*: often refers to the number of features/attributes

Major Tasks in Data Analytics

- Dimension Reduction
- Clustering
- Classification
- Regression
- Trend analysis
- ...

Numerical Linear Algebra

- Problems:
  - Linear systems
  - Least Squares
  - Eigenvalue problems
- Methods:
  - Direct: often involves Decomposition (Factorization) of a matrix, to transform the given problem into another problem which is easeir to solve: LU, QR, SVD, EVD, ...
  - Iterative
- Since the main topic is Constrained Low Rank Approximation, we will first focus on Rank and SVD

Singular Value Decomposition

For any matrix $A \in R^{m \times n}$, there exist matrices U, V, Σ such that
$A = U\Sigma V^T$,
where $U \in R^{m \times m}, U^T U = I_m$, $V \in R^{n \times n}, V^T V = I_n$,
$\Sigma = diag(\sigma_1, \sigma_2, \cdots) \in R^{m \times n}$ where

$$\Sigma = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ & 0 & \end{bmatrix} \text{ when } m \geq n,$$

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & 0 \\ & & \sigma_n & \end{bmatrix} \text{ when } m \leq n,$$

and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$ are singular values .

Properties of SVD

Suppose for $A \in R^{m\times n}(m \geq n)$, we have its SVD $A = U\Sigma V^T$.

- $A^T A = V\Sigma^T U^T U\Sigma V^T = V\Sigma^T\Sigma V^T$ where $\Sigma^T\Sigma = diag(\sigma_1^2, \cdots, \sigma_n^2)$
- $AA^T = U\Sigma V^T V\Sigma^T U^T = U\Sigma\Sigma^T U^T$ where $\Sigma^T\Sigma = diag(\sigma_1^2, \cdots, \sigma_n^2, 0, \cdots, 0)$
- If $\Sigma = diag(\sigma_1, \cdots, \sigma_n) = diag(\sigma_1, \cdots, \sigma_r, 0, \cdots, 0)$, i.e. $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_n = 0$, then $rank(A) = r$
- With $A = U\Sigma V^T = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \end{bmatrix}$ where

  $\Sigma_1 = diag(\sigma_1, \cdots, \sigma_r)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$,

  $Range(A) = span(U_1)$, $Null(A) = span(V_2)$.

  $Range(A^T) = span(V_1)$, $Null(A^T) = span(U_2)$.

QR Decomposition

For any matrix $A \in R^{m \times n}$**,** $\exists$ **orthogonal matrix** $Q \in R^{m \times m}$ $(Q^T Q = I_m)$ **and upper triangular matrix** $R \in R^{n \times n}$**, s.t.** $A = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$**.**

Theorem. If $A = [a_1 \cdots a_n] \in R^{m \times n}$ has $rank(A) = n$, and $A = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$, where $Q = (\underbrace{Q_1}_{n} \ \underbrace{Q_2}_{m-n}) = [q_1 \cdots q_n]$,

then $A = Q_1 R$ and

- $span\{a_1 \cdots a_k\} = span\{q_1 \cdots q_k\}$, for all $k = 1, \cdots, n$.
- $Range(A) = Range(Q_1)$ and $Range^{\perp}(A) = Range(Q_2)$.
- R^T in the QRD of A is the Cholesky factor of $A^T A$

SVD and QRD

Main differences between SVD and QRD?

Least Squares Problem - QRD

Linear System $Ax = b$ where $A : n \times n$ nonsingular and $b : n \times 1$
Least Squares $Ax \approx b$ where $A : m \times n$ with $m \geq n$ and $b : m \times 1$
For solving least squares (LS) problem, we need **orthogonalization** to reduce matrices to canonical forms : **QR factorization (decomposition)** or **SVD**.
$\|Ax - b\|_2 = \|Q^T Ax - Q^T b\|_2$ for any orthogonal matrix Q $(Q^T Q = I)$

Suppose there is an orthogonal matrix Q, $Q^T A = \begin{pmatrix} R \\ 0 \end{pmatrix}$, then

$\|Q^T Ax - Q^T b\|_2 = \| \begin{pmatrix} R \\ 0 \end{pmatrix} x - \begin{pmatrix} c \\ d \end{pmatrix} \|_2 = \| \begin{pmatrix} Rx - c \\ -d \end{pmatrix} \|_2$ where

$Q^T b = \begin{pmatrix} c \\ d \end{pmatrix}$
Solution x is obtained by solving $Rx = c$ when $rank(A) = n$
(When $rank(A) = n$, $rank(R) = n$)

Least Squares Problem – SVD

Solving LS
$\min_x \|Ax - b\|_2$, $A \in R^{m\times n}$, $b \in R^{m\times 1}$, $m \geq n$.

Let the SVD of A be

$$A = U\Sigma V^T = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1 & V_2 \end{bmatrix}^T$$

where $U_1 \in R^{m\times r}$, $U_2 \in R^{m\times(m-r)}$, $\Sigma_1 = diag(\sigma_1, \cdots, \sigma_r)$,
$\sigma_1 \geq \cdots \geq \sigma_r > 0$,
and $V_1 \in R^{n\times r}$, $V_2 \in R^{n\times(n-r)}$,i.e. $rank(A) = r$.

$$
\begin{aligned}
\|Ax-b\|_2 &= \left\|U\Sigma V^T x - b\right\|_2 = \left\|U^T(U\Sigma V^T x - b)\right\|_2 \\
&= \left\|\Sigma V^T x - U^T b\right\|_2 \\
& \begin{cases} \text{Letting } \; V^T x = \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} x = \begin{pmatrix} y \\ z \end{pmatrix} \begin{matrix} \} & r \\ \} & n-r \end{matrix} \\ U^T b = \begin{pmatrix} U_1^T \\ U_2^T \end{pmatrix} b = \begin{pmatrix} c \\ d \end{pmatrix} \begin{matrix} \} & r \\ \} & m-r \end{matrix} \end{cases} \\
&= \left\| \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} - \begin{bmatrix} c \\ d \end{bmatrix} \right\| = \left\| \begin{bmatrix} \Sigma_1 y - c \\ -d \end{bmatrix} \right\|_2
\end{aligned}
$$

Least Squares Problem – SVD

Since $\Sigma_1 \in R^{r \times r}$, non-singular, we can find the unique solution for $\Sigma_1 y - c = 0 \iff \Sigma_1 y = c \iff y = \Sigma_1^{-1} c$.

Letting $r(x) = \|Ax - b\|_2$, the residual $r(x_{LS}) = \|d\|$ where x_{LS} is the LS solution.

The solution is

$$x_{LS} = V \begin{bmatrix} y \\ z \end{bmatrix}$$

where $y = \Sigma_1^{-1} c$ and z can be anything. (if $rank(A) = n$, z is null).

$$x_{LS} = \begin{pmatrix} V_1 & V_2 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = V_1 y + V_2 z$$

Note $V_2 z \in null(A)$.

When $z = 0$, $x_{LS} = V \begin{bmatrix} \Sigma_1^{-1} c \\ 0 \end{bmatrix}$ is called **minimum-norm solution**.

Least Squares Problem – SVD

In some applications, just need to compute L_2 norm of the residual vector.

$\Longrightarrow$ Can be done **WITHOUT** computing the solution vector x.

$r = Ax_{LS} - b$
$\|r\|_2 = \|Ax_{LS} - b\|_2$

$$\begin{aligned} r &= U\Sigma V^T x_{LS} - b \\ &= U \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} - U \begin{pmatrix} c \\ d \end{pmatrix} \\ &= U \begin{pmatrix} \Sigma_1 y - c \\ -d \end{pmatrix} \\ &= U \begin{pmatrix} 0 \\ -d \end{pmatrix} \end{aligned}$$

$\therefore \|r\|_2 = \|U \begin{pmatrix} 0 \\ -d \end{pmatrix}\|_2 = \|d\|_2.$

Rank Decision in LS and SVD

$$A = U\Sigma V^T = U \begin{bmatrix} 1 & & & \\ & 0.5 & & \\ & & 10^{-14} & \\ & & & 10^{-16} \\ & & & \\ & & & \end{bmatrix} V^T$$

Depending on rank decision (2 or 3 or 4?), we obtain very different solutions.

If we consider the tolerance ϵ s.t. $10^{-16} < \epsilon$, and $rank(A) = 3$,

$$\Sigma_1 = \begin{bmatrix} 1 & & \\ & 0.5 & \\ & & 10^{-14} \end{bmatrix}, y = \begin{bmatrix} 1 & & \\ & 2 & \\ & & 10^{14} \end{bmatrix} \begin{bmatrix} x \\ x \\ x \end{bmatrix}.$$

If we consider the tolerance ϵ s.t. $10^{-14} < \epsilon$, and $rank(A) = 2$,

$$\Sigma_1 = \begin{bmatrix} 1 & \\ & 0.5 \end{bmatrix}, y = \begin{bmatrix} 1 & \\ & 2 \end{bmatrix} \begin{bmatrix} x \\ x \end{bmatrix}.$$

Rank Decision in LS and SVD

Min-norm solution:

the first case, $x_{LS} = V \begin{bmatrix} \begin{bmatrix} 1 & & \\ & 2 & \\ & & 10^{14} \end{bmatrix} \begin{bmatrix} x \\ x \\ x \end{bmatrix} \\ 0 \end{bmatrix}$

the second case, $x_{LS} = V \begin{bmatrix} \begin{bmatrix} 1 & \\ & 2 \end{bmatrix} \begin{bmatrix} x \\ x \end{bmatrix} \\ 0 \end{bmatrix}$

Determination of numerical rank can be difficult. Usually we find a large gap. $\begin{bmatrix} 1 & & & & \\ & 10^{-1} & & & \\ & & 10^{-2} & & \\ & & & 10^{-3} & \\ & & & & \ddots \end{bmatrix}$ no gap?

Ex.

$$A = \begin{bmatrix} 1 & -1 & -1 & -1 \\ & 1 & -1 & -1 \\ & & 1 & -1 \\ & & & 1 \end{bmatrix}, \ \det(A) = 1$$

$$A^{-1} = \begin{bmatrix} 1 & 2 & 2 & 4 \\ & 1 & 2 & 2 \\ & & 1 & 2 \\ & & & 1 \end{bmatrix}$$

In general $A^{-1}(1, n) = 2^{n-2}$ when $A = \begin{bmatrix} 1 & -1 & -1 & -1 \\ & 1 & -1 & -1 \\ & & 1 & -1 \\ & & & 1 \end{bmatrix}$

$K_1(A) = \|A\|_1 \left\|A^{-1}\right\|_1 \approx n \cdot 2^{n-2}$

The reason of "bad" solution:

1. Algorithm is bad? (unstable)
2. Problem difficult? (ill-conditioned)

Reduced Rank in Data Analytics

- In data analytics, reduced rank k of interest is the reduced dimension or the number of clusters, topics, communities
- Often k is much smaller than the rank of the data matrix r
- However, an optimal reduced rank k in data analytics is not easy to determine either: the optimal number of clusters? the optimal reduced dimension ?
- Will assume k is given and $k << r$: often requres very severe low rank approximation

QRD with Column Pivoting can Reveal Rank

If $A = QR$ **and** $rank(A) = n$**, then**

$span\{a_1, \cdots, a_k\} = span\{q_1, \cdots, q_k\}$, $1 \leq k \leq n$ **where**

$A = \begin{bmatrix} a_1 & \cdots & a_n \end{bmatrix}$, $Q = \begin{bmatrix} q_1 & \cdots & q_n \end{bmatrix}$.

Why QRD with Column Pivoting?

E.g. $A = \begin{bmatrix} 1 & 1 & 1 \\ & & 1 \\ & & 1 \end{bmatrix}$. $rank(A) = 2$.

Consider QRD of A

$$A = QR = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ & & 1 \\ & & 1 \end{bmatrix}$$

Although $rank(A) = 2$, we don't have $Range(A) = span\{q_i, q_j : i \neq j\}$. **QRD with C.P. can help us to maintain** $span\{a_1, \cdots, a_k\} = span\{q_1, \cdots, q_k\}$ **in rank deficient case.**

For any $A \in R^{m \times n}$, **QRD with Column Pivoting** computes

$$A\Pi = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$$

, where

$$R = \begin{pmatrix} R_{11} & R_{12} \\ \underbrace{0}_{(n-r)\times r} & \underbrace{0}_{(n-r)\times(n-r)} \end{pmatrix}$$

where $R_{11} \in \mathbb{R}^{r \times r}$ is upper triangular, $R_{12} \in \mathbb{R}^{r \times n-r}$,
$r = rank(A) = rank(R) = rank(R_{11})$.

$Q \in R^{m \times m}$, orthogonal; $\Pi \in R^{n \times n}$, permutation.

$$A\Pi = Q\begin{bmatrix} R \\ 0 \end{bmatrix} = Q\begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \Longleftrightarrow A = Q\begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \\ 0 & 0 \end{bmatrix}\Pi^T.$$

$$\|Ax - b\|_2 = \left\| Q\begin{bmatrix} R_{11} & R_{12} \\ & \end{bmatrix}\Pi^T x - b\right\|_2 = \left\|\begin{bmatrix} R_{11} & R_{12} \\ & \end{bmatrix}\Pi^T x - Q^T b\right\|_2$$

Letting $\Pi^T x = \begin{bmatrix} y \\ z \end{bmatrix} \begin{matrix} \} & r \\ \} & n-r \end{matrix}$, $Q^T b = \begin{bmatrix} c \\ d \end{bmatrix} \begin{matrix} \} & r \\ \} & m-r \end{matrix}$,

$$\|Ax - b\|_2 = \left\|\begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} y \\ z \end{bmatrix} - \begin{bmatrix} c \\ d \end{bmatrix}\right\|_2 = \left\|\begin{pmatrix} R_{11}y + R_{12}z - c \\ -d \end{pmatrix}\right\|_2$$

Least Squares Problem – Rank Deficient

z can be anything, and y can be chosen so that $R_{11}y = c - R_{12}z$.
Can set $z = 0$, then y satisfies $R_{11}y = c$.

$x = \Pi \begin{bmatrix} R_{11}^{-1}(c - R_{12}z) \\ z \end{bmatrix}$ where z is free.

If we set $z = 0$, we get basic solution $x = \Pi \begin{bmatrix} R_{11}^{-1}c \\ 0 \end{bmatrix}$.

When $rank(A) = n$, $A\Pi = Q \begin{bmatrix} R_{11} \\ 0 \end{bmatrix}$ and $R_{11} = R$.

QRD with Column Pivoting

A **can be nearly rank deficient without any** $fl(R_{22}^{(k)})$ **being very small.**

From V. Kahan

$$T_n(c) = diag(1, s, s^2, \cdots s^{n-1}) \begin{bmatrix} 1 & -c & \cdots & -c \\ & 1 & \ddots & \vdots \\ & & \ddots & -c \\ & & & 1 \end{bmatrix}$$

Least Squares Problem – Rank Deficient

$$T_5(c) = \begin{bmatrix} 1 & -c & -c & -c & -c \\ & s & -cs & -cs & -cs \\ & & s^2 & -cs^2 & -cs^2 \\ & & & s^3 & -cs^3 \\ & & & & s^4 \end{bmatrix}$$

$k=1$: all columns have norm 1 $\longrightarrow$ no permutation, no annihilation.

$k=2$: $c^2s^2 + s^4 = s^2(c^2+s^2) = s^2$ all columns have same norm $\longrightarrow$ no permutation, no annihilation.

For any k, $\left\| R_{22}^{(k+1)} \right\|_F \geq s^{n-1}$.

$T_{100}(0.2)$ has no very small trailing principal submatrix since $\left\| R_{22}^{(k+1)} \right\|_F \geq s^{99} \approx 0.13$, but $\sigma_{100} \approx 10^{-8}$.

QRD with column pivoting is not completely reliable for detecting near rank deficiency.

However in practice, QRD with column pivoting works well.

Eigenvalue Problem

Given a matrix $A \in C^{n\times n}$, $\exists$ n scalars λ_i(eigenvalues), n vectors $v_i \neq 0$(eigenvectors), s.t. $Av_i = \lambda_i v_i$.

Set of eigen values of A: $\lambda\{A\}$
Eigenvalues are the roots of **characteristic polynomial**
$P_A(\lambda) = \det(\lambda I - A)$ or $\det(A - \lambda I)$
e.g. $A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$, $\lambda I - A = \begin{bmatrix} \lambda - 1 & -2 \\ -3 & \lambda - 4 \end{bmatrix}$,
$\det(\lambda I - A) = (\lambda - 1)(\lambda - 4) - 6 = 0$

Eigenvalues of a diagonal matrix are the diagonal elements.
Eigenvalues of a triangular matrix are the diagonal elements.
$p(\lambda) = \det(\lambda I - A)$ has n roots.

Eigenvalue Problem

Definition: Two matrices A and B are **similar**, if $B = X^{-1}AX$ for a nonsingular matrix X. X is called **similarity transformation**.

Theorem. If A and B are similar, i.e. $\exists X$ is nonsingular, s.t. $B = X^{-1}AX$, then $\lambda\{A\} = \lambda\{B\}$.

Note that here X is not necessarily unitary.

Proof: $P_A(\lambda) = \det(\lambda I - A)$,
$P_B(\lambda) = \det(\lambda I - X^{-1}AX) = \det(X^{-1}(\lambda I - A)X) =$
$\det(X^{-1})\det(\lambda I - A)\det(X) = \det(\lambda I - A)$ as
$1 = \det(I) = \det(X^{-1}X) = \det(X^{-1})\det(X)$

To preserve eigen values, we have to use similarity transformations.

Schur Decomposition: For any $B \in C^{n \times n}$, there exists a unitary matrix $Q \in C^{n \times n}$ s.t. $Q^H BQ = T$ where $T \in C^{n \times n}$ is upper triangular and the diagonal elements of T are the eigenvalues of B.
Symmetric EVD: For any $B \in R^{n \times n}$ with $B^T = B$, there exists an orthogonal matrix $Q = \begin{bmatrix} q_1 & \cdots & q_n \end{bmatrix}$ s.t. $Q^T BQ = \Lambda = diag(\lambda_1, \cdots, \lambda_n)$, where λ_i are eigenvalues and q_i are eigenvectors.

$$Q^T BQ = \Lambda \Longleftrightarrow BQ = Q\Lambda \Longleftrightarrow$$

$$B \begin{bmatrix} q_1 & \cdots & q_n \end{bmatrix} = \begin{bmatrix} q_1 & \cdots & q_n \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

For a matrix A, $\|A\|_2 = \sigma_1(A)$ where $A = U\Sigma V^T \in R^{m\times n}$, $U^T U = V^T V = I$, $\Sigma = diag(\sigma_1, \cdots, \sigma_n)$, $\sigma_1 \geq \cdots \geq \sigma_n > 0$

$A^T A = V\Sigma^T \Sigma V^T$. Largest eigenvalue of $A^T A = \sigma_1^2$, $\|A\|_2 = \sqrt{(\text{largest eigen value of } A^T A)}$

Consider $Ax = b$, $A \in R^{n\times n}$. $Cond_p(A) = \|A\|_p \left\|A^{-1}\right\|_p$, $Cond_2(A) = \|A\|_2 \left\|A^{-1}\right\|_2 = \sigma_1 \times ?$

Assume $rank(A) = n$, $A = U\Sigma V^T$, $A^{-1} = V\Sigma^{-1}U^T$, hence $\left\|A^{-1}\right\|_2 = \frac{1}{\sigma_n}$,

$$Cond_2(A) = \sigma_1/\sigma_n$$

.

Pseudo-Inverse from SVD

Assume $A \in R^{m \times n}$has its SVD

$$A = U\Sigma V^T = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \\ 0 & 0 \\ & \end{bmatrix} \begin{bmatrix} V_1 & V_2 \end{bmatrix}^T \text{ where}$$

$\Sigma_1 = diag(\sigma_1, \cdots, \sigma_r)$, $\sigma_1 \geq \cdots \geq \sigma_r > 0$

The pseudo-inverse is $A^+ = V \begin{bmatrix} \Sigma_1^{-1} & \\ & \end{bmatrix} U^T$

which is the unique minimal Frobenius norm solution to $\min_{X \in \mathbf{R}^{n \times m}} \|AX - I_m\|_F$.

If $rank(A) = n$, $A^+ = (A^T A)^{-1} A^T$

If $rank(A) = n = m$, $A^+ = A^{-1}$

Moore-Penrose pseudo-inverse A^+ for $A \in \mathbf{R}^{m \times n}$ is a unique matrix X that satisfies:

1. $AXA = A$ 2. $XAX = X$ 3. $(AX)^T = AX$ 4. $(XA)^T = XA$

Note: LS solution for $\min \|Ax - b\|_2$: $x_{LS} = A^+ b$

For any matrix $A \in R^{m \times n}$, $\exists$ matrices U, V, Σ such that

$$A = U \Sigma V^T$$

where $U \in R^{m \times m}, U^T U = I_m$; $V \in R^{n \times n}, V^T V = I_n$, $\Sigma \in R^{m \times n}$ such that

$$\Sigma = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ & 0 & \end{bmatrix} \text{ when } m \geq n, \; \Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & 0 \\ & & \sigma_m & \end{bmatrix}$$

when $m \leq n$

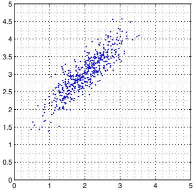
Let $U \Sigma V^T = \begin{bmatrix} U_k & \hat{U}_k \end{bmatrix} \begin{bmatrix} \Sigma_k & 0 \\ 0 & \hat{\Sigma}_k \end{bmatrix} \begin{bmatrix} V_k & \hat{V}_k \end{bmatrix}^T$ and

$A_k = U_k \Sigma_k V_k^T$: Truncated SVD

Then $\min_{rank(B)=k} \|A - B\|_F = \|A - A_k\|_F$ for $k \leq rank(A)$

Image Compression, Text Analysis (LSI), Signal Processing, ...

Consider data points in a two-dimensional space:



How can we use one variable to describe these data points?

Principal Component Analysis

Input: Data matrix $A_{m\times n}$ (m features, n data items)

Method 1 to compute PCA

1. Center the data matrix, and obtain $\tilde{A} = A - \frac{1}{n}Aee^T$ where $e = ones(n, 1)$
2. Compute SVD: $\tilde{A} = U\Sigma V^T$
3. Use U^T to transform centered data: $\tilde{A} \rightarrow U^T\tilde{A}$

Method 2 to compute PCA

1. Compute covariance matrix Ω from centered data: $\Omega = \tilde{A}\tilde{A}^T$
2. Compute SymEVD of $\Omega = U\Lambda U^T$
3. Use U^T to transform centered data: $\tilde{A} \rightarrow U^T\tilde{A}$

Dimension reduction by SVD computes SVD of A, not $\tilde{A}$

Avoid Squaring Matrices if possible!

- Example: $A = \begin{bmatrix} 1 & 1 \\ 10^{-3} & \\ & 10^{-3} \end{bmatrix}$, $b = \begin{bmatrix} 2 \\ 10^{-3} \\ 10^{-3} \end{bmatrix}$

  $x_{LS} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $K_2(A) \approx 1.4 \times 10^3$.
  Assume $\beta = 10,\ t = 6$, chopped arithmetic.

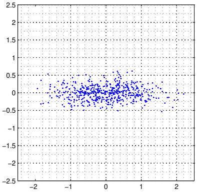
  $fl(A^T A) = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, $rank(A) = 2,\ rank(fl(A^T A)) = 1$.

  Assume $\beta = 10,\ t = 7,\ fl(A^T A) = \begin{bmatrix} 1 + 10^{-6} & 1 \\ 1 & 1 + 10^{-6} \end{bmatrix}$,
  $\hat{x} = \begin{bmatrix} 2.00001 \\ 0 \end{bmatrix}$ where $\hat{x}$ is solution for $fl(A^T A)x = fl(A^T b)$.

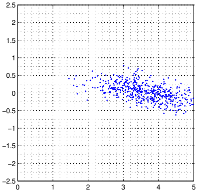
  $\frac{\|\hat{x} - x_{LS}\|_2}{\|x_{LS}\|_2} \approx \mu K_2(A^T A) = \mu (1.4 \times 10^3)^2$.

The previous example on two-dimensional data:

After PCA:



After SVD directly applied to A (instead of $\bar{A}$):

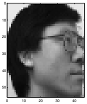


PCA and SVD for Image Compression

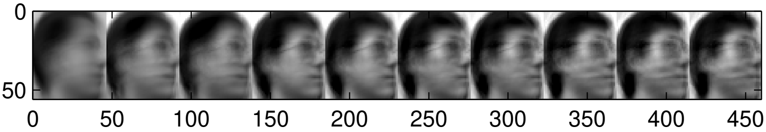
In a face data set, we have $n = 575$ images, each with $m = 56 \times 46 = 2576$ pixels.

We want to find lower rank approximation of the data matrix $A_{2576 \times 575}$ with $k = 2, 4, \cdots, 20$.

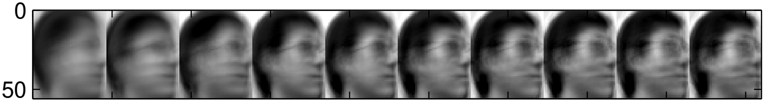
One of the original images:



After PCA (rank-k approximation of the covariance matrix):

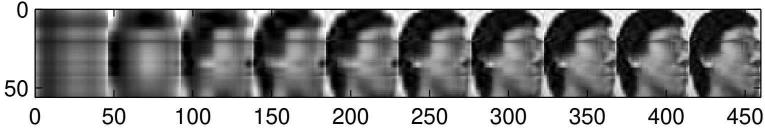


After SVD (rank-k approximation of the data matrix):



SVD for Image Compression (of *one* image)

Use a matrix $A_{56\times46}$ to represent one image.
Again, we use SVD to find the best rank-k approximation of A.
The images corresponding to best rank-k approximations $(k = 1, 2, \cdots, 10)$:

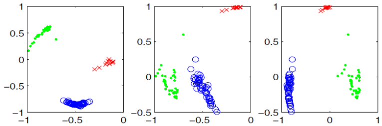


Apply SVD to the term-document matrix.
An example of term-document matrix: (from Wikipedia)

1. D1: "I like databases"
2. D2: "I hate hate databases"
3. ...

	D1	D2	...
I	1	1	...
like	1	0	...
hate	0	2	...
databases	1	1	...
⋮	⋮	⋮	⋱

LSI extracts k latent semantics represented by k orthogonal basis vectors: [Xu et al, 2003]



(b) Data distribution in the SVD subspace of $E_1 - E_2$, $E_1 - E_3$, and $E_2 - E_3$, respectively.

where E_1, E_2, E_3 are the first 3 columns of U in the SVD of term-document matrix A.

Orthogonal Procrustes Problem

$$\min_{Q, Q^T Q = I} \|AQ - B\|_F, \; A, B \in R^{m \times n}.$$

Solution is obtained from the Polar Decomposition of $A^T B$.

Polar Decomposition of a matrix $A \in \mathbf{R}^{m \times n}$ is:
$A = UP$
where $U \in \mathbf{R}^{m \times n}$ has orthonormal columns and
$P \in \mathbf{R}^{n \times n}$ is symmetric positive semidefinite.

Polar Decomposition can be computed from SVD:
$A = U \Sigma V^T = (UV^T)(V \Sigma V^T)$

QR Algorithm for Symmetric EVD

- Reduce A ($A = A^T$) to a tridiagonal matrix T: $U^T AU = T$, where U is an orthogonal matrix.
- Repeat:
  - Choose λ as an approximate eigenvalue of T
  - Compute QRD of $T - \lambda I$: $T - \lambda I = QR$,
  - $T_{new} := RQ + \lambda I$
- T_{new} is similar to T
- QRD of T is very fast: apply Givens rotations to make sub-diagonal entries of T zero
- Shift possibilities: $\lambda = T_{nn}$ or $\lambda = \mu$ where μ is the eigenvalue of $T(n-1:n, n-1:n)$ that is closer to T_{nn} (Wilkinson shift).
- Complexity of QR algorithm for Sym. EVD: $O(n^2)$ without eigenvectors and $O(n^3)$ with eigenvectors.

Jacobi Algorithm for Symmetric EVD

$A \in R^{n\times n}$, $A^T = A$, $Q^T AQ = D = diag(\lambda_1, \cdots, \lambda_n)$

1. QR algorithm, faster
2. Jacobi algorithm, **easy to parallelize**

After each step, the matrix becomes "more diagonal".

$A = \begin{bmatrix} x & y \\ y & z \end{bmatrix} \in R^{2\times 2}, \begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} x & y \\ y & z \end{bmatrix} \begin{bmatrix} c & s \\ -s & c \end{bmatrix} =$
$\begin{bmatrix} ? & 0 \\ 0 & ? \end{bmatrix}$
$\Rightarrow y(c^2 - s^2) + (x - z)cs = 0.$

Jacobi Algorithm

A measure to check how close a matrix is to a diagonal form:

$$off(A) = \sqrt{\sum_{j=1}^{n} \sum_{i=1, i \neq j}^{n} a_{ij}^2} = \|A\|_F^2 - \sum_{i=1}^{n} a_{ii}^2$$

- Jacobi algorithm decreases $off(A)$?

Let $B = J^T AJ$, where $J = J(p, q, \theta)$. $Off^2(B) = \|B\|_F^2 - \sum_{i=1}^{n} b_{ii}^2 = \|A\|_F^2 - \left(\sum_{i=1}^{n} a_{ii}^2 + 2a_{pq}^2\right) = off^2(A) - 2a_{pq}^2$, where (p, q) is two entries zeroed out.
Given that $a_{pq} \neq 0$, we have $off^2(B) \leq off^2(A)$ after 1 step.

Algorithms for SVD: Discussion

How do you use the ideas of QR algorithm or Jacobi algorithm for SymEVD to compute SVD?