Some NLA practice

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Numerical Linear Algebra. Skoltech

Lectures 7-8 recap

Matrix decompositions and linear systems

In a least-squares, or linear regression, problem, we have measurements $X \in \mathbb{R}^{m \times n}$ and $y \in \mathbb{R}^m$ and seek a vector $\theta \in \mathbb{R}^n$ such that $X\theta$ is close to y. Closeness is defined as the sum of the squared differences:

$$\sum_{i=1}^{m} (x_i^\top \theta - y_i)^2$$

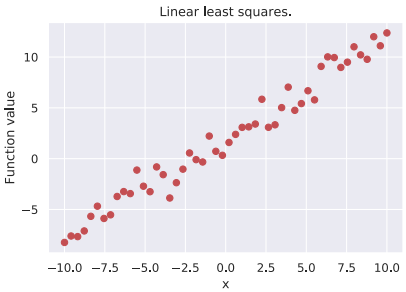
$$\|X\theta - y\|_2^2 \to \min_{\theta \in \mathbb{R}^n}$$

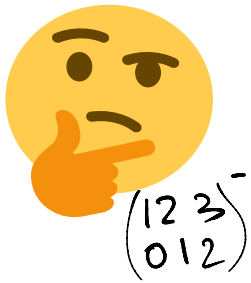
$$X\theta^* = y$$

is convex

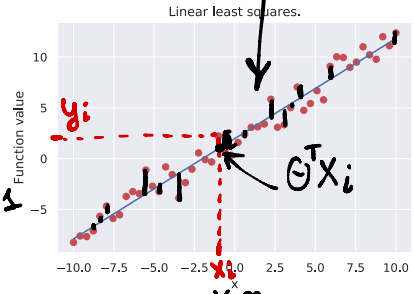
$Ax = b$

θ_0, θ_1





$\begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & 2 \end{pmatrix}^{-1}$



$X\theta = y$

$\rightarrow \theta = X^{-1} y$

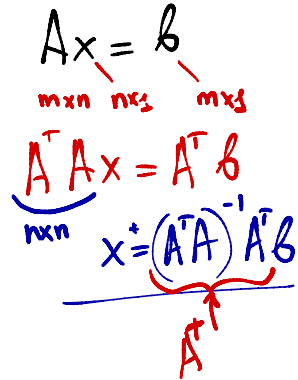
Figure 1: Illustration of linear system aka least squares

Matrix decompositions and linear systems. Approaches

Moore–Penrose inverse

If the matrix X is relatively small, we can write down and calculate exact solution:

$$\theta^* = (X^\top X)^{-1} X^\top y = X^\dagger y,$$



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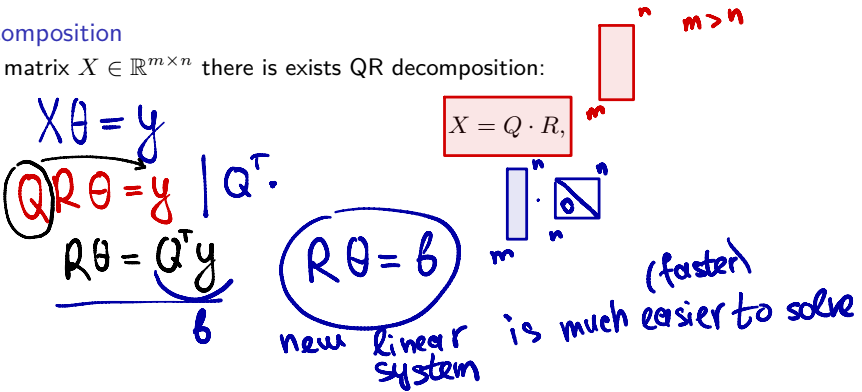
QR decomposition

For any matrix $X \in \mathbb{R}^{m \times n}$ there is exists QR decomposition:

$$X = Q \cdot R,$$



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where Q is an orthogonal matrix (its columns are orthogonal unit vectors) meaning $Q^\top Q = QQ^\top = I$ and R is an upper triangular matrix. It is important to notice, that since $Q^{-1} = Q^\top$, we have:

$$QR\theta = y \quad \longrightarrow \quad R\theta = Q^\top y$$

Now, process of finding theta consists of two steps:

1. Find the QR decomposition of X.

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1. Find the QR decomposition of X.
2. Solve triangular system $R\theta = Q^\top y$, which is triangular and, therefore, easy to solve.

Matrix decompositions and linear systems. Approaches

= LU in SPD case

Cholesky decomposition

For any positive definite matrix $A \in \mathbb{R}^{n \times n}$ there is exists Cholesky decomposition:

$$X^\top X = A = L^\top \cdot L,$$

where L is an lower triangular matrix. We have:

$$L^\top L\theta = y \quad \longrightarrow \quad L^\top z_\theta = y$$

Now, process of finding theta consists of two steps:

1. Find the Cholesky decomposition of $X^\top X$.

$X\theta = y$

$X^\top X\theta = X^\top y$

A $\quad$ b

$A\theta = b$

Note, that in this case the error stil proportional to the squared condition number.

why $X^\top X$ $\quad$ $X^\top X \geq 0$

$\forall y \in \mathbb{R}^n$: $\quad$ $y^\top X^\top X y \geq 0$

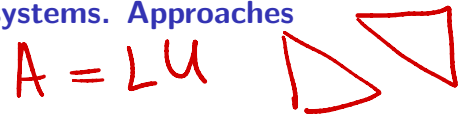
$y \neq 0$ $\quad$ $p^\top$ $\quad$ p $\quad$ $p \geq 0$

$p \neq 0$

for any X $\longrightarrow$ $A = X^\top X$

is SPD $\quad$ nxn

Matrix decompositions and linear systems. Approaches



Cholesky decomposition

For any positive definite matrix $A \in \mathbb{R}^{n \times n}$ there is exists Cholesky decomposition:

$$X^\top X = A = L^\top \cdot L,$$

if A is SPD

$A = LL^T$

where L is an lower triangular matrix. We have:

$$\boxed{L^\top L\theta = y} \quad \longrightarrow \quad \boxed{L^\top z_\theta = y}$$

z

we solve

$\Rightarrow z_\theta$

$L\theta = z$

Now, process of finding theta consists of two steps:

1. Find the Cholesky decomposition of $X^\top X$.
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3. Find the θ by solving triangular system $L\theta = z_\theta$

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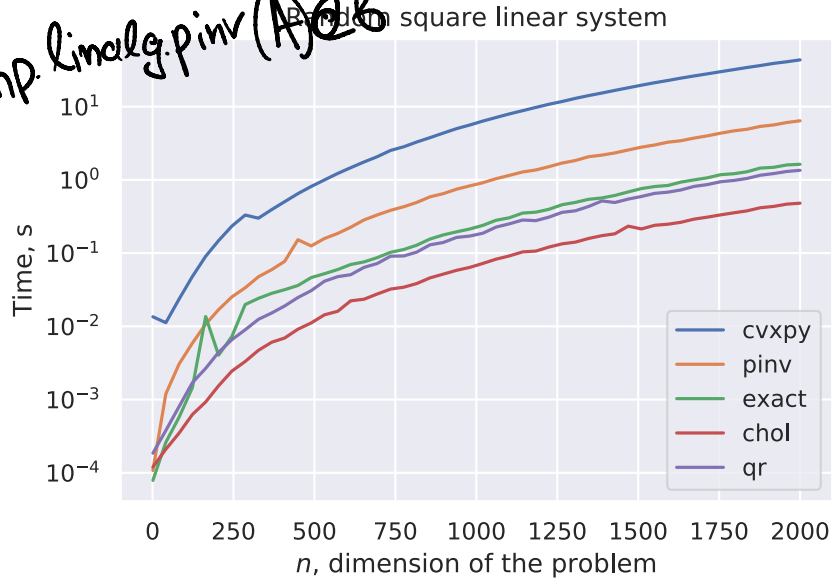
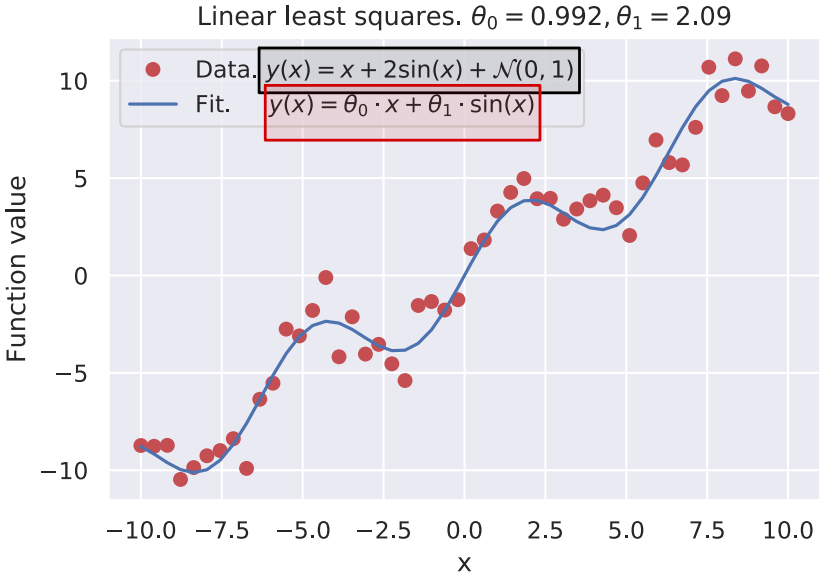
Matrix decompositions and linear systems. Approaches



Matrix decompositions and linear systems. Non-linear data



Gram–Schmidt process

Input: n linearly independent vectors $u_0, \ldots, u_{n-1}$.

Output: n linearly independent vectors, which are pairwise orthogonal $d_0, \ldots, d_{n-1}$.

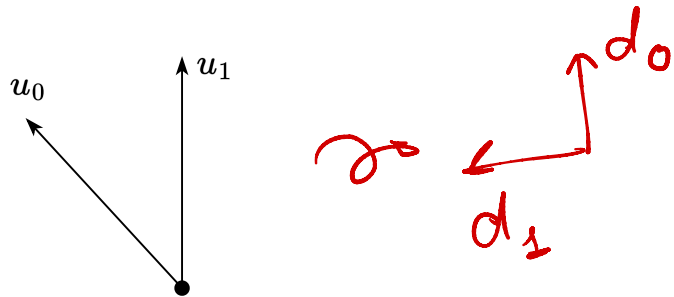


Figure 4: Illustration of Gram-Schmidt orthogonalization process

Gram–Schmidt process

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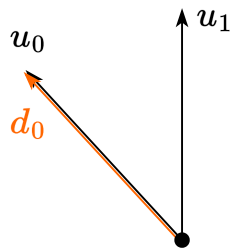

Figure 5: Illustration of Gram-Schmidt orthogonalization process

Gram–Schmidt process

Input: n linearly independent vectors $u_0, \ldots, u_{n-1}$.

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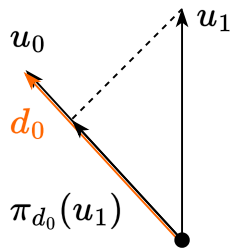

Figure 6: Illustration of Gram-Schmidt orthogonalization process

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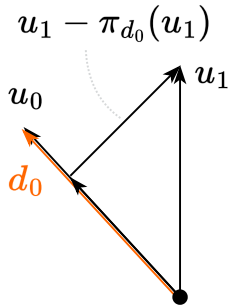

Figure 7: Illustration of Gram-Schmidt orthogonalization process

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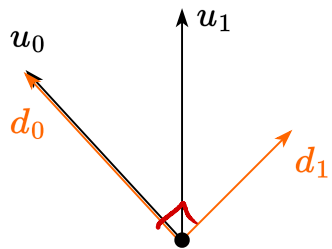

Figure 8: Illustration of Gram-Schmidt orthogonalization process

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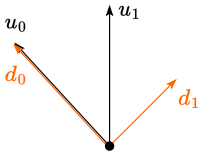
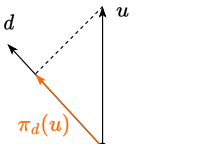
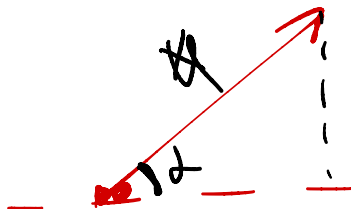
Input: n linearly independent vectors $u_0, \ldots, u_{n-1}$.





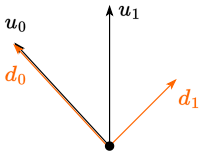
$$\pi_d(u) = \frac{\langle d, u \rangle}{\|d\|_2^2} d$$



$$\cos\alpha = \frac{\langle a, b \rangle}{\|a\| \cdot \|b\|}$$

$$\frac{d}{\|d\|} \cdot \|x\| \cdot \cos\alpha = \frac{d}{\|d\|} \cdot \|x\| \cdot \frac{\langle d, u \rangle}{\|d\| \cdot \|x\|}$$

Gram–Schmidt process



Input: n linearly independent vectors $u_0, \ldots, u_{n-1}$.
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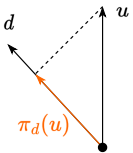
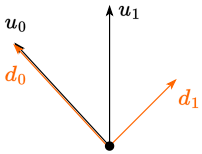
$$d_0 = u_0$$



$$\pi_d(u) = \frac{\langle d, u \rangle}{\|d\|_2^2} d$$

Gram–Schmidt process



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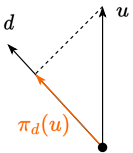

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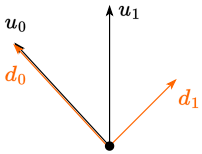

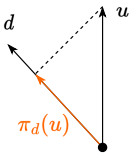

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$$d_1 = u_1 - \pi_{d_0}(u_1)$$
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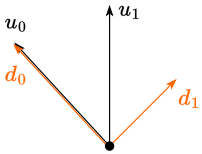
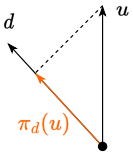
Gram–Schmidt process





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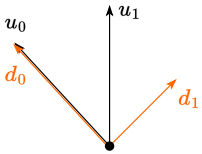
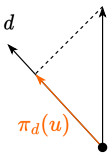
Gram–Schmidt process





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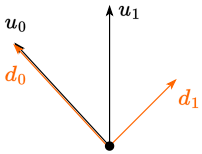
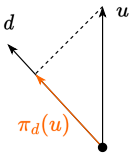
Gram–Schmidt process





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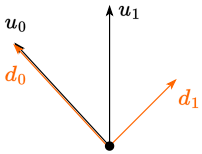
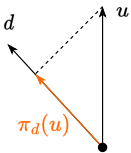
Gram–Schmidt process





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\end{aligned}$$

$$d_k = u_k + \sum_{i=0}^{k-1} \beta_{ik} d_i \qquad \beta_{ik} = -\frac{\langle d_i, u_k \rangle}{\langle d_i, d_i \rangle} \tag{1}$$

Here's how you can structure the final slide to illustrate the **Gram-Schmidt process** in matrix form via QR decomposition:

Gram–Schmidt process in Matrix Form via QR Decomposition

Step-by-step process in matrix notation:

- Given a matrix A with columns $u_0, u_1, \ldots, u_{n-1}$, the goal is to decompose A into:

$$A = QR$$

where:

Gram–Schmidt process in Matrix Form via QR Decomposition

Step-by-step process in matrix notation:

- Given a matrix A with columns $u_0, u_1, \ldots, u_{n-1}$, the goal is to decompose A into:

$$A = QR$$

where:

- Q: an orthogonal matrix whose columns are the orthonormal vectors $q_0, q_1, \ldots, q_{n-1}$.

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Gram-Schmidt ≃ QR decomp.

Illustration:

$$v_k = u_k - \sum_{i=0}^{k-1} \langle u_k, q_i \rangle q_i \qquad q_k = \frac{v_k}{\|v_k\|} \qquad R_{ij} = \langle u_j, q_i \rangle \qquad \text{for } i \leq j$$

$$\text{For } A = \begin{bmatrix} | & | & & | \\ u_0 & u_1 & \cdots & u_{n-1} \\ | & | & & | \end{bmatrix} \rightarrow Q = \begin{bmatrix} | & | & & | \\ q_0 & q_1 & \cdots & q_{n-1} \\ | & | & & | \end{bmatrix}, \quad R = \begin{bmatrix} r_{00} & r_{01} & \cdots & r_{0(n-1)} \\ 0 & r_{11} & \cdots & r_{1(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{(n-1)(n-1)} \end{bmatrix}$$

QR decomposition

GS is cool but not very practical (instability issues)

FASTEST

$$A = \begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}_{m \times n} \begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}_{n \times n} \qquad m \geq n$$

Q is left unitary

R

Givens rotations + Householder reflections

QR

there is stable modification of GS

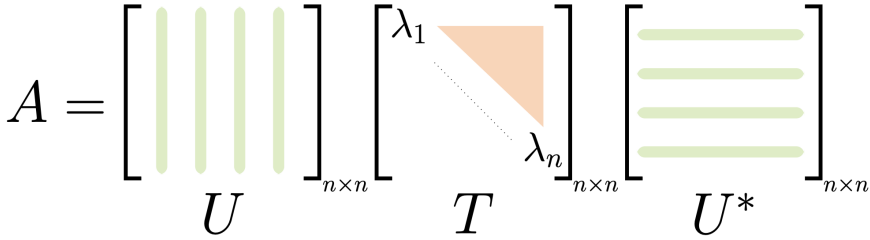
$$A = \begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}_{m \times m} \begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}_{m \times n} \qquad m < n$$

Q is unitary

R

Schur form

Schur



- U is unitary
- $\lambda_1, \ldots, \lambda_n$ are *eigenvalues*
- columns of U are *Schur vectors*

Figure 10: Decomposition

QR algorithm

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QR algorithm

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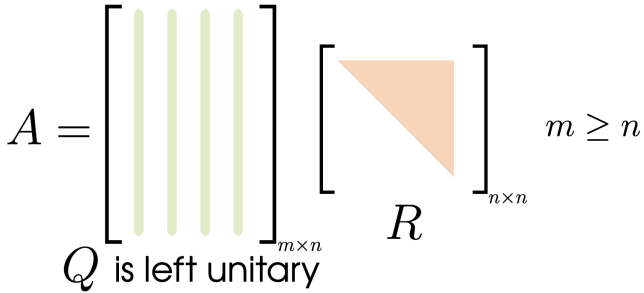
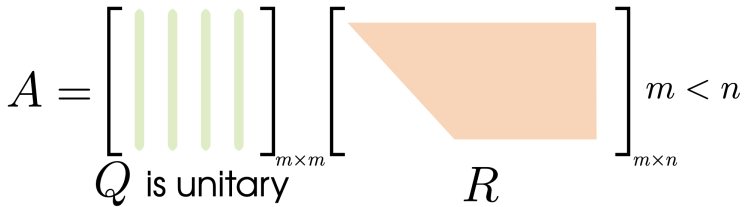
- Do not **mix** QR algorithm and QR decomposition!
- QR decomposition is the representation of a matrix, whereas QR algorithm uses QR decomposition to compute the eigenvalues!

SVD

QR

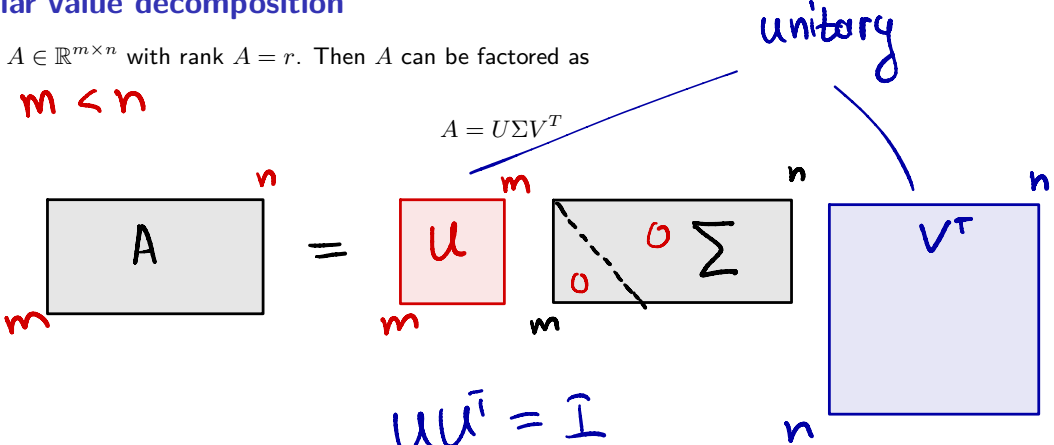

$A =$
$m \times n$
$n \times n$
$m \geq n$
Q is left unitary
R


$A =$
$m \times m$
$m \times n$
$m < n$
Q is unitary
R

Singular value decomposition

Suppose $A \in \mathbb{R}^{m \times n}$ with rank $A = r$. Then A can be factored as

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



$$UU^T = I$$

$$U^T U = I$$

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Suppose $A \in \mathbb{R}^{m \times n}$ with rank $A = r$. Then A can be factored as

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where $U \in \mathbb{R}^{m \times m}$ satisfies $U^T U = I$, $V \in \mathbb{R}^{n \times n}$ satisfies $V^T V = I$, and Σ is a matrix with non-zero elements on the main diagonal $\Sigma = \text{diag}(\sigma_1, ..., \sigma_r) \in \mathbb{R}^{m \times n}$, such that

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This factorization is called the **singular value decomposition (SVD)** of A. The columns of U are called left singular vectors of A, the columns of V are right singular vectors, and the numbers σ_i are the singular values. The singular value decomposition can be written as

$$A = \sum_{i=1}^{r} \sigma_i u_i v_i^T,$$

where $u_i \in \mathbb{R}^m$ are the left singular vectors, and $v_i \in \mathbb{R}^n$ are the right singular vectors.

Singular value decomposition

$S^n_{++} : A \in \mathbb{R}^{nn}$, $A \succ 0$

$A \in \mathbb{R}^{m \times n}$ $m > n$

$A^T A$ - full rank
$A A^T$ - singular

} square, symmetric, positive definite (semi)

Question

Suppose, matrix $A \in \mathbb{S}^n_{++}$. What can we say about the connection between its eigenvalues and singular values?

$\mathbb{S}^n_+ : A \succeq 0$

$\lambda(A^T A) =$

SPECTRAL DECOMP.:

$$A^T A = Q \cdot \Lambda \cdot Q^T$$

$U \; \Sigma \; V \quad \text{diag}(\lambda_1, \ldots, \lambda_n)$

Singular value decomposition

$A = U\Sigma V^*$

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

$A^*A = Q\Lambda Q^*$

$V\Sigma^T U^* \cdot U\Sigma V^* = V\Sigma^T\Sigma V^* = V\Sigma^2 V^*$ ($U^*U = I$)

Question

Suppose, matrix $A \in \mathbb{S}^n_{++}$. What can we say about the connection between its eigenvalues and singular values?

Question

How do the singular values of a matrix relate to its eigenvalues, especially for a symmetric matrix?

$Q\Lambda Q^* = V\Sigma^2 V^*$

$\sigma(A) = \sqrt{\lambda(A^*A)}$

$\lambda(A^TA) = \sigma^2(A)$

Skeleton decomposition

Simple, yet very interesting decomposition is Skeleton decomposition, which can be written in two forms:

$$A = UV^T \quad A = \hat{C}\hat{A}^{-1}\hat{R}$$

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Use cases for Skeleton decomposition are:

- Model reduction, data compression, and speedup of computations in numerical analysis: given rank-r matrix with $r \ll n, m$ one needs to store $\mathcal{O}((n+m)r) \ll nm$ elements.

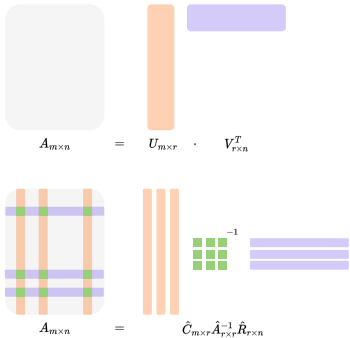

Figure 12: Illustration of Skeleton decomposition

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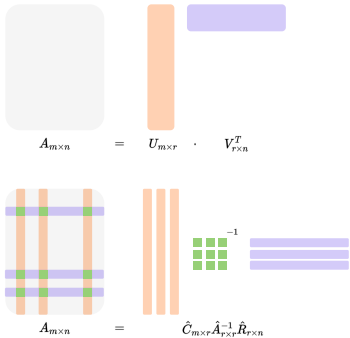

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- All applications where SVD applies, since Skeleton decomposition can be transformed into truncated SVD form.

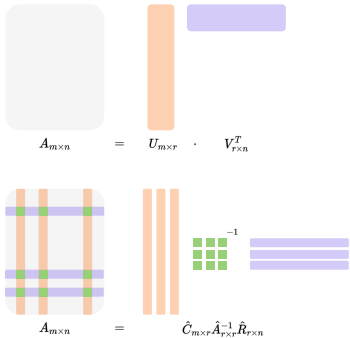

Figure 12: Illustration of Skeleton decomposition

Canonical tensor decomposition

One can consider the generalization of Skeleton decomposition to the higher order data structure, like tensors, which implies representing the tensor as a sum of r primitive tensors.

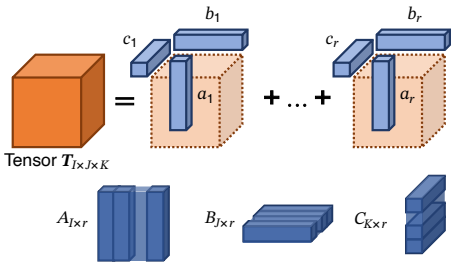

Figure 13: Illustration of Canonical Polyadic decomposition

Example

Note, that there are many tensor decompositions: Canonical, Tucker, Tensor Train (TT), Tensor Ring (TR), and others. In the tensor case, we do not have a straightforward definition of *rank* for all types of decompositions. For example, for TT decomposition rank is not a scalar, but a vector.

Problems

Example. Simple yet important idea on matrix computations.

Suppose, you have the following expression

$$b = A_1 A_2 A_3 x,$$

where the $A_1, A_2, A_3 \in \mathbb{R}^{3\times 3}$ - random square dense matrices and $x \in \mathbb{R}^n$ - vector. You need to compute b.

Which one way is the best to do it?

1. $A_1 A_2 A_3 x$ (from left to right)

Check the simple code snippet after all.

$$f(x) : \mathbb{R}^n \longrightarrow \mathbb{R}$$

$$f(x) = \frac{1}{2} x^T A^T A x - b^T x$$

$$A \qquad y = Ax$$

$$= \frac{1}{2} y^T y - b^T x$$

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3. It does not matter
4. The results of the first two options will not be the same.

Check the simple code snippet after all.

Problem 1

Find SVD of the following matrix:

$$A = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

3×1

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

$3 \times 3 \quad 3 \times 1 \quad 1 \times 1$

$$\Sigma = \begin{pmatrix} \sqrt{14} \\ 0 \\ 0 \end{pmatrix} \qquad V^T = 1$$

Solution

1. $A^T A$

$1 + 4 + 9 = 14 = \lambda(A^T A) = 14$

$\sigma(A) = \sqrt{\lambda(A^T A)} = \sqrt{14}$

2. We need to find eigenvectors of

$eig(A^T A) = 1$

$\lambda(AA^T) =$ AA^T

$(14, 0, 0)$

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 3 & 6 & 9 \end{pmatrix}$$

$\det(AA^T - \lambda I) =$

2. We need to find an eigenvec

Problem 1

Find SVD of the following matrix:

$$A = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = U \Sigma V^T = \begin{pmatrix} \frac{1}{\sqrt{14}} & & \\ \frac{2}{\sqrt{14}} & & \\ \frac{3}{\sqrt{14}} & & \end{pmatrix}_{3\times 3} \begin{pmatrix} \sqrt{14} \\ 0 \\ 0 \end{pmatrix} \cdot 1$$

Eigenvectors of $AA^T = \tilde{A}$

$\tilde{A}\ell = \lambda\ell$

1. Calculate λ using:

$\det(\tilde{A} - \lambda I) = 0$

$\hookrightarrow (14, 0, 0)$

2. $\begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 3 & 6 & 9 \end{pmatrix} \cdot \begin{pmatrix} \ell_1 \\ \ell_2 \\ \ell_3 \end{pmatrix} = 14 \begin{pmatrix} \ell_1 \\ \ell_2 \\ \ell_3 \end{pmatrix} \rightarrow$ solving $\rightarrow \begin{pmatrix} \ell_1 \\ \ell_2 \\ \ell_3 \end{pmatrix} \ell$

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Any vector e: $Ae = \lambda e$ will be an eigenvector, but typically we choose $\|e\|_2 = 1$

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Find SVD of the following matrix:

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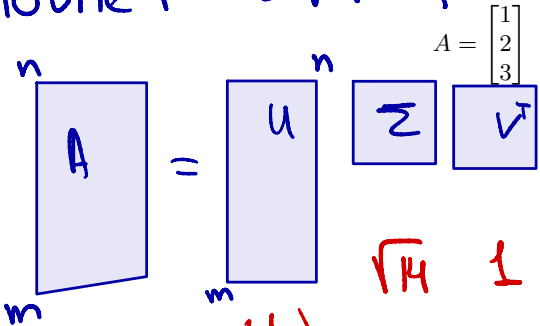
Another SVD form



$r = n$

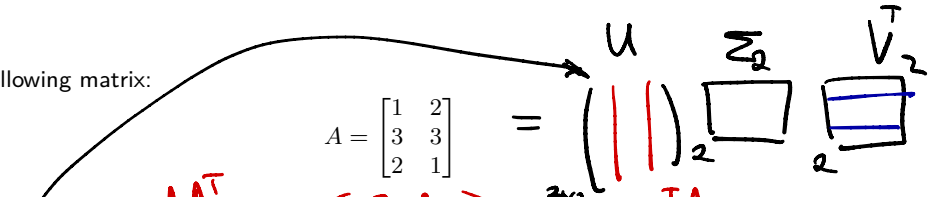
$\sqrt{14}$ 1

$\frac{1}{\sqrt{14}}$
$\frac{2}{\sqrt{14}}$
$\frac{3}{\sqrt{14}}$

Problem 2

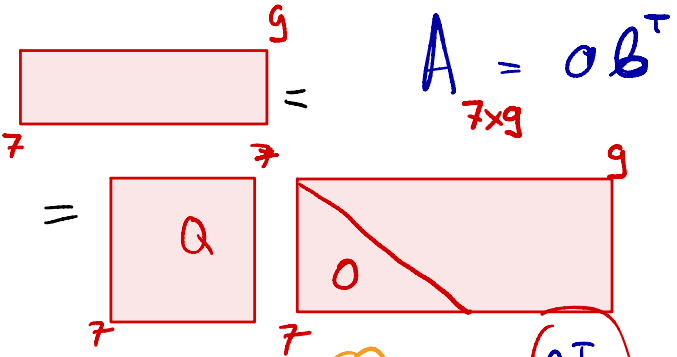
Find SVD of the following matrix:

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 3 \\ 2 & 1 \end{bmatrix}$$

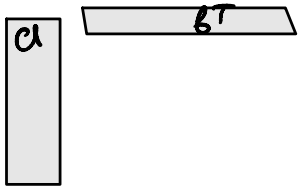


Problem 3

Find R matrix in QR decomposition for matrix $A = ab^T$, where $a = [1, 2, 1, 2, 1, 2, 1], b = [1, 2, 3, 4, 5, 6, 7, 8, 9]$



$A = aB^T$, 7×9



SVD of A:

$A = U \Sigma V^T$

7×7 7×7 7×9

$Q = U$ V

$R = \Sigma V^T$?

$SVD(aB^T) = \frac{a}{\|a\|} \|a\|\cdot\|b\| \frac{B^T}{\|b\|}$

U Σ V^T

Problem

$$\begin{pmatrix} \frac{a}{\|a\|} & 0 & 0 \\ & 0 & 0 \end{pmatrix}$$

U

$$a = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \qquad \|a\| = \sqrt{14}$$

$$\begin{pmatrix} \frac{1}{\sqrt{14}} & 0 & 0 & 0 & 0 \\ \frac{2}{\sqrt{14}} & 0 & 0 & 0 & 0 \\ \frac{3}{\sqrt{14}} & 0 & 0 & 0 & 0 \end{pmatrix}$$

Problem

$$A = a b^T = \frac{a}{\|a\|} \cdot \frac{\|a\| \cdot \|b\| \cdot b^T}{\|b\|} =$$

$$= \frac{a}{\|a\|} \cdot \|a\| \cdot b^T$$

Q R