



**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:

$$\sum_{i=1}^m (x_i^\top \theta - y_i)^2 \quad \|X\theta - y\|_2^2 \rightarrow \min_{\theta \in \mathbb{R}^n} \quad X\theta^* = y$$

Linear least squares.



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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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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:

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

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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

## Cholesky decomposition

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

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

where  $L$  is a lower triangular matrix. We have:

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

Now, the process of finding  $\theta$  consists of two steps:

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

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

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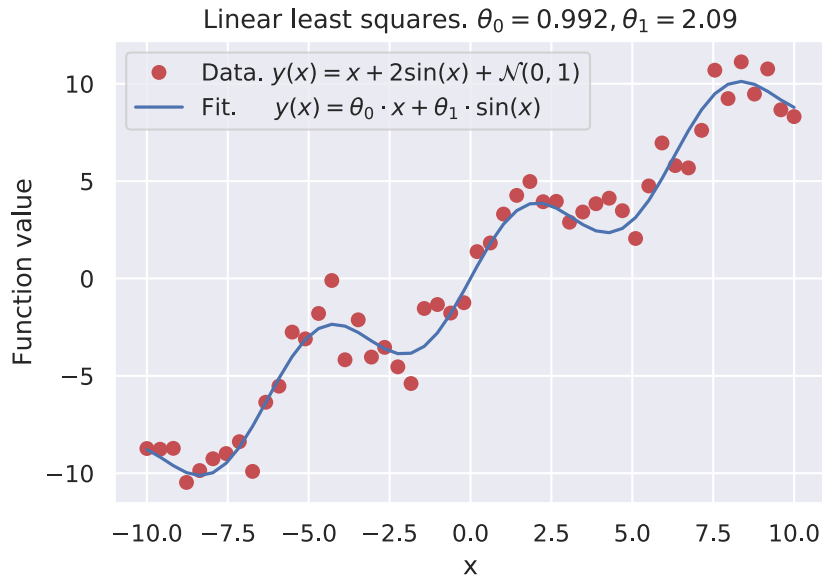
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# Matrix decompositions and linear systems. Approaches



## Matrix decompositions and linear systems. Non-linear data



## Gram–Schmidt process

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

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



Figure 4: Illustration of Gram-Schmidt orthogonalization process

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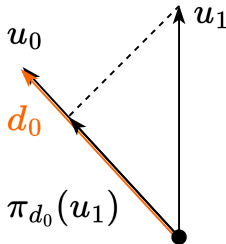


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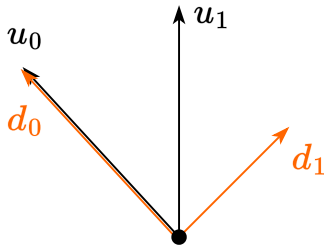
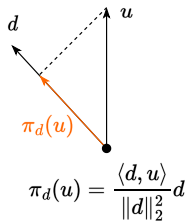
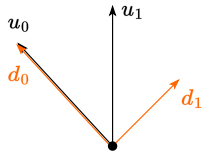


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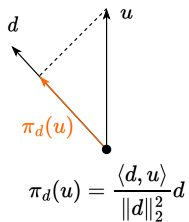


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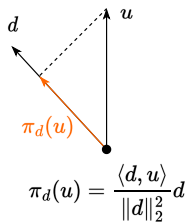
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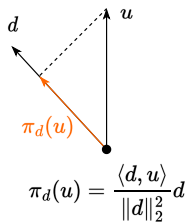
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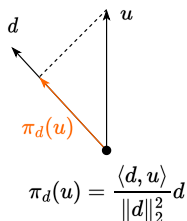
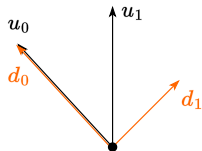
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$$d_k = u_k + \sum_{i=0}^{k-1} \beta_{ik} d_i \quad \beta_{ik} = -\frac{\langle d_i, u_k \rangle}{\langle d_i, d_i \rangle} \quad (1)$$

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  $u_0, u_1, \dots, u_{n-1}$ , the goal is to decompose  $A$  into:

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## Illustration:

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

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

# QR decomposition

QR

$$A = \begin{bmatrix} \text{4 green vertical bars} \end{bmatrix}_{m \times n} \begin{bmatrix} \text{orange triangle} \end{bmatrix}_{n \times n} \quad m \geq n$$

$Q$  is left unitary

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$U \qquad T \qquad U^*$

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

Figure 10: Decomposition

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$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0.$$

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  $\sigma_i$  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

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

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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.

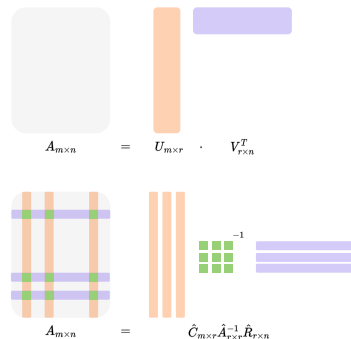


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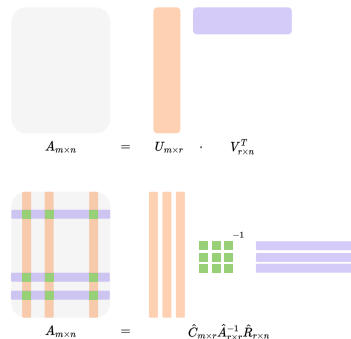


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- Feature extraction in machine learning, where it is also known as matrix factorization
- All applications where SVD applies, since Skeleton decomposition can be transformed into truncated SVD form.



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

### **i** 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?

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Check the simple  code snippet after all.

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3. It does not matter

Check the simple  code snippet after all.

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

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Find SVD of the following matrix:

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

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1. Compute  $A^T A$ :

$$A^T A = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = 1^2 + 2^2 + 3^2 = 14.$$

The singular values  $\sigma_i$  are the square roots of the eigenvalues of  $A^T A$ . Since  $A^T A$  is a  $1 \times 1$  matrix with value 14, the singular value is  $\sigma = \sqrt{14}$ .



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$$A = U \Sigma V^T = \begin{bmatrix} \frac{1}{\sqrt{14}} \\ \frac{2}{\sqrt{14}} \\ \frac{3}{\sqrt{14}} \end{bmatrix} \begin{bmatrix} \sqrt{14} \end{bmatrix} \begin{bmatrix} 1 \end{bmatrix}$$

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4. However, if you would like to use another form with square singular matrices:

$$A = U \Sigma V^T = \begin{bmatrix} \frac{1}{\sqrt{14}} \\ \frac{2}{\sqrt{14}} \\ \frac{3}{\sqrt{14}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{-5}{\sqrt{42}} \\ \frac{1}{\sqrt{3}} & \frac{4}{\sqrt{42}} \\ \frac{-1}{\sqrt{3}} & \frac{1}{\sqrt{42}} \end{bmatrix} \begin{bmatrix} \sqrt{14} \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \end{bmatrix}$$

## 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  $a = [1, 2, 1, 2, 1, 2, 1]$ ,  $b = [1, 2, 3, 4, 5, 6, 7, 8, 9]$

**Solution**