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:

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

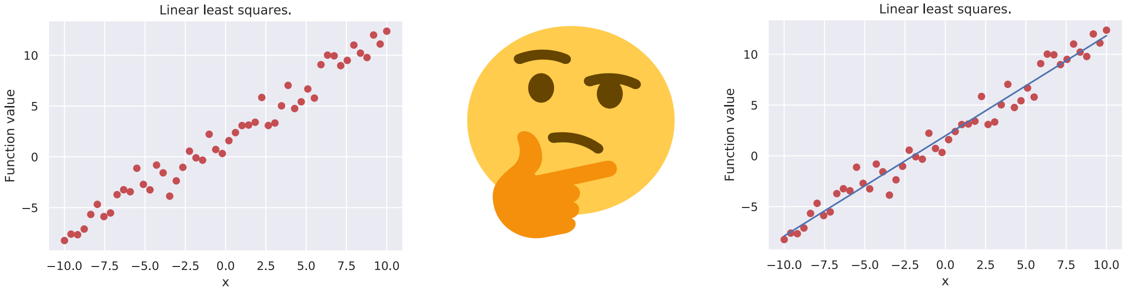

Figure 1: Illustration of linear system aka least squares

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

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

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:

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

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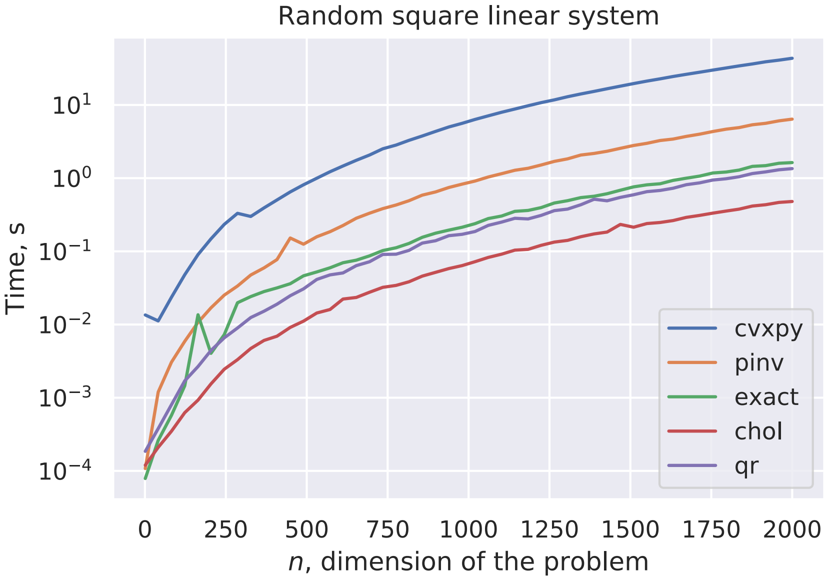
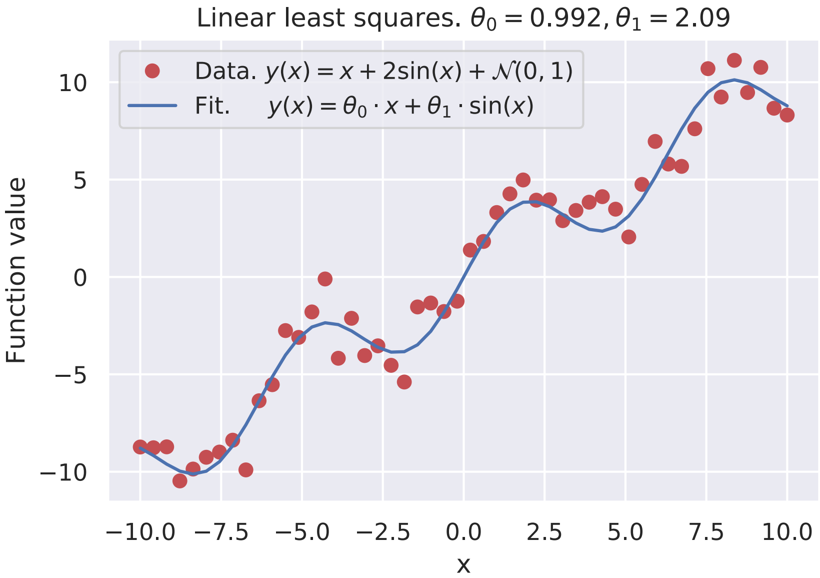
Matrix decompositions and linear systems. Approaches



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 $d_0, \ldots, d_{n-1}$.

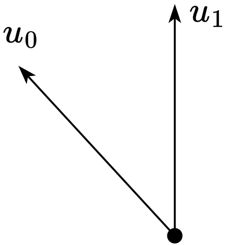


Figure 4: Illustration of Gram-Schmidt orthogonalization process

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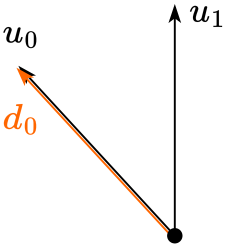

Figure 5: Illustration of Gram-Schmidt orthogonalization process

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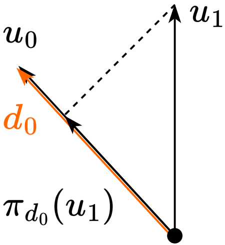

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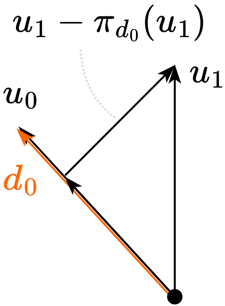

Figure 7: Illustration of Gram-Schmidt orthogonalization process

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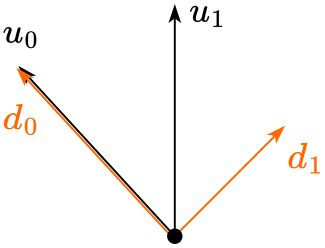
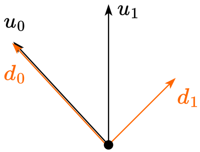
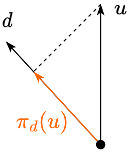


Figure 8: Illustration of Gram-Schmidt orthogonalization process

Gram–Schmidt process





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

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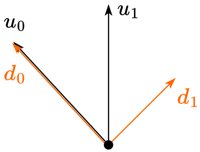

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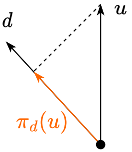

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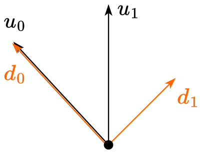

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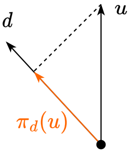

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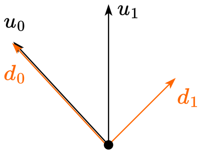

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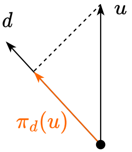

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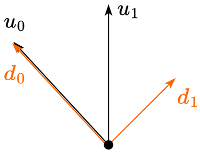

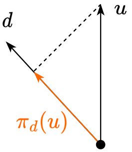

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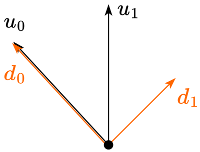

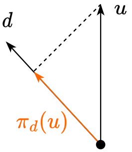

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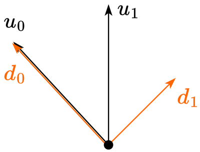

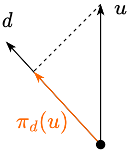

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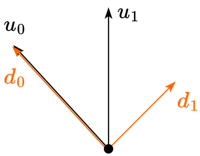

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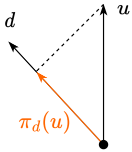

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$$
d_k = u_k + \sum_{i=0}^{k-1} \beta_{ik} d_i \qquad \beta_{ik} = -\frac{\langle d_i, u_k \rangle}{\langle d_i, d_i \rangle} \tag{1}
$$

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

$$A = QR$$

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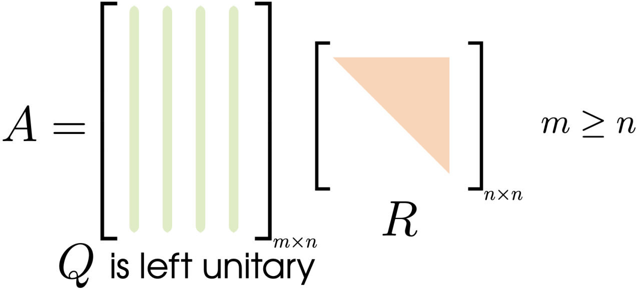
Illustration:

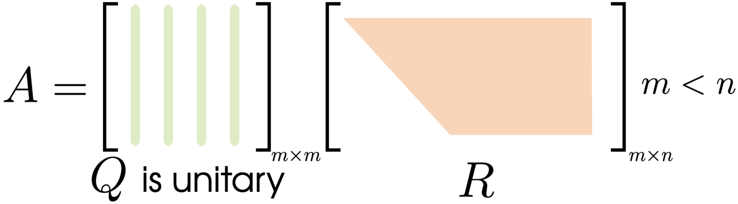
$$v_k = u_k - \sum_{i=0}^{k-1} \langle u_k, q_i \rangle q_i \qquad q_k = \frac{v_k}{\|v_k\|} \qquad R_{ij} = \langle u_j, q_i \rangle \qquad \text{for } i \leq j$$

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

QR decomposition

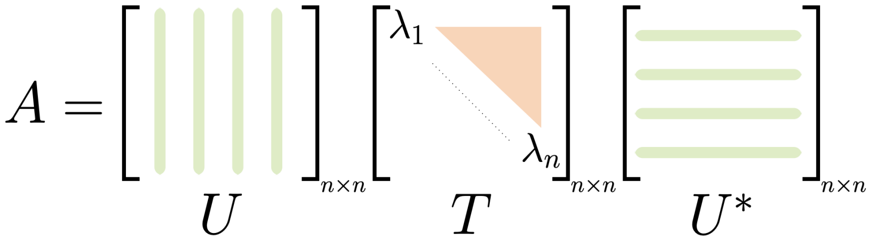
QR





Schur form

Schur



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

Figure 10: Decomposition

QR algorithm

- The QR algorithm was independently proposed in 1961 by Kublanovskaya and Francis.

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- Do not **mix** QR algorithm and QR decomposition!

QR algorithm

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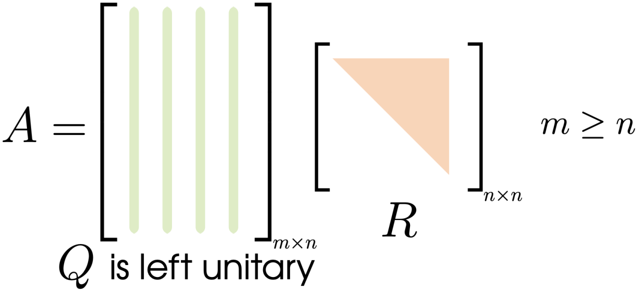
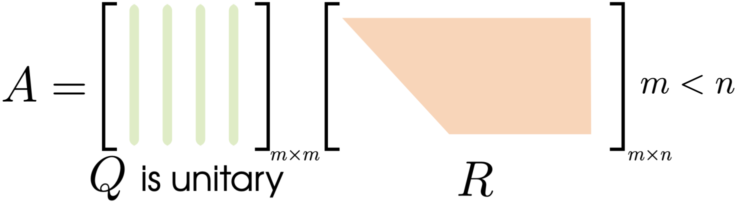
- Do not **mix** QR algorithm and QR decomposition!
- QR decomposition is the representation of a matrix, whereas QR algorithm uses QR decomposition to compute the eigenvalues!

SVD

QR


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


$A =$
$m \times m$
Q is unitary
R
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Singular value decomposition

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

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

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

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 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

Question

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

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Question

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

Skeleton decomposition

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- 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.

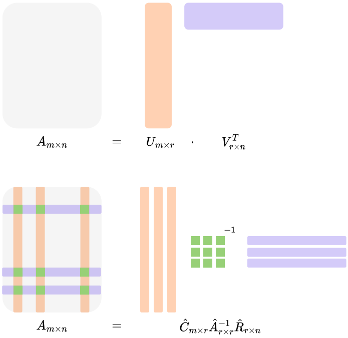

Figure 12: Illustration of Skeleton decomposition

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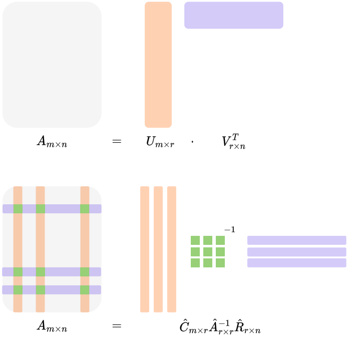

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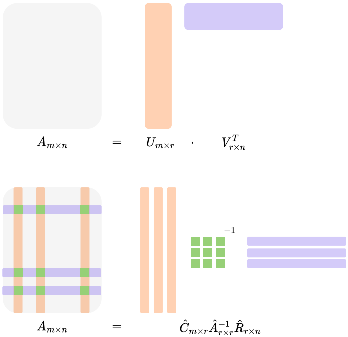
- All applications where SVD applies, since Skeleton decomposition can be transformed into truncated SVD form.



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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.

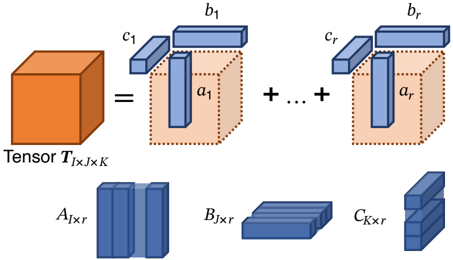

Figure 13: Illustration of Canonical Polyadic decomposition

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?

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Check the simple code snippet after all.

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3. It does not matter

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4. The results of the first two options will not be the same.

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Find SVD of the following matrix:

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

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1. Compute $A^T A$:

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

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3. The simplest form of SVD allows us to write:

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

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

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

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