# Computational Mathematics

**Adérito Araújo**
DMUC, University of Coimbra, Portugal


Coimbra, 2024

# Module Overview

# Numerical Linear Algebra

Computational Matehematics

Adérito Araújo (alma@mat.uc.pt)
February 7, 2024

## Syllabus

- What is numerical linear algebra?
  - Solving linear algebra problems using efficient algorithms on computers
- Module topics: direct and iterative methods for solving simultaneous linear equations ($Ax = b$)
  - Matrix factorization and decomposition.
  - Stationary iterative methods: Jacobi, Gauss-Seidel and relaxation methods
  - Non stationary iterative methods: Arnoldi and GMRES methods
  - The two-grid/multigrid and domain decomposition methods

## Syllabus

- Direct and iterative methods
  - Direct methods: solve the problem by a finite sequence of operations and in the absence of rounding errors, would deliver an exact solution; operate directly on elements of a matrix
  - Iterative methods: solve a problem by finding successive approximations to the solution starting from an initial guess, that hopefully converge to the true solution; often are easier to implement on parallel computers
- Prerequisite/co-requisite
  - Good knowledge in linear algebra
  - Programming experience in MATLAB (Fortran, C, C++)
  - Good numerical skils
- Required Textbook: Alfio Quarteroni, Riccardo Sacco, Fausto Saleri, Numerical Mathematics, Texts in Applied Mathematics Volume 37, 2007, ISBN: 978-1-4757-7394-1 (**Chapters 3 - 4**)
- Grading: Assignments ($5 \times 20\%$)

# Lecture 1

# Foundations of Matrix Analysis

Computational Mathematics

Adérito Araújo (alma@mat.uc.pt)
February 7, 2024

## Orthogonal Vectors and Matrices, Norms

## Transpose and Adjoint

- For real $A$, the transpose of $A$ is obtained by interchanging rows/columns

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} \Rightarrow A^T = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \end{bmatrix}$$

- The adjoint or hermitian conjugate also takes complex conjugates

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} \Rightarrow A^* = \begin{bmatrix} \bar{a}_{11} & \bar{a}_{21} & \bar{a}_{31} \\ \bar{a}_{21} & \bar{a}_{22} & \bar{a}_{32} \end{bmatrix}$$

- $A$ is symmetric (hermitian) if $A = A^T$ $(A = A^*)$

## Inner Product

- Inner product of two column vectors $x, y \in \mathbb{C}^n$

$$x^* y = \sum_{i=1}^{n} \bar{x}_i y_i$$

- Euclidean length of $x$

$$\|x\| = \sqrt{x^* x} = \left( \sum_{i=1}^{n} |x_i|^2 \right)$$

- Angle $\alpha$ between $x, y$

$$\cos \alpha = \frac{x^* y}{\|x\| \|y\|}$$

## Positive Definite Matrices

- A hermitian matrix A is symmetric (hermitian) positive definite if $x^T Ax > 0$ ($x^* Ax > 0$) for $x \neq 0$
- Exercise 1: $x^* Ax$ is always real
- Exercise 2: If $A \in \mathbb{C}^{m \times m}$ is PD and $X$ has full column rank, then $X^* AX$ is PD
- Any principal submatrix of a PD matrix $A$ is PD, and every diagonal entry $a_{ii} > 0$
- Exercise 3: PD matrices have positive real eigenvalues and orthogonal eigenvectors

## In MATLAB

| **Quantity** | **MATLAB Syntax** | **Comment** |
|---|---|---|
| Transpose of $A$ | `A.'` | Transpose only |
| Adjoint of $A$ | `A'` | Transpose + complex conjugate |
| Inner product $x^* y$ | `x'*y`<br>`dot(x,y)` | `'* assumes column vector` |
| Lenght $\|x\|$ | `sqrt(x'*x)`<br>`norm(x)` | `'* assumes column vector` |

## Orthogonal Vectors

- The vectors $x, y \in \mathbb{C}^n$ are orthogonal if

$$x^* y = 0$$

- The sets os vectors $X, Y$ are orthogonal of

every $x \in X$ is orthogonal to every $y \in Y$

- A set of (nonzero) vectors $S$ is orthogonal if

vectors pairwise orthogonal, i.e., for $x, y \in S$, $x \neq y \Rightarrow x^* y = 0$

and orthonormal if, in addition

every $x \in S$ has $\|x\| = 1$

## Orthogonal and Unitary Matrices

- A square matrix $Q \in \mathbb{C}^{n \times n}$ is unitary (orthogonal in real case) if

$$Q^* = Q^{-1}$$

- For unitary $Q$

$$Q^* Q = I \Leftrightarrow q_i^* q_j = \delta_{ij}$$

- Interpretation of unitary-times-vector product

$$\begin{aligned} x = Q^* b &= \text{solution to } Qx = b \\ &= \text{the vector of coefficients of the expansion of } b \\ &\quad \text{in the basis of columns of } Q \end{aligned}$$

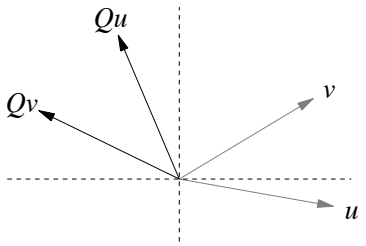
## Preservation of Geometry Structure

- Inner product is preserved under multiplication by unitary $Q$

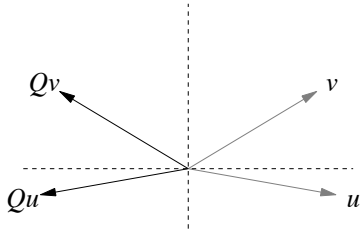
$$(Qx)^*(Qy) = x^*Q^*Qy = x^*y$$

- Therefore lengths of vectors and angles between vectors are preserved
- A real orthogonal $Q$ is either a rigid rotation or reflection

**Rotation**




**Reflection**




## Norms in MATLAB

| Quantity | MATLAB Syntax |
|---|---|
| $\|x\|_1$ | `sum(abs(x)) or norm(x,1)` |
| $\|x\|_2$ | `sqrt(x'*x) or norm(x)` |
| $\|x\|_p$ | `sum(abs(x).^p).^(1/p) or norm(x,p)` |
| $\|x\|_\infty$ | `max(abs(x)) or norm(x,inf)` |
| $\|A\|_1$ | `max(sum(abs(A),1)) or norm(A,1)` |
| $\|A\|_2$ | `norm(A)` |
| $\|A\|_\infty$ | `max(sum(abs(A),2)) or norm(A,inf)` |
| $\|A\|_F$ | `sqrt(A(:)'*A(:))  or norm(x,'fro')` |

# The Singular Value Decomposition

## Diagonalizable Matrices

- A square matrix $A$ is called diagonalizable or non-defective if it is similar to a diagonal matrix, i.e., there exists an invertible matrix $P$ and a diagonal matrix $D$ such that

$$P^{-1}AP = D$$

- Exercise 4: If $A \in \mathbb{C}^{n\times n}$ has $n$ linear independent columns, there exists an eigenvectors the eigenvalue decomposition (EVD)

$$X\Lambda X^{-1} = A$$

- If $A$ is real and symmetric, the EVD is always possible

$$A = U\Lambda U^T,$$

with $U$ an unitary matrix

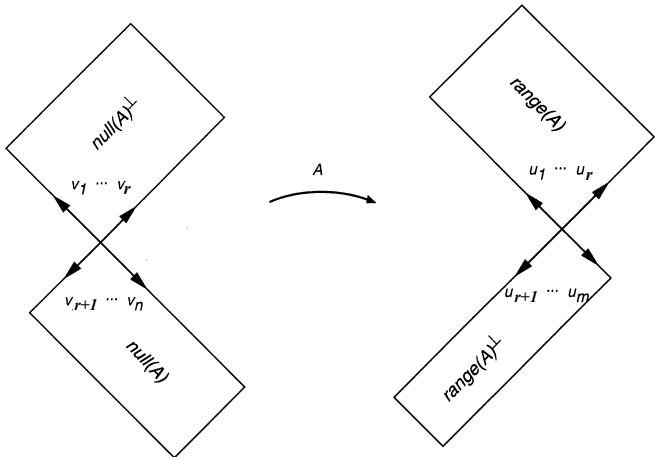
## The SVD - Brief Description

- Suppose that $A \in \mathbb{C}^{m \times n}$ with $m \geqslant n$ and full rank ($r = n$)
- Choose orthonormal basis

$$v_1, \ldots, v_n \text{ for the row space}$$

$$u_1, \ldots, u_n \text{ for the column space}$$

such that $Av_i$ is in the direction of $u_i$: $Av_i = \sigma_i u_i$




- The singular values $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_n > 0$

## The SVD - Brief Description

- In matrix form, $Av_i = \sigma_i u_i$ becomes

$$AV = \hat{U}\hat{\Sigma} \Leftrightarrow A = \hat{U}\hat{\Sigma}V^*$$

where $\hat{\Sigma} = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$

- This is the reduced singular value decomposition
- Add orthonormal extension to $\hat{U}$ and add rows to $\hat{\Sigma}$ to obtain the full sigular value decomposition

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

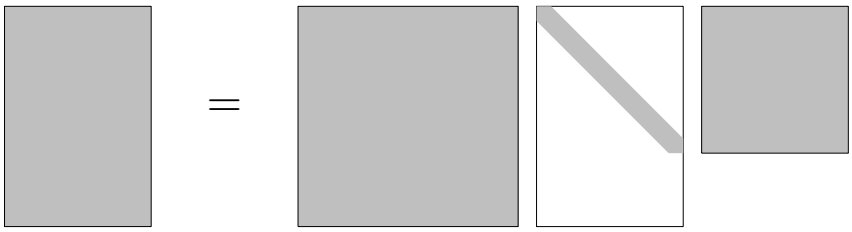
## The Full Singular Value Decomposition

- Let $A$ be an $m \times n$ matrix. The singular value decomposition of $A$ is the factorization $A = U\Sigma V^*$ where

  $U$ is $m \times m$ unitary (the left singular vectors of $A$)

  $V$ is $n \times n$ unitary (the right singular vectors of $A$)

  $U$ is $m \times m$ unitary (the left singular vectors of $A$)



$A \qquad\qquad U \qquad \Sigma \qquad V^*$

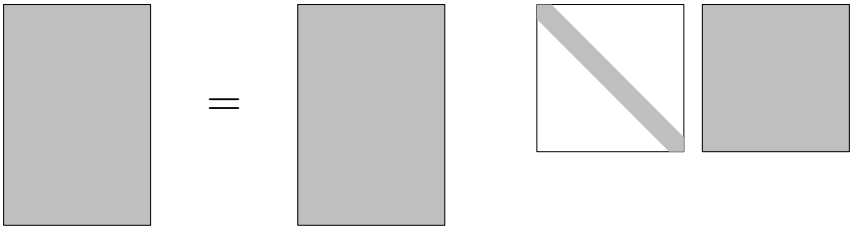
## The Reduced Singular Value Decomposition

- A more compact representation is the reduced SVD, for $m \geqslant n$:

$$A = \hat{U}\hat{\Sigma}V^*$$

where

$$U \text{ is } m \times n, \qquad V \text{ is } n \times n, \qquad \Sigma \text{ is } n \times n$$



$A \qquad\qquad \hat{U} \qquad \hat{\Sigma} \qquad V^*$

## The SVD and The Eigenvalue Decomposition

- The eigenvalue decomposition $A = X\Lambda X^{-1}$
  - uses the same basis $X$ for row and column space, but the SVD uses two different basis $V$ and $U$
  - generally does not use an orthonormal basis, but the SVD does
  - is only defined for square matrices, but the SVD exists for all matrices
- For symmetric positive definite matrices $A$, the EVD and SVD are equal

## Matrix Properties (Exercise 5)

1. The rank of $A$ is $r$, the number of nonzero singular values
2. range $(A) = \langle u_1, \ldots, u_r \rangle$ and null $(A) = \langle v_{r+1}, \ldots, v_n \rangle$
3. $\|A\|_2 = \sigma_1$ and $\|A\|_F = \sqrt{\sigma_1^2 + \sigma_2^2 \cdots + \sigma_r^2}$
4. Nonzero eigenvalues of $A^*A$ are nonzero $\sigma_j^2$, eigenvectors are $v_j$; Nonzero eigenvalues of $AA^*$ are nonzero $\sigma_j^2$, eigenvectors are $u_j$
5. In $A = A^*$, $\sigma_i = |\lambda_j|$, where $\lambda_j$ are eigenvalues of $A$
6. For square $A$, $|\det(A)| = \prod_{j=1}^{m} \sigma_j$

## Existence and Uniqueness

**Theorem 1.1: Existence**

Every matrix $A \in \mathbb{C}^{m \times n}$ has a SVD

**Theorem 1.2: Uniqueness**

The singular values $\{\sigma_j\}$ are uniquely determined. If $A$ is square and the $\sigma_j$ are distinct, the left and right singular vectors are uniquely determined **up to complex signs**

## Example: $A = \begin{bmatrix} 2 & 2 \\ 1 & -1 \end{bmatrix}$

- Prove that the eigenvalues of

$$A^T A = \begin{bmatrix} 5 & 3 \\ 3 & 5 \end{bmatrix},$$

are $\lambda_1 = 8$ and $\lambda_2 = 2$ and the (orthonormal) eigenvectors are

$$v_1 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \quad \text{and} \quad v_2 = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

- Then

$$\Sigma = \begin{bmatrix} \sigma_1 & \\ & \sigma_2 \end{bmatrix} = \begin{bmatrix} 2\sqrt{2} & \\ & \sqrt{2} \end{bmatrix} \text{ and } V = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

## Example: $A = \begin{bmatrix} 2 & 2 \\ 1 & -1 \end{bmatrix}$ (cont.)

- The columns of $U$ are obtained by

$$\sigma_1 u_1 = Av_1 = \begin{bmatrix} 2 & 2 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 2\sqrt{2} \\ 0 \end{bmatrix} \Rightarrow u_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

and

$$\sigma_2 u_2 = Av_2 = \begin{bmatrix} 2 & 2 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 0 \\ \sqrt{2} \end{bmatrix} \Rightarrow u_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- The SVD of $A = U\Sigma V^T$ is

$$\begin{bmatrix} 2 & 2 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 2\sqrt{2} & \\ & \sqrt{2} \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \quad \square$$

- Exercise 6: Obtain the SVD of $A = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$.

## Low-Rank Approximations

- The SVD can be written as a sum of rank-one matrices

$$A = \sum_{j=1}^{r} \sigma_j u_j v_j^*$$

- (Eckart-Young, 1936) The best rank $\eta$ approximation in the 2-norm is

$$A_\eta = \sum_{j=1}^{\eta} \sigma_j u_j v_j^*$$

with

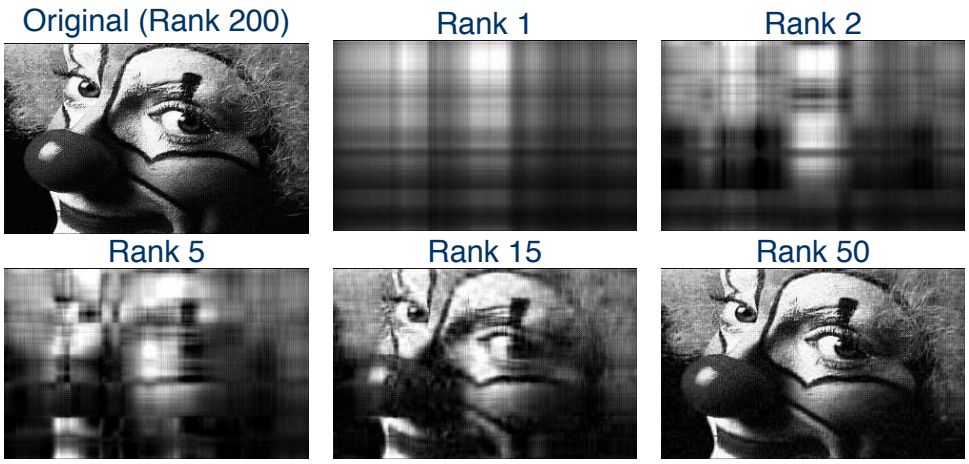
$$\|A - A_\eta\|_2 = \sigma_{\eta+1}$$

- Also true in the Frobenius norm, with

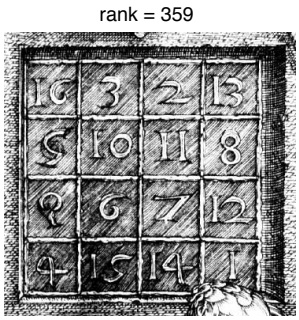
$$\|A - A_\eta\|_F = \sqrt{\sigma_{\eta+1}^2 + \cdots + \sigma_r^2}$$

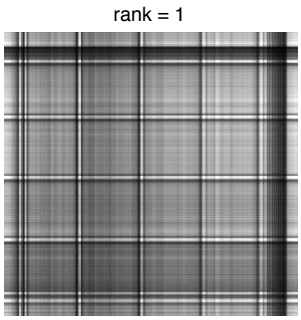
# Application: Image Compression

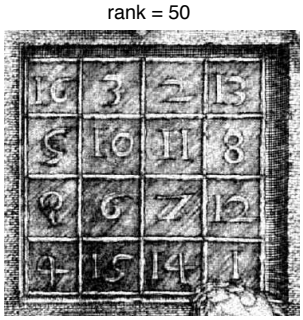
- View $m \times n$ image as a (real) matrix $A$, find best rank $\eta$ approximation by SVD
- Storage $\eta \times (m + n)$ instead of $m \times n$

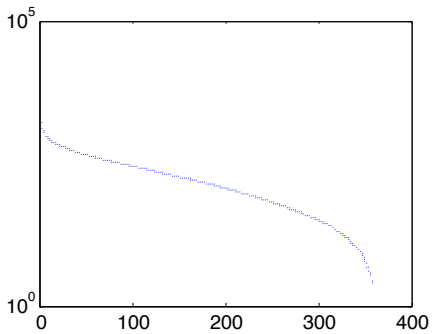



# Application: Image Compression




Cleave Moler Textbooks: `www.mathworks.com/moler/`

## Solving Systems of Linear Equations ($Ax = b$)

- Let $A = U\Sigma V^* = \hat{U}\hat{\Sigma}V^* \quad (\text{rank}(A) = r)$
- $Ax = b$ is solvable iif $b \perp \text{null}(A^*)$
- A solution of $Ax = b$, if exists, is given by

$$\hat{x} = \hat{V}\hat{\Sigma}^{-1}\hat{U}^*b = V\Sigma^+U^*b = A^+b,$$

  where $A^+ = V\Sigma^+U^*$ is the pseudo inverse of $A$
- The vector $\hat{x} = A^+b$ represents the uniquely determined solution of $Ax = b$ with minimal euclidean norm
- If $Ax = b$ has no solution, $\hat{x} = A^+b$ represents its least squares solution with minimal euclidean norm

## The QR Factorization

## The QR Factorization - Main Idea

- Find orthonormal vectors $q_j$ that span the successive spaces spanned by the columns of $A$:

$$\langle a_1 \rangle \subseteq \langle a_1, a_2 \rangle \subseteq \langle a_1, a_2, a_2 \rangle \subseteq \cdots$$

- This means that (for full rank $A$)

$$\langle q_1, q_2, \ldots q_j \rangle = \langle a_1, a_2, \ldots a_j \rangle, \qquad \text{for } j = 1, \ldots, n$$

## The QR Factorization - Matrix Form

- In matrix form $\langle q_1, q_2, \ldots q_j \rangle = \langle a_1, a_2, \ldots a_j \rangle$ becomes

$$\left[\begin{array}{c|c|c|c} a_1 & a_2 & \cdots & a_n \end{array}\right] = \left[\begin{array}{c|c|c|c} q_1 & q_2 & \cdots & q_n \end{array}\right] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}$$

or

$$A = \hat{Q}\hat{R}$$

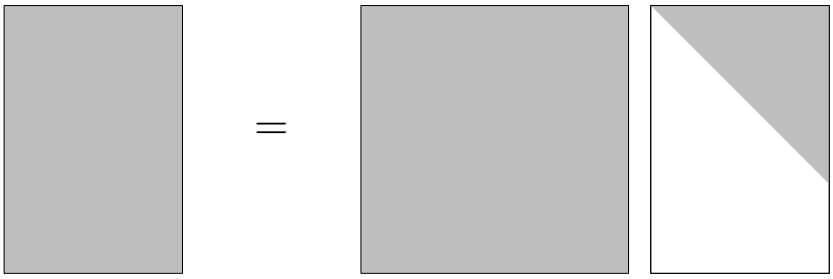
- This is the reduced QR factorization
- Add orthogonal extension to $\hat{Q}$ and add rows to $\hat{R}$ of obtain the full QR factorization

## The Full QR Factorization

- Let $A$ be an $m \times n$ matrix. The full QR factorization of $A$ is the factorization $A = QR$, where

  $Q$ is $m \times m$ unitary

  $R$ is $m \times n$ upper-triangular



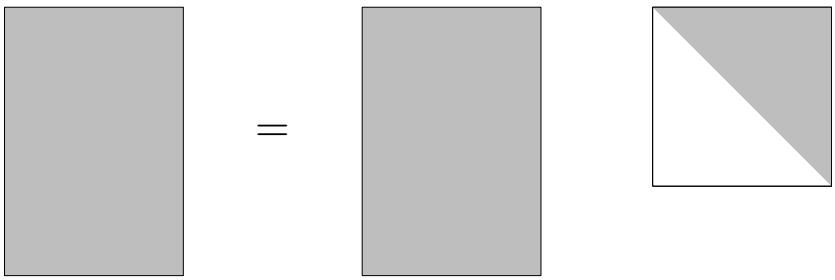
$A$ $Q$ $R$

## The Reduced QR Factorization

- A more compact representation is the reduced QR factorization $A = \hat{Q}\hat{R}$, where (for $m \geqslant n$)

  $\hat{Q}$ is $m \times n$ with orthonormal columns

  $R$ is $n \times n$ upper-triangular



$A$ $\hat{Q}$ $\hat{R}$

## Gram-Schmidt Orthogonalization (∗)

- Find new $q_j$ orthogonal to $q_1, \ldots, q_{j-1}$ by subtracting components along previous vectors

$$v_j = a_j - (q_1^* a_j)q_1 - (q_2^* a_j)q_2 - \cdots - (q_{j-1}^* a_j)q_{j-1}$$

- Normalize to get $q_j = v_j / \|v_j\|$
- We then obtain a reduced QR factorization $A = \hat{Q}\hat{R}$, with

$$r_{ij} = q_i^* a_j, \qquad (i \neq j)$$

and

$$|r_{jj}| = \left\| a_j - \sum_{i=1}^{j-1} r_{ij} q_i \right\|_2$$

- "Triangular Orthogonalization"

## Classical Gram-Schmidt (∗)

- Straight-forward application of Gram-Schmidt orthogonalization
- Numerically unstable
- Algorithm: Classical Gram-Schmidt

for $j = 1$ to $n$ do
  $v_j = a_j$
  for $i = 1$ to $j - 1$ do
    $r_{ij} = q_i^* a_j$
    $v_j = v_j - r_{ij} q_i$
  end for
  $r_{jj} = \|v_j\|_2$
  $q_j = v_j / r_{jj}$
end for

## Existence and Uniqueness

**Theorem 1.3: Existence**

Every $A \in \mathbb{C}^{m\times n}$ $(m \geqslant n)$ has a full QR factorization and a reduced QR factorization

Proof: For full rank $A$, Gram-Schmidt process gives the existence of $A = \hat{Q}\hat{R}$. Otherwise, when $v_j = 0$ choose arbitrary vector orthogonal to previous $q_1, \ldots, q_{j-1}$. For full QR, add orthogonal extension to $Q$ (silent columns) and zero rows to $R$. □

**Theorem 1.4: Uniqueness**

Each $A \in \mathbb{C}^{m\times n}$ $(m \geqslant n)$ of full rank has a unique $A = \hat{Q}\hat{R}$ with $r_{jj} > 0$

Proof: Again Gram-Schmidt, $r_{jj} > 0$ determines the sign. □

## Classical vs Modified Gram-Schmidt (∗)

- Some modifications of classical Gram-Schmidt gives modified Gram-Schmidt (but see next slide)
- Modified Gram-Schmidt is numerically stable (less sensitive to rounding errors)
- Algorithm: Classical/Modified Gram-Schmidt

for $j = 1$ to $n$ do
  $v_j = a_j$
  for $i = 1$ to $j - 1$ do
    $r_{ij} = q_i^* a_j$ (CGS)
    $r_{ij} = q_i^* v_j$ (MGS)
    $v_j = v_j - r_{ij} q_i$
  end for
  $r_{jj} = \|v_j\|_2$
  $q_j = v_j / r_{jj}$
end for

## Implementation of Modified Gram-Schmidt (∗)

- Algorithm: CGS

for $j = 1$ to $n$ do
  $v_j = a_j$
  for $i = 1$ to $j - 1$ do
    $r_{ij} = q_i^* a_j$
    $v_j = v_j - r_{ij} q_i$
  end for
  $r_{jj} = \|v_j\|_2$
  $q_j = v_j / r_{jj}$
end for

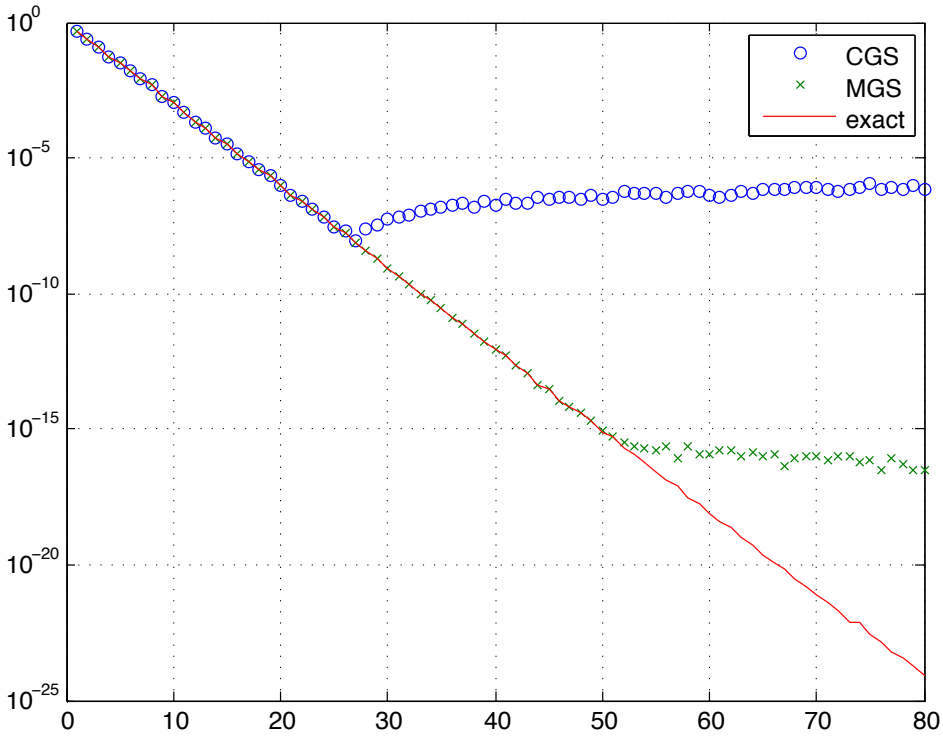
- Algorithm: MGS

for $i = 1$ to $n$ do
  $v_i = a_i$
end for
for $i = 1$ to $n$ do
  $r_{ii} = \|v_i\|_2$
  $q_i = v_i / r_{ii}$
  for $j = i + 1$ to $n$ do
    $r_{ij} = q_i^* v_j$
    $v_j = v_j - r_{ij} q_i$
  end for
end for

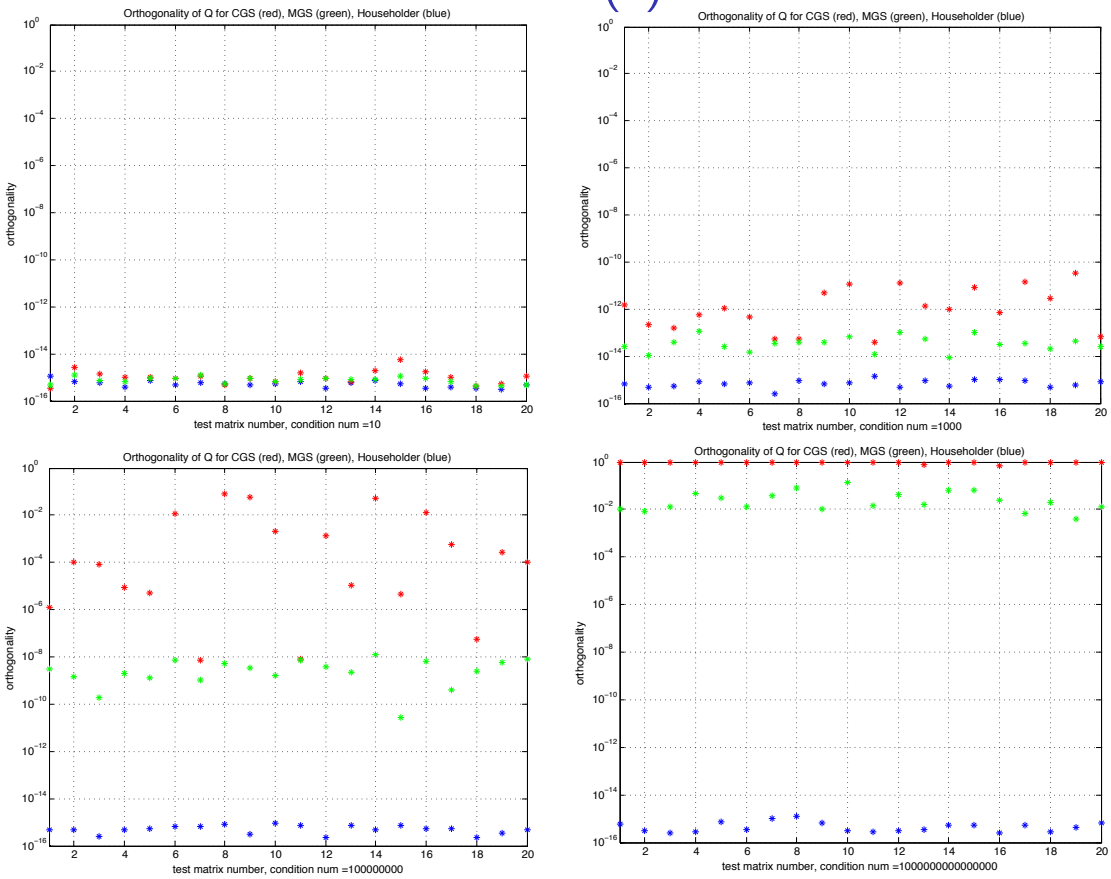
## Example: Classical vs Modified Gram-Schmidt (∗)

```
% Create a random orthogonal matrix Q
n = 80;
[Q,X] = qr(randn(n));
% Make an ill-conditioned R (with diagonal
% entries = 2^-j, j=1,...,n)
R = diag(2.^(-1:-1:-n))*triu(ones(n)+0.1*randn(n));
% Compute QR factorization with classical and with
% modified GS, compare diagonal elements of
% computed R's
A = Q*R;
[QC,RC] = clgs(A);
[QM,RM] = mgs(A);
semilogy(1:n,diag(RC),'o',1:n,diag(RM),'x',1:n,diag(R))
legend('CGS', 'MGS', 'exact')
grid on
```

# Example: Classical vs Modified Gram-Schmidt (∗)




# Gram-Schmidt vs Householder (∗)



# The LU Factorization

## The LU Factorization

- Transform $A = \mathbb{R}^{n \times n}$ into upper triangular $U$ by subtracting multiples of rows
- Each $L_i$ introduces zeros below diagonal of column $i$:

$$\underbrace{L_{n-1} \cdots L_2 L_1}_{L^{-1}} A = U \Rightarrow A = LU \text{ where } L = L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1}$$

$$\begin{bmatrix} \star & \star & \star & \star \\ \star & \star & \star & \star \\ \star & \star & \star & \star \\ \star & \star & \star & \star \end{bmatrix} \xrightarrow{L_1} \begin{bmatrix} \star & \star & \star & \star \\ 0 & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \end{bmatrix} \xrightarrow{L_2} \begin{bmatrix} \star & \star & \star & \star \\ & \star & \star & \star \\ & 0 & * & * \\ & 0 & * & * \end{bmatrix} \xrightarrow{L_3} \begin{bmatrix} \star & \star & \star & \star \\ & \star & \star & \star \\ & & \star & \star \\ & & 0 & * \end{bmatrix}$$

$A$ $\qquad$ $L_1 A$ $\qquad$ $L_2 L_1 A$ $\qquad$ $L_3 L_2 L_1 A$

- "Triangular triangularization"

## The Matrices $L_k$

- At step $k$, eliminate elements below $A_{kk}$:

$$x_k = \begin{bmatrix} x_{1k} & \cdots & x_{kk} & x_{k+1,k} & \cdots & x_{nk} \end{bmatrix}^T$$
$$L_k x_k = \begin{bmatrix} x_{1k} & \cdots & x_{kk} & 0 & \cdots & 0 \end{bmatrix}^T$$

- Each $L_i$ introduces zeros below diagonal of column $i$:

$$\underbrace{L_{n-1} \cdots L_2 L_1}_{L^{-1}} A = U \Rightarrow A = LU \text{ where } L = L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1}$$

- The multipliers $\ell_{jk} = x_{jk}/x_{kk}$ appear in $L_k$:

$$L_k = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -\ell_{k+1,k} & 1 & \\ & & \vdots & & \ddots \\ & & -\ell_{nk} & & 1 \end{bmatrix}$$

## Forming $L$

- The $L$ matrix contains all the multipliers in one matrix (with plus signs)

$$L = L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1} = \begin{bmatrix} 1 & & & & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & \vdots & \ddots & \ddots & \\ \ell_{n1} & \ell_{n2} & \cdots & \ell_{n,n-1} & 1 \end{bmatrix}$$

- Define $\ell_k = (0, \cdots, 0, \ell_{k+1,k}, \cdots, \ell_{nk})$. Then

$$L_k = I - \ell_k e_k^T,$$

where $e_k$ is the column vector with 1 in position $k$ and 0 elsewhere

  - First, $L_k^{-1} = I + \ell_k e_k^T$, since $e_k^T \ell_k = 0$ and

$$(I - \ell_k e_k^T)(I + \ell_k e_k^T) = I - \ell_k e_k^T \ell_k e_k^T = I$$

  - Also, $L_k^{-1} L_{k+1}^{-1} = I + \ell_k e_k^T + \ell_{k+1} e_{k+1}^T$, since $e_k^T \ell_{k+1} = 0$ and

$$(I - \ell_k e_k^T)(I + \ell_{k+1} e_{k+1}^T) = I + \ell_k e_k^T + \ell_{k+1} e_{k+1}^T$$

## Gaussian Elimination without Pivoting

- Factorize $A \in \mathbb{R}^{n \times n}$ into $A = LU$:
- Algorithm: Gaussian Elimination (no pivoting)

$U = A$, $L = I$
for $k = 1$ to $n - 1$ do
  for $j = k + 1$ to $n$ do
    $\ell_{jk} = u_{jk} / u_{kk}$
    $u_{j,k:n} = u_{j,k:n} - \ell_{jk} u_{k,k:n}$
  end for
end for

- The inner loop can be written using matrix operations instead of for-loop

## Pivoting ($*$)

- At step $k$, we used matrix element $k, k$ as pivot and introduced zeros in entry $k$ of remaining rows

$$\begin{bmatrix} \star & \star & \star & \star & \star \\ & x_{kk} & * & * & * \\ & \star & \star & \star & \star \\ & \star & \star & \star & \star \\ & \star & \star & \star & \star \end{bmatrix} \rightarrow \begin{bmatrix} \star & \star & \star & \star & \star \\ & x_{kk} & \star & \star & \star \\ & 0 & * & * & * \\ & 0 & * & * & * \\ & 0 & * & * & * \end{bmatrix}$$

- But any other element $i \leqslant k$ in column $k$ can be used as pivot:

$$\begin{bmatrix} \star & \star & \star & \star & \star \\ & \star & \star & \star & \star \\ & \star & \star & \star & \star \\ & x_{ik} & * & * & * \\ & \star & \star & \star & \star \end{bmatrix} \rightarrow \begin{bmatrix} \star & \star & \star & \star & \star \\ & 0 & * & * & * \\ & 0 & * & * & * \\ & x_{ik} & \star & \star & \star \\ & 0 & * & * & * \end{bmatrix}$$

## Pivoting (∗)

- Also, any other column $j \leqslant k$ can be used:

$$\begin{bmatrix} \star & \star & \star & \star & \star \\ & \star & \star & \star & \star \\ & \star & \star & \star & \star \\ & * & x_{ik} & * & * \\ & \star & \star & \star & \star \end{bmatrix} \rightarrow \begin{bmatrix} \star & \star & \star & \star & \star \\ & * & 0 & * & * \\ & * & 0 & * & * \\ & \star & x_{ik} & \star & \star \\ & * & 0 & * & * \end{bmatrix}$$

- Choosing different pivots means we can avoid zero or very small pivots
- Instead of using pivots at different entries, change rows or columns and use the standard triangular algorithm (pivoting)
- A computer code might account for the pivoting indirectly instead of actually moving the data

## Partial Pivoting (∗)

- Searching among all valid pivots is expensive (complete pivoting)
- Consider pivots in column k only and interchange rows (partial pivoting)

$$\begin{bmatrix} \star & \star & \star & \star & \star \\ & \star & \star & \star & \star \\ & \star & \star & \star & \star \\ & x_{ik} & * & * & * \\ & \star & \star & \star & \star \end{bmatrix} \xrightarrow{P_1} \begin{bmatrix} \star & \star & \star & \star & \star \\ & x_{ik} & * & * & * \\ & \star & \star & \star & \star \\ & * & * & * & * \\ & \star & \star & \star & \star \end{bmatrix} \xrightarrow{L_1} \begin{bmatrix} \star & \star & \star & \star & \star \\ & x_{ik} & \star & \star & \star \\ & 0 & * & * & * \\ & 0 & * & * & * \\ & 0 & * & * & * \end{bmatrix}$$

Pivot selection Row interchange Elimination

- In terms of matrices:

$$L_{n-1}P_{n-1}\cdots L_2P_2L_1P_1A = U$$

## The $PA = LU$ Factorization $(*)$

- To combine all $L_k$ and all $P_k$ into matrices, rewrite as

$$L_{n-1}P_{n-1}\cdots L_2P_2L_1P_1A = U$$
$$(\bar{L}_{n-1}\cdots\bar{L}_2\bar{L}_1)(P_{n-1}\cdots P_2P_1)A = U$$

  where
$$\bar{L}_k = P_{n-1}\cdots P_{k+1}L_kP_{k+1}^{-1}\cdots P_{n-1}^{-1}$$

- This gives the LU factorization of $A$

$$PA = LU$$

## Gaussian Elimination with Partial Pivoting $(*)$

- Factorize $A \in \mathbb{R}^{n\times n}$ into $PA = LU$:

- Algorithm: Gaussian Elimination (partial pivoting)

$U = A$, $L = I$, $P = I$
for $k = 1$ to $n-1$ do
  Select $i \geqslant k$ to maximize $|u_{ik}|$
  $u_{k,k:n} \leftrightarrow u_{i,k:n}$ % interchange two rows
  $\ell_{k,1:k-1} \leftrightarrow \ell_{i,1:k-1}$
  $p_{k,:} \leftrightarrow p_{i,:}$
  for $j = k+1$ to $n$ do
    $\ell_{jk} = u_{jk}/u_{kk}$
    $u_{j,k:n} = u_{j,k:n} - \ell_{jk}u_{k,k:n}$
  end for
end for

## Cholesky Factorization for SPD/HPD Matrices ($*$)

- Eliminate below pivot and to the right of pivot:

$$\begin{aligned} A &= \begin{bmatrix} a_{11} & \omega^* \\ \omega & K \end{bmatrix} = \begin{bmatrix} \alpha & 0 \\ \omega/\alpha & I \end{bmatrix} \begin{bmatrix} \alpha & \omega^*/\alpha \\ 0 & K - \omega\omega^*/a_{ii} \end{bmatrix} \\ &= \begin{bmatrix} \alpha & 0 \\ \omega/\alpha & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & K - \omega\omega^*/a_{ii} \end{bmatrix} \begin{bmatrix} \alpha & \omega^*/\alpha \\ 0 & I \end{bmatrix} \\ &= R_1^* A_1 R_1 \end{aligned}$$

  where $\alpha = \sqrt{a_{11}}$

- $K - \omega\omega^*/a_{11}$ is a principal submatrix of PD matrix $R_1^* A_1 R_1$, therefore its upper-left entry is positive
- Apply recursively to obtain

$$A = (R_1^* R_2^* \cdots R_n*)(R_n \cdots R_2 R_1) = R^* R, \qquad r_{jj} > 0$$

## The Cholesky Factorization Algorithm

- Factorize hermitian positive definite $A \in \mathbb{R}^{n \times n}$ into $A = R^* R$
- Algorithm: Cholesky Factorization ($*$)

```
R = A
for k = 1 to n do
        for j = k + 1 to n do
                r_{j,j:n} = r_{j,j:n} − r_{k,j:n} r*_{k,j} / r_{kk}
        end for
        r_{k,k:n} = r_{k,k:n} / √r_{kk}
        end for
end for
```

- Existence and uniqueness: Every PD matrix has a unique Choleskey factorization

## Backslash in MATLAB

- `x=A\b` for dense `A` performs these steps (stopping when successful):
  1. If `A` is upper or lower triangular, solve by back/forward substitution
  2. If `A` is permutation of triangular matrix, solve by permuted back substitution (useful for `[L,U]=lu(A)` since `L` is permuted)
  3. If `A` is symmetric
     - Check if all diagonal elements are positive
     - Try Cholesky, if successful solve by back substitutions
  4. If `A` is Hessenberg (upper triangular plus one subdiagonal), reduce to upper triangular then solve by back substitution
  5. If `A` is square, factorize $PA = LU$ and solve by back substitutions
  6. If `A` is not square, run Householder `QR`, solve least squares problem

## Conditioning and Condition Numbers

## Conditioning

- Absolute Condition Number of a differentiable problem $f$ at $x$:

$$\hat{k} = \lim_{\delta \to 0} \sup_{\|\delta x\| \leqslant \delta} \frac{\|\delta f\|}{\|\delta x\|} = \sup_{\delta x} \frac{\|\delta f\|}{\|\delta x\|} = \|J(x)\|,$$

  where the Jacobian $J_{ij} = \partial f_i / \partial x_j$, and the matrix norm is induced by the norms on $\delta f$ and $\delta x$

- Relative Condition Number:

$$k = \sup_{\delta x} \left( \frac{\|\delta f\|}{\|f(x)\|} \Big/ \frac{\|\delta x\|}{\|x\|} \right) = \frac{\|J(x)\|}{\|f(x)\|/\|x\|}$$

## Condition of Matrix-Vector Product

- Consider $f(x) = Ax$, with $A \in \mathbb{C}^{m \times n}$

$$k = \frac{\|J(x)\|}{\|f(x)\|/\|x\|} = \|A\| \frac{\|x\|}{\|Ax\|} = [Ax = b] = \|A\| \frac{\|x\|}{\|b\|}$$

- For $A$ square and nonsingular, use $\|x\|/\|Ax\| \leqslant \|A^{-1}\|$:

$$k \leqslant \|A\| \|A^{-1}\|$$

  (equality achieved for the last right singular vector $x = v_m$)

- The condition number of $Ax$ if $\infty$ if $x \in \text{null}(A)$

- Also the condition number for $f(b) = A^{-1}b$ (solution of linear system $Ax = b$):

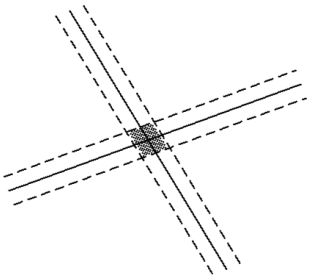
$$k = \|A^{-1}\| \frac{\|b\|}{\|x\|} \leqslant \|A\| \|A^{-1}\|$$

## Condition Number of a Matrix

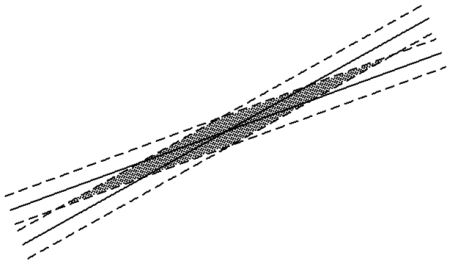
- Condition number of matrix $A$:

$$k(A) = \|A\|\|A^{-1}\| = [\text{for 2-norm}] = \frac{\sigma_1}{\sigma_m} \geqslant 1$$

- If $A$ is singular we consider, by convention, $k(A) = \infty$
- Measure of uncertainty



well-conditioned



ill-conditioned

## Condition of System of Equations

- Exercise 7: For fixed $A$, consider $f(b) = A^{-1}b$. Prove that

$$k = \frac{\|\delta x\|}{\|x\|} \Big/ \frac{\|\delta b\|}{\|b\|} \leqslant k(A).$$

Then, if the input data is accurate to the $\epsilon_{machine}$

$$\frac{\|\delta x\|}{\|x\|} \leqslant k(A)\epsilon_{machine}.$$

- Exercise 8 (Theorem 3.1 (QSS, page 60)): Let $A \in \mathbb{C}^{m\times m}$ be a non singular matrix and let $\delta A \in \mathbb{C}^{m\times m}$ be such that $\|A^{-1}\|\|\delta A\| < 1$. Let $Ax = b$ and $(A + \delta A)(x + \delta x) = b + \delta b$. Prove that

$$\frac{\|\delta x\|}{\|x\|} \leqslant \frac{k(A)}{1 - k(A)\frac{\|\delta A\|}{\|A\|}} \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|}\right),$$

where $k(A)$ is the condition number of the matrix $A$.

# Example: Condition of Hilbert system

```
% Initialise settings, constants and vectors

clc; clear; close all;

N = 12; error = zeros(1,N-1); estimate = zeros(1,N-1);

% Loop on the order of the matrix

for n = 2:N
    H = hilb(n);
    x = ones(n,1); b = H*x;     % Exact values
    xbar = H\b; bbar = H*xbar; % Computed values
    % Compute error and error estimate
    error(n-1) = norm(x-xbar)/norm(x);
    estimate(n-1) = cond(H)*norm(b-bbar)/norm(b);
end

semilogy(2:n,error,'-o',2:n,estimate,'-x')

legend('error', 'estimate')

xlabel('order'), ylabel('relative error')
```

# Example: Condition of Hilbert system