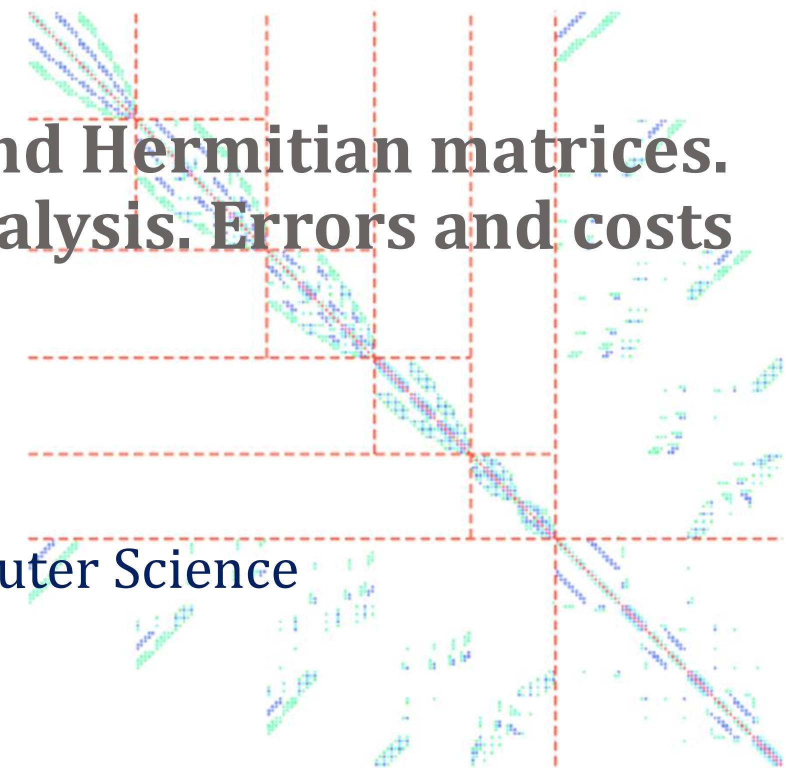
# Numerical Methods of Linear Algebra for Sparse Matrices

## Lecture 6

**Positive definite matrices. Normal and Hermitian matrices. Powers of matrices. Perturbation analysis. Errors and costs**



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# Outline

- Positive definite matrices
- Normal and Hermitian matrices
- Powers of matrices
- Perturbation analysis and condition number
- Errors and costs

# Positive definite matrices

- Real positive definite matrix $A \in \mathbb{R}^{n\times n}$

$(Au,u) > 0 \ \forall u \in \mathbb{R}^n$, $u \neq 0$. Recall that $(Au,u) = u^H Au$

- Real positive semidefinite matrix $A \in \mathbb{R}^{n\times n}$

$(Au,u) \geq 0 \ \forall u \in \mathbb{R}^n$

- Real symmetric positive definite matrix $A \in \mathbb{R}^{n\times n}$, $A = A^T$

$(Au,u) > 0 \ \forall u \in \mathbb{R}^n$, $u \neq 0$

Complex matrix can be positive definite only in the case, when it is Hermitian (Inner product $(Au,u)$ can be real only when $A = A^H$)

- Hermitian positive definite matrix $A \in \mathbb{C}^{n\times n}$, $A = A^H$

$(Au,u) > 0 \ \forall u \in \mathbb{C}^n$, $u \neq 0$

- Hermitian positive semidefinite matrix $A \in \mathbb{C}^{n\times n}$, $A = A^H$

$(Au,u) \geq 0 \ \forall u \in \mathbb{C}^n$

# Positive definite matrices: theorems

**Theorem 1**. Complex $A \in \mathbb{C}^{n\times n}$ is positive definite $\Leftrightarrow$ $A = A^H$ and the spectrum $\sigma(A) > 0$ (i.e. all eigenvalues are positive).

**Theorem 2**. If $A \in \mathbb{R}^{n\times n}$ is real positive definite, then

1) $\exists\, A^{-1}$

2) $\exists\ \alpha > 0:\ (Au, u) \geq \alpha \|u\|_2^2 \ \ \forall u \in \mathbb{R}^n$

**Theorem 3**. $\forall A \in \mathbb{C}^{n\times m}$ $A^H A$ is Hermitian positive semidefinite.

$\vartriangle$ $(A^H Au, u) = (Au, Au) \geq 0 \ \ \forall u \in \mathbb{C}^m$ $\square$

# Positive definite matrices: important notes

- Check positive definiteness in Matlab by Cholesky factorization: **chol(A)** or by computing eigenvalues **eig(A)**

```
A=rand(3)

A = 3x3
    0.4942    0.9037    0.6987
    0.7791    0.8909    0.1978
    0.7150    0.3342    0.0305
```

```
chol(A)

Error using chol
Matrix must be positive definite.
```

*Example.* Real matrix can be positive definite but nonsymmetric.

Take block-diagonal $A = \begin{pmatrix} 3 & 2 & 0 & 0 \\ 1 & 4 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 2 & 2 \end{pmatrix}$.

Its eigenvalues are $\{2, 5, 2, 2\}$ are all positive.

This matrix is positive definite, but $A \neq A^T$

```
[R,flag] = chol(A) % flag>0

R = 0.7030
flag = 2
```

```
eig(A)

ans = 3x1
    1.7988
   -0.5585
    0.1753
```

# Normal matrices: theorems

- Normal matrix $A \in \mathbb{C}^{n\times n}$

$A^H A = AA^H$

**Lemma**. A normal triangular matrix is diagonal.

**Theorem 1**. Any normal matrix has a diagonal form:

$A \in \mathbb{C}^{n\times n}$ is normal matrix $\Leftrightarrow$ A is unitarily similar to diagonal matrix:

$\exists Q: \; A = QDQ^H$, where $D = diag(\lambda_1, \dots, \lambda_n), \; \lambda_i \in \sigma(A)$

**Theorem 2**. $A \in \mathbb{C}^{n\times n}$ is normal $\Leftrightarrow$ any eigenvalue $\lambda \in \sigma(A)$ is an eigenvalue of $A^H$ $(\lambda \in \sigma(A^H))$

# Hermitian matrices: theorems

- Hermitian matrix $A \in \mathbb{C}^{n\times n}$ : $A = A^H$

**Proposition**. If inner product $(Az, z)$ is real for $\forall z \in \mathbb{C}^n$, then $A = A^H$ ($A$ is Hermitian)

**Lemma**. Any Hermitian matrix is normal.

**Theorem 1**. 1) Normal matrix with real eigenvalues is Hermitian.

2) Hermitian matrix has real eigenvalues.

**Theorem 2**. Any Hermitian matrix is unitarily similar to a real diagonal matrix: $A = A^H \;\Rightarrow\; A = QDQ^H$, where $D$ is real.

**Theorem 3**. $\forall A \in \mathbb{C}^{n\times n}$ there is decomposition of $A$: $A = H + iS$, where

$H = \frac{1}{2}(A + A^H)$, $S = \frac{1}{2i}(A - A^H)$; $H$, $S$ are Hermitian, $iS$ is skew-Hermitian

For eigenvalues $\lambda_i$, $i = \overline{1,n}$ of $A$ holds:

1) $\lambda_{\min}(H) \le \mathrm{Re}(\lambda_i) \le \lambda_{\max}(H)$

2) $\lambda_{\min}(S) \le \mathrm{Im}(\lambda_i) \le \lambda_{\max}(S)$

# Powers of matrices

**Theorem 1**. Sequence of matrix powers $\{A^k\}$ converges to zero matrix: $\{A^k\} \to 0 \;\Leftrightarrow\; \rho(A) < 1.$

Recall that $\rho(A)$ is the spectral radius of $A$: $\rho(A) = \max_{\lambda \in \sigma(A)} |\lambda|.$

**Theorem 2**. $\lim_{k\to\infty} \left\| A^k \right\|^{1/k} = \rho(A).$

**Theorem 3**. Series of matrix powers $\sum_{k=0}^{\infty} A^k$ converges $\Leftrightarrow\; \rho(A) < 1.$

# Perturbation analysis

Consider a linear system $Ax = b,\ A \in \mathbb{C}^{n \times n},\ b \in \mathbb{C}^n$

$x \in \mathbb{C}^n$ is the vector of unknowns

$x = A^{-1}b$ will be *exact* solution

Consider a pertubed system $(A + \delta A)\tilde{x} = b + \delta b$

$\tilde{x}$ is the solution of pertubed system

$\tilde{x}$ will be *approximate* solution to initial system $Ax = b$

$\delta x = \tilde{x} - x$ is an *error,* hence $\tilde{x} = x + \delta x$

Let us find estimation of the error $\|\delta x\|$

# Estimation of absolute error

Consider initial and pertubed systems:

1) $Ax = b$

2) $(A+\delta A)(x+\delta x) = b+\delta b$

$$Ax + A\cdot\delta x + \delta A\cdot(x+\delta x) = b+\delta b$$

Subtract (1) from (2):

$$Ax + A\cdot\delta x + \delta A\cdot(x+\delta x) - Ax = b+\delta b - b,\ x+\delta x = \tilde{x}$$

$$A\cdot\delta x + \delta A\cdot\tilde{x} = \delta b \ \Big|\cdot A^{-1}$$

$$\delta x + A^{-1}\cdot\delta A\cdot\tilde{x} = A^{-1}\cdot\delta b$$

$$\delta x = A^{-1}\cdot(\delta b - \delta A\cdot\tilde{x})$$

$$\|\delta x\| = \left\|A^{-1}\cdot(\delta b - \delta A\cdot\tilde{x})\right\| \le \left\|A^{-1}\right\|\cdot\left\|\delta b - \delta A\cdot\tilde{x}\right\| \le \left\|A^{-1}\right\|\cdot\left(\|\delta b\| + \left\|\delta A\cdot\tilde{x}\right\|\right),$$ that

follows from the properties of the norm: $\|Ax\|_p \le \|A\|_p\cdot\|x\|_p$, $\|a+b\| \le \|a\| + \|b\|$

Hence $\|\delta x\| \le \left\|A^{-1}\right\|\cdot\left(\|\delta b\| + \left\|\delta A\cdot\tilde{x}\right\|\right)$ is the estimation of absolute error

# Estimation of relative error

From the estimation of absolute error $\|\delta x\| \le \|A^{-1}\| \cdot \left(\|\delta b\| + \|\delta A \cdot \tilde{x}\|\right)$ let us derive the estimation of relative error

$$\|\delta x\| \le \|A^{-1}\| \cdot \|\delta b\| + \|A^{-1}\| \cdot \|\delta A\| \cdot \|\tilde{x}\| \quad \Big| \cdot \frac{1}{\|\tilde{x}\|}$$

$$\frac{\|\delta x\|}{\|\tilde{x}\|} \le \|A^{-1}\| \cdot \frac{\|\delta b\|}{\|\tilde{x}\|} + \|A^{-1}\| \cdot \|\delta A\| \quad \Big| \cdot \frac{\|A\|}{\|A\|}$$

$$\frac{\|\delta x\|}{\|\tilde{x}\|} \le \|A^{-1}\| \cdot \|A\| \cdot \left( \frac{\|\delta b\|}{\|\tilde{x}\| \cdot \|A\|} + \frac{\|\delta A\|}{\|A\|} \right)$$

$$\frac{\|\delta x\|}{\|\tilde{x}\|} \le cond(A) \cdot \left( \frac{\|\delta b\|}{\|\tilde{x}\| \cdot \|A\|} + \frac{\|\delta A\|}{\|A\|} \right)$$ is the estimation of relative error

where $cond(A) = \|A^{-1}\| \cdot \|A\|$ is the condition number of the matrix

# Estimation of relative error

$$\frac{\|\delta x\|}{\|\tilde{x}\|} \le cond(A) \cdot \left( \frac{\|\delta b\|}{\|\tilde{x}\| \cdot \|A\|} + \frac{\|\delta A\|}{\|A\|} \right)$$

When $\delta A = 0$

$$\frac{\|\delta x\|}{\|\tilde{x}\|} \le cond(A) \cdot \frac{\|\delta b\|}{\|\tilde{x}\| \cdot \|A\|}$$

$\frac{\|\delta x\|}{\|\tilde{x}\|} \le cond(A) \cdot \frac{\|\delta b\|}{\|b\|}$ is the estimation of relative error with respect to *approximate* solution.

In a similar way it can be derived that

$\frac{\|\delta x\|}{\|x\|} \le cond(A) \cdot \frac{\|\delta b\|}{\|b\|}$ is the estimation of relative error with respect to *exact* solution

# Condition number

- Condition number of the matrix $A \in \mathbb{C}^{n\times n}$

$$cond(A) = \left\|A^{-1}\right\| \cdot \left\|A\right\|$$

Condition number is relative to the matrix norm $cond_p(A) = \left\|A^{-1}\right\|_p \cdot \left\|A\right\|_p$

**Properties of condition number**

1) $1 \le cond(A) \le +\infty$

2) For singular matrix $cond(A) = +\infty$, otherwise $1 \le cond(A) < +\infty$

3) $cond(\alpha A) = cond(A)$ for $\forall \alpha \neq 0,\ \alpha \in \mathbb{C}$

4) For spectral and Eucledian matrix norms $cond(Q^H AQ) = cond(A)$, where $Q$ is unitary

5) $cond(A^{-1}) = cond(A)$

6) $cond(AB) \le cond(A) \cdot cond(B)$

7) $A = A^H \Rightarrow cond(A) = \left|\dfrac{\lambda_{\max}(A)}{\lambda_{\min}(A)}\right|$, where $\lambda_{\max}(A)$ and $\lambda_{\min}(A)$ are maximal and minimal eigenvalues of $A$

# Condition number and determinant

Condition number is used to estimate whether the problem is well- or ill-conditioned, and determinant cannot be used for such purpose.

- well-conditioned matrix

$cond(A) \sim 1$

- ill-conditioned matrix

$cond(A) \sim +\infty$

**Example**

Consider $A = \alpha I,\ A \in \mathbb{C}^{n\times n},\ \alpha \in \mathbb{C}$.

It is easy to show that $\det(A) = \alpha^n$

For $|\alpha| < 1$ $\det(A)$ is small, but for $|\alpha| \geq 1$ $\det(A)$ is large.

However, $cond(A) = 1$ for any norm,

thus $A = \alpha I$ is a well-conditioned matrix.

# Numerical errors: three types

1) Round-off errors, which appear because of finite precision of computer arithmetics

Example. $\pi \to fl(\pi)$ floating-point representation of $\pi$ in a computer

$\frac{1}{3} \to fl(\frac{1}{3})$ floating-point representation 0.33333...

2) Algorithmic errors, or trancation errors, which appear because the applied algorithm is not exact

Example. Consider a series expansion, such as Teylor series

$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(a)}{k!}(x-a)^k$. Suppose that the function $f(x)$ is infinitely differentiable at point $a$, but in a computer $f(x) \simeq \sum_{k=0}^{100} \frac{f^{(k)}(a)}{k!}(x-a)^k$

3) Propagated errors, which are the errors that spread during computations

Example. Input data x is stored as $fl(x)$ in a computer

$fl(x) = x(1+\varepsilon)$, where $|\varepsilon| \le \varepsilon_c$ (machine precision epsilon)

# Numerical errors and solution

Let $X$ be an input data, $R(X)$ is the problem solution.

Consider the problem of finding the solution of a linear system

$Mx = b,\ M \in \mathbb{C}^{n\times n},\ b \in \mathbb{C}^n$

Here $X = M,\ b$ is the input data, $R(x) = M^{-1}b$ is the solution.

Now let us consider real input data, stored in computer $X + \delta X,$ as there can be input error $\delta X$. Suppose that we apply the algorithm $A$ to solve the problem.

In reality we can deal with different solutions:

- $R(x)$ is the exact solution for exact input data $X$
- $R_A(x)$ is the solution by algorithm $A$ for exact input data $X$
- $R(x+\delta x)$ is the exact solution for real input data $X+\delta X$
- $R_A(x+\delta x)$ is the solution by algorithm $A$ for real input data $X+\delta X$

# Estimation of numerical errors

- $\|R_A(x) - R(x)\|$ is the absolute algorithmic error for exact solution or
- $\|R_A(x+\delta x) - R(x+\delta x)\|$ is the absolute algorithmic error for approximate

solution

- $\dfrac{\|R_A(x) - R(x)\|}{\|R(x)\|}$ is the relative algorithmic error for exact solution
- $\|R(x+\delta x) - R(x)\|$ is the absolute propagated error or
- $\|R_A(x+\delta x) - R_A(x)\|$ is the absolute propagated error for solution by algorithm
- $\dfrac{\|R(x+\delta x) - R(x)\|}{\|R(x)\|}$ is the relative propagated error

Note that in practice $\delta x$ is unavoidable, and all sorts of errors are combined.

In computer we cannot find $R(x)$, but only $R_A(x+\delta x)$.

Error of finding $R_A(x+\delta x)$ instead of $R(x)$ will be:

$$\|R_A(x+\delta x) - R(x)\| = \|R_A(x+\delta x) + R(x+\delta x) - R(x+\delta x) - R(x)\| \le$$

$$\le \|R_A(x+\delta x) - R(x+\delta x)\| + \|R(x+\delta x) - R(x)\|$$

# Conditioning of the problem and algorithm stability

Absolute propagated error shows how sensitive the problem is to small changes or errors in input data.

- well-conditioned problem: small error in input data leads to a small absolute propagated error $\|\delta x\| < \varepsilon \;\Rightarrow\; \|R(x+\delta x) - R(x)\| < \varepsilon$
- ill-conditioned problem: small error in input data leads to a large absolute propagated error $\|\delta x\| < \varepsilon \;\Rightarrow\; \|R(x+\delta x) - R(x)\| > \varepsilon$
- stable algorithm for a well-conditioned problem: small error in input data leads to a small absolute propagated error for solution obtained by algorithm $\|\delta x\| < \varepsilon \;\Rightarrow\; \|R_A(x+\delta x) - R_A(x)\| < \varepsilon$
- unstable algorithm: otherwise

**Dangerous situation** is to apply a stable algorithm to an ill-conditioned problem, because the error $\|R_A(x+\delta x) - R_A(x)\|$ can be small, but such answer will be wrong!

## Computational costs

- flops (floating-point operations per second) is a measure of computer performance, indicating the number of operations a processor can perform per second

**Examples**

1) $Ax+y,\ A\in\mathbb{R}^{m\times n},\ b\in\mathbb{R}^{n}$ requires $2mn$ flops.

2) $lu(A),\ A\in\mathbb{R}^{n\times n}$ requires $\frac{2}{3}n^3$ flops.

The aim is to choose an algorithm that requires minimal flops.

- Costs of algorithm are $O(f(n))$ flops, where $n$ is the size of the problem.

**Example**. If the first part of the algorithm is $O(n^2)$ flops and the second part is $O(n)$ flops, the total sum will be $O(n^2)$ flops.

**Properties.**

$$O(f(n))+O(g(n))=O(\max\{f(n),g(n)\})$$

$$O(f(n)\cdot g(n))=O(f(n))\cdot O(g(n))$$