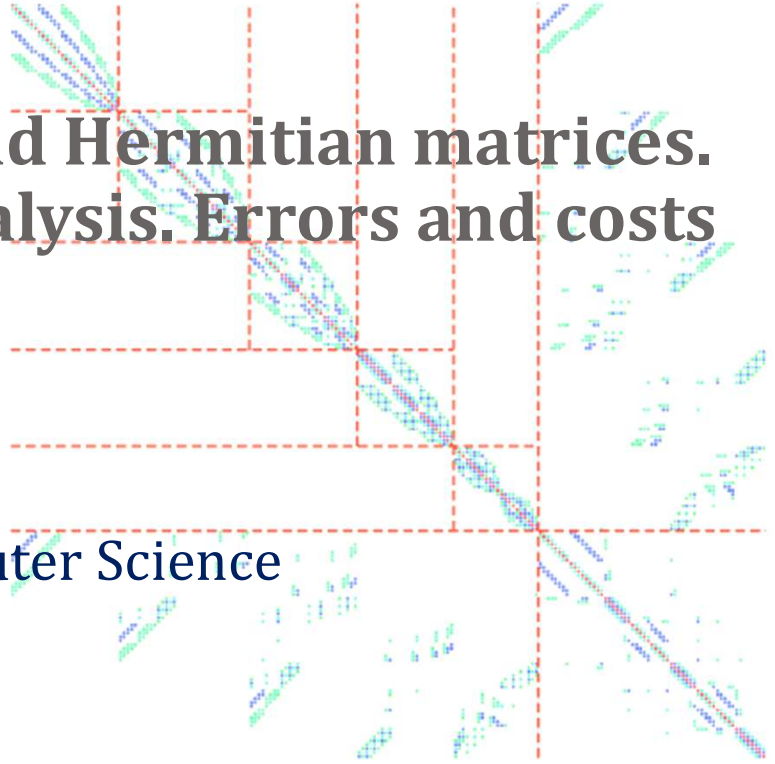
Numerical Methods of Linear Algebra for Sparse Matrices

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.

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

Theorem 4. $\forall A \in \mathbb{C}^{n\times n}$ 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) $\lambda_{\min}(H) \leq \mathrm{Re}(\lambda_i) \leq \lambda_{\max}(H)$

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

$H = \frac{1}{2}(A + A^H)$ is called Hermitian (symmetric in real case) part of A

If $A \in \mathbb{R}^{n\times n},\ u \in \mathbb{R}^n$ then $(Au,u) = (Hu,u)$

The definition of a real positive definite matrix

$(Au,u) > 0\ \forall u \in \mathbb{R}^n, u \neq 0\ \Leftrightarrow$ symmetric part of A is positive definite.

Positive definite matrices: important notes

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

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 $A \neq A^T$

```
A=rand(3)
```

```
A = 3×3
    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.
```

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

```
R = 0.7030
flag = 2
```

```
eig(A)
```

```
ans = 3×1
    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 $D = diag(\lambda_1,...,\lambda_n),\ \lambda_i \in \sigma(A)$

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 λ_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: $\rho(A) = \max\limits_{\lambda \in \sigma(A)} |\lambda|$.

Theorem 2. $\lim\limits_{k\to\infty} \|A^k\|^{1/k} = \rho(A).$

Theorem 3. Series of matrix powers $\sum\limits_{k=0}^{\infty} A^k$ 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 $A \in \mathbb{C}^{n\times n}$

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

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

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) $A = A^H \Rightarrow cond(A) = \left|\frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}\right|$, 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 π 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 δX. 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 δx 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.

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

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