MDI210 Numerical analysis and continuous optimisation Week 1 - Linear systems

Peter Brown

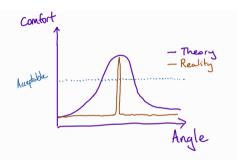
Télécom Paris peter.brown@telecom-paris.fr

September 13, 2022

We optimise all the time...

We optimise all the time...

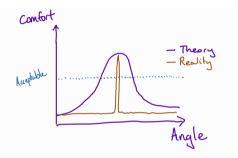
E.g., shower temperature:



We optimise all the time...

E.g., shower temperature:

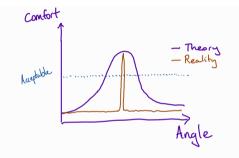
- How do we optimize?
- Efficient algorithms?
- Guaranteed optima?



We optimise all the time...

E.g., shower temperature:

- How do we optimize?
- Efficient algorithms?
- Guaranteed optima?



Course outline:

- Linear systems / eigenvalues / linear programming
- Optimization of continuous functions / constraints / convex functions

Notation

Given an $m \times n$ matrix $A = (a_{ij})_{\substack{1 \le i \le m \\ 1 \le j \le n}}$ we define

- Transpose: $A^t = (a_{ji})$.
- Adjoint: $A^* = (\overline{a_{ji}})$

(where \overline{x} is the complex conjugate of x)

Notation

Given an $m \times n$ matrix $A = (a_{ij})_{\substack{1 \le i \le m \\ 1 \le j \le n}}$ we define

- Transpose: $A^t = (a_{ji})$.
- Adjoint: $A^* = (\overline{a_{ji}})$

A real/complex square matrix A is:

- symmetric if $A^t = A$
- normal if $A^tA = AA^t$
- *orthogonal* if $A^tA = AA^t = \mathbb{I}$

(where \overline{x} is the complex conjugate of x)

Hermitian if
$$A^* = A$$

normal if
$$A^*A = AA^*$$

unitary if
$$A^*A = AA^* = \mathbb{I}$$

Notation

Given an $m \times n$ matrix $A = (a_{ij})_{\substack{1 \le i \le m \\ 1 \le j \le n}}$ we define

- Transpose: $A^t = (a_{ji})$.
- Adjoint: $A^* = (\overline{a_{ji}})$

(where \overline{x} is the complex conjugate of x)

A real/complex square matrix A is:

- symmetric if $A^t = A$
- *normal* if $A^tA = AA^t$
- *orthogonal* if $A^tA = AA^t = \mathbb{I}$

Hermitian if $A^* = A$

normal if $A^*A = AA^*$

unitary if $A^*A = AA^* = \mathbb{I}$

The *spectrum* of a matrix *A* is the set of its eigenvalues. The *spectral radius* is then

$$\rho(A) := \max\{|\lambda| : \lambda \in \operatorname{spectrum}(A)\}$$
 (1)

A motivating example

We're interested in solving linear systems given A, b such that Ax = b find x.

Example

We have a linear system

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix}$$

Solution:
$$x = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$
 (2)

A motivating example

We're interested in solving linear systems given A, b such that Ax = b find x.

Example

We have a linear system

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix}$$
 Solution: $x = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$

Potential numerical problems:

- Floating point errors finite precision / real data is noisy
- Truncation errors a useful algorithm must stop at a finite time

A motivating example

We're interested in solving linear systems given A, b such that Ax = b find x.

Example

We have a linear system

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix}$$

Solution:
$$x = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$
 (2)

Question

Suppose Ax = b. If $A' \approx A$, $b' \approx b$ and A'x' = b' then is $x' \approx x$?

Definition (Norm)

Let *V* be a vector space. Then $\|\cdot\|:V\to\mathbb{R}$ is a norm if

- $||x|| = 0 \iff x = 0$
- **3** $\|\alpha x\| = |\alpha| \|x\| \quad \forall x \in V \text{ and scalars } \alpha.$
- $||x + y|| \le ||x|| + ||y|| \quad \forall x, y \in V$

(non-negative) (positive definite) (absolute homogeneity) (triangle inequality)

Definition (Norm)

Let V be a vector space. Then $\|\cdot\|:V\to\mathbb{R}$ is a norm if

- $||x|| \ge 0 \qquad \forall x \in V$ $||x|| = 0 \iff x = 0$
- 3 $\|\alpha x\| = |\alpha| \|x\| \quad \forall x \in V \text{ and scalars } \alpha.$
- **4** $||x + y|| \le ||x|| + ||y|| \quad \forall x, y \in V$

(non-negative) (positive definite) (absolute homogeneity) (triangle inequality)

Example

Let $x = (x_i)_{1 \le i \le n}$ be a vector then

- $||x||_1 = \sum_{i=1}^{\overline{n}} |x_i|$
- $||x||_2 = \left(\sum_{i=1}^n |x_i|^2\right)^{1/2}$
- $\bullet \|x\|_{\infty} = \max_{1 \leq i \leq n} |x_i|$

(1-norm)

(2-norm / Euclidean norm)

(∞-norm / max-norm)

Definition (Norm)

Let V be a vector space. Then $\|\cdot\|:V\to\mathbb{R}$ is a norm if

- 3 $\|\alpha x\| = |\alpha| \|x\| \quad \forall x \in V \text{ and scalars } \alpha.$
- **4** $||x + y|| \le ||x|| + ||y|| \quad \forall x, y \in V$

(non-negative) (positive definite) (absolute homogeneity) (triangle inequality)

Example

Let $x = (x_i)_{1 \le i \le n}$ be a vector then

- $||x||_1 = \sum_{i=1}^n |x_i|$
- $||x||_2 = \left(\sum_{i=1}^n |x_i|^2\right)^{1/2}$
- $||x||_{\infty} = \max_{1 \leq i \leq n} |x_i|$

- (1-norm)
- (2-norm / Euclidean norm)
- $(\infty$ -norm / max-norm)

More generally we have a *p*-norm for $p \in [1, \infty)$ defined as $||x||_p := \left(\sum_{i=1}^n |x_i|^p\right)^{1/p}$.

Norms on square matrices can be defined a vector norm (subordinate norms)

$$||A|| := \sup_{x \neq 0} \frac{||Ax||}{||x||} = \sup_{x:||x||=1} ||Ax|| = \sup_{x:0 < ||x|| \le 1} \frac{||Ax||}{||x||}$$
(3)

These norms satisfy additional property $||AB|| \le ||A|| ||B||$ (submultiplicative) [Exercise: proof]

Norms on square matrices can be defined a vector norm (subordinate norms)

$$||A|| := \sup_{x \neq 0} \frac{||Ax||}{||x||} = \sup_{x: ||x|| = 1} ||Ax|| = \sup_{x: 0 < ||x|| \le 1} \frac{||Ax||}{||x||}$$
(3)

These norms satisfy additional property $||AB|| \le ||A|| ||B||$ (submultiplicative) [Exercise: proof]

Example

$$\begin{split} \|A\|_1 &= \sup_{x \neq 0} \frac{\|Ax\|_1}{\|x\|_1} = \max_{1 \leq j \leq n} \sum_{i=1}^n |a_{ij}| \\ \|A\|_2 &= \sup_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2} = \sqrt{\rho(A^TA)} \qquad \text{(largest singular value of } A\text{)} \\ \|A\|_\infty &= \sup_{x \neq 0} \frac{\|Ax\|_\infty}{\|x\|_\infty} = \max_{1 \leq i \leq n} \sum_{i=1}^n |a_{ij}| \end{split}$$

Not all matrix norms are subordinate norms

Example

A common matrix norm that is not subordinate is the *Frobenius* norm

$$\|A\|_F = \sqrt{\operatorname{Tr}\left[A^T A\right]}$$

Other examples include the *Schatten* norms $p \ge 1$

$$\|A\|_{(
ho)} := \left(\operatorname{Tr}\left[\left(A^TA\right)^{
ho/2}
ight]\right)^{1/
ho}$$

(matrix generalization of the p-norms).

Given a norm $\|\cdot\|$ we can then define a distance between x and y (or A and B) as

$$\operatorname{dist}(x,y) = \|x - y\| \tag{4}$$

this distance measure is called a metric.

Given a norm $\|\cdot\|$ we can then define a distance between x and y (or A and B) as

$$dist(x,y) = ||x - y|| \tag{4}$$

this distance measure is called a metric.

We can use this notion of distance to talk about *convergence*, a sequence of matrices A_k is said to converge to A (denoted $\lim_{k\to\infty} A_k = A$) if

$$\lim_{k} \|A_{k} - A\| = 0 \tag{5}$$

Given a norm $\|\cdot\|$ we can then define a distance between x and y (or A and B) as

$$dist(x,y) = ||x - y|| \tag{4}$$

this distance measure is called a metric.

We can use this notion of distance to talk about *convergence*, a sequence of matrices A_k is said to converge to A (denoted $\lim_{k\to\infty} A_k = A$) if

$$\lim_{k} \|A_{k} - A\| = 0 \tag{5}$$

All norms on finite dimensional spaces are equivalent! For any two norms $\|\cdot\|_a$ and $\|\cdot\|_b$ there exist constants $c_1, c_2 > 0$ such that

$$c_1 \|x\|_a \le \|x\|_b \le c_2 \|x\|_a \qquad \forall x$$
 (6)

Convergence doesn't depend on choice of norm!

ロト 4回 ト 4 重 ト 4 重 ト 3 重 9 9 9 9

Example

Let *A* be a matrix such that ||A|| < 1 for a submultiplicative norm $|| \cdot ||$ then

$$\lim_{k} A^{k} = 0.$$

Example

Let *A* be a matrix such that ||A|| < 1 for a submultiplicative norm $||\cdot||$ then

$$\lim_k A^k = 0.$$

This follows from

$$\|\mathbf{A}^k\| \leq \|\mathbf{A}\|^k \to 0$$
 as $k \to \infty$

therefore $\lim_{k} A^{k} = 0$.

Example

Let *A* be a matrix such that ||A|| < 1 for a submultiplicative norm $|| \cdot ||$ then

$$\lim_{k} A^{k} = 0.$$

This follows from

$$\|A^k\| \le \|A\|^k \to 0$$
 as $k \to \infty$

therefore $\lim_k A^k = 0$.

Take
$$A = \begin{pmatrix} a & a \\ a & a \end{pmatrix}$$
 for $a \in \mathbb{R}$. Then $||A||_1 = ||A||_2 = ||A||_{\infty} = 2|a|$ and so $A^k \to 0$ when $-1/2 < a < 1/2$.

Example

Let *A* be a matrix such that ||A|| < 1 for a submultiplicative norm $|| \cdot ||$ then

$$\lim_{k} A^{k} = 0.$$

This follows from

$$\|A^k\| \le \|A\|^k \to 0$$
 as $k \to \infty$

therefore $\lim_k A^k = 0$.

Take
$$A = \begin{pmatrix} a & a \\ a & a \end{pmatrix}$$
 for $a \in \mathbb{R}$. Then $||A||_1 = ||A||_2 = ||A||_\infty = 2|a|$ and so $A^k \to 0$ when $-1/2 < a < 1/2$.

This agrees with

$$A^n = 2^n \begin{pmatrix} a^n & a^n \\ a^n & a^n \end{pmatrix}$$

Back to the example

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix}$$
 Solution: $x = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$

Solution:
$$x = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$
 (7)

10/28

Back to the example

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix}$$
 Solution: $x = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$

Perturbing b we see

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \\ x'_4 \end{pmatrix} = \begin{pmatrix} 32.1 \\ 22.9 \\ 33.1 \\ 30.9 \end{pmatrix}$$
 Solution: $x' = \begin{pmatrix} 9.2 \\ -12.6 \\ 4.5 \\ -1.1 \end{pmatrix}$

Solution:
$$x' = \begin{pmatrix} 9.2 \\ -12.6 \\ 4.5 \\ -1.1 \end{pmatrix}$$
 (8)

The relative error on b is $\frac{\|b'-b\|}{\|b\|}$ of order 1/100 but the relative error on x is of order 10! (Order 1000 increase)

10/28

This large error increase is due to the *condition number* of *A*.

This large error increase is due to the *condition number* of *A*.

Let
$$\delta x = x' - x$$
 and $\delta b = b' - b$, then

$$\delta x = A^{-1} \delta b \tag{9}$$

Then for any *subordinate norm*

$$\|\delta \mathbf{x}\| \le \|\mathbf{A}^{-1}\| \|\delta \mathbf{b}\| \tag{10}$$

This large error increase is due to the *condition number* of *A*.

Let
$$\delta x = x' - x$$
 and $\delta b = b' - b$, then

$$\delta x = A^{-1} \delta b \tag{9}$$

Then for any *subordinate norm*

$$\|\delta x\| \le \|A^{-1}\| \|\delta b\|$$
 (10)

Moreover $||b|| \le ||A|| ||x||$, putting these together we get

$$\frac{\|\delta x\|}{\|x\|} \le \|A\| \|A^{-1}\| \frac{\|\delta b\|}{\|b\|} \tag{11}$$

This large error increase is due to the *condition number* of *A*.

Let
$$\delta x = x' - x$$
 and $\delta b = b' - b$, then

$$\delta \mathbf{x} = \mathbf{A}^{-1} \delta \mathbf{b} \tag{9}$$

Then for any *subordinate norm*

$$\|\delta x\| \le \|A^{-1}\| \|\delta b\|$$
 (10)

Moreover $||b|| \le ||A|| ||x||$, putting these together we get

$$\frac{\|\delta x\|}{\|x\|} \le \|A\| \|A^{-1}\| \frac{\|\delta b\|}{\|b\|}$$
 (11)

We call $cond(A) := ||A|| ||A^{-1}||$ the *conditioning of A* – relative error amplification depends on the conditioning!

For the example *A* we have $cond_2(A) \approx 2974$.

Properties of the conditioning

Recall cond(A) := $||A|| ||A^{-1}||$ for some subordinate norm $||\cdot||$.

Theorem

Let A be an invertible matrix. Then

- \bigcirc cond(A) \geq 1
- \bigcirc cond $(A) = \text{cond}(A^{-1})$
- **3** For $\alpha \neq 0$ we have $cond(\alpha A) = cond(A)$.
- 4 If U, V are orthogonal/unitary then $cond_2(UAV) = cond(A)$
- **5** If A is orthogonal/unitary then $cond_2(A) = 1$.

Properties of the conditioning

Recall cond(A) := $||A|| ||A^{-1}||$ for some subordinate norm $||\cdot||$.

Theorem

Let A be an invertible matrix. Then

- \bigcirc cond(A) \geq 1
- \bigcirc cond(A) = cond(A^{-1})
- **3** For $\alpha \neq 0$ we have $cond(\alpha A) = cond(A)$.
- 4) If U, V are orthogonal/unitary then $cond_2(UAV) = cond(A)$
- **5** If A is orthogonal/unitary then $cond_2(A) = 1$.

Remark (Geometric characterization of cond₂)

Let $\theta(A)$ be the smallest angle between vectors Ax and Ay where x and y are orthonormal. Then

$$\operatorname{cond}_2(A) = \frac{1}{\tan(\theta(A)/2)} \tag{12}$$

We can improve the conditioning of our problem by *rebalancing* the matrix *A*.

We can improve the conditioning of our problem by *rebalancing* the matrix A. Let D_1, D_2 be diagonal invertible matrices satisfying

$$\operatorname{cond}(D_1 A D_2) = \inf_{\Delta_1, \Delta_2 \text{invertible/diagonal}} \operatorname{cond}(\Delta_1 A \Delta_2)$$
(13)

We can improve the conditioning of our problem by *rebalancing* the matrix A. Let D_1, D_2 be diagonal invertible matrices satisfying

$$\operatorname{cond}(D_1 A D_2) = \inf_{\Delta_1, \Delta_2 \text{invertible/diagonal}} \operatorname{cond}(\Delta_1 A \Delta_2)$$
(13)

Then solve Ax = b in two steps:

- 1 Solve $D_1AD_2y = D_1b$ (receiving y)
- 2 Then compute $x = D_2 y$

We can improve the conditioning of our problem by *rebalancing* the matrix A. Let D_1, D_2 be diagonal invertible matrices satisfying

$$\operatorname{cond}(D_1 A D_2) = \inf_{\Delta_1, \Delta_2 \text{invertible/diagonal}} \operatorname{cond}(\Delta_1 A \Delta_2)$$
(13)

Then solve Ax = b in two steps:

- 1 Solve $D_1AD_2y = D_1b$ (receiving y)
- 2 Then compute $x = D_2 y$

Remark

In practice it is difficult to optimize the above so one can try to optimize the ratio

$$\frac{\max_{ij}|a'_{ij}|}{\min_{ij:a'_{ij}\neq 0}|a'_{ij}|} \qquad \qquad A' = \Delta_1 A \Delta_2$$

which can be treat as a linear program (see notes once studied LP).

Conditioning problem for eigenvalues

Question

How do the eigenvalues of a matrix A change if we perturb its entries?

Conditioning problem for eigenvalues

Question

How do the eigenvalues of a matrix A change if we perturb its entries?

Theorem

Let A be diagonalizable ($P^{-1}AP = \operatorname{diag}(\lambda_i)$). Let $\|\cdot\|$ be a matrix norm so that $\|\operatorname{diag}(\delta_i)\| = \max_i |\delta_i|$.

Then for any matrix δA we have

$$\operatorname{spectrum}(A + \delta A) \subset \bigcup_{i=1}^{n} D_{i}$$
 (14)

where

$$D_i = \{ z \in \mathbb{C} : |z - \lambda_i| \le \operatorname{cond}(P) \|\delta A\| \}. \tag{15}$$

Conditioning problem for eigenvalues

Question

How do the eigenvalues of a matrix A change if we perturb its entries?

Theorem

Let A be diagonalizable ($P^{-1}AP = \operatorname{diag}(\lambda_i)$). Let $\|\cdot\|$ be a matrix norm so that $\|\operatorname{diag}(\delta_i)\| = \max_i |\delta_i|$.

Then for any matrix δA we have

$$\operatorname{spectrum}(A + \delta A) \subset \bigcup_{i=1}^{n} D_{i}$$
 (14)

(16)

where

$$D_i = \{ z \in \mathbb{C} : |z - \lambda_i| \le \operatorname{cond}(P) \|\delta A\| \}. \tag{15}$$

We define the conditioning of A for the eigenvalue problem to be

$$\Gamma(A) = \min\{\operatorname{cond}(P) : P^{-1}AP \text{ is diagonal}\}\$$

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022

Solving linear systems

Problem

Let $A = (a_{ij})$ be an invertible square matrix and let x and b be column vectors such that

$$Ax = b ag{17}$$

Solve for x.

Solving linear systems

Problem

Let $A = (a_{ij})$ be an invertible square matrix and let x and b be column vectors such that

$$Ax = b ag{17}$$

Solve for x.

Numerical methods typically do not compute A^{-1} (we can be more efficient!)

Solving linear systems

Problem

Let $A = (a_{ij})$ be an invertible square matrix and let x and b be column vectors such that

$$Ax = b ag{17}$$

Solve for x.

Numerical methods typically do not compute A^{-1} (we can be more efficient!)

First let's think about a special case – *triangular matrices*.

Upper triangular A

Suppose A is an upper triangular matrix. Then we have the linear equations

$$a_{1,1}x_1 + \dots + a_{1,n-1}x_{n-1} + a_{1,n}x_n = b_1$$
...
$$a_{n-1,n-1}x_{n-1} + a_{n-1,n}x_n = b_{n-1}$$

$$a_{n,n}x_n = b_n$$

Upper triangular A

Suppose A is an upper triangular matrix. Then we have the linear equations

$$a_{1,1}x_1 + \dots + a_{1,n-1}x_{n-1} + a_{1,n}x_n = b_1$$
 \dots
 $a_{n-1,n-1}x_{n-1} + a_{n-1,n}x_n = b_{n-1}$
 $a_{n,n}x_n = b_n$

We can then use backwards substitution:

$$x_{n} = \frac{b_{n}}{a_{n,n}}$$

$$x_{n-1} = \frac{b_{n-1} - a_{n-1,n}x_{n}}{a_{n-1,n-1}}$$
...

Upper triangular *A* – efficiency

Question

How many operations needed to solve with backwards substitution?

Upper triangular *A* – efficiency

Question

How many operations needed to solve with backwards substitution?

Solution

$$a_{1,1}x_1 + \dots + a_{1,n-1}x_{n-1} + a_{1,n}x_n = b_1$$
...
$$a_{n-1,n-1}x_{n-1} + a_{n-1,n}x_n = b_{n-1}$$

$$a_{n,n}x_n = b_n$$

We have n(n-1)/2 additions, n(n-1)/2 multiplications and n divisions.

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022

Upper triangular A – efficiency

Ouestion

How many operations needed to solve with backwards substitution?

Solution

$$a_{1,1}x_1 + \dots + a_{1,n-1}x_{n-1} + a_{1,n}x_n = b_1$$
 \dots
 $a_{n-1,n-1}x_{n-1} + a_{n-1,n}x_n = b_{n-1}$
 $a_{n,n}x_n = b_n$

We have n(n-1)/2 additions, n(n-1)/2 multiplications and n divisions.

For comparison, computing the inverse is of order $O(n^3)$ operations.

Peter Brown (Télécom Paris) MDI210 - Optimisation

Reducing to upper triangular matrices

Triangular matrices are easy to solve. Can we reduce everything to triangular matrices?

Reducing to upper triangular matrices

Triangular matrices are easy to solve. *Can we reduce everything to triangular matrices?* Yes! Using *invertible* operations.

Theorem

Let $P \in \mathbb{R}^{n \times n}$ be an invertible matrix. Then

$${x : Ax = b} = {x : PAx = Pb}$$
 (18)

Reducing to upper triangular matrices

Triangular matrices are easy to solve. *Can we reduce everything to triangular matrices?* Yes! Using *invertible* operations.

Theorem

Let $P \in \mathbb{R}^{n \times n}$ be an invertible matrix. Then

$$\{x : Ax = b\} = \{x : PAx = Pb\}$$
 (18)

Gaussian Elimination: Use a sequence of invertible operators P_1, \ldots, P_k such that

$$P_n \dots P_2 P_1 A = U \tag{19}$$

where U is upper triangular. Then solve

$$Ux = P_n \dots P_2 P_1 b. \tag{20}$$

Gaussian elimination

The *elementary row operations* (all invertible) are

- Interchange any two rows.
- Multiply a row by a constant.
- Add a multiple of one row to another row.

Gaussian elimination

The *elementary row operations* (all invertible) are

- Interchange any two rows.
- Multiply a row by a constant.
- Add a multiple of one row to another row.

The algorithm:

- **1** For j ∈ {1, . . . n} repeat steps 2-4:
- 2 Choose a non-zero element (pivot) from column j below and including $a_{j,j}$.
- 3 If not row *j* then swap chosen elements row with row *j*.
- **4** Use linear combinations of rows to set all $a_{ij} = 0$ for i > j.

Consider the linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $4x_1 + x_2 + 5x_3 = -1$
 $10x_1 - 7x_2 + 13x_3 = -3$

Consider the linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $4x_1 + x_2 + 5x_3 = -1$
 $10x_1 - 7x_2 + 13x_3 = -3$

Step 1.2: Choose pivot.

20/28

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022

Consider the linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $4x_1 + x_2 + 5x_3 = -1$
 $10x_1 - 7x_2 + 13x_3 = -3$

Step 1.3: Swap chosen pivot row so pivot on diagonal. (done)

20/28

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022

Consider the linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $4x_1 + x_2 + 5x_3 = -1$
 $10x_1 - 7x_2 + 13x_3 = -3$

Step 1.4: Use row sums to remove below elements.

$$R_2 \mapsto R_2 - 2R_1$$
 and $R_3 \mapsto R_3 - 5R_1$

Consider the linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $4x_1 + x_2 + 5x_3 = -1$
 $10x_1 - 7x_2 + 13x_3 = -3$

Step 1.4: Use row sums to remove below elements.

$$R_2 \mapsto R_2 - 2R_1$$
 and $R_3 \mapsto R_3 - 5R_1$

$$2x_1 + x_2 - 3x_3 = 5$$

 $0 - x_2 + 11x_3 = -11$
 $0 - 12x_2 + 28x_3 = -28$

Consider the linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $0 - 1x_2 + 11x_3 = -11$
 $0 - 12x_2 + 28x_3 = -28$

Step 2.1: Choose pivot

Consider the linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $0 - 1x_2 + 11x_3 = -11$
 $0 - 12x_2 + 28x_3 = -28$

Step 2.2: Move to diagonal (done)

Consider the linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $0 - 1x_2 + 11x_3 = -11$
 $0 - 12x_2 + 28x_3 = -28$

Step 2.3: Remove zeros below pivot

$$R_3 \mapsto R_3 - 12R_2$$

20/28

September 13, 2022

Consider the linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $0 - 1x_2 + 11x_3 = -11$
 $0 - 12x_2 + 28x_3 = -28$

Step 2.3: Remove zeros below pivot

$$R_3 \mapsto R_3 - 12R_2$$

$$2x_1 + x_2 - 3x_3 = 5$$

 $0 - 1x_2 + 11x_3 = -11$
 $0 - 0 - 104x_3 = 104$

Now we're left with an upper triangular linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $0 - x_2 + 11x_3 = -11$
 $0 - 0 - 104x_3 = 104$

which we can compute like before!

Applying backward substitution we get

$$x_3 = -1, \qquad x_2 = 0, \qquad x_1 = 1$$

Now we're left with an upper triangular linear system

$$2x_1 + x_2 - 3x_3 = 5$$

 $0 - x_2 + 11x_3 = -11$
 $0 - 0 - 104x_3 = 104$

which we can compute like before!

Applying backward substitution we get

$$x_3 = -1, \qquad x_2 = 0, \qquad x_1 = 1$$

Remark

Whenever you exchange rows you flip the sign of the determinant. We can compute $\det(A)$ as

$$\det(A) = (-1)^q \times \Pi_i p_i$$

where p_i is the value of the *i*-th pivot.

Gauss method - choice of pivot

- Default strategy: Choose the term on the diagonal (or next available one).
- Partial pivot: Choose pivot with largest modulus in the current column.
- Total pivot: Choose pivot with largest modulus in the remaining residual matrix.

Choosing larger modulus reduces numerical instability due to divisions but is more expensive.

Gauss method - choice of pivot

- Default strategy: Choose the term on the diagonal (or next available one).
- Partial pivot: Choose pivot with largest modulus in the current column.
- Total pivot: Choose pivot with largest modulus in the remaining residual matrix.

Choosing larger modulus reduces numerical instability due to divisions but is more expensive.

Example (Choice of pivot)

Consider the system (solution $(x_1, x_2) = (1.0001, 0.9999)$)

$$10^{-4}x_1 + x_2 = 1$$
$$x_1 + x_2 = 2$$

After default pivoting we have

$$x_2 = \frac{2 - 10^4}{1 - 10^4} = \frac{9998}{9999} \approx_{\text{lose 1 digit}} 1 \implies x_1 = 0$$

Gauss method - choice of pivot

- Default strategy: Choose the term on the diagonal (or next available one).
- Partial pivot: Choose pivot with largest modulus in the current column.
- Total pivot: Choose pivot with largest modulus in the remaining residual matrix.

Choosing larger modulus reduces numerical instability due to divisions but is more expensive.

Example (Choice of pivot)

Consider the system (solution $(x_1, x_2) = (1.0001, 0.9999)$)

$$x_1 + x_2 = 2$$

 $10^{-4}x_1 + x_2 = 1$

After partial pivoting we have

$$x_2 = \frac{1 - 2 \times 10^{-4}}{1 - 10^{-4}} = \frac{0.9998}{0.9999} \approx_{\text{lose 1 digit }} 1 \implies x_1 = 1$$

We don't have to solve a single linear system

We can solve *n* systems at the same time and compute the inverse!

We don't have to solve a single linear system

We can solve *n* systems at the same time and compute the inverse!

Example: Compute the inverse of

$$A = \begin{pmatrix} 1 & -3 & 14 \\ 1 & -2 & 10 \\ -2 & 4 & -19 \end{pmatrix}$$

We don't have to solve a single linear system

We can solve *n* systems at the same time and compute the inverse!

Example: Compute the inverse of

$$A = \begin{pmatrix} 1 & -3 & 14 \\ 1 & -2 & 10 \\ -2 & 4 & -19 \end{pmatrix}$$

So we solve 3 systems simultaneously

So we solve 3 systems simultaneously

$$x_1$$
 - $3x_2$ + $14x_3$ = 1 | 0 | 0
 x_1 - $2x_2$ + $10x_3$ = 0 | 1 | 0
 $-2x_1$ + $4x_2$ - $19x_3$ = 0 | 0 | 1

So we solve 3 systems simultaneously

Step 1.1: Let's do a partial pivot

So we solve 3 systems simultaneously

Step 1.1: Let's do a partial pivot

Step 1.2: Remove the elements below pivot

$$R_2\mapsto R_2+\frac{1}{2}R_1 \qquad R_3\mapsto R_3+\frac{1}{2}R_1$$

September 13, 2022

Step 2.1: We do a total pivot (to demonstrate)

Step 2.1: We do a total pivot (to demonstrate)

Step 2.2: Remove coefficients above and below the pivot

$$R_1 \mapsto R_1 + \frac{38}{9}R_2 \qquad R_3 \mapsto R_39 - \frac{1}{9}R_2$$

Step 3.1: We choose a default pivot

Step 3.1: We choose a default pivot

Step 3.2: Remove coefficients above the pivot

$$R_1\mapsto R_1+2R_3 \qquad R_2\mapsto R_2+9R_3$$

Now we're almost done

Now we're almost done

Step 4: Solution

Now we're almost done

Step 4: Solution

and so

$$A^{-1} = \begin{pmatrix} -2 & -1 & -2 \\ -1 & 9 & 4 \\ 0 & 2 & 1 \end{pmatrix}$$

Suppose every pivot in the Gauss method was on the diagonal.

Suppose every pivot in the Gauss method was on the diagonal.

Consider the matrix P_k that does the linear combinations for column k, it takes the form

I.e., an identity matrix with coefficients under the *k*-th diagonal.

Therefore

$$P_n \dots P_1 A = U$$

where P_1, \ldots, P_n are *lower triangular* and *U* is *upper triangular*.

Therefore

$$P_n \dots P_1 A = U$$

where P_1, \ldots, P_n are *lower triangular* and U is *upper triangular*.

One can show P_k^{-1} is also lower triangular, therefore

$$A = P_1^{-1} \dots P_n^{-1} U = LU$$
 (21)

I.e., we can decompose A into the product of a lower triangular and upper triangular matrix!

Therefore

$$P_n \dots P_1 A = U$$

where P_1, \ldots, P_n are *lower triangular* and U is *upper triangular*.

One can show P_k^{-1} is also lower triangular, therefore

$$A = P_1^{-1} \dots P_n^{-1} U = LU$$
 (21)

I.e., we can decompose A into the product of a lower triangular and upper triangular matrix!

Question

What if the pivots are not on the diagonal?

Therefore

$$P_n \dots P_1 A = U$$

where P_1, \ldots, P_n are *lower triangular* and *U* is *upper triangular*.

One can show P_k^{-1} is also lower triangular, therefore

$$A = P_1^{-1} \dots P_n^{-1} U = LU$$
 (21)

I.e., we can decompose A into the product of a lower triangular and upper triangular matrix!

Question

What if the pivots are not on the diagonal?

Can rearrange rows/cols of A so all pivots on diagonal so

$$QAR = LU$$



Theorem

Let $A \in \mathbb{R}^{n \times n}$ be an invertible square matrix such that for $1 \le k \le n$ the submatrix

$$A_k = \begin{pmatrix} a_{11} & \dots & a_{1k} \\ \vdots & \ddots & \vdots \\ a_{k1} & \dots & a_{kk} \end{pmatrix}$$

is invertible. Then the Gauss method can be performed with all pivots on the diagonal and hence the LU decomposition exists for A.

Theorem

Let $A \in \mathbb{R}^{n \times n}$ be an invertible square matrix such that for $1 \le k \le n$ the submatrix

$$A_k = \begin{pmatrix} a_{11} & \dots & a_{1k} \\ \vdots & \ddots & \vdots \\ a_{k1} & \dots & a_{kk} \end{pmatrix}$$

is invertible. Then the Gauss method can be performed with all pivots on the diagonal and hence the LU decomposition exists for A.

Remark

The LU decomposition can be computed when trying to solve more than one linear system. Once you have the LU decomposition you need to solve two triangular systems per original system

$$Ly = b$$
 then $Ux = y$

Cholesky Decomposition

A matrix *A* is *positive definite* if it is symmetric and

$$x^T A x > 0, \qquad \forall x \neq 0$$
 (21)

For positive definite matrices we have a more efficient LU decomposition with $L = U^T$.

Example

We have
$$A = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}$$
, then $x^T A x = x_1^2 + (x_1 + x_2)^2 > 0$ and so A is positive definite.

24/28

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022

Cholesky Decomposition

A matrix *A* is *positive definite* if it is symmetric and

$$x^T A x > 0, \qquad \forall x \neq 0$$
 (21)

For positive definite matrices we have a more efficient LU decomposition with $L = U^T$.

Example

We have
$$A = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}$$
, then $x^T A x = x_1^2 + (x_1 + x_2)^2 > 0$ and so A is positive definite.

Theorem (Cholesky decomposition)

Let $A \in \mathbb{R}^{n \times n}$ be positive definite. Then there exists a lower triangular matrix $B \in \mathbb{R}^{n \times n}$ such that $A = BB^T$.

24/28

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022

Cholesky Decomposition

A matrix *A* is *positive definite* if it is symmetric and

$$x^T A x > 0, \qquad \forall x \neq 0$$
 (21)

24/28

For positive definite matrices we have a more efficient LU decomposition with $L = U^T$.

Example

We have
$$A = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}$$
, then $x^T A x = x_1^2 + (x_1 + x_2)^2 > 0$ and so A is positive definite.

Theorem (Cholesky decomposition)

Let $A \in \mathbb{R}^{n \times n}$ be positive definite. Then there exists a lower triangular matrix $B \in \mathbb{R}^{n \times n}$ such that $A = BB^T$.

Proof.

By induction...

Cholesky Decomposition – Proof

Base case n = 1 is trivial.

Cholesky Decomposition – Proof

Base case n = 1 is trivial. Consider general positive definite A and partition as

$$A = \begin{pmatrix} a_{11} & W^T \\ W & C \end{pmatrix}$$

where $W \in \mathbb{R}^{n \times 1}$ and $C \in \mathbb{R}^{n-1 \times n-1}$.

Cholesky Decomposition – Proof

Base case n = 1 is trivial. Consider general positive definite A and partition as

$$A = \begin{pmatrix} a_{11} & W^T \\ W & C \end{pmatrix}$$

where $W \in \mathbb{R}^{n \times 1}$ and $C \in \mathbb{R}^{n-1 \times n-1}$. By direct calculation we have

$$A = \begin{pmatrix} a_{11} & W^T \\ W & C \end{pmatrix} = \begin{pmatrix} \sqrt{a_{11}} & 0 \\ W/\sqrt{a_{11}} & I \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & C - WW^T/a_{11} \end{pmatrix} \begin{pmatrix} \sqrt{a_{11}} & W^T/\sqrt{a_{11}} \\ 0 & I \end{pmatrix}$$

Cholesky Decomposition - Proof

Base case n = 1 is trivial. Consider general positive definite A and partition as

$$A = \begin{pmatrix} a_{11} & W^T \\ W & C \end{pmatrix}$$

where $W \in \mathbb{R}^{n \times 1}$ and $C \in \mathbb{R}^{n-1 \times n-1}$. By direct calculation we have

$$A = \begin{pmatrix} a_{11} & W^T \\ W & C \end{pmatrix} = \begin{pmatrix} \sqrt{a_{11}} & 0 \\ W/\sqrt{a_{11}} & I \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & C - WW^T/a_{11} \end{pmatrix} \begin{pmatrix} \sqrt{a_{11}} & W^T/\sqrt{a_{11}} \\ 0 & I \end{pmatrix}$$

The middle matrix is block diagonal and positive definite therefore $C - WW^T/a_{11} = LL^T$ (Cholesky decomposition) by induction assumption. So

$$A = \begin{pmatrix} \sqrt{a_{11}} & 0 \\ W/\sqrt{a_{11}} & I \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & LL^T \end{pmatrix} \begin{pmatrix} \sqrt{a_{11}} & W^T/\sqrt{a_{11}} \\ 0 & I \end{pmatrix} \\ = \begin{pmatrix} \sqrt{a_{11}} & 0 \\ W/\sqrt{a_{11}} & L \end{pmatrix} \begin{pmatrix} \sqrt{a_{11}} & W^T/\sqrt{a_{11}} \\ 0 & L^T \end{pmatrix}$$

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022 25/28

Cholesky Decomposition - Algorithm

$$A = \begin{pmatrix} b_{11} & 0 & \dots & 0 \\ b_{21} & b_{22} & 0 & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \dots & b_{nn} \end{pmatrix} \begin{pmatrix} b_{11} & b_{21} & \dots & b_{n1} \\ 0 & b_{22} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & b_{nn} \end{pmatrix}$$

Cholesky Decomposition - Algorithm

$$A = \begin{pmatrix} b_{11} & 0 & \dots & 0 \\ b_{21} & b_{22} & 0 & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \dots & b_{nn} \end{pmatrix} \begin{pmatrix} b_{11} & b_{21} & \dots & b_{n1} \\ 0 & b_{22} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & b_{nn} \end{pmatrix}$$

and so

$$a_{ij} = \sum_{k=1}^{\min\{i,j\}} b_{ik}b_{jk} = \langle (b_{ik})_k, (b_{jk})_k \rangle = a_{ji}$$

Cholesky Decomposition – Algorithm

$$A = \begin{pmatrix} b_{11} & 0 & \dots & 0 \\ b_{21} & b_{22} & 0 & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \dots & b_{nn} \end{pmatrix} \begin{pmatrix} b_{11} & b_{21} & \dots & b_{n1} \\ 0 & b_{22} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & b_{nn} \end{pmatrix}$$

and so

$$a_{ij} = \sum_{k=1}^{\min\{i,j\}} b_{ik} b_{jk} = \langle (b_{ik})_k, (b_{jk})_k \rangle = a_{ji}$$

For the first column

$$b_{11} = \sqrt{a_{11}}$$
 and $b_{i1} = \frac{a_{i1}}{b_{11}}$ for $2 \le i \le n$

Cholesky Decomposition – Algorithm

$$A = \begin{pmatrix} b_{11} & 0 & \dots & 0 \\ b_{21} & b_{22} & 0 & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \dots & b_{nn} \end{pmatrix} \begin{pmatrix} b_{11} & b_{21} & \dots & b_{n1} \\ 0 & b_{22} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & b_{nn} \end{pmatrix}$$

and so

$$a_{ij} = \sum_{k=1}^{\min\{i,j\}} b_{ik}b_{jk} = \langle (b_{ik})_k, (b_{jk})_k \rangle = a_{ji}$$

For the first column

$$b_{11} = \sqrt{a_{11}}$$
 and $b_{i1} = \frac{a_{i1}}{b_{11}}$ for $2 \le i \le n$

For column $2 \le j \le n$

$$b_{jj} = \sqrt{a_{jj} - \sum_{k=1}^{j-1} b_{jk}^2}$$
 and $b_{ij} = \frac{a_{ij} - \sum_{k=1}^{j-1} b_{ik} b_{jk}}{b_{jj}}$

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022 26/2

Cholesky Decomposition – Algorithm II

Remark (Properties)

- **1** Suppose we solve Ax = b for a positive definite A.
 - Gaussian elimination approx $\frac{2n^3}{3}$ operations
 - Cholesky decomposition approx $\frac{n^3}{3}$ operations
- 2 If $A = BB^T$ then

$$\det(A) = \det(BB^T) = \det(B)\det(B^T) = (b_{11}b_{22}\dots b_{nn})^2$$

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022

Cholesky Decomposition – Algorithm II

Remark (Properties)

- **1** Suppose we solve Ax = b for a positive definite A.
 - Gaussian elimination approx $\frac{2n^3}{3}$ operations
 - Cholesky decomposition approx $\frac{n^3}{3}$ operations
- 2 If $A = BB^T$ then

$$\det(A) = \det(BB^T) = \det(B)\det(B^T) = (b_{11}b_{22}\dots b_{nn})^2$$

Example

We have

$$A = \begin{pmatrix} 4 & -2 & 0 \\ -2 & 2 & 3 \\ 0 & 3 & 10 \end{pmatrix}$$
$$x^{T}Ax = (2x_{1} - x_{2})^{2} + (x_{2} + 3x_{3})^{2} + x_{3}^{2} > 0$$

Cholesky Decomposition – Algorithm II

Remark (Properties)

- **1** Suppose we solve Ax = b for a positive definite A.
 - Gaussian elimination approx $\frac{2n^3}{3}$ operations
 - Cholesky decomposition approx $\frac{n^3}{3}$ operations
- 2 If $A = BB^T$ then

$$\det(A) = \det(BB^T) = \det(B)\det(B^T) = (b_{11}b_{22}\dots b_{nn})^2$$

Example

We have

$$A = \begin{pmatrix} 4 & -2 & 0 \\ -2 & 2 & 3 \\ 0 & 3 & 10 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 3 & 1 \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{pmatrix}$$
$$x^{T}Ax = (2x_{1} - x_{2})^{2} + (x_{2} + 3x_{3})^{2} + x_{3}^{2} > 0$$

Some exercises (working over \mathbb{R})

- Let V be an orthogonal matrix. Show that $cond_2(V) = 1$.
- 2 Let || · || be a subordinate norm. Show that

$$||Ax|| \le ||A|| ||x||$$
 and $||AB|| \le ||A|| ||B||$

- 3 Let $\alpha \neq 0$ and U, V be orthogonal. Prove
 - (a) cond(A) > 1

(b) $\operatorname{cond}(A) = \operatorname{cond}(A^{-1})$

- (c) $\operatorname{cond}(\alpha A) = \operatorname{cond}(A)$ (d) $\operatorname{cond}_2(A) = \operatorname{cond}_2(UAV)$
- 4 Let $A = \begin{pmatrix} 1 & \epsilon \\ \epsilon & 1 \end{pmatrix}$ for $0 < \epsilon < 1$ and let $b = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.
 - (a) Using Gauss' method solve Ax = b.
 - (b) Using Gauss-lacobi method compute A^{-1} .
 - (c) Compute $\operatorname{cond}_1(A)$ and $\operatorname{cond}_{\infty}(A)$. When is A well-conditioned? What happens at $\epsilon = 1$?
 - (d) For what values of ϵ is \boldsymbol{A} positive definite?
 - (e) Find the LU decomposition of A.
 - (f) Compute the Cholesky decomposition of A.
- Suppose Ax = b and A'x' = b. Show that

$$\frac{\|x'-x\|}{\|x'\|} \leq \operatorname{cond}(A) \frac{\|A'-A\|}{\|A\|}$$



28/28

Peter Brown (Télécom Paris) MDI210 - Optimisation September 13, 2022