Parallel Scientific Computing

Course AMS301 — Fall 2023 — Lecture 5

Direct methods for linear systems

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Solution procedures for linear systems — Recap

Find $\mathbf{x} \in \mathbb{R}^n$ such that $\mathbf{A}\mathbf{x} = \mathbf{b}$ with $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\mathbf{b} \in \mathbb{R}^n$.

Solution procedures

Direct methods: Factorization of A into triangular and diagonal matrices (ex. A = LU) and solution of simpler problems.

$$\mathbf{A}\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad \mathbf{L}\mathbf{U}\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad \begin{vmatrix} \mathbf{L}\mathbf{y} = \mathbf{b} \\ \mathbf{U}\mathbf{x} = \mathbf{y} \end{vmatrix}$$

Advantages: exact solution known after a given number of operations Difficulties: heavy computational cost (operations/memory), hard to parallelize

▶ Iterative methods: Iterative procedure to minimizing an error $\|\mathbf{x}^{(\ell)} - \mathbf{x}_{ref}\|$ and/or a residual $\|\mathbf{A}\mathbf{x}^{(\ell)} - \mathbf{b}\|$.

$$\begin{split} \mathbf{x}^{(0)} &= \mathrm{Iter}_{(0)}\left(\mathbf{A}, \mathbf{b}\right) \\ \mathbf{x}^{(\ell+1)} &= \mathrm{Iter}^{(\ell+1)}\left(\mathbf{x}^{(\ell)}, \mathbf{x}^{(\ell-1)}, \dots, \mathbf{A}, \mathbf{b}\right), \quad \text{pour } \ell \geq 0 \end{split}$$

Advantages: limited cost per iteration *(operations/memory)*, easy to parallelize Difficulties: approximate solution, control of the convergence of the process

Direct methods for linear systems Solution of triangular systems Gaussian elimination Matrix factorization

Triangular systems — Approaches by points [1/2]

Definitions

- ▶ Lower triangular matrix: $\mathbf{L} \in \mathbb{R}^{n \times n}$ with $L_{ij} = 0$ if i < j
- Upper triangular matrix: $\mathbf{U} \in \mathbb{R}^{n \times n}$ with $U_{ij} = 0$ if i > j

$$\mathbf{L} = \begin{bmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \qquad \mathbf{U} = \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

Properties

The determinant of a triangular matrix is the product of the diagonal elements:

$$\det(\mathbf{L}) = \prod_{i=1}^{n} L_{ii} \qquad \det(\mathbf{U}) = \prod_{i=1}^{n} U_{ii}$$

A triangular matrix is invertible if, and only if, its diagonal elements are nonzero.

Triangular systems — Approaches by points [2/2]

Procedure to solve $\mathbf{Lx} = \mathbf{b}$ (Forward substitution)Data: \mathbf{L} and \mathbf{b} Initialization: $\mathbf{x} \leftarrow 0$ for $i = 1, \dots, n$ do $\left| x_i \leftarrow \left[b_i - \sum_{j=1}^{i-1} L_{ij} x_j \right] / L_{ii} \right|$ end

Procedure to solve $\mathbf{Ux} = \mathbf{b}$ (Backward substitution)Data: \mathbf{U} et \mathbf{b} Initialization: $\mathbf{x} \leftarrow 0$ for $i = n, \dots, 1$ do $\left| x_i \leftarrow \left[b_i - \sum_{j=i+1}^n U_{ij} x_j \right] / U_{ii} \right|$ end

Algorithmic aspects

- Cost: n² operations
- Weak parallelization (computation of sums in parallel)

Triangular systems — Approaches by blocks [1/2]

Definitions

- ▶ Lower triangular matrix by blocks: $\mathbf{L} \in \mathbb{R}^{n \times n}$ with $\mathbf{L}_{IJ} = 0$ si I < J
- Upper triangular matrix by blocks: $\mathbf{U} \in \mathbb{R}^{n \times n}$ with $\mathbf{U}_{IJ} = 0$ si I > J

$$\mathbf{L} = \begin{bmatrix} \mathbf{L}_{11} & 0 & 0 \\ \mathbf{L}_{21} & \mathbf{L}_{22} & 0 \\ \mathbf{L}_{31} & \mathbf{L}_{32} & \mathbf{L}_{33} \end{bmatrix} \qquad \mathbf{U} = \begin{bmatrix} \mathbf{U}_{11} & \mathbf{U}_{12} & \mathbf{U}_{13} \\ 0 & \mathbf{U}_{22} & \mathbf{U}_{23} \\ 0 & 0 & \mathbf{U}_{33} \end{bmatrix}$$

The diagonal blocks are square. The other blocks may not be square.

Properties

The determinant of a triangular matrix by blocks is the product of the determinants of the diagonal blocks:

$$\det(\mathbf{L}) = \prod_{I=1}^{N} \det(\mathbf{L}_{II}) \qquad \det(\mathbf{U}) = \prod_{I=1}^{N} \det(\mathbf{U}_{II})$$

A diagonal or triangular matrix by blocks is invertible if, and only if, the diagonal blocks are invertible.

Triangular systems — Approaches by blocks [2/2]

Procedure to solve $\mathbf{L}\mathbf{x} = \mathbf{b}$	(Forward substitution)
Data: \mathbf{L} and \mathbf{b}	
Initialization: $\mathbf{x} \leftarrow 0$	
for $I=1,\ldots,N$ do	
$\mathbf{x}_{I} \leftarrow \mathbf{L}_{II}^{-1} \left[\mathbf{b}_{I} - \sum_{J=1}^{I-1} \mathbf{L}_{IJ} \mathbf{x}_{J} ight]$	
end	

Procedure to solve $\mathbf{U}\mathbf{x} = \mathbf{b}$	(Backward substitution)
Data: \mathbf{U} and \mathbf{b}	
Initialization: $\mathbf{x} \leftarrow 0$	
for $I = N, \dots, 1$ do	
$ \left \begin{array}{c} \mathbf{x}_{I} \leftarrow \mathbf{U}_{II}^{-1} \left[\mathbf{b}_{I} - \sum_{J=I+1}^{N} \mathbf{U}_{IJ} \mathbf{x}_{J} \right] \right. $	
end	

Algorithmic aspects

- Cost: N small system to solve and N(N-1)/2 matrix-vector products
- Better for parallel computing (computation of matrix-vector products in parallel)

Direct methods for linear systems

Solution of triangular systems

Gaussian elimination

Matrix factorization

General systems — Gaussian elimination [1/5]

 $\label{eq:Goal:Transform} \begin{array}{l} \mathbf{A}\mathbf{x}=\mathbf{b} \text{ into an equivalent system } \mathbf{U}\mathbf{x}=\mathbf{b}'. \end{array}$ Procedure

Initialization:

$$\begin{bmatrix} A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1n}^{(1)} \\ A_{21}^{(1)} & A_{22}^{(1)} & \cdots & A_{2n}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1}^{(1)} & A_{n2}^{(1)} & \cdots & A_{nn}^{(1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \\ \vdots \\ b_n^{(1)} \end{bmatrix}$$

Iteration 1:

$$\begin{bmatrix} A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1n}^{(1)} \\ 0 & A_{22}^{(2)} & \cdots & A_{2n}^{(2)} \\ \vdots & \vdots & & \vdots \\ 0 & A_{n2}^{(2)} & \cdots & A_{nn}^{(2)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(2)} \\ \vdots \\ b_n^{(2)} \end{bmatrix}$$

with

$$\begin{split} & \alpha_{i1} = A_{i1}^{(1)}/A_{11}^{(1)} & i = 2, \dots, n & \text{(multipliers)} \\ & A_{ij}^{(2)} = A_{ij}^{(1)} - \alpha_{i1}A_{1j}^{(1)} & i, j = 2, \dots, n \\ & b_i^{(2)} = b_i^{(1)} - \alpha_{i1}b_1^{(1)} & i = 2, \dots, n \end{split}$$

General systems — Gaussian elimination [2/5]

 $\label{eq:Goal:Transform} \begin{array}{l} \mathbf{A}\mathbf{x}=\mathbf{b} \text{ into an equivalent system } \mathbf{U}\mathbf{x}=\mathbf{b}'. \end{array}$ Procedure

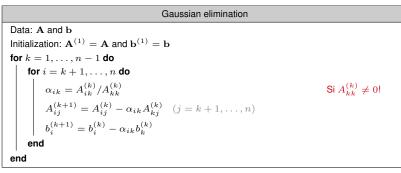
Iteration k:

$$\begin{bmatrix} A_{111}^{(1)} & A_{12}^{(1)} & \cdots & \cdots & A_{1n}^{(1)} \\ 0 & A_{22}^{(2)} & & & & & \\ \vdots & & \ddots & & & \vdots \\ 0 & \cdots & 0 & A_{k+1,k+1}^{(k)} & \cdots & A_{k+1,n}^{(k)} \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \cdots & 0 & A_{n,k+1}^{(k)} & \cdots & A_{n,n}^{(k)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{k+1} \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(2)} \\ \vdots \\ b_{k+1}^{(k)} \\ \vdots \\ b_n^{(k)} \end{bmatrix}$$

lteration n-1:

$$\begin{bmatrix} A_{11}^{(1)} & A_{12}^{(1)} & \cdots & \cdots & A_{1n}^{(1)} \\ 0 & A_{22}^{(2)} & & & A_{2n}^{(2)} \\ \vdots & & \ddots & & \vdots \\ 0 & & & \ddots & \vdots \\ 0 & & & & A_{nn}^{(n)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(2)} \\ \vdots \\ \vdots \\ \vdots \\ b_n^{(n)} \end{bmatrix}$$

General systems — Gaussian elimination [3/5]



Gaussian elimination (Rewriting)

```
Data: A and b

for k = 1, ..., n - 1 do

for i = k + 1, ..., n do

\begin{vmatrix} \alpha \leftarrow A_{ik}/A_{kk} & Si A_{kk} \neq 0! \\ A_{ij} \leftarrow A_{ij} - \alpha A_{kj} & (j = k + 1, ..., n) \\ A_{ik} \leftarrow 0 \\ b_i \leftarrow b_i - \alpha b_k \\ end

end
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General systems — Gaussian elimination [4/5]

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \quad \Leftrightarrow \quad \begin{bmatrix} A'_{11} & A'_{12} & A'_{13} \\ 0 & A'_{22} & A'_{23} \\ 0 & 0 & A'_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b'_1 \\ b'_2 \\ b'_3 \end{bmatrix}$$

Cost

- Gaussian elimination: 2(n-1)n(n+1)/3 + n(n-1) flop
- Backward substitution: n² flop
- ► Largest term: 2/3 n³ flop

Conditions of use

- The method must be modified if, at one step, $A_{kk}^{(k)} = 0$.
- The method can be used without modification ...
 - if A is diagonally dominant per line or per column
 - if A is symmetric positive definite
- For the other cases ⇒ Permutation of lines and/or columns

General systems — Gaussian elimination [5/5]

Gaussian elimination with pivoting Data: A and b for k = 1, ..., n - 1 do Find $r \in [k, ..., n]$ such that $|A_{rk}|$ is max. (if $\max_r |A_{rk}| = 0$, then A not invert.) Swap the r^{th} and k^{th} lines of A and b for i = k + 1, ..., n do $\alpha \leftarrow A_{ik}/A_{kk}$ $A_{ij} \leftarrow A_{ij} - \alpha A_{kj}$ $(j = k + 1, \dots, n)$ $\begin{vmatrix} A_{ik} \leftarrow 0 \\ b_i \leftarrow b_i - \alpha b_k \end{vmatrix}$ end end

Possible pivoting strategies

- Find $r \in [k, ..., n]$ such that $|A_{kr}|$ is maximum (partial pivoting)
- Find $r \in [k, ..., n]$ and $s \in [k, ..., n]$ such that $|A_{rs}|$ is maximum *(total pivoting)*

One can always find $r \in [k, ..., n]$ such that $|A_{rk}| > 0$, otherwise **A** is not invertible. \Rightarrow The Gaussian elimination with pivoting is applicable to every invertible matrix!

Direct methods for linear systems

Solution of triangular systems Gaussian elimination Matrix factorization

Generalities on matrix factorization [1/2]

Principle

Factorize A into triangular matrices:

$$\underbrace{\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}}_{\mathbf{A}} = \underbrace{\begin{bmatrix} \times & 0 & 0 \\ \times & \times & 0 \\ \times & \times & \times \end{bmatrix}}_{\mathbf{L}} \underbrace{\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \end{bmatrix}}_{\mathbf{U}}$$

Rewrite the problem with triangular matrices:

$$\mathbf{A}\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad \mathbf{L}\mathbf{U}\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad \begin{cases} \mathbf{L}\mathbf{y} = \mathbf{b} \\ \mathbf{U}\mathbf{x} = \mathbf{y} \end{cases}$$

and solve these problems with forward/back substitutions.

Comments

- A priori, same cost than Gaussian elimination.
- If the system must be solved with several right-hand sides, only one factorization is necessary.

Generalities on matrix factorization [2/2]

Several factorizations

If A is invertible and factorizable (to define later), one has:

$\mathbf{A} = \tilde{\mathbf{L}} \mathbf{U}$	(Gauss)	
$\mathbf{A} = \mathbf{L}\tilde{\mathbf{U}}$	(Gauss)	
$\mathbf{A} = \tilde{\mathbf{L}} \mathbf{D} \tilde{\mathbf{U}}$	(Gauss-Jordan)	
$\mathbf{A} = \tilde{\mathbf{L}} \mathbf{D} \tilde{\mathbf{L}}^T$	(Crout)	Si A symétrique.
$\mathbf{A} = \mathbf{L}\mathbf{L}^T$	(Cholesky)	Si A symétrique définie positive (SDP).

with

- D diagonal matrix
- L lower triangular matrix
- $\tilde{\mathbf{L}}~-$ lower triangular matrix with unit diagonal
- \mathbf{U} upper triangular matrix
- $\tilde{\mathbf{U}}$ upper triangular matrix with unit diagonal

Gaussian factorization $(\mathbf{A}=\tilde{\mathbf{L}}\mathbf{U})$ $_{[1/4]}$

Procedure

Initialization:

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1n}^{(1)} \\ A_{21}^{(1)} & A_{22}^{(1)} & \cdots & A_{2n}^{(1)} \\ \vdots & \vdots & & \vdots \\ A_{n1}^{(1)} & A_{n2}^{(1)} & \cdots & A_{nn}^{(1)} \end{bmatrix}$$

Iteration 1:

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ \alpha_{21} & 1 & & & 0 \\ \alpha_{31} & 0 & 1 & & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ \alpha_{n1} & 0 & \cdots & \cdots & 1 \end{bmatrix} \begin{bmatrix} A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1n}^{(1)} \\ 0 & A_{22}^{(2)} & \cdots & A_{2n}^{(2)} \\ 0 & A_{32}^{(2)} & \cdots & A_{3n}^{(2)} \\ \vdots & \vdots & & \vdots \\ 0 & A_{n2}^{(2)} & \cdots & A_{nn}^{(2)} \end{bmatrix}$$

with

$$\begin{aligned} \alpha_{i1} &= A_{i1}^{(1)} / A_{11}^{(1)} & i = 2, \dots, n \\ A_{ij}^{(2)} &= A_{ij}^{(1)} - \alpha_{i1} A_{1j}^{(1)} & i, j = 2, \dots, n \end{aligned}$$

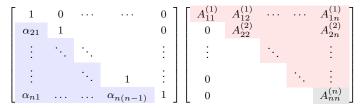
Gaussian factorization $(\mathbf{A} = \tilde{\mathbf{L}} \mathbf{U})$ [2/4]

Procedure (continuation)

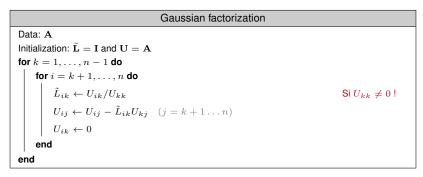
lteration k:

$$\begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ \alpha_{21} & \ddots & & & 0 \\ \vdots & \ddots & 1 & & \vdots \\ \vdots & & \vdots & 1 & & \vdots \\ \vdots & & \vdots & 1 & & \vdots \\ \alpha_{n1} & \cdots & \alpha_{nk} & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} A_{11}^{(1)} & A_{12}^{(1)} & \cdots & \cdots & A_{1n}^{(1)} \\ 0 & A_{22}^{(2)} & & & A_{2n}^{(2)} \\ \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & A_{k+1,k+1}^{(k)} & \cdots & A_{k+1,n}^{(k)} \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \cdots & 0 & A_{n,k+1}^{(k)} & \cdots & A_{nn}^{(k)} \end{bmatrix}$$

► Iteration n - 1:



Gaussian factorization $(\mathbf{A} = \tilde{\mathbf{L}} \mathbf{U})$ [3/4]



Gaussian factorization (Rewriting)

Data: A for k = 1, ..., n - 1 do for i = k + 1, ..., n do $\begin{vmatrix} for i = k + 1, ..., n \\ A_{ik} \leftarrow A_{ik}/A_{kk} \\ A_{ij} \leftarrow A_{ij} - A_{ik}A_{kj} \quad (j = k + 1 ... n) \end{vmatrix}$ end end

Gaussian factorization $(\mathbf{A} = \tilde{\mathbf{L}} \mathbf{U})$ [4/4]

Theorem – Unicity of the Gaussian factorization $(\mathbf{A} = \tilde{\mathbf{L}} \mathbf{U})$

The Gaussian factorization, if it exists, is unique.

Theorem – Existence of the Gaussian factorization $(\mathbf{A} = \tilde{\mathbf{L}} \mathbf{U})$

(not necessary)

Every matrix that is symmetric positive definite (SPD) is factorizable.

Theorem – Existence of the Gaussian factorization after permutation $(\mathbf{PA} = \mathbf{\tilde{L}U})$

For every invertible matrix, there exists a sequence of elementary permutations such that the permuted matrix admits a Gaussian factorization.

Permutation matrix

An elementary permutation matrix P^(i1,i2) is a matrix which the application on a matrix A permutes the lines i₁ and i₂:

ΓO	0	1	0]	A_{11}	A_{12}	A_{13}	A_{14}	$\begin{bmatrix} A_{31} \end{bmatrix}$	A_{32}	A ₃₃	A ₃₄]
0	1	0	0	A_{21}	A_{22}	A_{23}	A_{24}	$= \begin{bmatrix} A_{31} \\ A_{21} \\ A_{11} \\ A_{41} \end{bmatrix}$	A_{22}	A_{23}	A_{24}
1	0	0	0	A_{31}	A_{32}	A_{33}	A_{34}	- A ₁₁	A_{12}	A_{13}	A14
Lo	0	0	1	A_{41}	A_{42}	A_{43}	A_{44}	A_{41}	A_{42}	A_{43}	A_{44}

▶ The permutation matrix **P**^(i1,i2) is obtained by swapping the lines *i*₁ and *i*₂ and the columns *i*₁ and *i*₂ from the identity matrix.

Solution after factorization

 Gaussian factorization (Rewriting)

 Data: A

 for k = 1, ..., n - 1 do

 for i = k + 1, ..., n do

 $\begin{vmatrix} A_{ik} \leftarrow A_{ik}/A_{kk} \\ A_{ij} \leftarrow A_{ij} - A_{ik}A_{kj} \end{vmatrix}$ (j = k + 1...n)

 end

Cost of the entire solution procedure

- Gaussian or Gauss-Jordan factorization: $2/3 n^3$ operations
- Crout or Cholesky factorization: $1/3 n^3$ operations
- Forward and back substitution: $2 n^2$ operations
- Additional operations with pivoting strategies

Parallelization

- · Parallelization not easy for problems with dense matrices
- Strategies are possible with blocks approaches.
- Strategies are possible with sparse matrices.

Si $A_{kk} \neq 0$!

Summary

Triangular systems

- Simple computational procedures, but not suited for parallel computing!
- Computational cost:
 - By points: n^2 scalar operations
 - By blocks: N small systems to solve and $\mathcal{O}(N^2)$ matrix-vector products
- Parall. comp.: by-block strategy (dense mat.) or ad-hoc strategy (sparse mat.)

General systems

- Approaches:
 - Gaussian elimination \Rightarrow Gives the solution for a given vector ${\bf b}$
 - LU factorization + Two triangular systems to solve
 - \Rightarrow Factorization computed once and used for any vector \mathbf{b}
- For any invertible matrix A, \exists permutation matrix P such that $PA = \tilde{L}U$
- Different factorizations: $\tilde{\mathbf{L}}\mathbf{U}$, $\tilde{\mathbf{L}}\mathbf{D}\tilde{\mathbf{U}}$ (Gen), $\tilde{\mathbf{L}}\mathbf{D}\tilde{\mathbf{L}}^{\top}$ (Sym), $\mathbf{L}\mathbf{L}^{\top}$ (SDP)
- Computational cost: $\mathcal{O}(n^3)$ operations
- Parall. comp.: by-block strategy (dense mat.) or ad-hoc strategy (sparse mat.)

Resources

- Méthodes Numériques : Algorithmes, analyse et applications
 A. Quarteroni, R. Sacco, F. Saleri (2007), Springer
- Calcul scientifique parallèle
 F. Magoulès et F.-X. Roux (2017), Dunod
- Calcul scientifique parallèle
 P. Ciarlet et E. Jamelot, polycopié de cours