7. LU factorization

- triangular linear systems
- Gaussian elimination
- LU factorization
- positive definite matrices
- Cholesky factorization
- sparse linear equations

Solution of triangular linear equations

- if A is lower/upper triangular with nonzero diagonals
- $Ax = b$ can be solved using forward/back substitution

Forward substitution algorithm: assume A is *lower triangular*

$$
\begin{aligned}
x_1 &= b_1/A_{11} \\
x_2 &= (b_2 - A_{21}x_1)/A_{22} \\
x_3 &= (b_3 - A_{31}x_1 - A_{32}x_2)/A_{33} \\
&\vdots \\
x_n &= \left(b_n - A_{n1}x_1 - A_{n2}x_2 - \cdots - A_{n,n-1}x_{n-1}\right)/A_{nn}
\end{aligned}
$$

Back substitution algorithm: assume A is *upper triangular*

$$\begin{aligned}
x_n &= b_n / A_{nn} \\
x_{n-1} &= \left(b_{n-1} - A_{n-1,n}x_n\right)/A_{n-1,n-1} \\
x_{n-2} &= \left(b_{n-2} - A_{n-2,n-1}x_{n-1} - A_{n-2,n}x_n\right)/A_{n-2,n-2} \\
&\vdots \\
x_1 &= \left(b_1 - A_{12}x_2 - A_{13}x_3 - \cdots - A_{1n}x_n\right)/A_{11}
\end{aligned}$$

Complexity

$$1 + 3 + 5 + \cdots + (2n-1) = \sum_{k=1}^{n}(2k-1) = n^2 \text{ flops}$$

Example

$$\begin{aligned} 5x_1 &= 15 \\ x_1 + 2x_2 &= 7 \\ -x_1 + 3x_2 + 2x_3 &= 5 \end{aligned} \qquad A = \begin{bmatrix} 5 & 0 & 0 \\ 1 & 2 & 0 \\ -1 & 3 & 2 \end{bmatrix}, \; b = \begin{bmatrix} 15 \\ 7 \\ 5 \end{bmatrix}$$

applying the forward substitution algorithm, we get

$$\begin{aligned} x_1 &= \frac{15}{5} = 3 \\ x_2 &= \frac{7-3}{2} = 2 \\ x_3 &= \frac{5+3-6}{2} = 1 \end{aligned}$$

Inverse of triangular matrix

a triangular matrix A with nonzero diagonal elements is nonsingular:

$$Ax = 0 \quad \Longrightarrow \quad x = 0$$

this follows from forward or back substitution applied to the equation $Ax = 0$

- inverse of A can be computed by solving $AX = I$ column by column

$$A[x_1 \ \ x_2 \ \ \cdots \ \ x_n] = [e_1 \ \ e_2 \ \ \cdots \ \ e_n] \quad (x_i \text{ is column } i \text{ of } X)$$

  - inverse of lower triangular matrix is lower triangular
  - inverse of upper triangular matrix is upper triangular

- complexity of computing inverse of $n \times n$ triangular matrix

$$n^2 + (n-1)^2 + \cdots + 1 = \frac{n(n+1)(2n+1)}{6} \approx \frac{1}{3}n^3 \text{ flops}$$

- conclusion: solving using back/forward subs. is more efficient than inverse way

Outline

- triangular linear systems
- **Gaussian elimination**
- LU factorization
- positive definite matrices
- Cholesky factorization
- sparse linear equations

Elementary row operations

suppose A is an $n \times n$ invertible matrix, b is an n-vector

solution of $Ax = b$ is invariant under the elementary row operations:

1. *interchanging any two rows of the matrix* $[A \mid b]$
2. *multiplying one of its rows by a real nonzero number*
3. *adding a scalar multiple of one row to another row*

Elementary elimination matrix

for n-vector u, we can zero out elements below kth entry as follows:

$$G^{(k)}u = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -L_{k+1,k} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -L_{n,k} & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_k \\ u_{k+1} \\ \vdots \\ u_n \end{bmatrix} = \begin{bmatrix} u_1 \\ \vdots \\ u_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

- $L_{i,k} = u_i/u_k$ for $i = k+1, \ldots, n$
- the divisor u_k is called the *pivot*
- $G^{(k)}$ is lower triangular with unit (nonzero) diagonal, and hence nonsingular

Gaussian elimination procedure

Iteration 1

- zero out the first column below the main diagonal
- subtract $\frac{A_{i1}}{A_{11}}\times$ the first row from the ith row for all $i = 2, 3, \ldots, n$

$$\underbrace{\begin{bmatrix} 1 & 0 \\ -L_{2:n,1} & I \end{bmatrix}}_{G^{(1)}} [A \mid b] = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} & b_1 \\ 0 & A_{22}^{(1)} & \cdots & A_{2n}^{(1)} & b_2^{(1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & A_{n2}^{(1)} & \cdots & A_{nn}^{(1)} & b_n^{(1)} \end{bmatrix}$$

$$= \begin{bmatrix} A_{11} & A_{1,2:n} & b_1 \\ 0 & A_{2:n,2:n} - L_{2:n,1}A_{1,2:n} & b_{2:n} - L_{2:n,1}b_1 \end{bmatrix}$$

where $L_{2:n,1} = A_{2:n,1}/A_{11} = (A_{21}/A_{11}, \ldots, A_{n1}/A_{11})$

Iteration 2:

- zero out the second column below diagonal
- subtract $\frac{A_{i2}}{A_{22}}\times$ the second row from the ith row for all $i = 3, 4, \dots, n$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -L_{3:n,2} & I \end{bmatrix}}_{G^{(2)}} [A^{(1)}|b^{(1)}] = \begin{bmatrix} A_{11} & A_{12} & \cdots & \cdots & A_{1n} & b_1 \\ 0 & A_{22}^{(1)} & A_{23}^{(1)} & \cdots & A_{2n}^{(1)} & b_2^{(1)} \\ \vdots & 0 & A_{33}^{(2)} & \cdots & A_{3n}^{(2)} & b_3^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & A_{n3}^{(2)} & \cdots & A_{nn}^{(2)} & b_n^{(2)} \end{bmatrix}$$

$$= \begin{bmatrix} A_{11} & A_{12} & A_{1,3:n} & b_1 \\ 0 & A_{22}^{(1)} & A_{2,3:n}^{(1)} & b_2^{(1)} \\ 0 & 0 & A_{3:n,3:n}^{(1)} - L_{3:n,2}A_{2,3:n}^{(1)} & b_{3:n}^{(1)} - L_{3:n,2}b_2^{(1)} \end{bmatrix}$$

where $L_{3:n,2} = A_{3:n,2}^{(1)}/A_{22}^{(1)} = (A_{32}^{(1)}/A_{22}^{(1)}, \dots, A_{n2}^{(1)}/A_{22}^{(1)})$

Final iteration

- after $n-1$ iterations, we get the upper-triangular system

$$[A^{(n-1)}|b^{(n-1)}] = \begin{bmatrix} A_{11} & A_{12} & \cdots & \cdots & A_{1n} & b_1 \\ 0 & A_{22}^{(1)} & A_{23}^{(1)} & \cdots & A_{2n}^{(1)} & b_2^{(1)} \\ \vdots & 0 & A_{33}^{(2)} & \cdots & A_{3n}^{(2)} & b_3^{(2)} \\ \vdots & \vdots & \cdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & A_{nn}^{(n-1)} & b_n^{(n-1)} \end{bmatrix}$$

where

$$\begin{aligned} U = A^{(n-1)} &= G^{(n-1)} \cdots G^{(2)} G^{(1)} A \\ b^{(n-1)} &= G^{(n-1)} \cdots G^{(2)} G^{(1)} b \end{aligned}$$

- now, we solve $Ux = b^{(n-1)}$ using back substitution

Gaussian elimination algorithm

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given $Ax = b$ with nonsingular $A \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$; **set** $U = A$

for $k = 1, \ldots, n-1$

1. $L_{k+1:n,k} = U_{k+1:n,k}/U_{kk}$ then set $U_{k+1:n,k} = 0$
2. $U_{k+1:n,k+1:n} = U_{k+1:n,k+1:n} - L_{k+1:n,k}U_{k,k+1:n}$
3. $b_{k+1:n} = b_{k+1:n} - L_{k+1:n,k}b_k$

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next, apply the algorithm of back substitution to $Ux = b$

Complexity

- cost is approximately $(2/3)n^3$
- back substitution costs n^2
- cost of the Gaussian elimination phase dominates

Example

$$Ax = \begin{bmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 6 \\ 10 \end{bmatrix} = b$$

we subtract four times the first row from each of the second and third rows:

$$G^{(1)}A = \begin{bmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ -4 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & -2 & -4 \end{bmatrix}$$

$$G^{(1)}b = \begin{bmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ -4 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 6 \\ 10 \end{bmatrix} = \begin{bmatrix} 3 \\ -6 \\ -2 \end{bmatrix}$$

we subtract 0.5 times the second row from the third row:

$$G^{(2)}G^{(1)}A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{1}{2} & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & -2 & -4 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & 0 & -1 \end{bmatrix}$$

$$G^{(2)}G^{(1)}b = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{1}{2} & 1 \end{bmatrix} \begin{bmatrix} 3 \\ -6 \\ -2 \end{bmatrix} = \begin{bmatrix} 3 \\ -6 \\ 1 \end{bmatrix}$$

we have reduced the original system to the equivalent upper triangular system

$$Ux = \begin{bmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -6 \\ 1 \end{bmatrix}$$

which can now be solved by back-substitution to obtain $x = (-1, 3, -1)$

Inverse of elementary matrix

$$\begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -L_{k+1,k} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -L_{n,k} & 0 & \cdots & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & L_{k+1,k} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & L_{n,k} & 0 & \cdots & 1 \end{bmatrix} = L^{(k)}$$

- compactly: $(I - l_k e_k^T)^{-1} = I + l_k e_k^T$ where $l_k = (0, \ldots, 0, L_{k+1,k}, \ldots, L_{n,k})$
- inverse has same form as $G^{(k)}$ with subdiagonal entries negated
- for $k \le j$, we have $e_k^T l_j = 0$ and thus

$$L^{(1)} \cdots L^{(n-2)} L^{(n-1)} = I + l_1 e_1^T + \cdots + l_{n-1} e_{n-1}^T$$

which is also lower triangular

Gaussian elimination and LU factorization

Gaussian elimination produces

$$U = G^{(n-1)} \cdots G^{(2)} G^{(1)} A$$

or written equivalently

$$A = LU$$

- $L = L^{(1)} \cdots L^{(n-2)} L^{(n-1)}$ where $L^{(k)} = \left(G^{(k)}\right)^{-1}$
- L is lower triangular (see previous page)
- this is called *LU factorization* or *LU decomposition*
- requires pivot elements to be nonzero during the Gaussian elimination procedure

Example

consider A from previous example

$$A = \begin{bmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{bmatrix}$$

we have

$$G^{(1)} = \begin{bmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ -4 & 0 & 1 \end{bmatrix}, \quad G^{(2)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -0.5 & 1 \end{bmatrix}$$

hence,

$$L = \left(G^{(1)}\right)^{-1}\left(G^{(2)}\right)^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 4 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0.5 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 4 & 0.5 & 1 \end{bmatrix}$$

we thus have

$$A = \begin{bmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 4 & 0.5 & 1 \end{bmatrix}\begin{bmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & 0 & -1 \end{bmatrix} = LU$$

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LU factorization

LU factorization (no pivoting)

$$A = LU$$

- L unit lower triangular, U upper triangular
- does not always exist (even if A is nonsingular)

LU factorization with row pivoting

$$PA = LU$$

- P permutation matrix, L unit lower triangular, U upper triangular
- always exists if A is nonsingular
- not unique; there may be several possible choices for P, L, U
- interpretation: permute the rows of A and factor $PA = LU$

LU factorization and matrix inverse

let A is nonsingular and $n \times n$, with LU factorization

$$A = P^T LU$$

- inverse from LU factorization

$$A^{-1} = (P^T LU)^{-1} = U^{-1} L^{-1} P$$

- gives interpretation of solving $Ax = b$ steps: we evaluate

$$x = A^{-1} b = U^{-1} L^{-1} P b$$

  in three steps

$$z_1 = Pb, \quad z_2 = L^{-1} z_1, \quad x = U^{-1} z_2$$

Solving linear equations by LU factorization

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given $Ax = b$ with nonsingular $A \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$

1. factor A as $A = P^T LU$
2. solve $(P^T LU)x = b$ in three steps
   (a) permutation: $z_1 = Pb$ (0 flops)
   (b) forward substitution: solve $Lz_2 = z_1$
   (c) back substitution: solve $Ux = z_2$

Complexity:

- factorization requires $(2/3)n^3$flops
- forward and back substitution costs n^2 each
- total: $(2/3)n^3 + 2n^2 \approx (2/3)n^3$ flops

this is the standard method for solving $Ax = b$

Multiple right-hand sides

two equations with same non-singular $A \in \mathbb{R}^{n \times n}$ and different right-hand sides:

$$Ax = b, \quad A\tilde{x} = \tilde{b}$$

- factor A once
- forward/back substitution to get x
- forward/back substitution to get $\tilde{x}$

complexity: $(2/3)n^3 + 4n^2 \approx (2/3)n^3$

Computing the inverse

solve $AX = I$ column by column:

- one LU factorization of A: $(2/3)n^3$ flops
- n solve steps: $2n^3$ flops
- total: $(8/3)n^3$ flops

Conclusion: do not solve $Ax = b$ by multiplying A^{-1} with b

- $3\times$ more computationally expensive than going by the LU decomposition route
- forming A^{-1} is wasteful in storage
- it may give rise to a more pronounced presence of roundoff errors

Recursive computation of $A = LU$

$$\begin{bmatrix} A_{11} & A_{1,2:n} \\ A_{2:n,1} & A_{2:n,2:n} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ L_{2:n,1} & L_{2:n,2:n} \end{bmatrix} \begin{bmatrix} U_{11} & U_{1,2:n} \\ 0 & U_{2:n,2:n} \end{bmatrix}$$
$$= \begin{bmatrix} U_{11} & U_{1,2:n} \\ U_{11}L_{2:n,1} & L_{2:n,1}U_{1,2:n} + L_{2:n,2:n}U_{2:n,2:n} \end{bmatrix}$$

1. find the first row of U and the first column of L:
$$U_{11} = A_{11}, \quad U_{1,2:n} = A_{1,2:n}, \quad L_{2:n,1} = \frac{1}{A_{11}}A_{2:n,1}$$
2. factor the $(n-1) \times (n-1)$-matrix
$$L_{2:n,2:n}U_{2:n,2:n} = A_{2:n,2:n} - L_{2:n,1}U_{1,2:n} = A_{2:n,2:n} - \frac{1}{A_{11}}A_{2:n,1}A_{1,2:n}$$
this is an LU factorization of size $(n-1) \times (n-1)$
3. we can calculate $L_{2:n,2:n}$ and $U_{2:n,2:n}$ by repeating process on factored matrix

(this is basically Gaussian elimination)

Example

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix}$$

factor as $A = LU$ with L unit lower triangular, U upper triangular

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ L_{21} & 1 & 0 \\ L_{31} & L_{32} & 1 \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

Solution

- first row of U, first column of L:

$$\begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/4 & L_{32} & 1 \end{bmatrix} \begin{bmatrix} 8 & 2 & 9 \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

- second row of U, second column of L:

$$\begin{bmatrix} 9 & 4 \\ 7 & 9 \end{bmatrix} - \begin{bmatrix} 1/2 \\ 3/4 \end{bmatrix} \begin{bmatrix} 2 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ L_{32} & 1 \end{bmatrix} \begin{bmatrix} U_{22} & U_{23} \\ 0 & U_{33} \end{bmatrix}$$

$$\begin{bmatrix} 8 & -1/2 \\ 11/2 & 9/4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 11/16 & 1 \end{bmatrix} \begin{bmatrix} 8 & -1/2 \\ 0 & U_{33} \end{bmatrix}$$

- third row of U: $U_{33} = 9/4 + 11/32 = 83/32$

putting things together, we obtain

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/4 & 11/16 & 1 \end{bmatrix} \begin{bmatrix} 8 & 2 & 9 \\ 0 & 8 & -1/2 \\ 0 & 0 & 83/32 \end{bmatrix}$$

Factorization $A = LU$ may not exists

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ L_{21} & 1 & 0 \\ L_{31} & L_{32} & 1 \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

- first row of U, first column of L:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & L_{32} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

- second row of U, second column of L:

$$\begin{bmatrix} 0 & 2 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ L_{32} & 1 \end{bmatrix} \begin{bmatrix} U_{22} & U_{23} \\ 0 & U_{33} \end{bmatrix}$$

- issue: $U_{22} = 0$, $U_{23} = 2$, $L_{32} = 1/0$! (can be fixed via pivoting)

Effect of rounding error

$$\begin{bmatrix} 10^{-5} & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

solution is:

$$x_1 = \frac{-1}{1 - 10^{-5}}, \quad x_2 = \frac{1}{1 - 10^{-5}}$$

- let us solve using LU factorization for the two possible permutations:

$$P = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{or} \quad P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- we round intermediate results to four significant decimal digits

First choice: $P = I$ (no pivoting)

$$\begin{bmatrix} 10^{-5} & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix} \begin{bmatrix} 10^{-5} & 1 \\ 0 & 1 - 10^5 \end{bmatrix}$$

- L, U rounded to 4 significant decimal digits

$$L = \begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix}, \quad U = \begin{bmatrix} 10^{-5} & 1 \\ 0 & -10^5 \end{bmatrix}$$

- forward substitution

$$\begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \Longrightarrow \quad z_1 = 1, \quad z_2 = -10^5$$

- back substitution

$$\begin{bmatrix} 10^{-5} & 1 \\ 0 & -10^5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -10^5 \end{bmatrix} \quad \Longrightarrow \quad x_1 = 0, \quad x_2 = 1$$

error in x_1 is 100%

Second choice: interchange rows

$$\begin{bmatrix} 1 & 1 \\ 10^{-5} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 - 10^{-5} \end{bmatrix}$$

- L, U rounded to 4 significant decimal digits

$$L = \begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix}, \quad U = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

- forward substitution

$$\begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \Longrightarrow \quad z_1 = 0, \quad z_2 = 1$$

- back substitution

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \Longrightarrow \quad x_1 = -1, \quad x_2 = 1$$

error in x_1, x_2 is about 10^{-5}

Conclusion: rounding error and numerical instability

- for some P, small roundoff errors can cause very large errors in the solution
- this is called numerical instability:
  - for the first choice of P in the example, the algorithm is unstable
  - for the second choice of P, it is stable
- a simple rule for selecting a good permutation is via partial pivoting (see next)

Computing LU factorization with partial pivoting

Gaussian elimination with partial pivoting to compute $PA = LU$

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given nonsingular $A \in \mathbb{R}^{n \times n}$

set $P = I$, $L = 0$, $U = A$

for $k = 1, 2, \ldots, n-1$

1. select $q \geq k$ to maximize $|U_{qk}|$
   $P_{k,:} \leftrightarrow P_{q,:}$ (swap rows)
   $U = PU$ (swap rows)
   $L = PL$ (swap rows if $k \geq 2$)
2. set $L_{kk} = 1$
3. $L_{k+1:n,k} = U_{k+1:n,k} / U_{kk}$
   $U_{k+1:n,k+1:n} = U_{k+1:n,k+1:n} - L_{k+1:n,k} U_{k,k+1:n}$

Example

$$A = \begin{bmatrix} 0 & 5 & 5 \\ 2 & 3 & 0 \\ 6 & 9 & 8 \end{bmatrix}$$

since $A_{11} = 0$, we swap rows 1 and 3 using

$$U = P_1 A = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 5 & 5 \\ 2 & 3 & 0 \\ 6 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 6 & 9 & 8 \\ 2 & 3 & 0 \\ 0 & 5 & 5 \end{bmatrix}$$

set $L_{11} = 1$, $(L_{21}, L_{31}) = (\frac{2}{6}, \frac{0}{6})$, and

$$L^{(1)} = \begin{bmatrix} 1 & 0 & 0 \\ 1/3 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad U^{(1)}_{2:n,2:n} = \begin{bmatrix} 3 & 0 \\ 5 & 5 \end{bmatrix} - \begin{bmatrix} 1/3 \\ 0 \end{bmatrix} \begin{bmatrix} 9 & 8 \end{bmatrix} = \begin{bmatrix} 0 & -8/3 \\ 5 & 5 \end{bmatrix}$$

we swap the second and third row of $U^{(1)}$

$$U^{(2)}_{2:n,2:n} = P_2 U^{(1)}_{2:n,2:n} = \left[\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array}\right] \left[\begin{array}{cc} 0 & -8/3 \\ 5 & 5 \end{array}\right] = \left[\begin{array}{cc} 5 & 5 \\ 0 & -8/3 \end{array}\right]$$

we also swap the second and third rows of $L^{(1)}$ and set $L_{22} = 1$

$$L^{(2)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1/3 & 0 & 0 \end{bmatrix}$$

the matrix $U^{(2)}_{2:n,2:n}$ is upper triangular; hence $U^{(3)}_{3:n,3:n} = -8/3$ and

$$L^{(2)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1/3 & 0 & 1 \end{bmatrix}$$

the permutation matrix is (I swap rows $1 \leftrightarrow 3$ then $2 \leftrightarrow 3$)

$$P = \begin{bmatrix} 1 & 0 \\ 0 & P_2 \end{bmatrix} P_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

the LU factorization $A = P^T LU$ can now be assembled follows

$$\underbrace{\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}}_{P} \underbrace{\begin{bmatrix} 0 & 5 & 5 \\ 2 & 3 & 0 \\ 6 & 9 & 8 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1/3 & 0 & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 6 & 9 & 8 \\ 0 & 5 & 5 \\ 0 & 0 & -8/3 \end{bmatrix}}_{U}$$

Outline

- triangular linear systems
- Gaussian elimination
- LU factorization
- **positive definite matrices**
- Cholesky factorization
- sparse linear equations

Positive (semi)definite matrix

- a *symmetric* matrix $A \in \mathbb{R}^{n \times n}$ is *positive semidefinite* if

$$x^T A x \geq 0 \quad \text{for all } x$$

- a *symmetric matrix* $A \in \mathbb{R}^{n \times n}$ is *positive definite* if

$$x^T A x > 0 \quad \text{for all } x \neq 0$$

  this is a subset of the positive semidefinite matrices

note: if A is symmetric and $n \times n$, then the function

$$x^T A x = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j = \sum_{i=1}^{n} A_{ii} x_i^2 + 2 \sum_{i>j} A_{ij} x_i x_j$$

is called a *quadratic form*

Example

$$A = \begin{bmatrix} 9 & 6 \\ 6 & a \end{bmatrix}$$

$$x^T A x = 9x_1^2 + 12x_1x_2 + ax_2^2 = (3x_1 + 2x_2)^2 + (a-4)x_2^2$$

- A is positive definite for $a > 4$

$$x^T A x > 0 \text{ for all nonzero } x$$

- A is positive semidefinite but not positive definite for $a = 4$

$$x^T A x \geq 0 \quad \text{for all } x, \quad x^T A x = 0 \quad \text{for } x = (2, -3)$$

- A is not positive semidefinite for $a < 4$

$$x^T A x < 0 \quad \text{for } x = (2, -3)$$

Properties

- every positive definite matrix A is nonsingular

$$Ax = 0 \quad \Longrightarrow \quad x^T Ax = 0 \quad \Longrightarrow \quad x = 0$$

(last step follows from positive definiteness)

- every positive definite matrix A has positive diagonal elements

$$A_{ii} = e_i^T A e_i > 0$$

- every positive semidefinite matrix A has nonnegative diagonal elements

$$A_{ii} = e_i^T A e_i \geq 0$$

Schur complement

partition $n \times n$ symmetric matrix A as

$$A = \begin{bmatrix} A_{11} & A_{2:n,1}^T \\ A_{2:n,1} & A_{2:n,2:n} \end{bmatrix}$$

- the Schur complement of A_{11} is defined as the $(n-1) \times (n-1)$ matrix

$$S = A_{2:n,2:n} - \frac{1}{A_{11}} A_{2:n,1} A_{2:n,1}^T$$

- if A is positive definite, then S is positive definite

  to see this, take any $x \neq 0$ and define $y = -(A_{2:n,1}^T x)/A_{11}$, then

$$x^T S x = \begin{bmatrix} y \\ x \end{bmatrix}^T \begin{bmatrix} A_{11} & A_{2:n,1}^T \\ A_{2:n,1} & A_{2:n,2:n} \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} > 0$$

  because A is positive definite

Singular positive semidefinite matrices

if A is positive semidefinite, but not positive definite, then it is singular

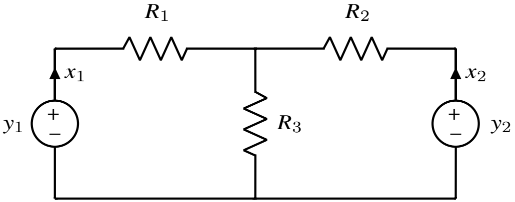
to see this, suppose A is positive semidefinite but not positive definite

- there exists a nonzero x with $x^T Ax = 0$
- since A is positive semidefinite the following function is nonnegative:

$$\begin{aligned} f(t) &= (x - tAx)^T A(x - tAx) \\ &= x^T Ax - 2tx^T A^2 x + t^2 x^T A^3 x \\ &= -2t\|Ax\|^2 + t^2 x^T A^3 x \end{aligned}$$

- $f(t) \geq 0$ for all t is only possible if $\|Ax\| = 0$; therefore $Ax = 0$
- hence there exists a nonzero x with $Ax = 0$, so A is singular

Example: resistor circuit



$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} R_1 + R_3 & R_3 \\ R_3 & R_2 + R_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

show that the matrix

$$A = \begin{bmatrix} R_1 + R_3 & R_3 \\ R_3 & R_2 + R_3 \end{bmatrix}$$

is positive definite if R_1, R_2, R_3 are positive

Solution

$$\begin{aligned} x^T A x &= (R_1 + R_3)\, x_1^2 + 2R_3 x_1 x_2 + (R_2 + R_3)\, x_2^2 \\ &= R_1 x_1^2 + R_2 x_2^2 + R_3\, (x_1 + x_2)^2 \\ &\geq 0 \end{aligned}$$

and $x^T A x = 0$ only if $x_1 = x_2 = 0$

Physics interpretation

- $x^T A x = y^T x$ is the power delivered by sources, dissipated by resistors
- power dissipated by the resistors is positive unless both currents are zero

Gram matrix

recall the definition of Gram matrix of a matrix B

$$A = B^T B$$

- every Gram matrix is positive semidefinite

$$x^T A x = x^T B^T B x = \|Bx\|^2 \geq 0 \quad \forall\, x$$

- a Gram matrix is positive definite if

$$x^T A x = x^T B^T B x = \|Bx\|^2 > 0 \quad \forall\, x \neq 0,$$

  i.e., B has linearly independent columns

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- triangular linear systems
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LU factorization for positive definite matrices

LU factorization of a symmetric positive definite matrix

$$A = LU$$

since U is upper triangular with diagonal elements $U_{kk} > 0$, we can write

$$U = \underbrace{\begin{bmatrix} U_{11} & & & & \\ & U_{22} & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & U_{nn} \end{bmatrix}}_{D} \underbrace{\begin{bmatrix} 1 & \frac{U_{12}}{U_{11}} & \cdots & \cdots & \frac{U_{1n}}{U_{11}} \\ & 1 & \frac{U_{23}}{U_{22}} & \cdots & \frac{U_{2n}}{U_{22}} \\ & & \ddots & & \vdots \\ & & & \ddots & \vdots \\ & & & & 1 \end{bmatrix}}_{\tilde{U}}$$

so the LU factorization reads

$$A = LD\tilde{U}$$

Symmetrizing the LU factorization

since A is symmetric, we have

$$L D \tilde{U} = A = A^T = \tilde{U}^T D L^T$$

since this factorization is unique, we have $L = \tilde{U}^T$ or

$$A = L D L^T$$

if we write $D = D^{1/2} D^{1/2}$ with

$$D^{1/2} = \text{diag}(\sqrt{U_{11}}, \ldots, \sqrt{U_{nn}})$$

we can express the LU as factorization

$$A = R^T R$$

with $R^T = L D^{1/2}$ a lower triangular matrix; this is called the *Cholesky factorization*

Cholesky factorization

every positive definite matrix $A \in \mathbb{R}^{n\times n}$ can be factored as

$$A = R^T R$$

where R is upper triangular with positive diagonal elements

- complexity of computing R is $(1/3)n^3$ flops
- R is called the *Cholesky factor* of A
- can be interpreted as "square root" of a positive definite matrix

Cholesky factorization algorithm

$$\begin{bmatrix} A_{11} & A_{1,2:n} \\ A_{2:n,1} & A_{2:n,2:n} \end{bmatrix} = \begin{bmatrix} R_{11} & 0 \\ R_{1,2:n}^T & R_{2:n,2:n}^T \end{bmatrix} \begin{bmatrix} R_{11} & R_{1,2:n} \\ 0 & R_{2:n,2:n} \end{bmatrix}$$
$$= \begin{bmatrix} R_{11}^2 & R_{11}R_{1,2:n} \\ R_{11}R_{1,2:n}^T & R_{1,2:n}^T R_{1,2:n} + R_{2:n,2:n}^T R_{2:n,2:n} \end{bmatrix}$$

---

given a symmetric positive definite matrix A

1. compute first row of R:

$$R_{11} = \sqrt{A_{11}}, \quad R_{1,2:n} = \frac{1}{R_{11}} A_{1,2:n}$$

2. compute 2,2 block $R_{2:n,2:n}$ from

$$A_{2:n,2:n} - R_{1,2:n}^T R_{1,2:n} = R_{2:n,2:n}^T R_{2:n,2:n}$$

this is a Cholesky factorization of order $n-1$

Example

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} R_{11} & 0 & 0 \\ R_{12} & R_{22} & 0 \\ R_{13} & R_{23} & R_{33} \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} & R_{13} \\ 0 & R_{22} & R_{23} \\ 0 & 0 & R_{33} \end{bmatrix}$$

- first row of R

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} 5 & 0 & 0 \\ 3 & R_{22} & 0 \\ -1 & R_{23} & R_{33} \end{bmatrix} \begin{bmatrix} 5 & 3 & -1 \\ 0 & R_{22} & R_{23} \\ 0 & 0 & R_{33} \end{bmatrix}$$

- second row of R

$$\begin{bmatrix} 18 & 0 \\ 0 & 11 \end{bmatrix} - \begin{bmatrix} 3 \\ -1 \end{bmatrix} \begin{bmatrix} 3 & -1 \end{bmatrix} = \begin{bmatrix} R_{22} & 0 \\ R_{23} & R_{33} \end{bmatrix} \begin{bmatrix} R_{22} & R_{23} \\ 0 & R_{33} \end{bmatrix}$$

$$\begin{bmatrix} 9 & 3 \\ 3 & 10 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 1 & R_{33} \end{bmatrix} \begin{bmatrix} 3 & 1 \\ 0 & R_{33} \end{bmatrix}$$

- third column of R : $10 - 1 = R_{33}^2$, so, $R_{33} = 3$

Example

we conclude

$$
\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} R_{11} & 0 & 0 \\ R_{12} & R_{22} & 0 \\ R_{13} & R_{23} & R_{33} \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} & R_{13} \\ 0 & R_{22} & R_{23} \\ 0 & 0 & R_{33} \end{bmatrix}
$$

$$
= \begin{bmatrix} 5 & 0 & 0 \\ 3 & 3 & 0 \\ -1 & 1 & 3 \end{bmatrix} \begin{bmatrix} 5 & 3 & -1 \\ 0 & 3 & 1 \\ 0 & 0 & 3 \end{bmatrix}
$$

Solving equations with positive definite A

given: $Ax = b$ with positive definite $A \in \mathbb{R}^{n\times n}$ and $b \in \mathbb{R}^n$

1. factor A as $A = R^TR$
2. solve $R^TRx = b$ in two steps
   (a) forward substitution: solve $R^Ty = b$
   (b) back substitution: solve $Rx = y$

Complexity: $(1/3)n^3 + 2n^2 \approx (1/3)n^3$ flops

(half the memory space and half the flops of the general LU factorization algorithm)

Outline

- triangular linear systems
- Gaussian elimination
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- **sparse linear equations**

Sparse linear equations

if A is sparse, it is usually factored as

$$P_1 A P_2 = LU$$

P_1 and P_2 are permutation matrices

- interpretation: permute rows and columns of A and factor $\tilde{A} = P_1 A P_2$

$$\tilde{A} = LU$$

- choice of P_1 and P_2 greatly affects the sparsity of L and U
- several heuristic methods exist for selecting good permutations
- in practice: #flops $\ll (2/3)n^3$; exact value depends on n, number of nonzero elements, sparsity pattern

Sparse Cholesky factorization

if A is sparse and positive definite, it is usually factored as

$$A = PR^TRP^T$$

P a permutation matrix; R upper triangular with positive diagonal elements

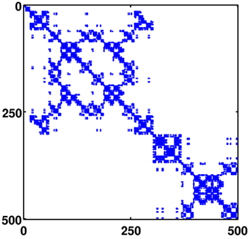
Interpretation: we permute the rows and columns of A and factor

$$P^TAP = R^TR$$

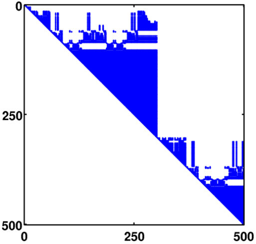
- if A is very sparse, R is often (but not always) sparse
- choice of permutation greatly affects the sparsity R
- there exist several heuristic methods for choosing a good permutation
- if R is sparse, the cost of the factorization is much less than $(1/3)n^3$

Example

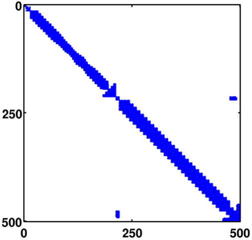
sparsity pattern of A



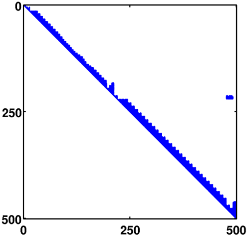
Cholesky factor of A



pattern of P^TAP



Cholesky factor of P^TAP



References and further readings

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