6. Cholesky factorization

- triangular matrices
- forward and backward substitution
- the Cholesky factorization
- solving $Ax = b$ with A positive definite
- inverse of a positive definite matrix
- permutation matrices
- sparse Cholesky factorization

Triangular matrix

a square matrix A is **lower triangular** if $a_{ij} = 0$ for $j > i$

$$A = \begin{bmatrix} a_{11} & 0 & \cdots & 0 & 0 \\ a_{21} & a_{22} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & 0 & 0 \\ a_{n-1,1} & a_{n-1,2} & \cdots & a_{n-1,n-1} & 0 \\ a_{n1} & a_{n2} & \cdots & a_{n,n-1} & a_{nn} \end{bmatrix}$$

A is **upper triangular** if $a_{ij} = 0$ for $j < i$ (A^T is lower triangular)

a triangular matrix is **unit upper/lower triangular** if $a_{ii} = 1$ for all i

Forward substitution

solve $Ax = b$ when A is lower triangular with nonzero diagonal elements

$$\begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

algorithm:

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

cost: $1 + 3 + 5 + \cdots + (2n-1) = n^2$ flops

Back substitution

solve $Ax = b$ when A is upper triangular with nonzero diagonal elements

$$\begin{bmatrix} a_{11} & \cdots & a_{1,n-1} & a_{1n} \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & a_{n-1,n-1} & a_{n-1,n} \\ 0 & \cdots & 0 & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_{n-1} \\ b_n \end{bmatrix}$$

algorithm:

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

cost: n^2 flops

Inverse of a triangular matrix

triangular matrix A with nonzero diagonal elements is nonsingular

- $Ax = b$ is solvable via forward/back substitution; hence A has full range
- therefore A has a zero nullspace, is invertible, etc. (see p.4-8)

inverse

- can be computed by solving $AX = I$ column by column

$$A \left[\begin{array}{cccc} X_1 & X_2 & \cdots & X_n \end{array} \right] = \left[\begin{array}{cccc} e_1 & e_2 & \cdots & e_n \end{array} \right]$$

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

Cholesky factorization

every positive definite matrix A can be factored as

$$A = LL^T$$

where L is lower triangular with positive diagonal elements

cost: $(1/3)n^3$ flops if A is of order n

- L is called the *Cholesky factor* of A
- can be interpreted as 'square root' of a positive define matrix

Cholesky factorization algorithm

partition matrices in $A = LL^T$ as

$$
\begin{aligned}
\begin{bmatrix} a_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} &= \begin{bmatrix} l_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} l_{11} & L_{21}^T \\ 0 & L_{22}^T \end{bmatrix} \\
&= \begin{bmatrix} l_{11}^2 & l_{11}L_{21}^T \\ l_{11}L_{21} & L_{21}L_{21}^T + L_{22}L_{22}^T \end{bmatrix}
\end{aligned}
$$

algorithm

1. determine l_{11} and L_{21}:

$$l_{11} = \sqrt{a_{11}}, \qquad L_{21} = \frac{1}{l_{11}} A_{21}$$

2. compute L_{22} from

$$A_{22} - L_{21}L_{21}^T = L_{22}L_{22}^T$$

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

proof that the algorithm works for positive definite A of order n

- step 1: if A is positive definite then $a_{11} > 0$

- step 2: if A is positive definite, then

$$A_{22} - L_{21}L_{21}^T = A_{22} - \frac{1}{a_{11}} A_{21}A_{21}^T$$

  is positive definite (see page 4-23)

- hence the algorithm works for $n = m$ if it works for $n = m - 1$

- it obviously works for $n = 1$; therefore it works for all n

Example

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

- first column of L

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} 5 & 0 & 0 \\ 3 & l_{22} & 0 \\ -1 & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 5 & 3 & -1 \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

- second column of L

$$\begin{bmatrix} 18 & 0 \\ 0 & 11 \end{bmatrix} - \begin{bmatrix} 3 \\ -1 \end{bmatrix} \begin{bmatrix} 3 & -1 \end{bmatrix} = \begin{bmatrix} l_{22} & 0 \\ l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{22} & l_{32} \\ 0 & l_{33} \end{bmatrix}$$

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

- third column of L: $10 - 1 = l_{33}^2$, *i.e.*, $l_{33} = 3$

conclusion:

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

Solving equations with positive definite A

$$Ax = b \qquad (A \text{ positive definite of order } n)$$

algorithm

- factor A as $A = LL^T$
- solve $LL^Tx = b$
  - forward substitution $Lz = b$
  - back substitution $L^Tx = z$

cost: $(1/3)n^3$ flops

- factorization: $(1/3)n^3$
- forward and backward substitution: $2n^2$

Inverse of a positive definite matrix

suppose A is positive definite with Cholesky factorization $A = LL^T$

- L is invertible (its diagonal elements are nonzero)
- $X = L^{-T}L^{-1}$ is a right inverse of A:

$$AX = LL^TL^{-T}L^{-1} = LL^{-1} = I$$

- $X = L^{-T}L^{-1}$ is a left inverse of A:

$$XA = L^{-T}L^{-1}LL^T = L^{-T}L^T = I$$

- hence, A is invertible and

$$A^{-1} = L^{-T}L^{-1}$$

Summary

if A is positive definite of order n

- A can be factored as LL^T
- the cost of the factorization is $(1/3)n^3$ flops
- $Ax = b$ can be solved in $(1/3)n^3$ flops
- A is invertible with inverse: $A^{-1} = L^{-T}L^{-1}$

Sparse positive definite matrices

- a matrix is *sparse* if most of its elements are zero
- a matrix is *dense* if it is not sparse

Cholesky factorization of dense matrices

- $(1/3)n^3$ flops
- on a current PC: a few seconds or less, for n up to a few 1000

Cholesky factorization of sparse matrices

- if A is very sparse, then L is often (but not always) sparse
- if L is sparse, the cost of the factorization is much less than $(1/3)n^3$
- exact cost depends on n, #nonzero elements, sparsity pattern
- very large sets of equations ($n \sim 10^6$) are solved by exploiting sparsity

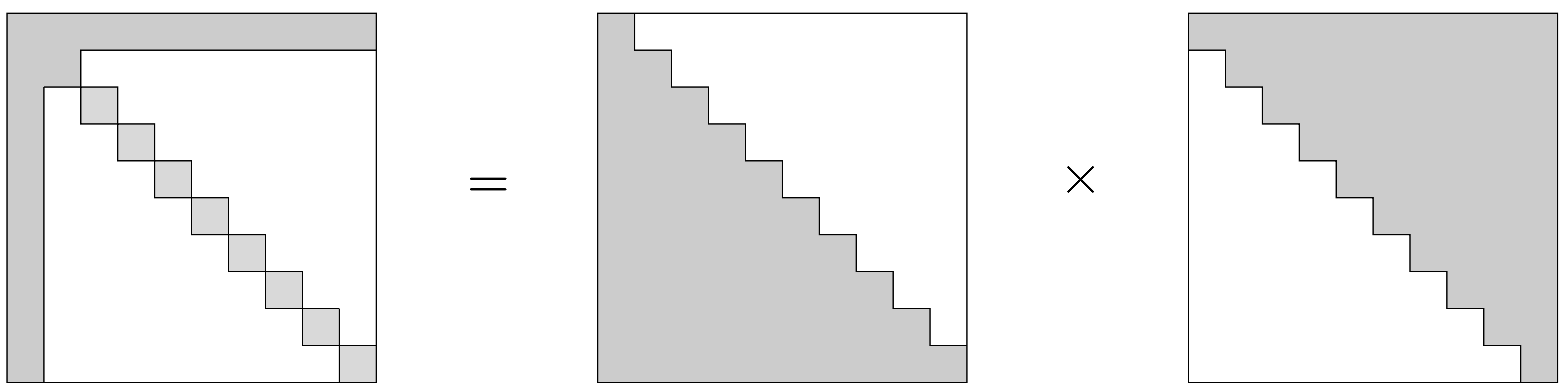
Effect of ordering

sparse equation (a is an $(n-1)$-vector with $\|a\| < 1$)

$$\begin{bmatrix} 1 & a^T \\ a & I \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} b \\ c \end{bmatrix}$$

factorization

$$\begin{bmatrix} 1 & a^T \\ a & I \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ a & L_{22} \end{bmatrix} \begin{bmatrix} 1 & a^T \\ 0 & L_{22}^T \end{bmatrix} \quad \text{where } I - aa^T = L_{22}L_{22}^T$$



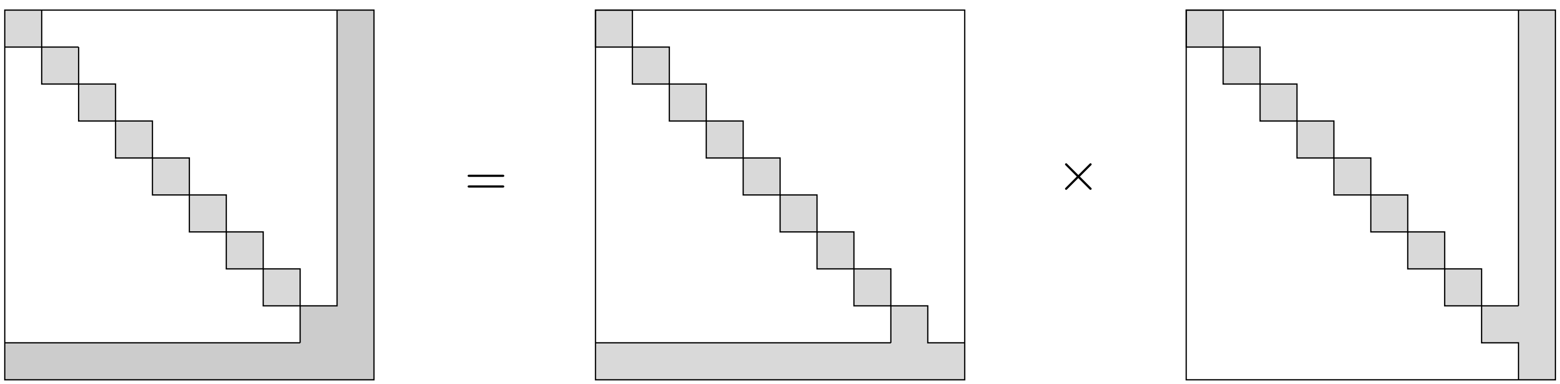
factorization with 100% fill-in

reordered equation

$$\begin{bmatrix} I & a \\ a^T & 1 \end{bmatrix} \begin{bmatrix} v \\ u \end{bmatrix} = \begin{bmatrix} c \\ b \end{bmatrix}$$

factorization

$$\begin{bmatrix} I & a \\ a^T & 1 \end{bmatrix} = \begin{bmatrix} I & 0 \\ a^T & \sqrt{1 - a^T a} \end{bmatrix} \begin{bmatrix} I & a \\ 0 & \sqrt{1 - a^T a} \end{bmatrix}$$



factorization with zero fill-in

Permutation matrices

a *permutation matrix* is the identity matrix with its rows reordered, $e.g.$,

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

- the vector Ax is a permutation of x

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_2 \\ x_3 \\ x_1 \end{bmatrix}$$

- $A^T x$ is the inverse permutation applied to x

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_3 \\ x_1 \\ x_2 \end{bmatrix}$$

- $A^T A = AA^T = I$, so A is invertible and $A^{-1} = A^T$

Solving $Ax = b$ when A is a permutation matrix

the solution of $Ax = b$ is $x = A^T b$

example

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 10.0 \\ -2.1 \end{bmatrix}$$

solution is $x = (-2.1, 1.5, 10.0)$

cost: zero flops

Sparse Cholesky factorization

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

$$A = PLL^T P^T$$

P a permutation matrix; L lower triangular with positive diagonal elements

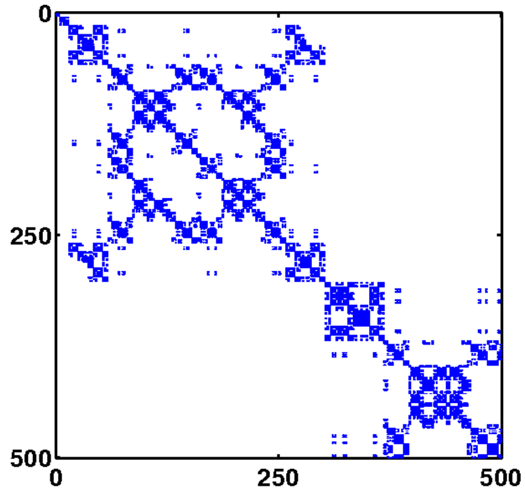
interpretation: we permute the rows and columns of A and factor

$$P^T AP = LL^T$$

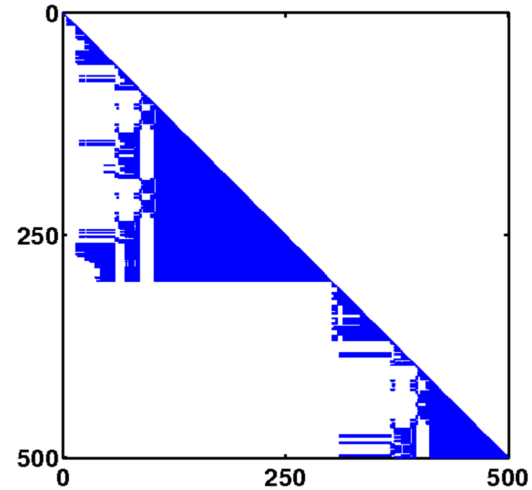
- choice of P greatly affects the sparsity L
- many heuristic methods (that we don't cover) exist for selecting good permutation matrices P

Example

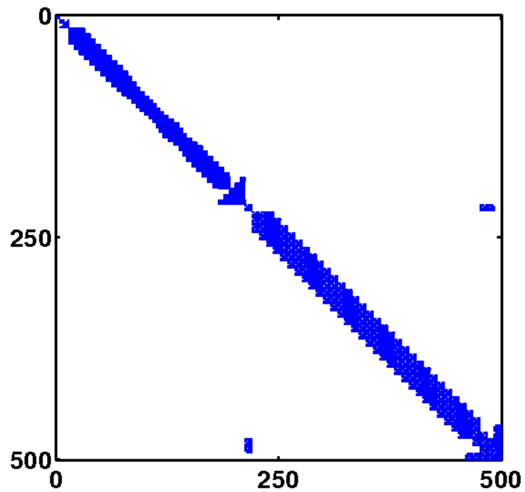
sparsity pattern of A



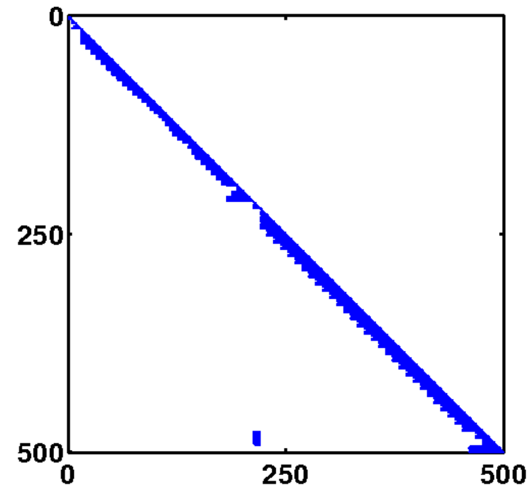
Cholesky factor of A



pattern of $P^T A P$



Cholesky factor of $P^T A P$



Solving sparse positive definite equations

solve $Ax = b$ via factorization $A = PLL^TP^T$

algorithm

1. $\tilde{b} := P^Tb$
2. solve $Lz = \tilde{b}$ by forward substitution
3. solve $L^Ty = z$ by back substitution
4. $x := Py$

interpretation: we solve

$$(P^TAP)\,y = \tilde{b}$$

using the Cholesky factorization of P^TAP