5. The Cholesky factorization

- positive (semi-)definite matrices
- examples
- the Cholesky factorization
- solving $Ax = b$ with A positive definite
- inverse of a positive definite matrix
- permutation matrices
- sparse Cholesky factorization

Positive (semi-)definite matrices

- A is *positive definite* if A is symmetric and

$$x^TAx > 0 \text{ for all } x \neq 0$$

- A is *positive semidefinite* if A is symmetric and

$$x^TAx \geq 0 \text{ for all } x$$

Note: if A is symmetric of order n, then

$$x^TAx = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_ix_j = \sum_{i=1}^{n} a_{ii}x_i^2 + 2\sum_{i>j} a_{ij}x_ix_j$$

Examples

$$A_1 = \begin{bmatrix} 9 & 6 \\ 6 & 5 \end{bmatrix}, \qquad A_2 = \begin{bmatrix} 9 & 6 \\ 6 & 4 \end{bmatrix}, \qquad A_3 = \begin{bmatrix} 9 & 6 \\ 6 & 3 \end{bmatrix}$$

- A_1 is positive definite:

$$x^TA_1x = 9x_1^2 + 12x_1x_2 + 5x_2^2 = (3x_1 + 2x_2)^2 + x_2^2$$

- A_2 is positive semidefinite but not positive definite:

$$x^TA_2x = 9x_1^2 + 12x_1x_2 + 4x_2^2 = (3x_1 + 2x_2)^2$$

- A_3 is not positive semidefinite:

$$x^TA_3x = 9x_1^2 + 12x_1x_2 + 3x_2^2 = (3x_1 + 2x_2)^2 - x_2^2$$

Examples

- $A = B^TB$ for some matrix B

$$x^TAx = x^TB^TBx = \|Bx\|^2$$

  A is positive semidefinite

  A is positive definite if B has a zero nullspace

- diagonal A

$$x^TAx = a_{11}x_1^2 + a_{22}x_2^2 + \cdots + a_{nn}x_n^2$$

  A is positive semidefinite if its diagonal elements are nonnegative

  A is positive definite if its diagonal elements are positive

Another example

$$A = \begin{bmatrix} 1 & -1 & \cdots & 0 & 0 \\ -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 2 & -1 \\ 0 & 0 & \cdots & -1 & 1 \end{bmatrix}$$

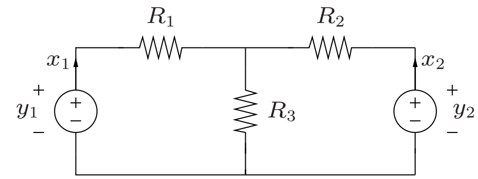
A is positive semidefinite:

$$x^TAx = (x_1 - x_2)^2 + (x_2 - x_3)^2 + \cdots + (x_{n-1} - x_n)^2 \geq 0$$

A is not positive definite:

$$x^TAx = 0 \text{ for } x = (1, 1, \ldots, 1)$$

Resistor circuit



Circuit model: $y = Ax$ with

$$A = \begin{bmatrix} R_1 + R_3 & R_3 \\ R_3 & R_2 + R_3 \end{bmatrix} \qquad (R_1, R_2, R_3 > 0)$$

Interpretation of $x^TAx = y^Tx$

x^TAx is the power delivered by the sources, dissipated by the resistors

A is positive definite, *i.e.*, $x^TAx > 0$ for all nonzero x

- proof from physics:

  power dissipated by the resistors is positive unless both currents are zero

- algebraic proof:

$$\begin{aligned} x^TAx &= (R_1 + R_3)x_1^2 + 2R_3x_1x_2 + (R_2 + R_3)x_2^2 \\ &= R_1x_1^2 + R_2x_2^2 + R_3(x_1 + x_2)^2 \\ &\geq 0 \end{aligned}$$

  and $x^TAx = 0$ only if $x_1 = x_2 = 0$

Properties

if A is positive definite of order n, then

- A has a zero nullspace

  proof: $x^TAx > 0$ for all nonzero x, hence $Ax \neq 0$ if $x \neq 0$

- the diagonal elements of A are positive

  proof: $a_{ii} = e_i^TAe_i > 0$ (e_i is the ith unit vector)

- $A_{22} - (1/a_{11})A_{21}A_{21}^T$ is positive definite, where $A = \begin{bmatrix} a_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix}$

  proof: take any $v \neq 0$ and $w = -(1/a_{11})A_{21}^Tv$

$$v^T\left(A_{22} - \frac{1}{a_{11}}A_{21}A_{21}^T\right)v = \begin{bmatrix} w & v^T \end{bmatrix} \begin{bmatrix} a_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} w \\ v \end{bmatrix} > 0$$

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

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

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

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 5–8)

- 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 substitution: n^2
- backward substitution: n^2

Inverse of a positive definite matrix

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

- L is invertible (its diagonal is nonzero; see lecture 4)
- $X = L^{-T}L^{-1}$ 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: $A^{-1} = L^{-T}L^{-1}$
- A has a full range: $Ax = b$ is solvable for all b
- A has a zero nullspace: $x^TAx > 0$ for all nonzero x

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

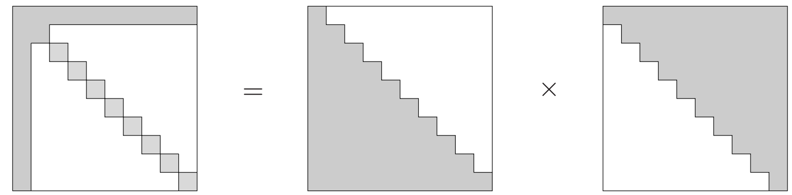
Effect of ordering

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

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



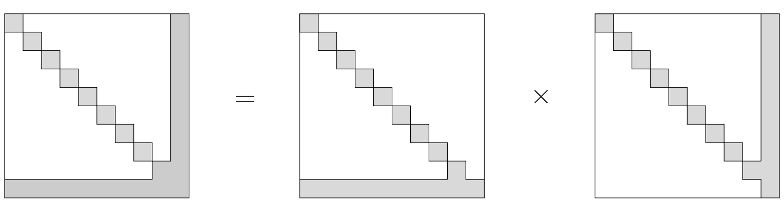
factorization with 100% fill-in

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

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

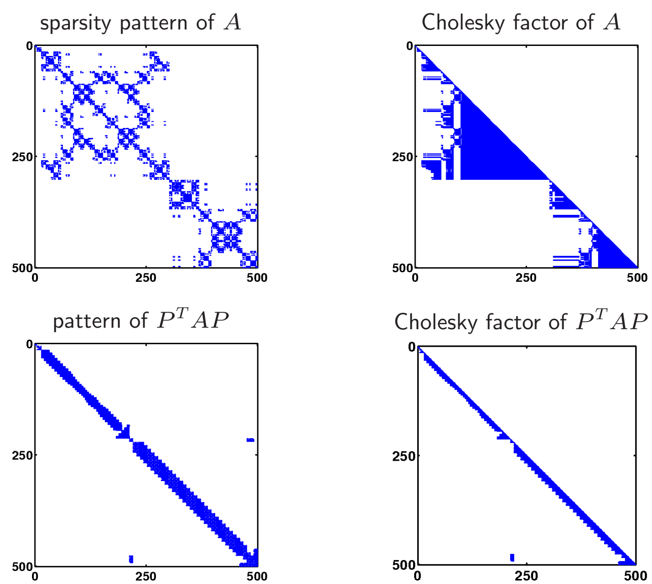
P a permutation matrix; L lower triangular with positive diagonal elements

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



Solving sparse positive definite equations

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

Algorithm

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

Interpretation: we solve

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

using the Cholesky factorization of $P^T AP$