The Cholesky decomposition

MATH 6610 Lecture 17

October 16, 2020

Trefethen & Bau: Lecture 23

Hermitian positive-definite matrices

Assume $A \in \mathbb{C}^{n\times n}$ is Hermitian positive definite. $\left(x^* A x > 0 \quad \forall\, x \in \mathbb{C}^n \setminus \{0\}\right)$

$A = A^*$

Our investigation of LU decompositions specializes considerably in this case.

Hermitian positive-definite matrices

Assume $A \in \mathbb{C}^{n \times n}$ is Hermitian positive definite.

Our investigation of LU decompositions specializes considerably in this case.

First we note some properties of A:

1. • A is invertible
2. • The diagonal entries of A are real and strictly positive
3. • If $B \in \mathbb{C}^{m \times n}$ with $m \leqslant n$ is of full rank, then BAB^* is positive-definite

1.) A is unitarily diagonalizable w/ positive eigenvalues.

2.) $e_j^* A e_j = A_{jj}$ (for any matrix A)

$e_j^* A e_j > 0$ ← A is Hermitian p.d.

3.) BAB^* is Hermitian

$y \in \mathbb{C}^m,\ y \neq 0$: $\quad y^* B A B^* y$

$$B^* = \begin{array}{cc} & m \\ n & \begin{pmatrix} & & \\ & & \\ & & \end{pmatrix} \end{array}$$

$\|$ $\Rightarrow B^* y \neq 0$ since $y \neq 0$ and $\ker(B^*) = \{0\}$

$(B^* y)^* A (B^* y) > 0.$

LU on (Hermitian) positive-definite matrices

A general positive-definite matrix A has the form

$$A = \begin{pmatrix} a & - & v^* & - \\ | & & & \\ v & & A_2 & \\ | & & & \end{pmatrix}.$$

$A_2 = A_2^*$

$a > 0$

Consider performing elimination on A:

Since $a > 0 \Rightarrow$ Gaussian elimination without pivoting

$$\begin{pmatrix} 1 & & & \\ | & 1 & & \\ -\frac{v}{a} & & 1 & \\ | & & & \ddots & \\ & & & & 1 \end{pmatrix} \begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix} = \begin{pmatrix} a & - & v^* & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix}$$

$$L_1^{-1} \Rightarrow L_1 = \begin{pmatrix} 1 & & & \\ | & 1 & & \\ \frac{v}{a} & & \ddots & \\ | & & & 1 \end{pmatrix}$$

$$A = L_1 \begin{pmatrix} a & — v^* — \\ | & \\ 0 & A_2 - \frac{vv^*}{a} \\ | & \end{pmatrix}$$

LU on positive-definite matrices

A general positive-definite matrix A has the form

$$A = \begin{pmatrix} a & - & v^* & - \\ | & & & \\ v & & A_2 & \\ | & & & \end{pmatrix}.$$

Consider performing elimination on A:

$$A = L_1 B^* = \begin{pmatrix} 1 & - & 0 & - \\ | & & & \\ \frac{v}{a} & I & & \\ | & & & \end{pmatrix} \underbrace{\begin{pmatrix} a & - & v^* & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix}}_{B^*}$$

Symmetric factorizations

$$A = L_1 B^*$$

We can perform a single step of Gaussian elimination on B:

$$B = \begin{pmatrix} a & - & 0 & - \\ | & & & \\ v & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix} \Longrightarrow B = L_1 \begin{pmatrix} a & - & 0 & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix}$$

first column of B = first column of A

$$\begin{cases} A = L_1 B^* \\ B = L_1 \begin{pmatrix} a & - & 0 & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix} \end{cases}$$

$$\longrightarrow \quad A = L_1 \begin{pmatrix} a & 0 \\ 0 & A_2 - \frac{vv^*}{a} \end{pmatrix} L_1^*$$

Last step: "factor out" $\sqrt{a}$

$$A = L_1 \begin{pmatrix} \sqrt{a} & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & A_2 - \frac{vv^*}{a} \end{pmatrix} \begin{pmatrix} \sqrt{a} & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}^* L_1^*$$

$$\tilde{L}_1 = L_1 \begin{pmatrix} \sqrt{a} & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix} \implies A = \tilde{L}_1 \begin{pmatrix} 1 & 0 \\ 0 & A_2 - \frac{vv^*}{a} \end{pmatrix} \tilde{L}_1^*$$

Symmetric factorizations

$$A = L_1 B^*$$

We can perform a single step of Gaussian elimination on B:

$$B = L_1 \begin{pmatrix} a & - & 0 & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix},$$

i.e.,

$$A = L_1 \begin{pmatrix} a & - & 0 & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix} L_1^* = \widetilde{L}_1 \begin{pmatrix} 1 & - & 0 & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix} \widetilde{L}_1^*.$$

The Cholesky factorization

$$A = \widetilde{L}_1 \begin{pmatrix} 1 & - & 0 & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix} \widetilde{L}_1^*.$$

Note that $A_2 - \frac{vv^*}{a}$ must be positive definite since $\widetilde{L}_1$ is invertible.

$\widetilde{L}_1$ invertible ✓

$$\widetilde{L}_1^{-1} A \widetilde{L}_1^{-*} = \begin{pmatrix} 1 & - & 0 & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix}$$

$$E = \begin{pmatrix} | & & | \\ e_2 & \cdots & e_n \\ | & & | \end{pmatrix} \in \mathbb{R}^{n\times(n-1)}$$

$$\underbrace{E^* \tilde{L}_1^{-1}}_{\text{full-rank}} A \tilde{L}_1^{-*} E = A_2 - \frac{vv^*}{a}$$

$A_2 - \frac{vv^*}{a}$ is a rank-$(n-1)$ compression of A

$\Rightarrow A_2 - \frac{vv^*}{a}$ is positive-definite.

The Cholesky factorization

$$A = \widetilde{L}_1 \begin{pmatrix} 1 & - & 0 & - \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix} \widetilde{L}_1^*.$$

Note that $A_2 - \frac{vv^*}{a}$ must be positive definite since $\widetilde{L}_1$ is invertible.

$\Rightarrow$ we can continue to eliminate without pivoting.

Thus, we can repeat this process:

$$\begin{aligned} A &= \left(\widetilde{L}_1 \widetilde{L}_2 \cdots \widetilde{L}_{n-1}\right) \overset{\substack{\wedge \\ \mathrm{I}}}{} \left(\widetilde{L}_1 \widetilde{L}_2 \cdots \widetilde{L}_{n-1}\right)^* \\ &=: LL^*. \end{aligned}$$

- Note: we <u>never</u> need to pivot!

The Cholesky factorization

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Note that $A_2 - \frac{vv^*}{a}$ must be positive definite since $\widetilde{L}_1$ is invertible.

Thus, we can repeat this process:

$$\begin{aligned} A &= \left(\widetilde{L}_1 \widetilde{L}_2 \cdots \widetilde{L}_{n-1}\right) \left(\widetilde{L}_1 \widetilde{L}_2 \cdots \widetilde{L}_{n-1}\right)^* \\ &=: LL^*. \end{aligned}$$

Theorem

Every Hermitian positive definite matrix A has a unique symmetric LU, or Cholesky, decomposition: $A = LL^*$, where L is lower-triangular and invertible.

Pivoted Cholesky

One can perform symmetric pivoting on a Hermitian positive-definite matrix A: $A = PLL^*P^*$.

This could be used to pivot maximum-magnitude diagonal entries to the front.

Pivoted Cholesky

One can perform symmetric pivoting on a Hermitian positive-definite matrix A: $A = PLL^*P^*$.

This could be used to pivot maximum-magnitude diagonal entries to the front.

However, pivoted Cholesky decompositions have another use:

Theorem

$x^*Ax \geq 0$

Every Hermitian positive semi-definite matrix A has a pivoted Cholesky decomposition: $A = PLL^*P^*$, where L is lower-triangular but need not invertible. This decomposition is in general not unique.

E.g.: $A = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \Rightarrow A = \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{P} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}}_{L} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}}_{L^*} \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{P^*}$

Aside: $A = \begin{pmatrix} | & | & | & \cdots & | \end{pmatrix} \in \mathbb{C}^{m \times n}$, $m > n$

a_j : jth column of A.

$A = QR$

G : "Gramian" $(G)_{i,j} = \langle a_i, a_j \rangle$

If A is full rank, then G is positive-definite

$G = LL^*$

vs.

$A = QR \longrightarrow G = A^*A = R^*R$

$\Longrightarrow R^* = L$

This is useful since in some cases we have G, but <u>not</u> A.