C S C I 5304 Fall 2021

COMPUTATIONAL ASPECTS OF MATRIX THEORY

Class time	:	*MW 4:00 – 5:15 pm*
Room	:	*Keller 3-230 or Online*
Instructor	:	*Daniel Boley*

Lecture notes: http://www-users.cselabs.umn.edu/classes/Fall-2021/csci5304/

August 27, 2021

SYMMETRIC POSITIVE DEFINITE (SPD) MATRICES

SPD LINEAR SYSTEMS

- **Symmetric positive definite matrices.**
- **The LDL^T decomposition; The Cholesky factorization**

Positive-Definite Matrices

➤ A real matrix is said to be positive definite if

$$(Au, u) > 0 \text{ for all } u \neq 0 \; u \in \mathbb{R}^n$$

➤ Let A be a real positive definite matrix. Then there is a scalar $\alpha > 0$ such that

$$(Au, u) \geq \alpha \|u\|_2^2.$$

- Consider now the case of Symmetric Positive Definite (SPD) matrices.
- Consequence 1: A is nonsingular
- Consequence 2: the eigenvalues of A are (real) positive

A few properties of SPD matrices

➤ Diagonal entries of A are positive

➤ Recall: the k-th principal submatrix A_k is the $k \times k$ submatrix of A with entries a_{ij}, $1 \le i, j \le k$ (Matlab: $A(1:k, 1:k)$).

✍1 Each A_k is SPD

✍2 Consequence: $Det(A_k) > 0$ for $k = 1, \cdots, n$. In fact A is SPD iff this condition holds.

3 If A is SPD then for any $n \times k$ matrix X of rank k, the matrix $X^T A X$ is SPD.

➤ The mapping : $\quad x, y \quad \rightarrow \quad (x, y)_A \equiv (Ax, y)$

defines a proper inner product on $\mathbb{R}^n$. The associated norm, denoted by $\|.\|_A$, is called the energy norm, or simply the A-norm:

$$\|x\|_A = (Ax, x)^{1/2} = \sqrt{x^T A x}$$

➤ Related measure in Machine Learning, Vision, Statistics: the Mahalanobis distance between two vectors:

$$d_A(x, y) = \|x - y\|_A = \sqrt{(x - y)^T A (x - y)}$$

Appropriate distance (measured in # standard deviations) if x is a sample generated by a Gaussian distribution with covariance matrix A and center y.

More terminology

- A matrix is Positive Semi-Definite if: $(Au, u) \geq 0$ *for all* $u \in \mathbb{R}^n$

- Eigenvalues of symmetric positive semi-definite matrices are real nonnegative, i.e., ...

- ... A can be singular [If not, A is SPD]

- A matrix is said to be Negative Definite if $-A$ is positive definite. Similar definition for Negative Semi-Definite

➤ A matrix that is neither positive semi-definite nor negative semi-definite is indefinite

✍4 Show that if $A^T = A$ and $(Ax, x) = 0 \ \forall x$ then $A = 0$

✍5 Show: $A \neq 0$ is indefinite iff $\exists\, x, y : (Ax, x)(Ay, y) < 0$

The LDL^T and Cholesky factorizations

✍6 The (standard) LU factorization of an SPD matrix A exists

➤ Let $A = LU$ and $D = diag(U)$ and set $M \equiv (D^{-1}U)^T$.

Then $$A = LU = LD(D^{-1}U) = LDM^T$$

➤ Both L and M are unit lower triangular

➤ Consider $\boxed{L^{-1}AL^{-T} = DM^TL^{-T}}$

➤ Matrix on the right is upper triangular. But it is also symmetric. Therefore $M^TL^{-T} = I$ and so $M = L$

➤ Alternative proof: exploit uniqueness of LU factorization without pivoting + symmetry: $A = LDM^T = MDL^T \rightarrow M = L$

➤ The diagonal entries of D are positive [Proof: consider $L^{-1}AL^{-T} = D$]. In the end:

$$A = LDL^T = GG^T \text{ where } G = LD^{1/2}$$

➤ Cholesky factorization is a specialization of the LU factorization for the SPD case. Several variants exist.

First algorithm: row-oriented LDLT

Adapted from Gaussian Elimination. Main observation: The working matrix $\boldsymbol{A(k+1:n, k+1:n)}$ in standard LU remains symmetric.
$\longrightarrow$ Work only on its upper triangular part & ignore lower part

1. For $k = 1 : n - 1$ Do:
2. For $i = k + 1 : n$ Do:
3. $piv := a(k, i)/a(k, k)$
4. $a(i, i : n) := a(i, i : n) - piv * a(k, i : n)$
5. End
6. End

➤ This will give the U matrix of the LU factorization. Therefore $D = diag(U)$, $L^T = D^{-1}U$.

Row-Cholesky (outer product form)

Scale the rows as the algorithm proceeds. Line 4 becomes

$$a(i,:) := a(i,:) - [a(k,i)/\sqrt{a(k,k)}] * \left[a(k,:)/\sqrt{a(k,k)}\right]$$

ALGORITHM : 1. *Outer product Cholesky*

1. *For* $k = 1 : n$ *Do:*
2. $\quad A(k, k:n) = A(k, k:n)/\sqrt{A(k,k)}$;
3. $\quad$ *For* $i := k+1 : n$ *Do :*
4. $\qquad A(i, i:n) = A(i, i:n) - A(k,i) * A(k, i:n);$
5. $\quad$ *End*
6. *End*

➤ Result: Upper triangular matrix U such $A = U^T U$.

Example:

$$A = \begin{pmatrix} 1 & -1 & 2 \\ -1 & 5 & 0 \\ 2 & 0 & 9 \end{pmatrix}$$

✍7 Is A symmetric positive definite?

✍8 What is the LDL^T factorization of A ?

✍9 What is the Cholesky factorization of A ?

Column Cholesky. Let $A = GG^T$ with G = lower triangular. Then equate j-th columns:

$$a(:,j) = \sum_{k=1}^{j} g(:,k) g^T(k,j) \rightarrow$$

$$\begin{aligned} A(:,j) &= \sum_{k=1}^{j} G(j,k) G(:,k) \\ &= G(j,j) G(:,j) + \sum_{k=1}^{j-1} G(j,k) G(:,k) \rightarrow \\ G(j,j) G(:,j) &= A(:,j) - \sum_{k=1}^{j-1} G(j,k) G(:,k) \end{aligned}$$

- Assume that first $j-1$ columns of G already known.
- Compute unscaled column-vector:

$$v = A(:,j) - \sum_{k=1}^{j-1} G(j,k)G(:,k)$$

- Notice that $v(j) \equiv G(j,j)^2$.
- Compute $\sqrt{v(j)}$ and scale v to get j-th column of G.

ALGORITHM : 2. *Column Cholesky*

1. *For* $j = 1 : n$ *do*
2. *For* $k = 1 : j-1$ *do*
3. $A(j:n, j) = A(j:n, j) - A(j,k) * A(j:n, k)$
4. *EndDo*
5. *If* $A(j,j) \leq 0$ *ExitError("Matrix not SPD")*
6. $A(j,j) = \sqrt{A(j,j)}$
7. $A(j+1:n, j) = A(j+1:n, j)/A(j,j)$
8. *EndDo*

✍10 Try algorithm on:

$$A = \begin{pmatrix} 1 & -1 & 2 \\ -1 & 5 & 0 \\ 2 & 0 & 9 \end{pmatrix}$$