Lecture Notes 18: Direct Methods for Linear Systems

CPSC 302: Numerical Computation for Algebraic Problems

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Chapter 4: Direct Methods for Linear Systems

- Gaussian Elimination and Backward Substitution
- LU Decomposition
- Pivoting Strategies
- Efficient Implementation
- Estimating Errors and Condition Number

- Cholesky Decomposition

- Sparse Matrices

Outline

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The "Square Root" of a Symmetric Positive Definite Matrix

- Recall that symmetric positive definite is the concept extension of a positive scalar to square real matrices A.
- For a scalar $a > 0$ there is a real square root, i.e., a real scalar g s.t. $g^2 = a$.
- For a symmetric positive definite matrix A, the Cholesky decomposition is written as

$$A = GG^T$$

  where G is a *lower triangular matrix*.
- Obtain Cholesky as a special case of LU decomposition, utilizing both symmetry of A and the assurance that no partial pivoting is needed.

Outline

Example

Consider the symmetric positive definite matrix

$$A = \begin{pmatrix} 1 & \mathbf{w}^T \\ \mathbf{w} & K \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

A single step of Gaussian elimination (introduce zeros in the 1st column) results in

$$A = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{w} & I \end{pmatrix} \begin{pmatrix} 1 & \mathbf{w}^T \\ \mathbf{0} & K - \mathbf{w}\mathbf{w}^T \end{pmatrix} = \left[M^{(1)} \right]^{-1} A^{(1)}.$$

Gaussian elimination would now continue to introduce zeros in the 2nd column. However, in order to maintain **symmetry**, Cholesky factorization first **introduces zeros in the 1st row** to match the zeros just introduced in the 1st column.

$$A^{(1)} = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & K - \mathbf{w}\mathbf{w}^T \end{pmatrix} \begin{pmatrix} 1 & \mathbf{w}^T \\ \mathbf{0} & I \end{pmatrix} = \tilde{A}^{(1)} \left[M^{(1)} \right]^{-T}.$$

Example (cont.)

Combining the operations on the previous slide, we find that A has been factored into 3 terms:

$$
\begin{aligned}
A &= \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{w} & I \end{pmatrix} \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & K - \mathbf{w}\mathbf{w}^T \end{pmatrix} \begin{pmatrix} 1 & \mathbf{w}^T \\ \mathbf{0} & I \end{pmatrix} \\
&= \left[M^{(1)} \right]^{-1} \tilde{A}^{(1)} \left[M^{(1)} \right]^{-T}.
\end{aligned}
$$

The idea of Cholesky factorization is to continue this process, zeroing one column and one row symmetrically until it is reduced to the identity.

Generalization of the Previous Example

Consider the symmetric positive definite matrix

$$A = \begin{pmatrix} a_{11} & \mathbf{w}^T \\ \mathbf{w} & K \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

Note that $a_{11} > 0$. The generalization of the previous slide is

$$\begin{aligned} A &= \begin{pmatrix} \sqrt{a_{11}} & \mathbf{0}^T \\ \frac{1}{\sqrt{a_{11}}}\mathbf{w} & I \end{pmatrix} \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & K - \frac{1}{a_{11}}\mathbf{w}\mathbf{w}^T \end{pmatrix} \begin{pmatrix} \sqrt{a_{11}} & \frac{1}{\sqrt{a_{11}}}\mathbf{w}^T \\ \mathbf{0} & I \end{pmatrix} \\ &= \left[M^{(1)}\right]^{-1} \tilde{A}^{(1)} \left[M^{(1)}\right]^{-T}. \end{aligned}$$

The second step reads

$$A = \left[M^{(1)}\right]^{-1} \left[M^{(2)}\right]^{-1} \tilde{A}^{(2)} \left[M^{(2)}\right]^{-T} \left[M^{(1)}\right]^{-T},$$

and so on, until we reach step n

$$\begin{aligned} A &= \left[M^{(1)}\right]^{-1} \cdots \left[M^{(n)}\right]^{-1} I \left[M^{(n)}\right]^{-T} \cdots \left[M^{(1)}\right]^{-T} \\ &= GG^T. \end{aligned}$$

Outline

Cholesky Decomposition

- Since A is symmetric positive definite, we can stably write

$$A = LU.$$

- Factor out the diagonal of U

$$U = \begin{pmatrix} u_{11} & & & & \\ & u_{22} & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & u_{nn} \end{pmatrix} \begin{pmatrix} 1 & \frac{u_{12}}{u_{11}} & \cdots & \cdots & \frac{u_{1n}}{u_{11}} \\ & 1 & \frac{u_{23}}{u_{22}} & \cdots & \frac{u_{2n}}{u_{22}} \\ & & \ddots & & \vdots \\ & & & \ddots & \vdots \\ & & & & 1 \end{pmatrix} = D\tilde{U}.$$

- So $A = LD\tilde{U}$, and by symmetry, $A = LDL^T$.

Cholesky Decomposition (cont.)

- By an elementary linear algebra theorem, $u_{kk} > 0$, $k = 1, \ldots, n$, so can define

$$D^{1/2} = diag\{\sqrt{u_{11}},\ \ldots\ , \sqrt{u_{nn}}\}.$$

- Obtain $A = GG^T$ with $G = LD^{1/2}$.
- Compute directly, using symmetry, in $\frac{1}{3}n^3 + \mathcal{O}(n^2)$ flops.
- In MATLAB, `R = chol(A)` gives $R = G^T$.

Cholesky Algorithm

Given a symmetric positive definite $n \times n$ matrix A, this algorithm overwrites its lower part with its Cholesky factor.

$$
\begin{array}{l}
\text{for } k = 1 : n \\
\quad a_{kk} = \sqrt{a_{kk}} \\
\quad \text{for } i = k+1 : n \\
\quad\quad a_{ik} = \dfrac{a_{ik}}{a_{kk}} \\
\quad \text{end} \\
\quad \text{for } j = k+1 : n \\
\quad\quad \text{for } i = j : n \\
\quad\quad\quad a_{ij} = a_{ij} - a_{ik} a_{jk} \\
\quad\quad \text{end} \\
\quad \text{end} \\
\text{end}
\end{array}
$$