Mathematical Tripos Part IB: Easter 2001

Numerical Analysis – Lecture 2[1]

2 Factorization of structured matrices

2.1 Symmetric matrices

Let A be an $n \times n$ symmetric matrix (i.e., $A_{k,\ell} = A_{\ell,k}$). An analogue of LU factorization takes advantage of symmetry: we express A in the form of the product LDL^{T}, where L is $n \times n$ lower triangular, with ones on its diagonal, whereas D is a diagonal matrix. Subject to its existence, we can write this factorization as

$$A = \begin{bmatrix} \boldsymbol{l}_1 & \boldsymbol{l}_2 & \cdots \boldsymbol{l}_n \end{bmatrix} \begin{bmatrix} D_{1,1} & 0 & \cdots & 0 \\ 0 & D_{2,2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & D_{n,n} \end{bmatrix} \begin{bmatrix} \boldsymbol{l}_1^{\mathrm{T}} \\ \boldsymbol{l}_2^{\mathrm{T}} \\ \vdots \\ \boldsymbol{l}_n^{\mathrm{T}} \end{bmatrix} = \sum_{k=1}^{n} D_{k,k} \boldsymbol{l}_k \boldsymbol{l}_k^{\mathrm{T}}$$

where, as before, $\boldsymbol{l}_k$ is the kth column of L.
The analogy with the algorithm of Section 1.2 becomes obvious by letting $U = DL^{\mathrm{T}}$, but the present form lends itself better to exploitation of symmetry. Specifically, to compute this factorization, we let $A_0 = A$ and for $k = 1, 2, \ldots, n$ let $\boldsymbol{l}_k$ be the multiple of the kth column of A_{k-1} such that $L_{k,k} = 1$. Set $D_{k,k} = (A_{k-1})_{k,k}$ and form $A_k = A_{k-1} - D_{k,k} \boldsymbol{l}_k \boldsymbol{l}_k^{\mathrm{T}}$.

Example Let $A = A_0 = \begin{bmatrix} 2 & 4 \\ 4 & 11 \end{bmatrix}$. Hence $\boldsymbol{l}_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$, $D_{1,1} = 2$ and

$$A_1 = A_0 - D_{1,1} \boldsymbol{l}_1 \boldsymbol{l}_1^{\mathrm{T}} = \begin{bmatrix} 2 & 4 \\ 4 & 11 \end{bmatrix} - 2 \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 3 \end{bmatrix}.$$

We deduce that $\boldsymbol{l}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $D_{2,2} = 3$ and $A = \begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}$.

2.2 Symmetric positive definite matrices

Recall that A is positive definite if $\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x} > 0$ for all $\boldsymbol{x} \neq \boldsymbol{0}$.

Theorem Let A be a real $n \times n$ symmetric matrix. It is positive definite if and only if it has an LDL^{T} factorization in which the diagonal elements of D are all positive.

Proof. Suppose that $A = LDL^{\mathrm{T}}$ and let $\boldsymbol{x} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}$. Since L is nonsingular, $\boldsymbol{y} := L^{\mathrm{T}} \boldsymbol{x} \neq \boldsymbol{0}$. Then $\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x} = \boldsymbol{y}^{\mathrm{T}} D \boldsymbol{y} = \sum_{k=1}^{n} D_{k,k} y_k^2 > 0$, hence A is positive definite.
Conversely, suppose that A is positive definite. We wish to demonstrate that an LDL^{T} factorization exists. We denote by $\boldsymbol{e}_k \in \mathbb{R}^n$ the kth unit (a.k.a. coordinate) vector. Hence $\boldsymbol{e}_1^{\mathrm{T}} A \boldsymbol{e}_1 = A_{1,1} > 0$ and $\boldsymbol{l}_1$ & $D_{1,1}$ are well defined. We now show that $(A_{k-1})_{k,k} > 0$ for $k = 1, 2, \ldots$. The result is true for $k = 1$ and we continue by induction (hence may assume that $A_{k-1} = A - \sum_{j=1}^{k-1} D_{j,j} \boldsymbol{l}_j \boldsymbol{l}_j^{\mathrm{T}}$ has been computed successfully).
We define $\boldsymbol{x} \in \mathbb{R}^n$ as follows. The bottom $n - k$ components are zero, $x_k = 1$ and $x_1, x_2, \ldots, x_{k-1}$ are calculated in a reverse order, each x_j being chosen so that $\boldsymbol{l}_j^{\mathrm{T}} \boldsymbol{x} = 0$ for $j = k-1, k-2, \ldots, 1$.

[1] Corrections and suggestions to these notes should be emailed to `a.shadrin@damtp.cam.ac.uk`. All handouts are available on the WWW at the URL `http://www.damtp.cam.ac.uk/user/na/PartIB/Handouts.html`.

In other words, since $0 = \boldsymbol{l}_j^{\mathrm{T}}\boldsymbol{x} = \sum_{i=1}^{n} L_{i,j}x_i = \sum_{i=j}^{k} L_{i,j}x_i$, we let $x_j = -\sum_{i=j+1}^{k} L_{i,j}x_i$, $j = k-1, k-2, \ldots, 1$.
Since the first $k-1$ rows & columns of A_{k-1} vanish, our choice implies that $(A_{k-1})_{k,k} = \boldsymbol{x}^{\mathrm{T}}A_{k-1}\boldsymbol{x}$. Thus, from the definition of A_{k-1} and the choice of $\boldsymbol{x}$,

$$(A_{k-1})_{k,k} = \boldsymbol{x}^{\mathrm{T}}A_{k-1}\boldsymbol{x} = \boldsymbol{x}^{\mathrm{T}}\left(A - \sum_{j=1}^{k-1} D_{j,j}\boldsymbol{l}_j\boldsymbol{l}_j^{\mathrm{T}}\right)\boldsymbol{x} = \boldsymbol{x}^{\mathrm{T}}A\boldsymbol{x} - \sum_{j=1}^{k-1} D_{j,j}(\boldsymbol{l}_j^{\mathrm{T}}\boldsymbol{x})^2 = \boldsymbol{x}^{\mathrm{T}}A\boldsymbol{x} > 0,$$

as required. Hence $(A_{k-1})_{k,k} > 0$, $k = 1, 2, \ldots, n$, and the factorization exists. □

Conclusion It is possible to check if a symmetric matrix is positive definite by trying to form its LDL^{T} factorization.

Cholesky factorization Define $D^{1/2}$ as the diagonal matrix whose (k,k) element is $D_{k,k}^{1/2}$, hence $D^{1/2}D^{1/2} = D$. Then, A being positive definite, we can write

$$A = (LD^{1/2})(D^{1/2}L^{\mathrm{T}}) = (LD^{1/2})(LD^{1/2})^{\mathrm{T}}.$$

In other words, letting $\tilde{L} := LD^{1/2}$ by L, we obtain the *Cholesky factorization* $A = \tilde{L}\tilde{L}^{\mathrm{T}}$.

2.3 Sparse matrices

Frequently it is required to solve *very* large systems $A\boldsymbol{x} = \boldsymbol{b}$ ($n = 10^5$ is considered small in this context!) where nearly all the elements of A are zero. Such a matrix is called *sparse* and efficient solution of $A\boldsymbol{x} = \boldsymbol{b}$ should exploit sparsity. In particular, we wish the matrices L and U to inherit as much as possible of the sparsity of A. The only tool at our disposal at the moment is the freedom to exchange rows and columns to minimise *fill-in.* To this end the following theorem is useful.

Theorem Let $A = LU$ be an LU factorization (without pivoting) of a sparse matrix. Then all leading zeros in the rows of A to the left of the diagonal are inherited by L and all the leading zeros in the columns of A above the diagonal are inherited by U.

Proof Follows from Question 2 on Examples' Sheet 1. □

This theorem suggests that if one requires a factorization of a sparse matrix then one might try to reorder its rows and columns by a preliminary calculation so that many of the zero elements are leading zero elements in rows and columns. This will reduce the fill-in.

Example 1 The LU factorisation of

$$\begin{bmatrix} -3 & 1 & 1 & 2 & 0 \\ 1 & -3 & 0 & 0 & 1 \\ 1 & 0 & 2 & 0 & 0 \\ 2 & 0 & 0 & 3 & 0 \\ 0 & 1 & 0 & 0 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 1 & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{8} & 1 & 0 & 0 \\ -\frac{2}{3} & -\frac{1}{4} & \frac{6}{19} & 1 & 0 \\ 0 & -\frac{3}{8} & \frac{1}{19} & \frac{4}{81} & 1 \end{bmatrix} \begin{bmatrix} -3 & 1 & 1 & 2 & 0 \\ 0 & -\frac{8}{3} & \frac{1}{3} & \frac{2}{3} & 1 \\ 0 & 0 & \frac{19}{8} & \frac{3}{4} & \frac{1}{8} \\ 0 & 0 & 0 & \frac{81}{19} & \frac{4}{19} \\ 0 & 0 & 0 & 0 & \frac{272}{81} \end{bmatrix},$$

has significant fill-in. However, reordering (symmetrically) rows and columns yields

$$\begin{bmatrix} 2 & 0 & 1 & 0 & 0 \\ 0 & 3 & 2 & 0 & 0 \\ 1 & 2 & -3 & 0 & 1 \\ 0 & 0 & 0 & 3 & 1 \\ 0 & 0 & 1 & 1 & -3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{2}{3} & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -\frac{6}{29} & \frac{1}{3} & 1 \end{bmatrix} \begin{bmatrix} 2 & 0 & 1 & 0 & 0 \\ 0 & 3 & 2 & 0 & 0 \\ 0 & 0 & -\frac{29}{6} & 0 & 1 \\ 0 & 0 & 0 & 3 & 1 \\ 0 & 0 & 0 & 0 & -\frac{272}{87} \end{bmatrix}.$$

Example 2 If the nonzeros of A occur only on the diagonal, in one row and in one column, then the full row and column should be placed at the bottom and on the right of A, respectively.