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MAT 610
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Lecture 7 Notes

These notes correspond to Sections 4.2 and 4.3 in the text.

Positive Definite Systems

A real, $n \times n$ symmetric matrix A is *symmetric positive definite* if $A = A^T$ and, for any nonzero vector \mathbf{x} ,

$$\mathbf{x}^T A \mathbf{x} > 0.$$

A symmetric positive definite matrix is the generalization to $n \times n$ matrices of a positive number.

If A is symmetric positive definite, then it has the following properties:

- A is nonsingular; in fact, $\det(A) > 0$.
- All of the diagonal elements of A are positive.
- The largest element of the matrix lies on the diagonal.
- All of the eigenvalues of A are positive.

In general it is not easy to determine whether a given $n \times n$ symmetric matrix A is also positive definite. One approach is to check the matrices

$$A_k = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{bmatrix}, \quad k = 1, 2, \dots, n,$$

which are the *leading principal minors* of A . It can be shown that A is positive definite if and only if $\det(A_k) > 0$ for $k = 1, 2, \dots, n$.

One desirable property of symmetric positive definite matrices is that Gaussian elimination can be performed on them without pivoting, and all pivot elements are positive. Furthermore, Gaussian elimination applied to such matrices is robust with respect to the accumulation of roundoff error. However, Gaussian elimination is not the most practical approach to solving systems of linear equations involving symmetric positive definite matrices, because it is not the most efficient approach in terms of the number of floating-point operations that are required.

Instead, it is preferable to compute the *Cholesky factorization* of A ,

$$A = GG^T,$$

where G is a lower triangular matrix with positive diagonal entries. Because A is factored into two matrices that are the transpose of one another, the process of computing the Cholesky factorization requires about half as many operations as the LU decomposition.

The algorithm for computing the Cholesky factorization can be derived by matching entries of GG^T with those of A . This yields the following relation between the entries of G and A ,

$$a_{ik} = \sum_{j=1}^k g_{ij}g_{kj}, \quad i, k = 1, 2, \dots, n, \quad i \geq k.$$

From this relation, we obtain the following algorithm.

```

for  $j = 1, 2, \dots, n$  do
     $g_{jj} = \sqrt{a_{jj}}$ 
    for  $i = j + 1, j + 2, \dots, n$  do
         $g_{ij} = a_{ij} / g_{jj}$ 
        for  $k = j + 1, \dots, i$  do
             $a_{ik} = a_{ik} - g_{ij}g_{kj}$ 
        end
    end
end

```

The innermost loop subtracts off all terms but the last (corresponding to $j = k$) in the above summation that expresses a_{ik} in terms of entries of G . Equivalently, for each j , this loop subtracts the matrix $\mathbf{g}_j\mathbf{g}_j^T$ from A , where \mathbf{g}_j is the j th column of G . Note that based on the outer product view of matrix multiplication, the equation $A = GG^T$ is equivalent to

$$A = \sum_{j=1}^n \mathbf{g}_j\mathbf{g}_j^T.$$

Therefore, for each j , the contributions of all columns \mathbf{g}_ℓ of G , where $\ell < j$, have already been subtracted from A , thus allowing column j of G to easily be computed by the steps in the outer loops, which account for the last term in the summation for a_{ik} , in which $j = k$.

Example Let

$$A = \begin{bmatrix} 9 & -3 & 3 & 9 \\ -3 & 17 & -1 & -7 \\ 3 & -1 & 17 & 15 \\ 9 & -7 & 15 & 44 \end{bmatrix}.$$

A is a symmetric positive definite matrix. To compute its Cholesky decomposition $A = GG^T$, we

equate entries of A to those of GG^T , which yields the matrix equation

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} g_{11} & 0 & 0 & 0 \\ g_{21} & g_{22} & 0 & 0 \\ g_{31} & g_{32} & g_{33} & 0 \\ g_{41} & g_{42} & g_{43} & g_{44} \end{bmatrix} \begin{bmatrix} g_{11} & g_{21} & g_{31} & g_{41} \\ 0 & g_{22} & g_{32} & g_{42} \\ 0 & 0 & g_{33} & g_{43} \\ 0 & 0 & 0 & g_{44} \end{bmatrix},$$

and the equivalent scalar equations

$$\begin{aligned} a_{11} &= g_{11}^2, \\ a_{21} &= g_{21}g_{11}, \\ a_{31} &= g_{31}g_{11}, \\ a_{41} &= g_{41}g_{11}, \\ a_{22} &= g_{21}^2 + g_{22}^2, \\ a_{32} &= g_{31}g_{21} + g_{32}g_{22}, \\ a_{42} &= g_{41}g_{21} + g_{42}g_{22}, \\ a_{33} &= g_{31}^2 + g_{32}^2 + g_{33}^2, \\ a_{43} &= g_{41}g_{31} + g_{42}g_{32} + g_{43}g_{33}, \\ a_{44} &= g_{41}^2 + g_{42}^2 + g_{43}^2 + g_{44}^2. \end{aligned}$$

We compute the nonzero entries of G one column at a time. For the first column, we have

$$\begin{aligned} g_{11} &= \sqrt{a_{11}} = \sqrt{9} = 3, \\ g_{21} &= a_{21}/g_{11} = -3/3 = -1, \\ g_{31} &= a_{31}/g_{11} = 3/3 = 1, \\ g_{41} &= a_{41}/g_{11} = 9/3 = 3. \end{aligned}$$

Before proceeding to the next column, we first subtract all contributions to the remaining entries of A from the entries of the first column of G . That is, we update A as follows:

$$\begin{aligned} a_{22} &= a_{22} - g_{21}^2 = 17 - (-1)^2 = 16, \\ a_{32} &= a_{32} - g_{31}g_{21} = -1 - (1)(-1) = 0, \\ a_{42} &= a_{42} - g_{41}g_{21} = -7 - (3)(-1) = -4, \\ a_{33} &= a_{33} - g_{31}^2 = 17 - 1^2 = 16, \\ a_{43} &= a_{43} - g_{41}g_{31} = 15 - (3)(1) = 12, \\ a_{44} &= a_{44} - g_{41}^2 = 44 - 3^2 = 35. \end{aligned}$$

Now, we can compute the nonzero entries of the second column of G just as for the first column:

$$\begin{aligned} g_{22} &= \sqrt{a_{22}} = \sqrt{16} = 4, \\ g_{32} &= a_{32}/g_{22} = 0/4 = 0, \\ g_{42} &= a_{42}/g_{22} = -4/4 = -1. \end{aligned}$$

We then remove the contributions from G 's second column to the remaining entries of A :

$$\begin{aligned} a_{33} &= a_{33} - g_{32}^2 = 16 - 0^2 = 16, \\ a_{43} &= a_{43} - g_{42}g_{32} = 12 - (-1)(0) = 12, \\ a_{44} &= a_{44} - g_{42}^2 = 35 - (-1)^2 = 34. \end{aligned}$$

The nonzero portion of the third column of G is then computed as follows:

$$\begin{aligned} g_{33} &= \sqrt{a_{33}} = \sqrt{16} = 4, \\ g_{43} &= a_{43}/g_{33} = 12/4 = 3. \end{aligned}$$

Finally, we compute g_{44} :

$$a_{44} = a_{44} - g_{43}^2 = 34 - 3^2 = 25, \quad g_{44} = \sqrt{a_{44}} = \sqrt{25} = 5.$$

Thus the complete Cholesky factorization of A is

$$\begin{bmatrix} 9 & -3 & 3 & 9 \\ -3 & 17 & -1 & -7 \\ 3 & -1 & 17 & 15 \\ 9 & -7 & 15 & 44 \end{bmatrix} = \begin{bmatrix} 3 & 0 & 0 & 0 \\ -1 & 4 & 0 & 0 \\ 1 & 0 & 4 & 0 \\ 3 & -1 & 3 & 5 \end{bmatrix} \begin{bmatrix} 3 & -1 & 1 & 3 \\ 0 & 4 & 0 & -1 \\ 0 & 0 & 4 & 3 \\ 0 & 0 & 0 & 5 \end{bmatrix}.$$

□

If A is not symmetric positive definite, then the algorithm will break down, because it will attempt to compute g_{jj} , for some j , by taking the square root of a negative number, or divide by a zero g_{jj} .

Example The matrix

$$A = \begin{bmatrix} 4 & 3 \\ 3 & 2 \end{bmatrix}$$

is symmetric but not positive definite, because $\det(A) = 4(2) - 3(3) = -1 < 0$. If we attempt to compute the Cholesky factorization $A = GG^T$, we have

$$\begin{aligned} g_{11} &= \sqrt{a_{11}} = \sqrt{4} = 2, \\ g_{21} &= a_{21}/g_{11} = 3/2, \\ a_{22} &= a_{22} - g_{21}^2 = 2 - 9/4 = -1/4, \\ g_{22} &= \sqrt{a_{22}} = \sqrt{-1/4}, \end{aligned}$$

and the algorithm breaks down. \square

In fact, due to the expense involved in computing determinants, the Cholesky factorization is also an efficient method for checking whether a symmetric matrix is also positive definite. Once the Cholesky factor G of A is computed, a system $A\mathbf{x} = \mathbf{b}$ can be solved by first solving $G\mathbf{y} = \mathbf{b}$ by forward substitution, and then solving $G^T\mathbf{x} = \mathbf{y}$ by back substitution.

This is similar to the process of solving $A\mathbf{x} = \mathbf{b}$ using the LDL^T factorization, except that there is no diagonal system to solve. In fact, the LDL^T factorization is also known as the “square-root-free Cholesky factorization”, since it computes factors that are similar in structure to the Cholesky factors, but without computing any square roots. Specifically, if $A = GG^T$ is the Cholesky factorization of A , then $G = LD^{1/2}$. As with the LU factorization, the Cholesky factorization is unique, because the diagonal is required to be positive.

Banded Systems

An $n \times n$ matrix A is said to have *upper bandwidth* p if $a_{ij} = 0$ whenever $j - i > p$. Similarly, A has *lower bandwidth* q if $a_{ij} = 0$ whenever $i - j > q$. A matrix that has upper bandwidth p and lower bandwidth q is said to have *bandwidth* $w = p + q + 1$.

Any $n \times n$ matrix A has a bandwidth $w \leq 2n - 1$. If $w < 2n - 1$, then A is said to be *banded*. However, cases in which the bandwidth is $O(1)$, such as when A is a *tridiagonal* matrix for which $p = q = 1$, are of particular interest because for such matrices, Gaussian elimination, forward substitution and back substitution are much more efficient. This is because

- If A has lower bandwidth q , and $A = LU$ is the LU decomposition of A (without pivoting), then L has lower bandwidth q , because at most q elements per column need to be eliminated.
- If A has upper bandwidth p , and $A = LU$ is the LU decomposition of A (without pivoting), then U has upper bandwidth p , because at most p elements per row need to be updated.

It follows that if A has $O(1)$ bandwidth, then Gaussian elimination, forward substitution and back substitution all require only $O(n)$ operations each, provided no pivoting is required.

Example The matrix

$$A = \begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix},$$

which arises from discretization of the second derivative operator, is banded with lower bandwidth

and upper bandwidth 1, and total bandwidth 3. Its LU factorization is

$$\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 & 0 & 0 \\ 0 & -\frac{2}{3} & 1 & 0 & 0 \\ 0 & 0 & -\frac{3}{4} & 1 & 0 \\ 0 & 0 & 0 & -\frac{4}{5} & 1 \end{bmatrix} \begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 0 & -\frac{3}{2} & 1 & 0 & 0 \\ 0 & 0 & -\frac{4}{3} & 1 & 0 \\ 0 & 0 & 0 & -\frac{5}{4} & 1 \\ 0 & 0 & 0 & 0 & -\frac{6}{5} \end{bmatrix}.$$

We see that L has lower bandwidth 1, and U has upper bandwidth 1. \square

When a matrix A is banded with bandwidth w , it is wasteful to store it in the traditional 2-dimensional array. Instead, it is much more efficient to store the elements of A in w vectors of length at most n . Then, the algorithms for Gaussian elimination, forward substitution and back substitution can be modified appropriately to work with these vectors. For example, to perform Gaussian elimination on a tridiagonal matrix, we can proceed as in the following algorithm. We assume that the main diagonal of A is stored in the vector \mathbf{a} , the *subdiagonal* (entries $a_{j+1,j}$) is stored in the vector \mathbf{l} , and the *superdiagonal* (entries $a_{j,j+1}$) is stored in the vector \mathbf{u} .

```
for  $j = 1, 2, \dots, n-1$  do
     $l_j = l_j / a_j$ 
     $a_{j+1} = a_{j+1} - l_j u_j$ 
end
```

Then, we can use these updated vectors to solve the system $A\mathbf{x} = \mathbf{b}$ using forward and back substitution as follows:

```
 $y_1 = b_1$ 
for  $i = 2, 3, \dots, n$  do
     $y_i = b_i - l_{i-1} y_{i-1}$ 
end
 $x_n = y_n / a_n$ 
for  $i = n-1, n-2, \dots, 1$  do
     $x_i = (y_i - u_i x_{i+1}) / a_i$ 
end
```

After Gaussian elimination, the components of the vector \mathbf{l} are the subdiagonal entries of L in the LU decomposition of A , and the components of the vector \mathbf{u} are the superdiagonal entries of U .

Pivoting can cause difficulties for banded systems because it can cause *fill-in*: the introduction of nonzero entries outside of the band. For this reason, when pivoting is necessary, pivoting schemes that offer more flexibility than partial pivoting are typically used. The resulting trade-off is that the entries of L are permitted to be somewhat larger, but the sparsity (that is, the occurrence of zero entries) of A is preserved to a greater extent.