Queens College, CUNY, Department of Computer Science

Numerical Methods

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12 Lecture 12

12.1 Applied linear algebra Part 4

- We conclude our study of applied linear algebra by listing some additional topics.
- The topics are important, but they are beyond the scope of these lectures.

12.2 Banded matrices

- An $n \times n$ square matrix M is called a **banded matrix** if all the nonzero matrix elements lie on only a few diagonals on or near the main diagonal. More precisely, there is a constant integer $c \geq 0$ such that

$$M_{ij} = 0 \qquad \text{if } |i - j| > c. \tag{12.2.1}$$

- A diagonal matrix is a banded matrix with $c = 0$.

- A tridiagonal matrix is a banded matrix with $c = 1$.

- A banded matrix has nonzero elements on $2c + 1$ diagonals.

- It is also possible to define constant integers c_1 and c_2 so that there are nonzero elements only up to c_1 diagonals below (and c_2 diagonals above) the main diagonal.

$$M_{ij} = 0 \qquad \text{if } i - j > c_1 \text{ or } j - i > c_2. \tag{12.2.2}$$

- Obviously this classification is most useful if $c \ll n$ or $c_{1,2} \ll n$, so that most of the matrix elements are zero.

- There are algorithms to solve sets of coupled linear equations with banded matrices, but we shall not discuss them.

12.3 Iterative methods

- Similar to root finding techniques for real solutions of nonlinear equations, we can solve the equation $A\boldsymbol{x} = \boldsymbol{b}$ iteratively. We write the equation in the form

$$F(\boldsymbol{x}) \equiv A\boldsymbol{x} - \boldsymbol{b} = \boldsymbol{0}\,. \tag{12.3.1}$$

- We search for a column vector $\boldsymbol{x}$ which a root of the equation $F(\boldsymbol{x}) = \boldsymbol{0}$.
- We begin with an initial guess $\boldsymbol{x}_0$ and iterate to obtain successive approximations $\boldsymbol{x}_1, \boldsymbol{x}_2, \dots$
- A tolerance parameter must be specified, to determine convergence.
- The iterative procedure may or may not converge.
- Some algorithms will converge if the matrix A is strongly diagonally dominant.
- We shall not discuss iterative methods in these lectures.

12.4 Singular Value Decomposition

- **Singular Value Decomposition (SVD)** is a very important technique when the equations are not linearly independent, or when there are fewer equations than unknowns.
- SVD is an important technique for the least squares fitting of data.
- However, we shall not discuss SVD in these lectures.

12.5 QR decomposition

- In additon to LU decomposition, there is another technique called **QR decomposition.**
- The technique is also called **QR factorization.**
- In QR decomposition, we factorize the matrix A in the form $A = QR$, where R is an upper triangular matrix and Q is an **orthogonal matrix**, i.e. $Q^T Q = I_{n\times n}$.
- Then the equations can be set up and solved as follows

$$\begin{aligned} A\boldsymbol{x} &= \boldsymbol{b}\,, \\ QR\boldsymbol{x} &= \boldsymbol{b}\,, \\ Q^T QR\boldsymbol{x} &= Q^T\boldsymbol{b} \qquad\qquad (\text{use } Q^TQ = I)\,, \\ R\boldsymbol{x} &= Q^T\boldsymbol{b}\,. \end{aligned} \tag{12.5.1}$$

- The final equation $R\boldsymbol{x} = Q^T\boldsymbol{b}$ is solved by backsubstitution, because R is upper triangular.
- Just as with LU decomposition, multiple right hand sides can be solved simultaneously. We write the original equations as $AX = B$ and we solve the equations via

$$RX = Q^T B\,. \tag{12.5.2}$$

- If we set $B = I$ then the solution for X is the inverse matrix $A^{-1} = X$.
- The determinant of an orthogonal matrix equals ± 1, hence

$$\det(A) = \det(Q)\det(R) = \pm\det(R)\,. \tag{12.5.3}$$

- We shall not discuss QR decomposition in these lectures.

12.6 Cholesky decomposition

- The technique of **Cholesky decomposition** (or **Cholesky factorization**) is applicable to **symmetric positive definite matrices.**
- A **symmetric positive definite matrix** is obviously symmetric, and "positive definite" means all of its eigenvalues are positive.
- A **symmetric positive semi-definite matrix** is a symmetric matrix all of whose eigenvalues are ≥ 0.
- Unfortunately, to make sense of the above statements, we need to know the concept of eigenvalues, which is beyond the scope of these lectures.
- Hence Cholesky decomposition will not be discussed in these lectures.
- We can give a summary of the technique. For a symmetric positive definite matrix A, the LU factorization can be formulated in such a way that $U = L^T$, the transpose of L, so

$$A = LL^T \,. \tag{12.6.1}$$

- Hence only one matrix L needs to be computed.
- Some authors say the matrix L is effectively a "square root" of the matrix A.
- A simple example of a symmetric positive definite matrix is the following.
  Let ρ be real and $\rho^2 < 1$. Then

$$A = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \,. \tag{12.6.2}$$

  1. The matrix is clearly symmetric.
  2. The eigenvalues of A are $1+\rho$ and $1-\rho$, which are both positive because $-1 < \rho < 1$.
  3. Then the matrix L is given by

$$L = \begin{pmatrix} 1 & 0 \\ \rho & \sqrt{1-\rho^2} \end{pmatrix} \,. \tag{12.6.3}$$

  4. We verify this as follows:

$$LL^T = \begin{pmatrix} 1 & 0 \\ \rho & \sqrt{1-\rho^2} \end{pmatrix} \begin{pmatrix} 1 & \rho \\ 0 & \sqrt{1-\rho^2} \end{pmatrix} = \begin{pmatrix} 1 & \rho \\ \rho & \rho^2 + (1-\rho^2) \end{pmatrix} = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \,. \tag{12.6.4}$$

- Cholesky decomposition also works if the matrix A is **complex valued.**
  In that case A must be a **Hermitian matrix** with all positive eigenvalues.
- If A is a **Hermitian positive definite matrix,** then $U = L^\dagger$, the **Hermitian conjugate** of L, and

$$A = LL^\dagger \,. \tag{12.6.5}$$