Queens College, CUNY, Department of Computer Science

Numerical Methods

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11 Lecture 11

11.1 Applied linear algebra Part 3

- We continue the study how to solve a set of coupled linear equations in several variables.
- In this lecture we study (some more) matrix algorithms.

11.2 Matrix equations: review

- We wish to solve a set of n coupled linear equations, which are expressed in matrix form as

$$AX = B\,. \tag{11.2.1}$$

- Here A is an $n \times n$ square matrix, while X and B are $n \times k$ matrices.
- We employ the $PA = LU$ **algorithm with partial pivoting.**
- The matrix A is decomposed into lower and upper triangular matrices L and U, respectively.
- No extra storage is required: the matrices L and U are stored in the memory occupied by A. The original matrix A is overwritten.
- The partial pivoting permutes the rows of the matrix A, so the algorithm also returns an array of the swap indices and the number of swaps performed.
- The array of swap indices can be formed into a permutation matrix P. The relation between the original matrix A and the LU factorization and the permutation matrix P is

$$PA = LU\,. \tag{11.2.2}$$

- Any square matrix can be factorized in this way. The algorithm is computationally stable.
- Since $PA = LU$, the equations to be solved using the LU decomposition are

$$LUX = PB\,. \tag{11.2.3}$$

  1. We first solve the following equation for a temporary matrix Y

$$LY = PB\,. \tag{11.2.4}$$

  2. We then solve the following equation to obtain the solution matrix X

$$UX = Y\,. \tag{11.2.5}$$

  3. Both sets of equations are solved using backsubstitution. The LU factorization is performed only once. After that, multiple sets of equations with different right-hand sides can be solved.

- The PA=LU algorithm can be used to calculate the inverse matrix A^{-1}, if A is non-singular, we set $B = I_{n\times n}$ and solve the equation

$$LUX = P\,. \tag{11.2.6}$$

  The solution for X yields the inverse matrix: $A^{-1} = X$.

- The PA=LU algorithm can be used to calculate the determinant of A via

$$\det(A) = (-1)^{\text{number of swaps}} \det(U)\,. \tag{11.2.7}$$

11.3 Special cases

- Although it may seem foolish, let us list some obvious special cases where a lot of theory or formalism is not required

- Suppose the matrix A is **diagonal**, say $A = D$ where

$$D = \begin{pmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \cdots & d_n \end{pmatrix} . \tag{11.3.1}$$

  The solution of the equations is obvious. The inverse matrix is

$$D^{-1} = \begin{pmatrix} d_1^{-1} & 0 & \dots & 0 \\ 0 & d_2^{-1} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \cdots & d_n^{-1} \end{pmatrix} . \tag{11.3.2}$$

- Suppose the matrix A is **upper triangular.** Say $A = U$ where U is upper triangular. Then the equations are already in LU form and can be solved immediately

$$UX = B\,. \tag{11.3.3}$$

  There is no need for pivoting and swapping of rows, etc.

- Conversely, suppose the matrix A is **lower triangular.** Say $A = L$ where L is lower triangular. Then the equations are already in LU form and can be solved immediately

$$LX = B\,. \tag{11.3.4}$$

  This can be solved "as is" via backsubstitution.

- **If A is already lower triangular, *there is no need to rearrange the rows to make the matrix upper triangular.***

- **Pay attention to the structure of the matrix A.**

- Do not automatically rush to a $PA = LU$ formalism.

11.4 Tridiagonal matrices

- Let us now analyze another special structure of the matrix A, very important in practice.
- The matrix A is **tridiagonal.**
- A tridiagonal matrix has nonzero elements only on the main diagonal and the two neighboring diagonals immediately above and below the main diagonal.
- In other words, $a_{ij} = 0$ if $|i - j| > 1$.
- The structure of a tridiagonal matrix T is shown below.

$$T = \begin{pmatrix} a_1 & c_1 & 0 & & & \dots & 0 \\ b_2 & a_2 & c_2 & 0 & & \dots & 0 \\ 0 & b_3 & a_3 & c_3 & 0 & \dots & 0 \\ & & & \ddots & & & \\ & & & & \ddots & & \\ 0 & & \dots & 0 & b_{n-1} & a_{n-1} & c_{n-1} \\ 0 & & \dots & & 0 & b_n & a_n \end{pmatrix}. \tag{11.4.1}$$

- This looks messy. Let us clean it up by replacing all the zeroes with blanks.
- Then the matrix equation $T\boldsymbol{x} = \boldsymbol{r}$ looks like this ("$\boldsymbol{r}$" for right hand side).

$$\begin{pmatrix} a_1 & c_1 & & & & & \\ b_2 & a_2 & c_2 & & & & \\ & b_3 & a_3 & c_3 & & & \\ & & & \ddots & & & \\ & & & & \ddots & & \\ & & & & b_{n-1} & a_{n-1} & c_{n-1} \\ & & & & & b_n & a_n \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ \vdots \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \\ \vdots \\ r_{n-1} \\ r_n \end{pmatrix}. \tag{11.4.2}$$

- For formal purposes, we set $b_1 = 0$ and $c_n = 0$.
  Then we can write general formulas for $i = 1, \dots, n$ without special cases for $i = 1$ and $i = n$.
- For a tridiagonal matrix, we only need to store the elements in the three diagonals, which is totally $3n$ elements (actually $3n - 2$). We do not need storage space for n^2 matrix elements.
- All the calculations can be formulated using only the elements in three diagonals.
- A tridiagonal set of equations can be solved using $O(n)$ computations. By comparison, LU factorization requires $O(n^3)$ computations. This saving in computation time is important in practical applications.

11.5 Tridiagonal algorithm Part 1

- The matrix equation to solve is $T\boldsymbol{x} = \boldsymbol{r}$, shown in eq. (11.4.2).
- The problem can be solved in $O(n)$ steps as follows.
  1. We use the first equation to express x_1 in terms of x_2.
  2. We substitute for x_1 in the second equation, to obtain an equation in x_2 and x_3.
  3. Then we express x_2 in terms of x_3.
  4. Then we substitute for x_2 in the third equation, obtain an equation involving x_3 and x_4, and use that to express x_3 in terms of x_4.
  5. We repeat the process until we reach the last equation. We substitute for x_{n-1} in the last equation, and we obtain an equation **involving x_n only.**
  6. Hence we solve for x_n.
  7. Then we work backwards (backsubstitution) to compute the values of $x_{n-1}, \dots, x_1$ in reverse order.
  8. There are totally $n-1$ elimination steps for $x_1, \dots, x_{n-1}$, one step to solve for x_n, then $n-1$ backsubstitution steps for $x_{n-1}, \dots, x_1$.
  9. Hence there are totally $2n-1$ equations to process, i.e. the tridiagonal equations are solved in $O(n)$ steps.
- We can obviously formulate the algorithm in the opposite direction.
  We eliminate $x_n, \dots, x_2$, solve for x_1, then perform backsubstitution to solve for $x_2, \dots, x_n$.
- **There is no pivoting** in the tridiagonal algorithm.
- For this reason the tridiagonal algorithm can fail even if the matrix is non-singular.
- In most practical applications, the lack of pivoting is not a serious problem.
- Unlike LU decomposition, the original matrix T is **not overwritten.**
- The same problems of inconsistent or ill-conditioned equations (or not linearly independent) also exist for tridiagonal matrix equations. Such difficulties are connected with the structure of the equations themselves, not with a computational algorithm.
- The tridiagonal algorithm is a good choice, if it is applicable to a problem. If it fails, one can use the $PA = LU$ algorithm.

11.6 Tridiagonal algorithm Part 2

11.6.1 Elimination of unknowns

- The equation in the first row is

$$a_1x_1 + c_1x_2 = r_1\,. \tag{11.6.1.1}$$

- We express x_1 in terms of r_1 and x_2 as follows

$$x_1 = \frac{r_1}{a_1} - \frac{c_1}{a_1}\,x_2 \;\equiv\; \beta_1 - \alpha_1\,x_2\,. \tag{11.6.1.2}$$

- The equation in the second row is

$$b_2x_1 + a_2x_2 + c_2x_3 = r_2\,. \tag{11.6.1.3}$$

- We substitute $x_1 = \beta_1 - \alpha_1x_2$ into the above equation, to obtain an equation in two unknowns x_2 and x_3.

$$\begin{aligned} b_2(\beta_1 - \alpha_1x_2) + a_2x_2 + c_2x_3 &= r_2 \\ (a_2 - b_2\alpha_1)x_2 + c_2x_3 &= r_2 - b_2\beta_1\,. \end{aligned} \tag{11.6.1.4}$$

- We follow the pattern and express x_2 in terms of r_2 and x_3 as follows

$$x_2 = \frac{r_2 - b_2\beta_1}{a_2 - b_2\alpha_1} - \frac{c_2}{a_2 - b_2\alpha_1}\,x_3 \;\equiv\; \beta_2 - \alpha_2\,x_3\,. \tag{11.6.1.5}$$

- This is the general pattern: for row i ($2 \le i \le n-1$), we write

$$x_i = \beta_i - \alpha_i\,x_{i+1}\,. \tag{11.6.1.6}$$

- The parameters β_i and γ_i are given by

$$\alpha_i = \frac{c_i}{a_i - b_i\alpha_{i-1}}\,, \qquad \beta_i = \frac{r_i - b_i\beta_{i-1}}{a_i - b_i\alpha_{i-1}}\,. \tag{11.6.1.7}$$

- If we define $b_1 = 0$ and $c_n = 0$ then we can extend the above expressions to all $i = 1, \dots, n$.
- **Note that if $a_1 = 0$ or $a_i - b_i\alpha_{i-1} = 0$ for $i = 2, \dots, n$, the algorithm will encounter a division by zero and will fail. The tridiagonal algorithm has no pivoting.**
- Although this is a weak point, it is not a serious problem in most practical applications.

11.6.2 Solution: backsubstitution

- Finally we reach the last equation, which is

$$b_n x_{n-1} + a_n x_n = r_n \,. \tag{11.6.2.1}$$

- We eliminate x_{n-1} by using $x_{n-1} = \beta_{n-1} - \alpha_{n-1} x_n$. This yields an equation in x_n only.

$$\begin{aligned} b_n(\beta_{n-1} - \alpha_{n-1} x_n) + a_n x_n &= r_n \\ (a_n - b_n \alpha_{n-1}) x_n &= r_n - b_n \beta_{n-1} \ ,. \end{aligned} \tag{11.6.2.2}$$

- The solution for x_n is

$$x_n = \frac{r_n - b_n \beta_{n-1}}{a_n - b_n \alpha_{n-1}} \,. \tag{11.6.2.3}$$

- We now work backwards by backsubstitution to calculate $x_{n-1}, \dots, x_1$ in reverse order.

$$\begin{aligned} x_{n-1} &= \beta_{n-1} - \alpha_{n-1}\, x_n \,, \\ &\vdots \\ x_i &= \beta_i - \alpha_i\, x_{i+1} \,, \\ &\vdots \\ x_1 &= \beta_1 - \alpha_1\, x_2 \,. \end{aligned} \tag{11.6.2.4}$$

11.7 Tridiagonal algorithm Part 3

- A careful examination of the algorithm in Sec. 11.6 shows that an array to hold the values of β_i is unnecessary. We can use the elements of the solution vector x_i to hold β_i.
- The only temporary storage required is to hold the values of α_i, $i = 1, \dots, n-1$.
- For computational purposes we can therefore restructure the algorithm as follows.
- **Elimination**
  1. Row 1 ($i = 1$)
  $$x_1 = \frac{r_1}{a_1}\,, \qquad \alpha_1 = \frac{c_1}{a_1}\,. \tag{11.7.1}$$
  2. Rows $i = 2, \dots, n-1$. It is convenient to define a temporary local variable γ.
  $$\gamma = a_i - b_i\alpha_{i-1}\,, \qquad x_i = \frac{r_i - b_i x_{i-1}}{\gamma}\,, \qquad \alpha_i = \frac{c_i}{\gamma}\,. \tag{11.7.2}$$
- **Backsubstitution**
  1. Final row ($i = n$).
  $$x_n = \frac{r_n - b_n\beta_{n-1}}{a_n - b_n\alpha_{n-1}}\,. \tag{11.7.3}$$
  2. Rows $i = n-1, \dots, 1$.
  $$\begin{aligned} x_{n-1} &:= x_{n-1} - \alpha_{n-1}\,x_n\,, \\ &\vdots \\ x_i &=: x_i - \alpha_i\,x_{i+1}\,, \\ &\vdots \\ x_1 &:= x_1 - \alpha_1\,x_2\,. \end{aligned} \tag{11.7.4}$$

11.8 Diagonal dominance

- A square matrix M (not necessarily tridiagonal) is called **strongly diagonally dominant** if for every row the magnitude of the diagonal element exceeds the sum of the amplitues of all the other elements in that row

$$|m_{ii}| > \sum_{j\neq i} |m_{ij}| \qquad (i = 1, \dots, n)\,. \tag{11.8.1}$$

- Then **weak diagonal dominance** means

$$|m_{ii}| \geq \sum_{j\neq i} |m_{ij}| \qquad (i = 1, \dots, n)\,. \tag{11.8.2}$$

- Some authors use the term "**diagonal dominance**" without a "atrong" or "weak" qualifier. It that case they mean strong diagonal dominance. We shall append the qualifier "atrong" or "weak" in these lectures.

- A tridiagonal matrix is (strongly) diagonally dominant if for every row

$$|a_i| > |b_i| + |c_i| \qquad (i = 1, \dots, n)\,. \tag{11.8.3}$$

- If a tridiagonal matrix is strongly diagonally dominant, then a zero pivot cannot occur in the elimination process in Sec. 11.7.

- For many practical applications involving tridiagonal matrices, the matrix is strongly diagonally dominant. Hence a zero pivot does not occur.

- There is a related concept called **strong column diagonal dominance** where for every column the magnitude of the diagonal element exceeds the sum of the amplitues of all the other elements in that column

$$|m_{jj}| > \sum_{i\neq j} |m_{ij}| \qquad (j = 1, \dots, n)\,. \tag{11.8.4}$$

11.9 Tridiagonal matrix: inverse

- The inverse of a tridiagonal matrix T is obtained by solving the equation

$$TX = I_{n\times n} \,. \tag{11.9.1}$$

- Each column of X is calculated using the algorithm in Sec. 11.7.
- The solution for X is the matrix inverse $T^{-1} = X$.
- In general, the inverse of a tridiagonal matrix is a full matrix, which has nonzero elements in every row and every column.

1. Consider the following 5×5 tridiagonal matrix (which is strongly diagonally dominant)

$$T = \begin{pmatrix} 1 & -0.25 & & & \\ 0.25 & 1 & -0.25 & & \\ & 0.25 & 1 & -0.25 & \\ & & 0.25 & 1 & -0.25 \\ & & & 0.25 & 1 \end{pmatrix} . \tag{11.9.2}$$

2. The inverse matrix is

$$T^{-1} = \begin{pmatrix} 0.944272 & 0.22291 & 0.0526316 & 0.0123839 & 0.00309598 \\ -0.22291 & 0.891641 & 0.210526 & 0.0495356 & 0.0123839 \\ 0.0526316 & -0.210526 & 0.894737 & 0.210526 & 0.0526316 \\ -0.0123839 & 0.0495356 & -0.210526 & 0.891641 & 0.22291 \\ 0.00309598 & -0.0123839 & 0.0526316 & -0.22291 & 0.944272 \end{pmatrix} . \tag{11.9.3}$$

- It is therefore a ***bad idea*** to solve the tridiagonal matrix equation $T\boldsymbol{x} = \boldsymbol{r}$ by computing the inverse and solving for $\boldsymbol{x}$ via

$$\boldsymbol{x} = T^{-1}\boldsymbol{r} \,. \tag{11.9.4}$$

- The calculation of $T^{-1}\boldsymbol{r}$ requires n^2 computations.
- By contrast, the solving for $\boldsymbol{x}$ by applying the tridiagonal algorithm to the equation $T\boldsymbol{x} = \boldsymbol{r}$ requires $O(n)$ computations.

11.10 Tridiagonal matrix: determinant

- The determinant of a tridiagonal matrix can be computed by solving a recurrence.
- Using eq. (11.4.1), let us define Δ_{n-i} to be the determinant of the bottom right $(n-i)\times(n-i)$ tridiagonal matrix.
- Hence we wish to compute $\det(T) = \Delta_n$.
- The recurrence is

$$\Delta_{n-i} = a_{i+1}\Delta_{n-i-1} - b_{i+2}c_{i+1}\Delta_{n-i-2} \qquad (i = 0, \dots, n-3)\,. \tag{11.10.1}$$

- The initial values are

$$\Delta_1 = a_n\,, \qquad \Delta_2 = a_{n-1}a_n - b_nc_{n-1}\,. \tag{11.10.2}$$

- The recurrence can be computed in $n-3$ steps to obtain $\det(T)$.
- The determinant of the matrix in eq. (11.9.2) is 1.26172 to five decimal places.

11.11 C++ code

- Examples of working C++ functions to implement the tridiagonal algorithm are given below.
- Note that the indexing of all the arrays follows the C/C++ convention.
- **Hence the indices run from 0 through $n-1$ for an array of length n.**

11.11.1 C++ code: Tridiagonal algorithm

```
int Tridiagonal_solve(const int n,
                      const std::vector<double> & a,
                      const std::vector<double> & b,
                      const std::vector<double> & c,
                      const std::vector<double> & rhs,
                      std::vector<double> & x)
{
  const double tol = 1.0e-14;
  x.clear();
  if ((n < 1) || (a.size() < n) || (b.size() < n) || (c.size() < n)
             || (rhs.size() < n)) return 1;   // fail
  double alpha[n]; // temporary storage

  x.resize(n, 0.0);

  // initial equation i = 0
  int i = 0;
  double gamma = a[i];
  if (std::abs(gamma) <= tol) return 1; // fail
  x[i] = rhs[i]/gamma;
  alpha[i] = c[i]/gamma;

  // forward pass: elimination
  for (i = 1; i < n-1; ++i) {
    gamma = a[i] - b[i]*alpha[i-1];
    if (std::abs(gamma) <= tol) return 1; // fail
    x[i] = (rhs[i] - b[i]*x[i-1])/gamma;
    alpha[i] = c[i]/gamma;
  }

  // solve final equation i = n-1
  i = n-1;
  gamma = a[i] - b[i]*alpha[i-1];
  if (std::abs(gamma) <= tol) return 1; // fail
  x[i] = (rhs[i] - b[i]*x[i-1])/gamma;

  // backward substitution
  for (i = n-2; i >= 0; --i) {
    x[i] -= alpha[i]*x[i+1];
  }
  return 0;
}
```

11.11.2 C++ code: Tridiagonal inverse

```
int Tridiagonal_inverse(const int n,
                        const std::vector<double> & a,
                        const std::vector<double> & b,
                        const std::vector<double> & c,
                        std::vector<std::vector<double>> & inv_matrix)
{
  if (n < 1) return 1;   // fail

  for (int j = 0; j < n; ++j) {
    std::vector<double> rhs(n, 0.0);
    std::vector<double> x(n, 0.0);
    rhs[j] = 1.0;

    inv_matrix[j].clear();

    int rc = Tridiagonal_solve(n, a, b, c, rhs, x);
    if (rc) {
      for (j = 0; j < n; ++j) {
        inv_matrix[j].clear(); // fail, clear everything
      }
      return rc; // fail
    }

    for (int i = 0; i < n; ++i) {
      inv_matrix[i][j] = x[i];
    }
  }

  return 0;
}
```

11.11.3 C++ code: Tridiagonal determinant

```
int Tridiagonal_determinant(const int n,
                            const std::vector<double> & a,
                            const std::vector<double> & b,
                            const std::vector<double> & c,
                            double & det)
{
  det = 0;
  if (n < 1) return 1;   // fail

  double F[n];    // temporary storage
  F[0] = a[n-1];
  if (n == 1) {
    det = F[n-1];
    return 0;
  }
  F[1] = a[n-2]*a[n-1] - b[n-1]*c[n-2];
  if (n == 2) {
    det = F[n-1];
    return 0;
  }

  for (int j = 2; j < n; ++j) {
    F[j] = a[n-1-j]*F[j-1] - b[n-j]*c[n-1-j]*F[j-2];
  }
  det = F[n-1];
  return 0;
}
```