# Numerical Analysis Mathematics of Scientific Computing

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## Solving Systems of Linear Equations

- Pivoting and Constructing an algorithm
  - Basic Gaussian Elimination
  - Pivoting
  - Gaussian Elimination with Scaled Row Pivoting
  - Factorizations PA = LU
  - Operation Counts
  - Diagonally Dominant Matrices
  - Tridiagonal System

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## Basic Gaussian Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}$$

$$Ax = b$$

• For the process, there are n-1 principal steps. In the first step, we refer to the first equation as the first pivot equation and to  $a_{11}$  as the first pivot element. For the remaining equations  $(2 \le i \le n)$ ,

$$\begin{cases} a_{ij} \leftarrow a_{ij} - \left(\frac{a_{i1}}{a_{11}}\right) a_{1j} & (1 \leq j \leq n) \\ b_i \leftarrow b_i - \left(\frac{a_{i1}}{a_{11}}\right) b_1 \end{cases}$$

Note that the quantities  $(a_{i1}/a_{11})$  are the multipliers.

• Just prior to the kth step in the forward elimination, the system will appear as follows:

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• We compute for each remaining equation  $(k+1 \le i \le n)$ 

$$\begin{cases} a_{ij} \leftarrow a_{ij} - \left(\frac{a_{ik}}{a_{kk}}\right) a_{kj} & (k \leq j \leq n) \\ b_i \leftarrow b_i - \left(\frac{a_{ik}}{a_{kk}}\right) b_k \end{cases}$$

• Obviously, we must assume that all the divisors in this algorithm are nonzero.

#### Pseudocode

```
input n, (a_{ij}), (b_i)
for k = 1 to n-1 do
for i = k + 1 to n do
z \leftarrow a_{ik}/a_{kk}
a_{ik} \leftarrow 0
for j = k + 1 to n do
a_{ij} \leftarrow a_{ij} - z a_{kj}
end do
b_i \leftarrow b_i - zb_k
end do
end do
output (a_{ij}), (b_i)
```

```
function a=Gaussian(a)
   n=length(a);
   for k=1:n-1
       for i=k+1:n
            z=a(i,k)/a(k,k);
5
            a(i,k)=0;
6
            for j=k+1:n
                a(i,j)=a(i,j)-z*a(k,j);
8
            end
9
       end
10
   end
11
```

```
function x=GaussianBacksub(a,b)
   n=length(a);
   for k=1:n-1
       for i=k+1:n
4
            z=a(i,k)/a(k,k);a(i,k)=0;
5
            for j=k+1:n
6
                 a(i,j)=a(i,j)-z*a(k,j);
            end
8
            b(i)=b(i)-z*b(k);
9
       end
10
   end
11
   for i=n:-1:1
12
       s=b(i);
13
       for j=i+1:1:n
14
            s=s-a(i,j)*x(j);
15
       end
16
       x(i)=s/a(i,i);
17
   end
18
```

• 
$$A = A^{(1)} \to A^{(2)} \to \dots \to A^{(n)}$$

$$\begin{bmatrix} a_{11}^{(k)} & \dots & a_{1,k-1}^{(k)} & a_{1k}^{(k)} & \dots & a_{1j}^{(k)} & \dots & a_{1n}^{(k)} \\ \vdots & \ddots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & a_{k-1,k-1}^{(k)} & a_{k-1,k}^{(k)} & \dots & a_{k-1,j}^{(k)} & \dots & a_{k-1,n}^{(k)} \\ 0 & \dots & 0 & a_{kk}^{(k)} & \dots & a_{kj}^{(k)} & \dots & a_{kn}^{(k)} \\ 0 & \dots & 0 & a_{k+1,k}^{(k)} & \dots & a_{k+1,j}^{(k)} & \dots & a_{k+1,n}^{(k)} \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & 0 & a_{ik}^{(k)} & \dots & a_{ij}^{(k)} & \dots & a_{in}^{(k)} \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & 0 & a_{nk}^{(k)} & \dots & a_{nj}^{(k)} & \dots & a_{nn}^{(k)} \end{bmatrix}$$

• Our task is to describe how  $A^{(k+1)}$  is obtained from  $A^{(k)}$ . The formula is

$$a_{ij}^{(k+1)} = \begin{cases} a_{ij}^{(k)} & \text{if } i \leqslant k \\ a_{ij}^{(k)} - (a_{ik}^{(k)}/a_{kk}^{(k)})a_{kj}^{(k)} & \text{if } i \geqslant k+1 \\ 0 & \text{if } i \geqslant k+1 \\ 0 & \text{if } i \geqslant k+1 \\ \end{cases}$$

Then we set  $U = A^{(n)}$  and define L by

$$l_{ik} = \begin{cases} a_{ik}^{(k)} / a_{kk}^{(k)} & \text{if } i \geqslant k+1\\ 1 & \text{if } i = k\\ 0 & \text{if } i \leqslant k-1 \end{cases}$$

#### Basic Gaussian Elimination

#### THEOREM 1 (Theorem on Nonzero Privots)

If all the pivot elements  $a_{kk}^{(k)}$  are nonzero in the process just described, then A = LU.

#### Proof.

Observe that  $a_{ij}^{(k+1)} = a_{ij}^{(k)}$  if  $i \le k$  or  $j \le k-1$ . Note  $u_{kj} = a_{kj}^{(n)} = a_{kj}^{(k)}$ ,  $l_{ik} = 0$  if k > i, and  $u_{kj} = 0$  if k > j. Now let  $i \le j$ . We have

$$(LU)_{ij} = \sum_{k=1}^{n} l_{ik} u_{kj} = \sum_{k=1}^{i} l_{ik} u_{kj}^{(k)} = \sum_{k=1}^{i} l_{ik} a_{kj}^{(k)}$$
$$= \sum_{k=1}^{i-1} l_{ik} a_{kj}^{(k)} + l_{ii} a_{ij}^{(i)}$$

#### Proof.

$$= \sum_{k=1}^{i-1} (a_{ik}^{(k)}/a_{kk}^{(k)}) a_{kj}^{(k)} + a_{ij}^{(i)}$$

$$= \sum_{k=1}^{i-1} (a_{ij}^{(k)} - a_{ij}^{(k+1)}) + a_{ij}^{(i)}$$

$$= a_{ij}^{(1)} = a_{ij}$$



#### Proof.

If i > j, then

$$(LU)_{ij} = \sum_{k=1}^{n} l_{ik} u_{kj} = \sum_{k=1}^{j} l_{ik} a_{kj}^{(k)}$$

$$= \sum_{k=1}^{j} (a_{ij}^{(k)} - a_{ij}^{(k+1)})$$

$$= a_{ij}^{(1)} - a_{ij}^{j+1}$$

$$= a_{ij}^{(1)} = a_{ij}$$

Since  $a_{ii}^{(k)} = 0$  if  $i \ge j + 1$  and  $k \ge j + 1$ .



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# Pivoting

• The first example

$$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

The algorithm fails because  $a_{11} = 0$ .

## Pivoting

• Another example, which  $\varepsilon$  is a small number different from 0.

$$\begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

The solution is

$$\begin{cases} x_2 = (2 - \varepsilon^{-1})/(1 - \varepsilon^{-1}) \approx 1 \\ x_1 = (1 - x_2)\varepsilon^{-1} \approx 0 \end{cases}$$

But the correct solution is

$$\left\{ \begin{array}{l} x_1 = 1/(1-\varepsilon) \approx 1 \\ x_2 = (1-2\varepsilon)/(1-\varepsilon) \approx 1 \end{array} \right.$$

• Interchanging the two equaions in example 1

$$\begin{bmatrix} 1 & 1 \\ \varepsilon & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

The solution is

$$\begin{cases} x_2 = (1 - 2\varepsilon)/(1 - \varepsilon) \approx 1 \\ x_1 = (2 - x_1) \approx 1 \end{cases}$$

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$$Ax = b$$

The algorithm has two parts: a factorization phase and a solution phase.

- The factorization phase is designed to produce the LU-decomposition of PA, the permuted linear system is PAx = Pb. P is a permutation matrix.
  - The factorization is obtained from a modified Gaussian elimination algorithm to be explained below.
- In the solution phase, we consider two equations Lz = Pb and Ux = z.
  - b is rearranged according to P and  $b \leftarrow Pb$ .
  - Lz = b is solved for z and  $b \leftarrow L^{-1}b$ .
  - Then back substitution is used to solve Ux = b for  $x_n, x_{n-1}, \ldots, x_1$ .

• Computing the scale of each row. We put

$$s_i = \max_{1 \le j \le n} |a_{ij}| = \max\{|a_{i1}|, |a_{i2}|, \dots, |a_{in}|\} \qquad (1 \le i \le n)$$

These *n* numbers are recorded in the scale vector  $s = [s_1, s_2, \dots, s_n]$ .

- Firstly, define the index vector p to be  $[p_1, p_2, \ldots, p_n] = [1, 2, \ldots, n]$ . Selecting an index j for which  $|a_{i1}|/s_i$  is largest. Interchanging  $p_j$  with  $p_1$  in the index vector. Next, use multipliers  $(a_{p_i1}/a_{p_11})$  times row 1, and subtract from equations  $p_i$  for  $2 \le i \le n$ .
- At step k, select j to be the first index corresponding to the largest of the ratios,  $\{|a_{p_ik}|/s_{p_i} \mid k \leq i \leq n\}$ , interchanging  $p_j$  with  $p_k$  in p.

# Pseudocode for Factorization phase

```
• input n, (a_{ij})

for i=1 to n do

p_i \leftarrow i

smax \leftarrow 0

for j=1 to n do

smax \leftarrow max(smax, |a_{ij}|)

end do

s_i \leftarrow smax

end do
```

• for k=1 to n-1 do  $rmax \leftarrow 0$ for i = k to n do  $r \leftarrow |a_{p_i k}/s_{p_i}|$ if (r > rmax) then  $rmax \leftarrow r \quad j \leftarrow i$ end if end do  $p_i \leftrightarrow p_k$ for i = k + 1 to n do  $z \leftarrow a_{p,k}/a_{p,k}; a_{p,k} \leftarrow z$ for j = k + 1 to n do  $a_{p_ij} \leftarrow a_{p_ij} - z a_{p_kj}$ end do end do end do output  $(a_{ij}), (p_i)$ 

# Pseudocode for Solution phase

• for k=1 to n-1 do for i=k+1 to n do  $b_{p_i} \leftarrow b_{p_i} - a_{p_i k} b_{p_k}$ end do end do for i=n to 1 step -1 do  $x_i \leftarrow (b_{p_i} - \sum_{j=i+1}^n a_{p_i j} x_j)/a_{p_i i}$ end do output  $(x_i)$ 

```
function x=ScaleGaussian(a,b)
   n=length(a);
   for i=1:n
       p(i)=i;
4
       smax=0;
5
6
       for j=1:n
        smax=max(smax, abs(a(i,j)));
       end
8
       s(i)=smax;
9
   end
10
   for k=1:n-1
11
       format rat rmax=0;
12
       for i=k:n
13
            r=abs(a(p(i),k))/s(p(i))
14
            if r>rmax
15
                 rmax=r; j=i;
16
            end
17
        end
18
```

```
c=p(k);p(k)=p(j);p(j)=c;
1
        for i=k+1 \cdot n
2
            z=a(p(i),k)/a(p(k),k);a(p(i),k)=z;
3
            for j=k+1:n
4
                 a(p(i),j)=a(p(i),j)-z*a(p(k),j);
5
            end
6
        end
        for i=k+1:n
8
            b(p(i))=b(p(i))-a(p(i),k)*b(p(k));
9
        end
10
   end
11
   for i=n:-1:1
12
        q=b(p(i));
13
        for j=i+1:1:n
14
            q=q-a(p(i),j)*x(j);
15
        end
16
        x(i)=q/a(p(i),i);
17
   end
18
```

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• Let  $p_1, p_2, \ldots, p_n$  be the indices of the rows in the order in which they become pivoting rows. Let  $A^{(1)} = A$ , and define  $A^{(2)}, A^{(3)}, \ldots, A^{(n)}$  recursively by the formula

$$a_{p_{i}j}^{(k+1)} = \begin{cases} a_{p_{i}j}^{(k)} & \text{if } i \leq k \text{ or } i > k > j \\ a_{p_{i}j}^{(k)} - (a_{p_{i}k}^{(k)}/a_{p_{k}k}^{(k)}) a_{p_{k}j}^{(k)} & \text{if } i > k \text{ and } j > k \\ a_{p_{i}k}^{(k)}/a_{p_{k}k}^{(k)} & \text{if } i > k \text{ and } j = k \end{cases}$$

#### THEOREM 2 (Theorem on LU Factorization of PA)

Define a permutation matrix P whose elements are  $P_{ij} = \delta_{p,j}$ . Define an upper triangular matrix U whose elements are  $u_{ij} = a_{p,j}^{(n)}$  if  $j \ge i$ . Define a unit lower triangular matrix L whose elements are  $l_{ij} = a_{p,j}^{(n)}$  if j < i. Then PA = LU.

#### Proof.

From the recursive formula, we have

$$u_{kj} = a_{p_k j}^{(n)} = a_{p_k j}^{(k)} (j \ge k)$$

$$l_{ik} = a_{p_i k}^{(n)} = a_{p_i k}^{(k+1)} = a_{p_i k}^{(k)} / a_{p_k k}^{(k)} (i \ge k)$$

Because the row  $p_k$  in  $A^{(n)}$  became fixed in step k, and column k in  $A^{(n)}$  became fixed in step k+1. Thus

$$a_{p_k j}^{(n)} = a_{p_k j}^{(k)}$$
  $a_{p_i k}^{(n)} = a_{p_i k}^{(k+1)}$ 



## Factorizations PA = LU

#### Proof.

Suppose that  $i \leq j$ .

$$(LU)_{ij} = \sum_{k=1}^{i} l_{ik} u_{kj}$$

$$= \sum_{k=1}^{i-1} (a_{p_i k}^{(k)} / a_{p_k k}^{(k)}) a_{p_k j}^{(k)} + l_{ii} a_{p_i j}^{(i)}$$

$$= \sum_{k=1}^{i-1} (a_{p_i j}^{(k)} - a_{p_i j}^{(k+1)}) + a_{p_i j}^{(i)}$$

$$= a_{p_i j}^{(1)} = a_{p_i j}$$

## Factorizations PA = LU

#### Proof.

If i > j, then

$$(LU)_{ij} = \sum_{k=1}^{j} l_{ik} u_{kj}$$

$$= \sum_{k=1}^{j-1} (a_{p_i k}^{(k)} / a_{p_k k}^{(k)}) a_{p_k j}^{(k)}) + (a_{p_i j}^{(j)} / a_{p_j j}^{(j)})$$

$$= \sum_{k=1}^{j-1} (a_{p_i j}^{(k)} - a_{p_i j}^{(k+1)}) + a_{p_i j}^{(j)}$$

$$= a_{p_i j}^{(1)} = a_{p_i j}$$

## Factorizations PA = LU

#### Proof.

And,

$$(PA)_{ij} = \sum_{k=1}^{n} P_{ik} a_{kj} = \sum_{k=1}^{n} \delta_{p_{ik}} a_{kj} = a_{p_{ij}}$$

So for all pairs (i, j), that

$$(PA)_{ij} = (LU)_{ij}$$



## Factorizations PA = LU

## THEOREM 3 (Theorem on Solving PA = LU)

If the factorization PA = LU is produced from the Gaussian algorithm with scaled row pivoting, then the solution of Ax = b is obtained by first solving Lz = Pb and then solving Ux = z. Similarly, the solution of  $y^TA = c^T$  is obtained by solving  $U^Tz = c$  and then  $L^TPy = z$ .

## Pseudocode in terms of L and U

• input  $n, (l_{ij}), (u_{ij}), (b_i), (p_i)$  for i=1 to n do  $z_i \leftarrow b_{p_i} - \sum_{j=1}^{i-1} l_{ij} z_j$  end do for i=n to 1 step -1 do  $x_i \leftarrow (z_i - \sum_{j=i+1}^n u_{ij} x_j) / u_{ii}$  end do output  $(x_i)$ 

## Pseudocode in terms of L and U

• input  $n, (a_{ij}), (b_i), (p_i)$ for i=1 to n do  $z_i \leftarrow b_{p_i} - \sum_{j=1}^{i-1} a_{p_i j} z_j$ end do for i=n to 1 step -1 do  $x_i \leftarrow (z_i - \sum_{j=i+1}^n a_{p_i j} x_j) / a_{p_i i}$ end do output  $(x_i)$  Factorizations PA = LU

## Pseudocode for $y^T A = c^T$

• input  $n, (a_{ij}), (c_i), (p_i)$ for j=1 to n do  $z_j \leftarrow (c_i - \sum_{i=1}^{j-1} a_{p_i j} z_i) / a_{p_j j}$ end do for j=n to 1 step -1 do  $y_{p_j} \leftarrow z_j - \sum_{i=j+1}^n a_{p_i j} y_{p_i}$ end do output  $(x_i)$  Operation Counts

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## Operation Counts

#### THEOREM 4 (Theorem on Long Operations)

If Gaussian elimination is used with scaled row pivoting, then the solution of the system Ax = b, with fixed A, and m different vectors b, involves approximately

$$\frac{1}{3}n^3 + (\frac{1}{2} + m)n^2$$

long operations (multiplications or divisions).

### Factorizations PA = LU

#### Proof.

Consider the first major step.

- Define  $p_1$  involves n divisions (n ops).
- For each of the n-1 rows, a multiplier is computed (1 op), then a multiple of row  $p_1$  is subtracted from  $p_i$  for  $2 \le i \le n$ . So the multiplier and the elimination process consume n ops per row.
- Since n-1 rows are processed, we have n(n-1) ops. So the total is  $n^2$  ops.

For the entire calculation, the factorization requires

$$n^{2} + (n-1)^{2} + \ldots + 2^{2} = \frac{1}{3}n^{3} + \frac{1}{2}n^{2} + \frac{1}{6}n - 1 \approx \frac{1}{3}n^{3} + \frac{1}{2}n^{2}$$

long operations.



## Operation Counts

#### Proof.

• In updating the b, there are n-1 steps. In the first, there are n-1 long operations. In the second, there are n-2, and so on. The total is

$$(n-1) + (n-2) + \ldots + 1 = \frac{1}{2}n^2 - \frac{1}{2}n$$

• In the back substitution, there is one long operation in the first step (computing  $x_n$ ). Then there are successively 2, 3,..., n long operations. The total is

$$1 + 2 + \ldots + n = \frac{1}{2}n^2 + \frac{1}{2}n$$

The grand total is  $n^2$ .

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## Diagonally Dominant Matrices

The property of **diagonally dominant matrices** is expressed by the inequality  $|a_{ii}| > \sum_{\substack{j=2\\ i\neq i}}^{n} |a_{ij}|$   $(1 \le i \le n)$ .

It has the property that Gaussian elimination without pivoting can be safely used.

#### THEOREM 5 (Theorem on Preserving Diagonal Dominance)

Gaussian elimination without pivoting preserves the diagonal dominance of a matrix.

#### Proof.

It suffices to consider the first step in Gaussian elimination, so we have to prove that for i = 2, 3, ..., n,

$$|a_{ii}^{(2)}| > \sum_{\substack{j=2\\j\neq i}}^{n} |a_{ij}^{(2)}|$$

In terms of A, this means  $|a_{ii} - (a_{i1}/a_{11})a_{1i}| > \sum_{\substack{j=2 \ j \neq i}}^{n} |a_{ij} - (a_{i1}/a_{11})a_{1j}|$ 

It suffices to prove the stronger inequality

$$|a_{ii}| - |(a_{i1}/a_{11})a_{1i}| > \sum_{\substack{j=2\\j\neq i}}^{n} \{|a_{ij}| + |(a_{i1}/a_{11})a_{1j}|\}$$

An equivalent inequality is  $|a_{ii}| - \sum_{\substack{j=2 \ j \neq i}}^{n} |a_{ij}| > \sum_{\substack{j=2 \ j \neq i}}^{n} |(a_{i1}/a_{11})a_{1j}|$ 

Form the diagonal dominance in the *i*th row, we know that

$$|a_{ii}| - \sum_{\substack{j=2\\i\neq i}}^{n} |a_{ij}| > |a_{i1}|$$

Hence, it suffices to prove that  $|a_{i1}| \ge \sum_{j=2}^{n} |(a_{i1}/a_{11})a_{1j}|$ 

This is true because of the diagonal dominance in row 1:

$$|a_{11}| > \sum_{i=2}^{n} |a_{1i}| \Longrightarrow 1 > \sum_{i=2}^{n} |a_{1i}/a_{11}|$$

## Diagonally Dominant Matrices

#### COROLLARY 1 (First Corollary on Diagonally Dominant Matrix)

Every diagonally dominant matrix is nonsingular and has an LU-factorization.

# COROLLARY 2 (Second Corollary on Diagonally Dominant Matrix)

If the scaled row pivoting version of Gaussian elimination recomputes the scale array after each major step and is applied to a diagonally dominant matrix, then the pivots will be the natural ones: 1, 2, ..., n. Hence, the work of choosing the pivots can be omitted in this case.

## Diagonally Dominant Matrices

#### Proof.

By Theorem 5, we only need to prove that the first pivot chosen in the algorithm is 1. So we should prove  $|a_{11}|/s_1 > |a_{i1}|/s_i$   $(2 \le i \le n)$ .

By the diagonal dominance,  $|a_{ii}| = max_j |a_{ij}| = s_i$  for all i.

Hence,  $|a_{11}|/s_1 = 1$ .

For 
$$i \ge 2$$
, We have  $|a_{i1}| \le \sum_{\substack{j=1 \ j \ne i}}^n |a_{ij}| < |a_{ii}| = s_i$ 

Thus,  $|a_{i1}|/s_i < 1$ .



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• A square matrix  $A = (a_{ij})$  is said to be tridiagonal if  $a_{ij} = 0$  for all pairs (i, j) that satisfy |i - j| > 1.

• Step 1 consists of these replacements:

$$d_2 \leftarrow d_2 - (a_1/d_1)c_1$$
  
 $b_2 \leftarrow b_2 - (a_1/d_1)b_1$ 

In the back substitution phase, the first step is

$$x_n \leftarrow b_n/d_n$$

The next step is

$$x_{n-1} \leftarrow (b_{n-1} - c_{n-1}x_n)/d_{n-1}$$

```
input n, (a_i), (b_i), (c_i), (d_i)

for i = 2 to n do

d_i \leftarrow d_i - (a_{i-1}/d_{i-1})c_{i-1}

b_i \leftarrow b_i - (a_{i-1}/d_{i-1})b_{i-1}

end do

x_n \leftarrow b_n/d_n

for i = n - 1 to 1 step -1 do

x_i \leftarrow (b_i - c_i x_{i+1})/d_i

end do

output(x_i)
```

## Tridiagonal System

```
1 function x=tri(a,b,c,d)
2 n=length(d);
3 for i=2:n
4     d(i)=d(i)-(a(i-1)/d(i-1))*c(i-1);
5     b(i)=b(i)-(a(i-1)/d(i-1))*b(i-1);
6 end
7 x(n)=b(n)/d(n);
8 for i=n-1:-1:1
9     x(i)=(b(i)-c(i)*x(i+1))/d(i);
10 end
```