线性方程组的直接解法

- ◆Gauss消元法
- ◆LU三角分解
- ◆范数/误差
- ◆部分主元Gauss消元法
- ◆LU分解与Gauss消元法的联系

理论基础

- 求解$n \times n$线性方程组

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n \end{cases}$$

定义：$x = [x_1, x_2, \ldots, x_n]^T, b = [b_1, b_2, \ldots, b_n]^T$

$$A = \begin{bmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{bmatrix}$$

方程组可表示为$Ax = b$

理论基础

- 如何求解$Ax = b$？

1. 如果$|A| \neq 0, x = A^{-1}b$

2. 如果$|A| \neq 0$，由Cramer法则知：

$$x_k = \frac{|A_k|}{|A|}$$

- 有没有更简单实用的求解方法？

理论基础

- 容易求解的情况

$$A = I = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

$$A = D = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & d_n \end{bmatrix}$$

$$A = L = \begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \ddots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix}$$

$$A = U = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \ddots & u_{2n} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

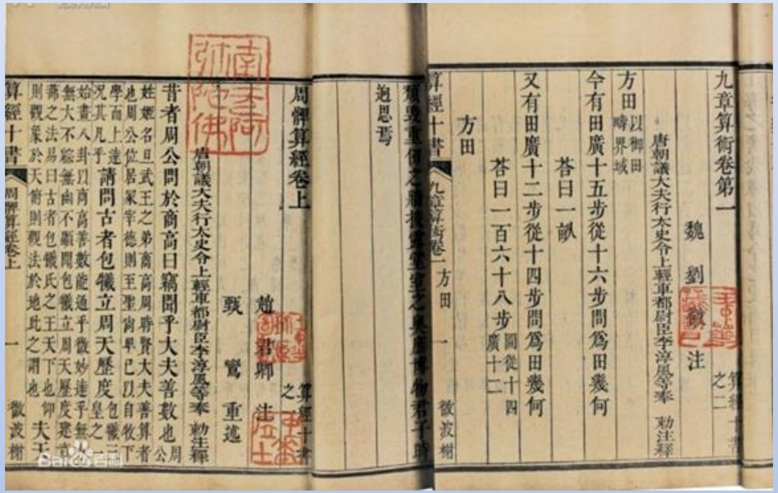
$$A = L^* = \begin{bmatrix} l^*_{11} & l^*_{12} & \cdots & l^*_{1n} \\ l^*_{21} & l^*_{22} & ⋰ & 0 \\ \vdots & ⋰ & \vdots & \vdots \\ l^*_{n1} & 0 & \cdots & 0 \end{bmatrix}$$

$$A = U^* = \begin{bmatrix} 0 & 0 & \cdots & u^*_{1n} \\ 0 & 0 & ⋰ & u^*_{2n} \\ \vdots & ⋰ & \vdots & \vdots \\ u^*_{n1} & u^*_{n2} & \cdots & u^*_{nn} \end{bmatrix}$$

高斯消元

- 核心思想：将方程组化简为三角形方程组

高斯1777-1855



九章算术成书于约公元前150年

- 理论支撑：对一个方程组做有限次行初等运算得到的方程与原方程同解
  - ➢交换方程组中的两个方程
  - ➢用一个非零数乘一个方程
  - ➢一个方程加上某个其它方程的倍数

高斯消元

- 具体操作

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

$$a_{ij} \leftarrow a_{ij} - \left(\frac{a_{i1}}{a_{11}}\right) a_{1j} \quad \Downarrow \quad b_i \leftarrow b_i - \left(\frac{a_{i1}}{a_{11}}\right) b_1, a_{11} \neq 0$$

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ 0 & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

高斯消元

- 经过$n-1$轮操作后

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1 \\ a_{22}x_2 + a_{23}x_3 + \dots + a_{2n}x_n = b_2 \\ \vdots \\ a_{n-1,n-1}x_{n-1} + a_{n-1,n}x_n = b_{n-1} \\ a_{nn}x_n = b_n \end{cases}$$

- 回代求解

$$x_n = b_n / a_{nn}$$

$$x_{n-1} = \left(b_{n-1} - a_{n-1,n}x_n\right) / a_{n-1,n-1}$$

$$x_i = \left(b_i - \sum_{j=i+1}^{n} a_{ij}x_j\right) / a_{ii}, i = n-1, n-2, \dots, 1$$

高斯消元

- 例：求解线性方程组

$$\begin{cases} x + 2y - z = 3 \\ 2x + y - 2z = 3 \\ -3x + y + z = -6 \end{cases}$$

高斯消元

- 伪代码(pseudocode)

消元

回代

```
procedure Naive_Gauss(n, (a_ij), (b_i), (x_i))
integer i, j, k, n;    real sum, xmult
real array (a_ij)_{1:n×1:n}, (b_i)_{1:n}, (x_i)_{1:n}
for k = 1 to n − 1 do
    for i = k + 1 to n do
        xmult ← a_ik/a_kk
        a_ik ← xmult
        for j = k + 1 to n do
            a_ij ← a_ij − (xmult)a_kj
        end for
        b_i ← b_i − (xmult)b_k
    end for
end for
x_n ← b_n/a_nn
for i = n − 1 to 1 step −1 do
    sum ← b_i
    for j = i + 1 to n do
        sum ← sum − a_ij x_j
    end for
    x_i ← sum/a_ii
end for
end procedure Naive_Gauss
```

$$\tilde{a}_{ij} = a_{ij} - \left(\frac{a_{ik}}{a_{kk}}\right) a_{kj}$$

$$\tilde{b}_i = b_i - \left(\frac{a_{ik}}{a_{kk}}\right) b_k$$

$$x_n = b_n / a_{nn}$$

$$x_i = \left(b_i - \sum_{j=i+1}^{n} a_{ij} x_j\right) / a_{ii}$$

高斯消元

- 第一轮消元计算量

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

$$a_{ij} \leftarrow a_{ij} - \left(\frac{a_{i1}}{a_{11}}\right) a_{1j} \quad \Downarrow \quad b_i \leftarrow b_i - \left(\frac{a_{i1}}{a_{11}}\right) b_1, a_{11} \neq 0$$

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ 0 & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

消去一个元的计算量：1次除法，n次乘法，n次减法（加法）

高斯消元

- 消元总体计算量(N_e)

$$\begin{bmatrix} 0 & & & & \\ 2n+1 & 0 & & & \\ 2n+1 & 2(n-1)+1 & \ddots & & \\ \vdots & \vdots & \ddots & 0 & \\ 2n+1 & 2(n-1)+1 & \dots & 2(2)+1 & 0 \end{bmatrix}$$

$$N_e = \sum_{j=1}^{n}(2j+1)(j-1) = \frac{2}{3}n^3 + \frac{1}{2}n^2 - \frac{7}{6}n = O(n^3)$$

高斯消元

- 回代计算量(N_b)

$$x_n = b_n / a_{nn}$$

$$x_i = \left(b_i - \sum_{j=i+1}^{n} a_{ij} x_j \right) / a_{ii}, i = n-1, n-2, \dots, 1$$

$$N_b = \sum_{i=1}^{n} [2(n-i)+1] = n^2 = O(n^2)$$

高斯消元

- 例：估算在求解一个规模为500×500个未知量的系统时，计算机系统消元过程和回代过程所花的时间之比。

$$\frac{t_b}{t_e} \approx \frac{N_b}{N_e} \approx \frac{500^2}{\frac{2}{3} \times 500^3} = 0.003$$

LU分解

- 什么是矩阵A的LU分解？
- LU分解有什么用？
- 怎么分解？

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & \cdots & 0 \\ l_{31} & l_{32} & l_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & l_{nn} \end{bmatrix} \cdot \begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

$$a_{ij} = \sum_{s=1}^{s=n} l_{is}u_{sj} = \sum_{s=1}^{s=\min(i,j)} l_{is}u_{sj}$$

n^2个方程，n^2+n个未知数

LU分解

- Doolittle分解

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{bmatrix} \cdot \begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

- Crout分解

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & \cdots & 0 \\ l_{31} & l_{32} & l_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & l_{nn} \end{bmatrix} \cdot \begin{bmatrix} 1 & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & 1 & u_{23} & \cdots & u_{2n} \\ 0 & 0 & 1 & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

LU分解

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & \cdots & 0 \\ l_{31} & l_{32} & l_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & l_{nn} \end{bmatrix} \cdot \begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

$$a_{11} = \sum_{s=1}^{s=\min(1,1)} l_{1s}u_{s1} = l_{11}u_{11} \rightarrow l_{11} \backslash u_{11}$$

$$a_{1j} = \sum_{s=1}^{s=\min(1,j)} l_{1s}u_{sj} = l_{11}u_{1j} \rightarrow u_{1j} \quad (2 \le j \le n)$$

$$a_{i1} = \sum_{s=1}^{s=\min(i,1)} l_{is}u_{s1} = l_{i1}u_{11} \rightarrow l_{i1} \quad (2 \le i \le n)$$

LU分解

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & \cdots & 0 \\ l_{31} & l_{32} & l_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & l_{nn} \end{bmatrix} \cdot \begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

$$a_{22} = \sum_{s=1}^{s=\min(2,2)} l_{2s}u_{s2} = l_{21}u_{12} + l_{22}u_{22} \to l_{22}\backslash u_{22}$$

$$a_{2j} = \sum_{s=1}^{s=\min(2,j)} l_{2s}u_{sj} = l_{21}u_{1j} + l_{22}u_{2j} \to u_{2j} \ \ (3 \le j \le n)$$

$$a_{i2} = \sum_{s=1}^{s=\min(i,2)} l_{is}u_{s2} = l_{i1}u_{12} + l_{i2}u_{22} \to l_{i2} \ \ (3 \le i \le n)$$

LU分解

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & 0 & \cdots & 0 \\ l_{k-1,1} & \cdots & l_{k-1,k-1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & \cdots & l_{n,k-1} & \cdots & l_{nn} \end{bmatrix} \cdot \begin{bmatrix} u_{11} & \cdots & u_{1,k-1} & \cdots & u_{1n} \\ 0 & \ddots & \vdots & \cdots & \vdots \\ 0 & 0 & u_{k-1,k-1} & \cdots & u_{k-1,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

$$a_{k,k} = \sum_{s=1}^{s=\min(k,k)} l_{ks}u_{sk} = \sum_{s=1}^{k-1} l_{ks}u_{sk} + l_{kk}u_{kk} \to l_{kk} \backslash u_{kk}$$

$$a_{kj} = \sum_{s=1}^{s=\min(k,j)} l_{ks}u_{sj} = \sum_{s=1}^{k-1} l_{ks}u_{sj} + l_{kk}u_{k,j} \to u_{kj}\ (k < j \le n)$$

$$a_{ik} = \sum_{s=1}^{s=\min(i,k)} l_{is}u_{sk} = \sum_{s=1}^{k-1} l_{is}u_{sk} + l_{ik}u_{kk} \to l_{ik}\ (k < i \le n)$$

LU分解

- $A = LU$分解过程

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & \dots & 0 \\ l_{21} & l_{22} & 0 & \dots & 0 \\ l_{31} & l_{32} & l_{33} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \dots & l_{nn} \end{bmatrix} \cdot \begin{bmatrix} u_{11} & u_{12} & u_{13} & \dots & u_{1n} \\ 0 & u_{22} & u_{23} & \dots & u_{2n} \\ 0 & 0 & u_{33} & \dots & u_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \boxed{u_{nn}} \end{bmatrix}$$

求解顺序:$u_{11} \to l_{i1}, u_{1j} \to u_{22} \to l_{i2}, u_{2j} \to \cdots \to u_{nn}$

显式求解:

$$u_{kj} = \left(a_{kj} - \sum_{s=1}^{k-1} l_{ks} u_{sj} \right) / l_{kk}$$

$$l_{ik} = \left(a_{ik} - \sum_{s=1}^{k-1} l_{is} u_{sk} \right) / u_{kk}$$

LU分解

- 例：3 × 3矩阵的Doolittle分解

$$A=\begin{bmatrix}1 & 2 & -1\\ 2 & 1 & -2\\ -3 & 1 & 1\end{bmatrix}=LU=\begin{bmatrix}1 & 0 & 0\\ l_{21} & 1 & 0\\ l_{31} & l_{32} & 1\end{bmatrix}\begin{bmatrix}u_{11} & u_{12} & u_{13}\\ 0 & u_{22} & u_{23}\\ 0 & 0 & u_{33}\end{bmatrix}$$

$$=\begin{bmatrix}u_{11} & u_{12} & u_{13}\\ l_{21}u_{11} & l_{21}u_{12}+u_{22} & l_{21}u_{13}+l_{22}u_{23}\\ l_{31}u_{11} & l_{31}u_{12}+l_{32}u_{22} & l_{31}u_{13}+l_{32}u_{23}+u_{33}\end{bmatrix}$$

- 求解

$$\begin{bmatrix}1 & 2 & -1\\ 2 & 1 & -2\\ -3 & 1 & 1\end{bmatrix}\begin{bmatrix}x_1\\ x_2\\ x_3\end{bmatrix}=\begin{bmatrix}3\\ 3\\ -6\end{bmatrix}$$

LU分解

- Doolittle分解的伪代码

integer i, k, n;   **real array** $(a_{ij})_{1:n\times 1:n}, (\ell_{ij})_{1:n\times 1:n}, (u_{ij})_{1:n\times 1:n}$

for $k = 1$ **to** n **do**

  $\ell_{kk} \leftarrow 1$ 把1赋值给L的对角元

  for $j = k$ **to** n **do**

    $$u_{kj} \leftarrow a_{kj} - \sum_{s=1}^{k-1} \ell_{ks} u_{sj}$$ 更新U的第k行

  end do

  for $i = k + 1$ **to** n **do**

    $$\ell_{ik} \leftarrow \left(a_{ik} - \sum_{s=1}^{k-1} \ell_{is} u_{sk} \right) \Big/ u_{kk}$$ 更新L的第k列

  end do

end do

LU分解

- Doolittle分解计算量？

integer i, k, n; **real array** $(a_{ij})_{1:n\times 1:n}, (\ell_{ij})_{1:n\times 1:n}, (u_{ij})_{1:n\times 1:n}$

for $k = 1$ **to** n **do**

  $\ell_{kk} \leftarrow 1$

  for $j = k$ **to** n **do**

    $u_{kj} \leftarrow a_{kj} - \sum_{s=1}^{k-1} \ell_{ks} u_{sj}$ $k-1$次乘法，$k-1$次减法

  end do

  for $i = k+1$ **to** n **do**

    $\ell_{ik} \leftarrow \left(a_{ik} - \sum_{s=1}^{k-1} \ell_{is} u_{sk}\right) \Big/ u_{kk}$ $k-1$次乘法，$k-1$次减法，1次除法

  end do

end do

总计算量= $\sum_{k=1}^{n} [2(k-1)(n-k+1) + (2k-1)(n-k)] = \frac{2}{3}n^3 - \frac{1}{2}n^2 - \frac{1}{6}n$

LU分解

- LU分解的存在性？
- LU分解定理：若$n \times n$矩阵A的n个前主子式非奇异，则A有LU分解。

A的第k个前主子式定义为：

$$A_k = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1k} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2k} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3k} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{k1} & a_{k2} & a_{k3} & \dots & a_{kk} \end{bmatrix}$$

- LU分解相比Gauss消元有什么优势？

误差

- 直接法有误差吗？
- 如何衡量误差？
- 向量$x \in \mathbb{R}^n$的范数$\|x\| \in \mathbb{R}$满足

1. 正定性：$\|x\| \geq 0$，仅当$x = 0$时等号成立
2. 齐次性： $\|\alpha x\| = |\alpha| \cdot \|x\|$
3. 三角不等式： $\|x + y\| \leq \|x\| + \|y\|$

- 例：

$$\|x\|_1 = |x_1| + \cdots + |x_n|$$

$$\|x\|_2 = \sqrt{x_1^2 + \cdots + x_n^2}$$

$$\|x\|_\infty = \max_{1 \leq i \leq n} |x_i|$$

误差

- 矩阵A的范数$\|A\| \in \mathbb{R}$满足

1. 正定性：$\|A\| \geq 0$，仅当$A = 0$时等号成立
2. 齐次性： $\|\alpha A\| = |\alpha| \cdot \|A\|$
3. 三角不等式： $\|A + B\| \leq \|A\| + \|B\|$

- 算子（从属矩阵）范数：$\|A\| = max \frac{\|Ax\|}{\|x\|}$ $(\forall x \in \mathbb{R}^n, x \neq 0)$

性质1. $\|I\| = 1$

性质2. $\|A\| \cdot \|x\| \geq \|Ax\|, \forall x \in \mathbb{R}^n$

性质3. $\|A\| \cdot \|B\| \geq \|AB\|$

误差

- 算子范数的例子

1. $\|A\|_1 = \max_{1\le j\le n}\left(\left|a_{1j}\right| + \cdots + \left|a_{nj}\right|\right)$， 最大绝对列和

2. $\|A\|_2 = \sqrt{\rho(A^T A)}$， $A^T A$的谱半径（特征值的最大模）的平方根

3. $\|A\|_\infty = \max_{1\le i\le n}\left(|a_{i1}| + \cdots + |a_{in}|\right)$， 最大绝对行和

误差

- 求解$Ax = b$的误差定义：

1. 近似解x_a的前向误差$\|x_a - x\|_\infty$

2. 后向误差$\|b - Ax_a\|_\infty = \|r\|_\infty$

3. 误差放大因子$= \frac{\|x_a - x\|_\infty / \|x\|_\infty}{\|r\|_\infty / \|b\|_\infty}$

4. 也可以采用其它范数来定义误差

误差

- 定义：n阶可逆方阵A的条件数$cond(A)$为求解$Ax = b$时，对于所有$b \neq 0$可能出现的最大误差放大因子，即：

$$cond(A) = \max_{b \in \mathbb{R}^n, b \neq 0} \frac{\|x_a - x\|_\infty / \|x\|_\infty}{\|r\|_\infty / \|b\|_\infty}$$

- 定理：可逆方阵A的条件数$cond(A) = \|A\|_\infty \ \|A^{-1}\|_\infty$，即：

$$\frac{\|x_a - x\|_\infty}{\|x\|_\infty} \leq \|A\|_\infty \ \|A^{-1}\|_\infty \frac{\|r\|_\infty}{\|b\|_\infty}$$

误差

- 定理：求解方程$Ax = b$时，前向误差和后向误差满足：

$$\frac{1}{cond(A)}\frac{\|r\|_\infty}{\|b\|_\infty} \le \frac{\|x_a - x\|_\infty}{\|x\|_\infty} \le cond(A)\ \frac{\|r\|_\infty}{\|b\|_\infty}$$

- 大条件数的矩阵是病态的。

误差

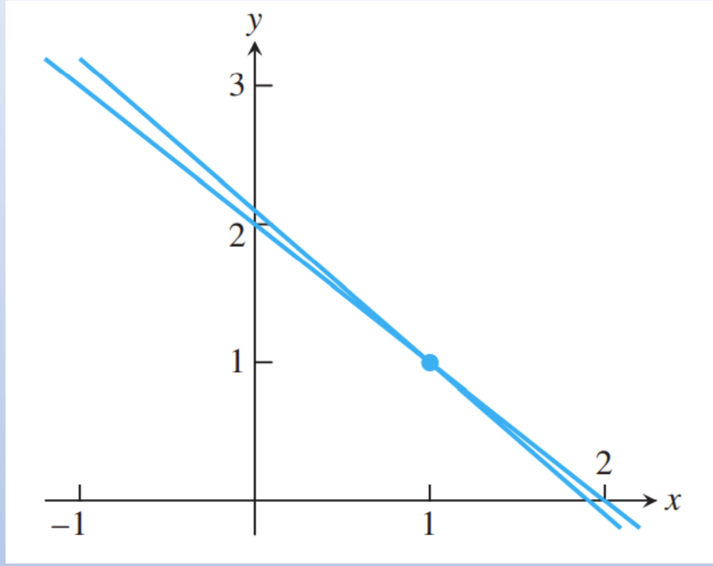
- 例：$\begin{cases} x_1 + x_2 = 2 \\ 1.0001x_1 + x_2 = 2.0001 \end{cases}$

近似解$x_a = [-1,3.0001]^T$的前向误差与后向误差？

系数矩阵条件数？

$$A = \begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix}, A^{-1} = \begin{bmatrix} -10000 & 10000 \\ 10001 & -10000 \end{bmatrix}$$

$$cond(A) = \|A\|_\infty \|A^{-1}\|_\infty \approx 40000$$



问题的几何解释

```
>> A = [1 1;1.0001 1]; b=[2;2.0001];
>> xa = A\b
xa =
    1.0000000000222
    0.9999999999778
```

11位

Matlab求解

误差

- Hilbert矩阵$H\left(h_{ij}=\frac{1}{i+j-1}\right)$是有名的病态矩阵

$$H_5=\begin{bmatrix}1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5}\\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6}\\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7}\\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} & \frac{1}{8}\\ \frac{1}{5} & \frac{1}{6} & \frac{1}{7} & \frac{1}{8} & \frac{1}{9}\end{bmatrix}$$

Matlab实验

```
>> n=10;H=hilb(n);
>> cond(H,inf)      条件数
ans =
     3.535371683074594e+013
>> b=H*ones(n,1);
>> xa=H\b
xa =
   0.99999999875463
   1.00000010746631
   0.99999771299818
   1.00002077769598
   0.99990094548472
   1.00027218303745
   0.99955359665722
   1.00043125589482
   0.99977366058043
   1.00004976229297
```

误差

- 例：$\begin{cases} 10^{-20}x_1 + x_2 = 1 \\ x_1 + 2x_2 = 4 \end{cases}$，精确解为$x_1 = \frac{2}{1-2\times10^{-20}}, x_2 = \frac{1-4\times10^{-20}}{1-2\times10^{-20}}$

顺序高斯消元：$\hat{x}_1 = 0, \hat{x}_2 = 1$

系数矩阵条件数？

$$A = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 2 \end{bmatrix}, A^{-1} = \frac{1}{2\times10^{-20}-1}\begin{bmatrix} 2 & -1 \\ -1 & 10^{-20} \end{bmatrix}$$

调换方程顺序消元：$\hat{x}_1 = 2, \hat{x}_2 = 1$

‘淹没’引起的误差放大可以通过列主消元避免

误差

- 列主消元：在消除第i列元素前找到绝对值最大的元素$a_{ji}(i \le j \le n)$

交换第i行和第j行

$$\begin{bmatrix} a_{11} & \cdots & a_{1i} & \cdots & a_{1j} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & a_{ii} & \cdots & a_{ij} & \cdots & a_{in} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \cdots & a_{ji} & \cdots & a_{jj} & \cdots & a_{jn} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & a_{ni} & \cdots & a_{nj} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_i \\ \vdots \\ x_j \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_i \\ \vdots \\ b_j \\ \vdots \\ b_n \end{bmatrix}$$

LU分解与高斯消元的联系

- 高斯消元基本的行变换操作与左乘初等矩阵对应

1. 交换第i行和第j行⟺左乘初等矩阵

$$
P = \begin{array}{cc}
\left[\begin{array}{ccccccc}
1 & \dots & 0 & \dots & 0 & \dots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \dots & \vdots \\
0 & \dots & 0 & \dots & 1 & \dots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \dots & 1 & \dots & 0 & \dots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \dots & 0 & \dots & 0 & \dots & 1
\end{array}\right]
&
\begin{array}{c}
\\ \\ \text{第}i\text{行} \\ \\ \text{第}j\text{行} \\ \\ \\
\end{array}
\\
\begin{array}{ccccccc}
 & & \text{第}i\text{列} & & \text{第}j\text{列} & &
\end{array}
&
\end{array}
$$

LU分解与高斯消元的联系

2. 非零数λ乘第i行加到第j行$\Leftrightarrow$左乘初等矩阵

$$E=\begin{array}{cc}\begin{bmatrix}1 & \dots & 0 & \dots & 0 & \dots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \dots & \vdots\\ 0 & \dots & 1 & \dots & 0 & \dots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ 0 & \dots & \lambda & \dots & 1 & \dots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ 0 & \dots & 0 & \dots & 0 & \dots & 1\end{bmatrix} & \begin{array}{l} \\ \\ \text{第}i\text{行} \\ \\ \text{第}j\text{行} \\ \\ \\ \end{array}\\ \begin{array}{ccccccc} & & \text{第}i\text{列} & & \text{第}j\text{列} & & \end{array} & \end{array}$$

LU分解与高斯消元的联系

- 顺序高斯消元$\Leftrightarrow E_m \dots E_1 A = U \Leftrightarrow A = E_1^{-1} \dots E_m^{-1} U, m \le \frac{n(n-1)}{2}$
- $E_1^{-1} \dots E_m^{-1} = L\,?$

$$\begin{bmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & \dots & 1 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \lambda & \dots & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & \dots & 1 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & -\lambda & \dots & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{bmatrix}$$

LU分解与高斯消元的联系

$$E_1^{-1}\dots E_m^{-1}=E_1^{-1}\dots E_{m-1}^{-1}\cdot\begin{bmatrix}1&\dots&0&0&0\\0&\ddots&\vdots&0&0\\\vdots&\ddots&1&\vdots&\vdots\\0&\ddots&0&1&0\\0&\dots&0&c_{n,n-1}&1\end{bmatrix}=E_1^{-1}\dots E_{m-2}^{-1}\cdot\begin{bmatrix}1&\dots&0&0&0\\0&\ddots&\vdots&0&0\\\vdots&\ddots&1&\vdots&\vdots\\0&\ddots&0&1&0\\0&\dots&c_{n,n-2}&c_{n,n-1}&1\end{bmatrix}$$

$$=E_1^{-1}\dots E_{m-3}^{-1}\cdot\begin{bmatrix}1&\dots&0&0&0\\0&\ddots&\vdots&0&0\\\vdots&\ddots&1&\vdots&\vdots\\0&\ddots&c_{n-1,n-2}&1&0\\0&\dots&c_{n,n-2}&c_{n,n-1}&1\end{bmatrix}=E_1^{-1}\dots E_{n-2}^{-1}\cdot\begin{bmatrix}1&\dots&0&0&0\\0&\ddots&\vdots&0&0\\\vdots&\ddots&1&\vdots&\vdots\\0&\ddots&c_{n-1,n-2}&1&0\\c_{n,1}&\dots&c_{n,n-2}&c_{n,n-1}&1\end{bmatrix}$$

$$=E_1^{-1}\dots E_{n-3}^{-1}\cdot\begin{bmatrix}1&\dots&0&0&0\\0&\ddots&\vdots&0&0\\\vdots&\ddots&1&\vdots&\vdots\\c_{n-1,1}&\ddots&c_{n-1,n-2}&1&0\\c_{n,1}&\dots&c_{n,n-2}&c_{n,n-1}&1\end{bmatrix}=\begin{bmatrix}1&\dots&0&0&0\\c_{21}&\ddots&\vdots&0&0\\\vdots&\ddots&1&\vdots&\vdots\\c_{n-1,1}&\ddots&c_{n-1,n-2}&1&0\\c_{n,1}&\dots&c_{n,n-2}&c_{n,n-1}&1\end{bmatrix}$$

LU分解与高斯消元的联系

- 例：推导A的LU分解

$$A=\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix}$$

LU分解与高斯消元的联系

- 伪代码

procedure **LU_Factorization** $\left(\left(a_{ij}\right)\right)$
integer i, j, k, n; **real** $xmult$
real array $\left(a_{ij}\right)_{1:n\times 1:n}$
for $k = 1$ **to** $n-1$ **do**
    for $i = k+1$ **to** n **do**
        $xmult \leftarrow a_{ik}/a_{kk}$
        $a_{ik} \leftarrow xmult$
        for $j = k+1$ **to** n **do**
            $a_{ij} \leftarrow a_{ij} - (xmult)a_{kj}$
        end for
    end for
end for

$$l_{ik} = \frac{a_{ik}}{a_{kk}}$$

LU分解与高斯消元的联系

- 列主高斯消元$\Leftrightarrow$ $E_{n(n-1)/2}P_{n-1}\dots E_{2n-3}\dots E_nP_2E_{n-1}\dots E_1P_1A=U$

$$A=P_1^{-1}E_1^{-1}\dots E_{n-1}^{-1}P_2^{-1}E_n^{-1}\dots E_{2n-3}^{-1}\dots P_{n-1}^{-1}E_{n(n-1)/2}^{-1}U$$

- $P_i^{-1}=P_i$

$$P_1^{-1}E_1^{-1}\dots E_{n-1}^{-1}P_2^{-1}E_n^{-1}\dots E_{2n-3}^{-1}\dots P_{n-1}^{-1}E_{n(n-1)/2}^{-1}$$

$$=P_1^{-1}E_1^{-1}\dots E_{n-1}^{-1}P_2^{-1}E_n^{-1}\dots E_{2n-3}^{-1}\dots P_{n-1}^{-1}\begin{bmatrix}1&\dots&0&0&0\\0&\ddots&\vdots&0&0\\\vdots&\ddots&1&\vdots&\vdots\\0&\ddots&0&1&0\\0&\dots&0&c_{n,n-1}&1\end{bmatrix}$$

$$=P_1^{-1}E_1^{-1}\dots E_{n-1}^{-1}P_2^{-1}E_n^{-1}\dots E_{2n-3}^{-1}\dots P_{n-2}^{-1}\begin{bmatrix}1&\dots&0&0&0\\0&\ddots&\vdots&0&0\\\vdots&\ddots&1&\vdots&\vdots\\0&\ddots&c_{n,n-2}&c_{n,n-1}&1\\0&\dots&c_{n-1,n-2}&1&0\end{bmatrix}$$

$P_{n-1}\dots P_1A=LU\Longrightarrow PA=LU,P=P_{n-1}\dots P_1$

LU分解与高斯消元的联系

- $PA = LU$回代求解$Ax = b$

$$PAx = Pb \;\rightarrow\; LUx = Pb \;\rightarrow \begin{cases} Ly = Pb \\ Ux = y \end{cases}$$

- 例：用$PA = LU$分解求解

$$\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 5 \\ 0 \\ 6 \end{bmatrix}$$

LU分解与高斯消元的联系

- 定义：严格行对角占优矩阵是指

$$|a_{ii}| > \sum_{j=1, j\neq i}^{n} |a_{ij}|, \qquad (1 \leq i \leq n)$$

- 定理：不选主元Gauss消元法保持矩阵的严格行对角占优性质。
- 推论：行对角占优矩阵非奇异且有LU分解。

LU分解与高斯消元的联系

- 例：

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

带状方程组的求解

- 三对角方程组

$$
\begin{bmatrix}
d_1 & c_1 & & & & & & \\
a_1 & d_2 & c_2 & & & & & \\
 & a_2 & d_3 & c_3 & & & & \\
 & & \ddots & \ddots & \ddots & & & \\
 & & & a_{i-1} & d_i & c_i & & \\
 & & & & \ddots & \ddots & \ddots & \\
 & & & & & a_{n-2} & d_{n-1} & c_{n-1} \\
 & & & & & & a_{n-1} & d_n
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_i \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix}
=
\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_i \\ \vdots \\ b_{n-1} \\ b_n \end{bmatrix}
$$

带状方程组的求解

- 高斯消元法（追赶法）

$$
\begin{bmatrix}
d_1 & c_1 & & & & & & \\
0 & d_2 & c_2 & & & & & \\
 & 0 & d_3 & c_3 & & & & \\
 & & \ddots & \ddots & \ddots & & & \\
 & & & 0 & d_i & c_i & & \\
 & & & & \ddots & \ddots & \ddots & \\
 & & & & & 0 & d_{n-1} & c_{n-1} \\
 & & & & & & 0 & d_n
\end{bmatrix}
\begin{bmatrix}
x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_i \\ \vdots \\ x_{n-1} \\ x_n
\end{bmatrix}
=
\begin{bmatrix}
b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_i \\ \vdots \\ b_{n-1} \\ b_n
\end{bmatrix}
$$

带状方程组的求解

- 追赶法的伪代码

procedure $Tri(n, (a_i), (d_i), (c_i), (b_i), (x_i))$
integer i, n; **real** $xmult$
real array $(a_i)_{1:n}, (d_i)_{1:n}, (c_i)_{1:n}, (b_i)_{1:n}, (x_i)_{1:n}$

消元

for $i = 2$ **to** n **do**
  $xmult \leftarrow a_{i-1}/d_{i-1}$
  $d_i \leftarrow d_i - (xmult)c_{i-1}$
  $b_i \leftarrow b_i - (xmult)b_{i-1}$
end for

回代

$x_n \leftarrow b_n/d_n$
for $i = n - 1$ **to** 1 **step** -1 **do**
  $x_i \leftarrow (b_i - c_i x_{i+1})/d_i$
end for
end procedure Tri

计算量$O(n)$

思考与练习

- 给定方程组$\begin{bmatrix} 1 & 1 \\ 1+\delta & 1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 2+\delta \end{bmatrix}$,$\delta > 0.1$、计算系数矩阵的条件数。2、计算近似解$x_a = [-1, 3+\delta]$的误差放大因子。

- 用Gauss消元法、列主消元法、LU分解法、$PA = LU$分解法求解下列方程组

$$\begin{bmatrix} 3 & 1 & 2 \\ 6 & 3 & 4 \\ 3 & 2 & 5 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 11 \\ 24 \\ 22 \end{bmatrix}$$

- 编写通用的Gauss消元法和LU分解法程序:1、求解以上方程组对程序进行验证；2、用程序求解$Hx = b$，H设置为12阶和20阶Hilbert矩阵，$b = H \cdot [1, \dots, 1]^T$。