# 作业三:线性方程组求解

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## 1 引言

在解决实际问题的时候,常常会遇到求解线性方程组的问题,比如使用有限差分法解偏微分方程. 往往线性方程组的个数会达到上万个,因此研究高效的算法很有必要. 这次作业主要使用 Gauss 消元法、Doolittle 分解法、Gauss-Seidel 迭代法和超松弛迭代法来解线性方程组.

## 2 问题描述

问题 1. 分别使用 Gauss 消元法、Doolittle 分解法、超松弛 Gauss-Seidel 迭代法解以下方程组

$$\mathbf{A}\mathbf{x} = \begin{bmatrix} -15 \\ 27 \\ -23 \\ 0 \\ -20 \\ 12 \\ -7 \\ 10 \end{bmatrix} \quad \mathbf{A} = \begin{bmatrix} 31 & -13 & 0 & 0 & 0 & -10 & 0 & 0 & 0 \\ -13 & 35 & -9 & 0 & -11 & 0 & 0 & 0 & 0 \\ 0 & -9 & 31 & -10 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -10 & 79 & -30 & 0 & 0 & 0 & -9 \\ 0 & 0 & 0 & -30 & 57 & -7 & 0 & -5 & 0 \\ 0 & 0 & 0 & 0 & -7 & 47 & -30 & 0 & 0 \\ 0 & 0 & 0 & 0 & -30 & 41 & 0 & 0 \\ 0 & 0 & 0 & 0 & -5 & 0 & 0 & 27 & -2 \\ 0 & 0 & 0 & -9 & 0 & 0 & 0 & -2 & 29 \end{bmatrix}$$

## 3 程序实现

为了方便,使用拓展矩阵来储存线性方程组的全部信息. 由于上面提到的所有方法都不希望 对角元出现 0,因此在计算之前,先对矩阵做列主元变换. 代码见 Listing 1.

Listing 1: 列主元变换

```
subroutine pivot_exchange(matrix, ndim1, ndim2)
2
        implicit none
3
        integer(8), intent(in) :: ndim1, ndim2
4
        real(8), dimension(ndim1, ndim2) :: matrix
5
6
        integer :: col, i
7
        real(8), dimension(ndim2) :: tmp_row
8
9
        do col = 1, ndim2
10
           do i = col, ndim1
11
               if (matrix(i, col) > matrix(col, col)) then
12
                   tmp_row = matrix(col, :)
13
                  matrix(col, :) = matrix(i, :)
14
                   matrix(i, :) = tmp_row
15
               end if
16
           end do
```

```
17 end do
18
19 return
20 end subroutine
```

所有的求解方法都被封装在一个叫做 linear\_eqs\_solver 的 module 里. 其中还包含了一个常数 EPSILON ,用来控制求解的精度,默认为 1e-3. 完整代码见附录.

### 3.1 Gauss 消元法

Gauss 消元法每次消元后矩阵大部分的值都改变了,所以 Gauss 消元法时不用上面这个列主元变换子程序,而是内置一个,即在每次消某一列之前对这一列做列主元变换. 流程图如图1所示. 代码见 Listing 2.

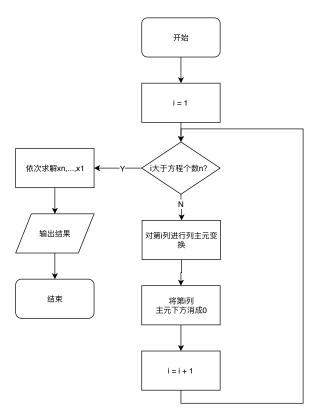


图 1: Gauss 消元法流程图

Listing 2: Gauss 消元法

```
1 subroutine gauss_elimination(co_matrix, ndim, solution)
2   implicit none
3   integer(8), intent(in) :: ndim
4   real(8), dimension(ndim, ndim+1), intent(in) :: co_matrix
```

```
5
        type(result), dimension(ndim), intent(out) :: solution
6
7
       real(8), dimension(ndim, ndim+1) :: A
8
        real(8), dimension(ndim) :: tmp_row, X
9
        integer(8) :: t, i
10
11
        A = co_matrix
12
        do t = 1, ndim
           ! pivot exchange
13
           do i = t, ndim
14
               if (abs(A(i, t)) > abs(A(t, t))) then
15
                  tmp_row = A(t, :)
16
                  A(t, :) = A(i, :)
17
18
                  A(i, :) = tmp_row
19
               end if
20
           end do
21
           ! Gauss elimination
22
           do i = t+1, ndim
23
               A(i, :) = A(i, :) - A(i, t) / A(t, t) * A(t, :)
24
           end do
25
        end do
26
27
        print "('The Gauss-eliminated extented coefficients matrix is')"
28
       print "(10f7.2)", (A(i, :), i=1,9)
29
       X = 0.0d0
30
31
       do t = ndim, 1, -1
32
           X(t) = (A(t, ndim+1) - dot_product(A(t, t+1:ndim), X(t+1:ndim))) / A(t, t)
        end do
33
34
35
        solution%value = X
        solution%error = 0.0d0
36
37
38
       return
39
   end subroutine
```

#### 3.2 Doolittle 分解法

Doolittle 分解法将系数矩阵分解为一个下三角矩阵和一个上三角矩阵的乘积.

$$A = LU$$

#### L 和 U 各分量的值可以由下式得到

$$u_{kj} = a_{kj} - \sum_{r=1}^{k-1} l_{kr} u_{rj} \quad j = k, \dots, n$$
$$l_{ik} = \frac{a_{ik} - \sum_{r=1}^{k-1} l_{ir} u_{rk}}{u_{kk}} \quad i = k+1, \dots, n$$

方程最终的解分两步得到

$$y_i = b_i - \sum_{j=1}^{i-1} I_{ij} y_j \quad i = 1, \dots, n$$
 
$$x_i = \frac{y_i - \sum_{j=i+1}^{n} u_{ij} x_j}{u_{ii}} \quad i = n, \dots, 1$$

由于 Gauss 消元法和 Doolittle 分解法都是精确的算法,因此最后输出的结果误差为 0 (实际上不是严格的 0,但是误差会比双精度浮点数最小的那个数小).流程图见图2.代码见 Listing 3.

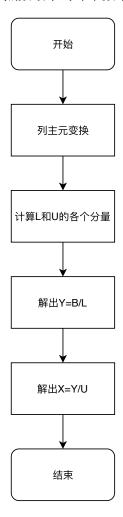


图 2: Doolittle 分解法流程图

Listing 3: **Doolittle 分解法** 

```
subroutine doolittle(co_matrix, ndim, solution)
1
2
        implicit none
3
       integer(8), intent(in) :: ndim
       real(8), dimension(ndim, ndim+1), intent(in) :: co_matrix
4
        type(result), dimension(ndim), intent(out) :: solution
5
7
       real(8), dimension(ndim, ndim+1) :: A
8
       real(8), dimension(ndim, ndim) :: L, U
       real(8), dimension(ndim) :: X, Y
10
       integer(8) :: i, j, k
11
12
       A = co_matrix
       L = 0.0d0; U = 0.0d0;
13
14
15
        call pivot_exchange(A, ndim, ndim+1)
16
       do k = 1, ndim
17
18
           do j = k, ndim
19
              U(k, j) = A(k, j) - dot_product(L(k, :k-1), U(:k-1, j))
20
           end do
21
           L(k, k) = 1.0d0
22
           do i = k+1, ndim
23
               L(i, k) = (A(i, k) - dot_product(L(i, :k-1), U(:k-1, k))) / U(k, k)
24
           end do
25
       end do
26
27
       do i = 1, ndim
28
           Y(i) = A(i, ndim+1) - dot_product(L(i, :i-1), Y(:i-1))
29
       end do
       do i = ndim, 1, -1
30
           X(i) = (Y(i) - dot_product(U(i, i+1:), X(i+1:))) / U(i, i)
31
32
       end do
33
34
        solution%value = X
        solution%error = 0.0d0
35
36
37
       return
    end subroutine
38
```

#### 3.3 Gauss-Seidel 迭代法

Gauss-Seidel 迭代法的子程序其中的参数 omega 是可选参数. 如果不输入 omega, 那么默认 omega 的值为 1, 即 Gauss-Seidel 迭代; 如果输入 omega, 若大于 1 则是 overrelaxation 迭代, 若小于 1 则是 underrelaxation 迭代. 迭代初值设置为零向量. 迭代结果的误差大小取的是最后两次迭代的差值. 流程图见图3. 代码见 Listing 4.

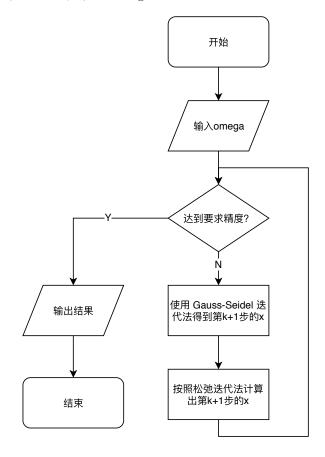


图 3: 使用松弛迭代的 Gauss-Seidel 迭代法流程图

Listing 4: Gauss-Seidel 迭代法

```
subroutine gauss_seidel_iteration(co_matrix, ndim, solution, omega)
1
2
       implicit none
3
       integer(8), intent(in) :: ndim
4
       real(8), optional, intent(in) :: omega
       real(8), dimension(ndim, ndim+1), intent(in) :: co_matrix
5
6
       type(result), dimension(ndim), intent(out) :: solution
8
       real(8), dimension(ndim, ndim+1) :: A
9
       real(8) :: lambda = 1.0d0
10
       real(8), dimension(ndim) :: X, X_tmp, Error
```

```
11
        integer(8) :: iter, i
12
13
        A = co_matrix
14
        call pivot_exchange(A, ndim, ndim+1)
15
16
        if (present(omega)) then
           lambda = omega
17
18
        end if
19
        X = 0.0d0
20
21
        do iter = 1, 10000
22
           X_{tmp} = X
23
           do i = 1, ndim
               X(i) = -(dot_product(A(i, :ndim), X) - A(i, i) * X(i) - A(i, ndim+1)) / A(i, i)
24
25
           X = (1 - lambda) * X_tmp + lambda * X
26
           Error = abs(X - X_tmp)
27
28
29
           if (maxval(Error) < EPSILON) then</pre>
30
31
           end if
32
        end do
        print "('Iter: ',i4)", iter
34
        solution%value = X
35
        solution%error = Error
36
37
38
        return
39
   end subroutine
```

## 4 运行时结果

#### 4.1 Gauss 消元法

Gauss 消元法的运行时结果如图4所示. 得到的结果为

```
\mathbf{x} = \begin{bmatrix} -0.2892 & 0.3454 & -0.7128 & -0.2206 & -0.4304 & 0.1543 & -0.0578 & 0.2011 & 0.2982 \end{bmatrix}^T
```

命令行中 Checking results... 的下一行是将数值结果代回原方程得到的值,可见完全满足方程组 (也就是和拓展矩阵的最后一列相等)

#### 4.2 Doolittle 分解法

Doolittle 分解法的运行时结果如图5,结果与 Gauss 消元法完全一致.

图 4: Gauss 消元法

```
zipwin@WorldGate: ~/WorkPlace/fortran/computational_physics/assignment3/task0
文件(F) 编辑(E) 查看(V) 搜索(S) 终端(T) 帮助(H)
           gfortran linear_eqs_solver.f90 -o linear_eqs_solve
./linear_eqs_solver
  task0
                  0.00 0.00 0.00
-9.00 0.00 -11.00
31.00 -10.00 0.00
                                                       0.00
                                             -7.00
47.00
-30.00
                                     -7.00
0.00
                                                      30.00
                                                      41.00
                                      0.00
                                               0.00
                                                        0.00
   solution vector is
.2892 0.3454 -0.7128 -0.2206 -0.4304 0.1543 -0.0578
 0.0000 0.0000 0.0000 0.0000 0.0000
                                                                       0.0000
```

图 5: Doolittle 分解法

#### 4.3 超松弛 Gauss-Seidel 迭代法

设置 omega 为 1.5, 使用 Gauss-Seidel 迭代法的运行时结果如图6所示. 得到的结果为

$$\mathbf{x} = \begin{bmatrix} -0.2895 & 0.3455 & -0.7128 & -0.2206 & -0.4304 & 0.1543 & -0.0578 & 0.2011 & 0.2982 \end{bmatrix}^T$$

除第一个数有 0.0007 的误差外, 其他的都没有误差. 达到需求的精度迭代了 19 次. 代回方程组 检验发现, 第一个方程有 0.01 的偏差.

图 6: 超松弛 Gauss-Seidel 迭代法

## 附录

代码可在https://github.com/ZipWin/computational\_physics/tree/master/assignments/assignment3找到.

Listing 5: linear\_eqs\_solver.f90

```
1
    module utils
2
        implicit none
3
        type result
           real(8) :: value
4
           real(8) :: error
5
6
        end type
7
8
        contains
9
        subroutine pivot_exchange(matrix, ndim1, ndim2)
10
           implicit none
           integer(8), intent(in) :: ndim1, ndim2
11
           real(8), dimension(ndim1, ndim2) :: matrix
12
13
14
           integer :: col, i
15
           real(8), dimension(ndim2) :: tmp_row
16
17
           do col = 1, ndim2
               do i = col, ndim1
18
19
                   if (matrix(i, col) > matrix(col, col)) then
                      tmp_row = matrix(col, :)
20
                      matrix(col, :) = matrix(i, :)
21
```

```
22
                      matrix(i, :) = tmp_row
23
                   end if
24
               end do
25
           end do
26
27
           return
28
        end subroutine
29
30
    end module
31
32
33
   module linear_eqs_solver
34
        use utils
35
        implicit none
36
        real(8), parameter :: EPSILON = 1e-3
37
38
39
        subroutine gauss_elimination(co_matrix, ndim, solution)
40
           implicit none
           integer(8), intent(in) :: ndim
41
42
           real(8), dimension(ndim, ndim+1), intent(in) :: co_matrix
           type(result), dimension(ndim), intent(out) :: solution
43
44
45
           real(8), dimension(ndim, ndim+1) :: A
           real(8), dimension(ndim) :: tmp_row, X
46
           integer(8) :: t, i
47
48
49
           A = co_matrix
           do t = 1, ndim
50
51
               ! pivot exchange
52
               do i = t, ndim
                   if (abs(A(i, t)) > abs(A(t, t))) then
53
54
                      tmp_row = A(t, :)
                      A(t, :) = A(i, :)
55
                      A(i, :) = tmp_row
56
57
                   end if
58
               end do
               ! Gauss elimination
59
60
               do i = t+1, ndim
                   A(i, :) = A(i, :) - A(i, t) / A(t, t) * A(t, :)
61
62
               end do
63
           end do
64
65
           print "('The Gauss-eliminated extented coefficients matrix is')"
```

```
66
            print "(10f7.2)", (A(i, :), i=1,9)
67
68
            X = 0.0d0
69
            do t = ndim, 1, -1
                X(t) = (A(t, ndim+1) - dot_product(A(t, t+1:ndim), X(t+1:ndim))) / A(t, t)
70
71
            end do
72
73
            solution%value = X
74
            solution%error = 0.0d0
75
76
            return
77
         end subroutine
78
79
         subroutine doolittle(co_matrix, ndim, solution)
80
            implicit none
            integer(8), intent(in) :: ndim
81
            real(8), dimension(ndim, ndim+1), intent(in) :: co_matrix
82
83
            type(result), dimension(ndim), intent(out) :: solution
84
85
            real(8), dimension(ndim, ndim+1) :: A
86
            real(8), dimension(ndim, ndim) :: L, U
            real(8), dimension(ndim) :: X, Y
87
88
            integer(8) :: i, j, k
89
90
            A = co_matrix
            L = 0.0d0; U = 0.0d0;
91
92
93
            call pivot_exchange(A, ndim, ndim+1)
94
            do k = 1, ndim
95
                do j = k, ndim
96
97
                   U(k, j) = A(k, j) - dot_product(L(k, :k-1), U(:k-1, j))
98
                end do
                L(k, k) = 1.0d0
99
                do i = k+1, ndim
100
101
                   L(i, k) = (A(i, k) - dot_product(L(i, :k-1), U(:k-1, k))) / U(k, k)
                end do
102
103
            end do
104
105
            do i = 1, ndim
106
                Y(i) = A(i, ndim+1) - dot_product(L(i, :i-1), Y(:i-1))
107
            end do
108
            do i = ndim, 1, -1
109
                X(i) = (Y(i) - dot_product(U(i, i+1:), X(i+1:))) / U(i, i)
```

```
110
            end do
111
112
            solution%value = X
            solution%error = 0.0d0
113
114
115
            return
116
         end subroutine
117
118
119
         subroutine jacobi_iteration(co_matrix, ndim, solution)
120
            implicit none
121
            integer(8), intent(in) :: ndim
122
            real(8), dimension(ndim, ndim+1), intent(in) :: co_matrix
123
            type(result), dimension(ndim), intent(out) :: solution
124
125
            real(8), dimension(ndim, ndim+1) :: A
126
            real(8), dimension(ndim) :: X, X_tmp, Error
127
            integer(8) :: iter, i
128
129
            A = co_matrix
130
            call pivot_exchange(A, ndim, ndim+1)
131
132
            X = 0.0d0
133
            do iter = 1, 10000
134
                do i = 1, ndim
                    X_{tmp}(i) = -(dot_{product}(A(i, :ndim), X) - A(i, i) * X(i) - A(i, ndim+1)) / A(i, i)
135
                         , i)
136
                end do
137
                Error = abs(X - X_tmp)
138
                X = X_{tmp}
139
140
                if (maxval(Error) < EPSILON) then</pre>
141
142
                end if
143
144
            end do
            print *, iter
145
146
            solution%value = X
147
            solution%error = Error
148
149
            return
150
         end subroutine
151
152
```

```
153
         subroutine gauss_seidel_iteration(co_matrix, ndim, solution, omega)
154
            implicit none
155
            integer(8), intent(in) :: ndim
156
            real(8), optional, intent(in) :: omega
157
            real(8), dimension(ndim, ndim+1), intent(in) :: co_matrix
158
            type(result), dimension(ndim), intent(out) :: solution
159
160
            real(8), dimension(ndim, ndim+1) :: A
161
            real(8) :: lambda = 1.0d0
162
            real(8), dimension(ndim) :: X, X_tmp, Error
163
            integer(8) :: iter, i
164
165
            A = co_matrix
166
            call pivot_exchange(A, ndim, ndim+1)
167
168
            if (present(omega)) then
169
                lambda = omega
170
            end if
171
172
            X = 0.0d0
173
            do iter = 1, 10000
174
                X_{tmp} = X
175
                do i = 1, ndim
176
                    X(i) = -(dot_{product}(A(i, :ndim), X) - A(i, i) * X(i) - A(i, ndim+1)) / A(i, i)
177
                end do
178
                X = (1 - lambda) * X_tmp + lambda * X
179
                Error = abs(X - X_tmp)
180
181
                if (maxval(Error) < EPSILON) then</pre>
182
183
                end if
184
185
            end do
186
            print "('Iter: ',i4)", iter
187
            solution%value = X
            solution%error = Error
188
189
190
            return
191
        end subroutine
192
193
    end module
194
195
196 program main
```

```
197
        use utils
198
        use linear_eqs_solver
199
        implicit none
200
        integer(8), parameter :: ndim = 9
201
        real(8), dimension(ndim, ndim+1) :: A
202
        type(result), dimension(ndim) :: solution
203
        integer(8) :: i
204
205
        A(1, :9) = (/31.0d0, -13.0d0, 0.0d0, 0.0d0, -10.0d0, 0.0d0, 0.0d0, 0.0d0)
        A(2, :9) = (/-13.040, 35.040, -9.040, 0.040, -11.040, 0.040, 0.040, 0.040, 0.040/)
206
207
        A(3, :9) = (/0.0d0, -9.0d0, 31.0d0, -10.0d0, 0.0d0, 0.0d0, 0.0d0, 0.0d0, 0.0d0)
208
        A(4, :9) = (/0.0d0, 0.0d0, -10.0d0, 79.0d0, -30.0d0, 0.0d0, 0.0d0, 0.0d0, -9.0d0/)
        A(5, :9) = (/0.0d0, 0.0d0, 0.0d0, -30.0d0, 57.0d0, -7.0d0, 0.0d0, -5.0d0, 0.0d0/)
209
210
        A(6, :9) = (/0.0d0, 0.0d0, 0.0d0, 0.0d0, -7.0d0, 47.0d0, -30.0d0, 0.0d0, 0.0d0/)
211
        A(7, :9) = (/0.0d0, 0.0d0, 0.0d0, 0.0d0, 0.0d0, -30.0d0, 41.0d0, 0.0d0, 0.0d0/)
212
        A(8, :9) = (/0.0d0, 0.0d0, 0.0d0, 0.0d0, -5.0d0, 0.0d0, 0.0d0, 27.0d0, -2.0d0/)
        A(9, :9) = (/0.0d0, 0.0d0, 0.0d0, -9.0d0, 0.0d0, 0.0d0, 0.0d0, -2.0d0, 29.0d0/)
213
        A(:, 10) = (/-15.0d0, 27.0d0, -23.0d0, 0.0d0, -20.0d0, 12.0d0, -7.0d0, 7.0d0, 10.0d0/)
214
215
216
        print "('The extented coefficients matrix is')"
217
        print "(10f7.2)", (A(i, :), i=1,9)
218
219
        call gauss_seidel_iteration(A, ndim, solution)
220
221
        print "('The solution vector is')"
222
        print "(9f8.4)", (solution(i)%value, i=1,9)
223
        print "('The errors are')"
224
        print "(9f8.4)", (solution(i)%error, i=1,9)
225
        print "('Checking result...')"
226
227
        print "(9f8.2)", (dot_product(A(i, :9), solution%value), i=1,9)
228
229 end program
```