

数値計算・講義資料 (QR 法)

担当：緒方秀教 (e-mail) ogata@im.uec.ac.jp

2016 年 2 月 3 日 (水)

3 重対角行列

$$A = \begin{bmatrix} 4 & -1 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & -1 & 4 \end{bmatrix}$$

の固有値を QR 法で計算した.

計算に用いた MATLAB プログラムは, <http://www.im.uec.ac.jp/~ogata/numcomp2015/numcomp2015.html> に載せてある.

シフトなし QR 法 計算結果

A =

4	-1	0	0	0
-1	4	-1	0	0
0	-1	4	-1	0
0	0	-1	4	-1
0	0	0	-1	4

epsilon = 1.000e-015

|A(n,n)| < epsilon になったら, QR 法反復を止め deflation を行う.

step 10

A =

5.6085	-0.2821	-0.0000	-0.0000	-0.0000
-0.2821	5.0348	-0.2975	0.0000	-0.0000
0	-0.2975	4.0644	-0.1579	0.0000
0	0	-0.1579	3.0162	-0.0774
0	0	0	-0.0774	2.2761

step 20

A =

5.7229	-0.0815	-0.0000	-0.0000	-0.0000
-0.0815	5.0082	-0.0317	0.0000	-0.0000
0	-0.0317	4.0009	-0.0087	0.0000
0	0	-0.0087	3.0000	-0.0047
0	0	0	-0.0047	2.2680

step 30

A =

5.7314	-0.0210	-0.0000	-0.0000	0.0000
-0.0210	5.0006	-0.0034	0.0000	-0.0000
0	-0.0034	4.0000	-0.0005	0.0000
0	0	-0.0005	3.0000	-0.0003
0	0	0	-0.0003	2.2679

step 40

A =

5.7320	-0.0054	-0.0000	-0.0000	0.0000
-0.0054	5.0000	-0.0004	0.0000	-0.0000
0	-0.0004	4.0000	-0.0000	0.0000
0	0	-0.0000	3.0000	-0.0000
0	0	0	-0.0000	2.2679

step 50

A =

5.7320	-0.0014	-0.0000	-0.0000	0.0000
-0.0014	5.0000	-0.0000	0.0000	-0.0000
0	-0.0000	4.0000	-0.0000	0.0000
0	0	-0.0000	3.0000	-0.0000
0	0	0	-0.0000	2.2679

step 60

A =

5.7321	-0.0003	-0.0000	-0.0000	0.0000
-0.0003	5.0000	-0.0000	0.0000	-0.0000
0	-0.0000	4.0000	-0.0000	0.0000
0	0	-0.0000	3.0000	-0.0000
0	0	0	-0.0000	2.2679

step 70

A =

5.7321	-0.0001	-0.0000	-0.0000	0.0000
-0.0001	5.0000	-0.0000	0.0000	-0.0000
0	-0.0000	4.0000	-0.0000	0.0000
0	0	-0.0000	3.0000	-0.0000

0	0	0	-0.0000	2.2679
---	---	---	---------	--------

step 80

A =

5.7321	-0.0000	-0.0000	-0.0000	0.0000
-0.0000	5.0000	-0.0000	0.0000	-0.0000
0	-0.0000	4.0000	-0.0000	0.0000
0	0	-0.0000	3.0000	-0.0000
0	0	0	-0.0000	2.2679

step 90

A =

5.7321	-0.0000	-0.0000	-0.0000	0.0000
-0.0000	5.0000	-0.0000	0.0000	-0.0000
0	-0.0000	4.0000	-0.0000	0.0000
0	0	-0.0000	3.0000	-0.0000
0	0	0	-0.0000	2.2679

step 100

A =

5.7321	-0.0000	-0.0000	-0.0000	0.0000
-0.0000	5.0000	-0.0000	0.0000	-0.0000
0	-0.0000	4.0000	-0.0000	0.0000
0	0	-0.0000	3.0000	-0.0000
0	0	0	-0.0000	2.2679

step 110

A =

5.7321	-0.0000	-0.0000	-0.0000	0.0000
-0.0000	5.0000	-0.0000	0.0000	-0.0000
0	-0.0000	4.0000	-0.0000	0.0000
0	0	-0.0000	3.0000	-0.0000
0	0	0	-0.0000	2.2679

step 120

A =

5.7321	-0.0000	-0.0000	-0.0000	0.0000
--------	---------	---------	---------	--------

-0.0000	5.0000	-0.0000	0.0000	-0.0000
0	-0.0000	4.0000	-0.0000	0.0000
0	0	-0.0000	3.0000	-0.0000
0	0	0	-0.0000	2.2679

step 125
deflation n=5 to 4
step 126
deflation n=4 to 3
step 130

A =

5.7321	-0.0000	0.0000
-0.0000	5.0000	0.0000
0	0.0000	4.0000

step 140

A =

5.7321	-0.0000	0.0000
-0.0000	5.0000	0.0000
0	0.0000	4.0000

step 150

A =

5.7321	-0.0000	0.0000
-0.0000	5.0000	0.0000
0	0.0000	4.0000

step 160

A =

5.7321	-0.0000	0.0000
-0.0000	5.0000	0.0000
0	0.0000	4.0000

step 165
deflation n=3 to 2
step 170

A =

5.7321	-0.0000
-0.0000	5.0000

step 180

A =

5.7321	-0.0000
-0.0000	5.0000

step 190

A =

5.7321	-0.0000
-0.0000	5.0000

step 200

A =

5.7321	-0.0000
-0.0000	5.0000

step 210

A =

5.7321	-0.0000
-0.0000	5.0000

step 220

A =

5.7321	-0.0000
-0.0000	5.0000

step 230

A =

5.7321	-0.0000
-0.0000	5.0000

step 240

A =

5.7321	-0.0000
-0.0000	5.0000

step 250

A =

5.7321	-0.0000
-0.0000	5.0000

step 260

deflation n=2 to 1

固有値 (計算値)

5.732050807568872e+000 5.000000000000000e+000 3.999999999999990e+000
3.000000000000000e+000 2.267949192431125e+000

固有値 (厳密値)

2.267949192431123e+000 3.000000000000000e+000 4.000000000000000e+000
5.000000000000000e+000 5.732050807568877e+000

シフト付き QR 法 (1) シフトは右下行列成分を用いた.

計算結果

A =

4	-1	0	0	0
-1	4	-1	0	0
0	-1	4	-1	0
0	0	-1	4	-1
0	0	0	-1	4

epsilon = 1.000e-015

|A(n,n)|<epsilon となったら, QR 法反復を止め deflation を行う.

step 1

shift = 4.000000

A =

4.0000	1.4142	0	0.0000	0
1.4142	4.0000	0.7071	0	0
0	0.7071	4.0000	1.2247	0.0000
0	0	1.2247	4.0000	0
0	0	0	0	4.0000

step 2

deflation n=5 to 4
shift = 4.000000

A =

4.0000	-1.5811	0	-0.0000
-1.5811	4.0000	-0.5477	0
0	-0.5477	4.0000	1.0954
0	0	1.0954	4.0000

step 3
shift = 4.000000

A =

4.0000	1.6733	0	0.0000
1.6733	4.0000	0.3586	0
0	0.3586	4.0000	1.0351
0	0	1.0351	4.0000

step 4
shift = 4.000000

A =

4.0000	-1.7113	0	-0.0000
-1.7113	4.0000	-0.2169	0
0	-0.2169	4.0000	1.0121
0	0	1.0121	4.0000

step 5
shift = 4.000000

A =

4.0000	1.7250	0	0.0000
1.7250	4.0000	0.1273	-0.0000
0	0.1273	4.0000	1.0041
0	0	1.0041	4.0000

step 6
shift = 4.000000

A =

4.0000	-1.7297	-0.0000	-0.0000
-1.7297	4.0000	-0.0739	0.0000

0	-0.0739	4.0000	1.0014
0	0	1.0014	4.0000

★ (4,3) 成分より先に (3,2) 成分が減衰し始めた !?
(中略)

step 20
shift = 4.000000

A =

4.0000	-1.7321	-0.0000	-0.0000
-1.7321	4.0000	-0.0000	0.0000
0	-0.0000	4.0000	1.0000
0	0	1.0000	4.0000

★ 2×2 小行列を並べたブロック対角行列になってしまった.
(中略)

step 33
shift = 3.997742

A =

4.0068	1.7320	-0.0000	0.0000
1.7320	3.9932	0.0000	-0.0000
0	0.0000	4.0068	1.0000
0	0	1.0000	3.9932

step 34
shift = 3.993227

A =

4.0203	-1.7319	-0.0000	-0.0000
-1.7319	3.9797	-0.0000	0.0000
0	-0.0000	4.0203	0.9998
0	0	0.9998	3.9797

★ ようやく (4,3) 成分が減衰し始めた.

step 35
shift = 3.979684

A =

4.0609	1.7310	-0.0000	0.0000
--------	--------	---------	--------

1.7310	3.9391	0.0000	-0.0000
0	0.0000	4.0609	0.9981
0	0	0.9981	3.9391

(中略)

step 39
shift = 3.071719

A =

5.6814	0.4157	-0.0000	0.0000
0.4157	2.3186	0.0000	0.0000
0	0.0000	4.9999	0.0143
0	0	0.0143	3.0001

step 40
shift = 3.000103

A =

5.7284	-0.1129	-0.0000	-0.0000
-0.1129	2.2716	-0.0000	0.0000
0	-0.0000	5.0000	0.0000
0	0	0.0000	3.0000

step 41
shift = 3.000000

A =

5.7318	0.0303	-0.0000	0.0000
0.0303	2.2682	0.0000	0.0000
0	0.0000	5.0000	0.0000
0	0	0.0000	3.0000

step 42
deflation n=4 to 3
shift = 5.000000

A =

5.7284	-0.1129	0.0000
-0.1129	2.2716	0.0000
0	0.0000	5.0000

step 43

```
deflation n=3 to 2
shift = 2.271635
```

A =

```
5.7321 -0.0001
-0.0001 2.2679
```

```
step 44
shift = 2.267949
```

A =

```
5.7321 -0.0000
-0.0000 2.2679
```

```
step 45
shift = 2.267949
```

A =

```
5.7321 0.0000
-0.0000 2.2679
```

```
step 46
deflation n=2 to 1
```

固有値 (計算値)

```
5.732050807568882e+000 2.267949192431123e+000 5.000000000000000e+000
3.000000000000000e+000 4.000000000000000e+000
```

固有値 (厳密値)

```
2.267949192431123e+000 3.000000000000000e+000 4.000000000000000e+000
5.000000000000000e+000 5.732050807568877e+000
```

シフト付き QR 法 (2) シフトは Wilkinson シフトを用いた.
計算結果

A =

```
4    -1    0    0    0
-1    4    -1    0    0
0    -1    4    -1    0
0    0    -1    4    -1
0    0    0    -1    4
```

```
epsilon = 1.000e-015
|A(n,n)|<epsilon  となったら, QR 法反復を止め deflation を行う.
```

step 1
shift = 5.000000

A =

3.0000	0.7071	0	-0.0000	-0.0000
0.7071	4.0000	1.2247	-0.0000	-0.0000
0	1.2247	4.3333	-0.9428	-0.0000
0	0	-0.9428	3.6667	-0.0000
0	0	0	0	5.0000

step 2
deflation n=5 to 4
shift = 3.000000

A =

4.0000	-1.4142	0.0000	0.0000
-1.4142	4.0000	-1.0000	-0.0000
0	-1.0000	4.0000	0.0000
0	0	0.0000	3.0000

step 3
deflation n=4 to 3
shift = 5.000000

A =

2.6667	0.9428	0.0000
0.9428	4.8333	-0.8660
0	-0.8660	4.5000

step 4
shift = 3.784750

A =

2.6378	-1.0664	-0.0000
-1.0664	5.3536	0.1376
0	0.1376	4.0086

step 5
shift = 3.994720

A =

2.6385	1.0707	0.0000
--------	--------	--------

1.0707	5.3615	-0.0004
0	-0.0004	4.0000

step 6

shift = 4.000000

A =

2.6385	-1.0707	-0.0000
-1.0707	5.3615	0.0000
0	0.0000	4.0000

step 7

shift = 4.000000

A =

2.6385	1.0707	0.0000
1.0707	5.3615	0.0000
0	0.0000	4.0000

step 8

deflation n=3 to 2

shift = 5.732051

A =

2.2679	-0.0000
-0.0000	5.7321

step 9

deflation n=2 to 1

固有値 (計算値)

2.267949192431123e+000 5.732050807568878e+000 4.000000000000000e+000
3.000000000000000e+000 5.000000000000000e+000

固有値 (厳密値)

2.267949192431123e+000 3.000000000000000e+000 4.000000000000000e+000
5.000000000000000e+000 5.732050807568877e+000