

计算物理 HW4 Problem1

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题目 1: 利用 QR 算法、Jacobi 算法、Sturm 序列 + 对分法, 求下列矩阵的本征值

解答: (a)QR 算法结果如下图1.

图 1: QR 算法迭代后的矩阵 T_k

第5次迭代后的矩阵 T_5 为:

```
[[ 4.29276628e+00 -7.21313977e-01 -8.18666697e-17 -5.43358514e-16]
 [-7.21313977e-01  3.55611356e+00 -3.34967464e-01  2.34289842e-16]
 [-4.81736808e-17 -3.34967464e-01  1.89640130e+00 -3.99652715e-04]
 [-2.29665523e-16  2.47087812e-17 -3.99652715e-04  2.54718859e-01]]
```

第10次迭代后的矩阵 T_{10} 为:

```
[[ 4.73418406e+00 -1.31448547e-01 -1.93246264e-16 -5.88422845e-16]
 [-1.31448547e-01  3.18812610e+00 -1.85822775e-02 -5.23882601e-17]
 [-4.91447089e-17 -1.85822775e-02  1.82297108e+00 -2.07643132e-08]
 [-2.15069804e-16 -8.42262145e-17 -2.07643133e-08  2.54718760e-01]]
```

第15次迭代后的矩阵 T_{15} 为:

```
[[ 4.74507887e+00 -1.78120256e-02 -2.13428616e-16 -5.83027491e-16]
 [-1.78120256e-02  3.17748431e+00 -1.15075434e-03 -9.57586083e-17]
 [-4.90024094e-17 -1.15075434e-03  1.82271806e+00 -1.10653406e-12]
 [-2.08367533e-16 -9.96575175e-17 -1.10658672e-12  2.54718760e-01]]
```

第20次迭代后的矩阵 T_{20} 为:

```
[[ 4.74527757e+00 -2.39738535e-03 -2.16210952e-16 -5.82057684e-16]
 [-2.39738535e-03  3.17728658e+00 -7.14944440e-05 -1.01528010e-16]
 [-4.90014462e-17 -7.14944440e-05  1.82271708e+00 -6.32650951e-18]
 [-2.07377671e-16 -1.01701275e-16 -5.89837548e-17  2.54718760e-01]]
```

第50次迭代后的矩阵 T_{50} 为:

```
[[ 4.74528124e+00 -1.42415346e-08 -2.16652277e-16 -5.81901771e-16]
 [-1.42415347e-08  3.17728292e+00 -4.11284268e-12 -1.02420601e-16]
 [-4.90014291e-17 -4.11313580e-12  1.82271708e+00  5.26572381e-17]
 [-2.07221933e-16 -1.02018224e-16 -3.04354935e-28  2.54718760e-01]]
```

第100次迭代后的矩阵 T_{100} 为:

```
[[ 4.74528124e+00  1.05745153e-16 -2.16652279e-16 -5.81901770e-16]
 [-2.77493838e-17  3.17728292e+00  2.93120804e-16 -1.02420607e-16]
 [-4.90014291e-17 -3.52648320e-24  1.82271708e+00  5.26572381e-17]
 [-2.07221932e-16 -1.02018226e-16 -2.60945089e-40  2.54718760e-01]]
```

(b) Jacobi 算法结果如下图2.

图 2: QR 算法迭代后的矩阵 T_k

第5次迭代后的矩阵T_5为:

$$\begin{bmatrix} 3.02671876e-01 & 1.98877843e-01 & 2.83269704e-17 & 3.90083050e-01 \\ 1.98877843e-01 & 3.15387625e+00 & -1.13689848e-01 & 1.15838509e-16 \\ 6.75012884e-17 & -1.13689848e-01 & 1.84612375e+00 & 1.98877843e-01 \\ 3.90083050e-01 & 2.65066327e-18 & 1.98877843e-01 & 4.69732812e+00 \end{bmatrix}$$

第10次迭代后的矩阵T_10为:

$$\begin{bmatrix} 2.54777527e-01 & 8.28956379e-04 & -9.51832874e-03 & -1.84018719e-03 \\ 8.28956379e-04 & 3.17728268e+00 & -4.96426137e-06 & 1.61604514e-18 \\ -9.51832874e-03 & -4.96426137e-06 & 1.82265953e+00 & 8.17755211e-04 \\ -1.84018719e-03 & -1.19810643e-16 & 8.17755211e-04 & 4.74528026e+00 \end{bmatrix}$$

第15次迭代后的矩阵T_15为:

$$\begin{bmatrix} 2.54718760e-01 & -2.52080934e-12 & 3.41591974e-07 & 1.92963626e-10 \\ -2.52071295e-12 & 3.17728292e+00 & -3.08506021e-22 & -3.41591974e-07 \\ 3.41591974e-07 & -2.28100143e-17 & 1.82271708e+00 & -2.52080926e-12 \\ 1.92963590e-10 & -3.41591974e-07 & -2.52086171e-12 & 4.74528124e+00 \end{bmatrix}$$

第20次迭代后的矩阵T_20为:

$$\begin{bmatrix} 2.54718760e-01 & -2.27191941e-28 & 1.89259166e-22 & 9.69352252e-27 \\ 9.63916993e-17 & 3.17728292e+00 & -1.09861777e-18 & -1.42358096e-22 \\ 4.94031311e-17 & -2.39083332e-17 & 1.82271708e+00 & -2.01948392e-28 \\ -3.66087544e-17 & -1.21403863e-16 & -5.24559053e-17 & 4.74528124e+00 \end{bmatrix}$$

第50次迭代后的矩阵T_50为:

$$\begin{bmatrix} 2.54718760e-001 & -6.38693976e-109 & 3.87209453e-121 & -4.72728505e-124 \\ 9.63916993e-017 & 3.17728292e+000 & -1.28675627e-120 & 5.94464077e-229 \\ 4.94029418e-017 & -2.28097154e-017 & 1.82271708e+000 & 0.00000000e+000 \\ -3.66087544e-017 & -1.21403720e-016 & -5.24559053e-017 & 4.74528124e+000 \end{bmatrix}$$

第100次迭代后的矩阵T_100为:

$$\begin{bmatrix} 2.54718760e-001 & -5.09847511e-157 & -7.94920474e-169 & -5.82682870e-156 \\ 9.63916993e-017 & 3.17728292e+000 & 0.00000000e+000 & 2.33073148e-156 \\ 4.94029418e-017 & -2.28097154e-017 & 1.82271708e+000 & -5.82682870e-157 \\ -3.66087544e-017 & -1.21403720e-016 & -5.24559053e-017 & 4.74528124e+000 \end{bmatrix}$$

(c) Sturm 序列 + 对分法

本征值范围: 0.000000~5.000000

第 5 次迭代后的本征值为:

4.765625, 3.203125, 1.796875, 0.234375

第 10 次迭代后的本征值为:

4.74365234375, 3.17626953125, 1.82373046875, 0.25634765625

第 15 次迭代后的本征值为:

4.7452545166015625, 3.1772613525390625, 1.8227386474609375, 0.2547454833984375

第 20 次迭代后的本征值为:

4.745280742645264, 3.1772828102111816, 1.8227171897888184, 0.25471925735473633

第 50 次迭代后的本征值为:

4.745281240174137, 3.1772829191128937, 1.8227170808871063, 0.2547187598258627

第 100 次迭代后的本征值为:

4.745281240174139, 3.1772829191128915, 1.822717080887108, 0.254718759825861