

Universidade de São Paulo

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Lista 4

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1 Matrix Operations

1.1 Exercício 1

Tarefa: Calcule todos os autovalores da matriz simétrica e tridiagonal A , definida por:

$$A_{mm} = -2, \quad A_{m,m-1} = A_{m-1,m} = 1$$

a qual está relacionada à discretização da derivada segunda em uma dimensão:

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

Use as seguintes relações de recorrência para o polinômio característico $P_n(\lambda) = \det(A - \lambda I)$:

$$\begin{aligned} P_1(\lambda) &= A_{11} - \lambda, \\ P_2(\lambda) &= (A_{22} - \lambda)P_1(\lambda) - A_{21}A_{12}, \\ P_3(\lambda) &= (A_{33} - \lambda)P_2(\lambda) - A_{32}A_{23}P_1(\lambda), \\ &\vdots \\ P_m(\lambda) &= (A_{mm} - \lambda)P_{m-1}(\lambda) - A_{m,m-1}A_{m-1,m}P_{m-2}(\lambda), \\ &\vdots \\ P_n(\lambda) &= (A_{nn} - \lambda)P_{n-1}(\lambda) - A_{n,n-1}A_{n-1,n}P_{n-2}(\lambda). \end{aligned}$$

Use o método de Newton-Raphson para calcular numericamente as raízes de $P_n(\lambda)$, ou seja, os autovalores da matriz A .

Sugestão: escreva uma relação de recorrência também para as derivadas primeira e segunda, em relação à variável λ , das funções $P_m(\lambda)$. Considere o caso $n \times n$, onde n é uma entrada (input) do código.

Compare os resultados numéricos com o resultado exato:

$$\lambda_m = -4 \sin^2 \left(\frac{m\pi}{2(n+1)} \right), \quad m = 1, 2, \dots, n.$$

Sugestão: use as desigualdades

$$\max_{j=1,\dots,n} \left(A_{jj} + \sum_{k \neq j} |A_{jk}| \right) \geq \lambda_m \geq \min_{j=1,\dots,n} \left(A_{jj} - \sum_{k \neq j} |A_{jk}| \right)$$

para organizar a busca inicial das raízes de $P_n(\lambda)$.

Derivando a relação de recorrência com relação a λ , obtemos:

$$P'_m(\lambda) = (A_{mm} - \lambda)P'_{m-1}(\lambda) - A_{m,m-1}A_{m-1,m}P'_{m-2}(\lambda) - P_{m-1}(\lambda)$$

Para determinar o chute inicial do Newton-Raphson, temos:

$$\begin{aligned} A_{jj} &= -2, \\ \sum_{k \neq j} |A_{jk}| &= |A_{j,j-1}| + |A_{j,j+1}| = 1 + 1 = 2, \quad \text{para } j = 2, \dots, n-1, \\ \sum_{k \neq j} |A_{jk}| &= 1, \quad \text{para } j = 1 \text{ ou } j = n, \end{aligned}$$

E, utilizando a desigualdade dada, temos:

$$-4 \geq \lambda_{\max} \geq 0$$

Logo, é razoável começar com o chute inicial entre 0 e -4.

O código foi compilado com o comando:

```
gfortran L4-5255417-ex-1.f90 -Wall -Wextra -pedantic -ffree-form -o L4-
```

Resultados:

Testou-se os seguintes casos:

```
> $ ./L4-5255417-ex-1.exe
Insert matrix dimension:
2
Insert tolerance
1.0e-10
```

Figura 1: Dimensão da Matriz = 2

Com o resultado:

```
1 eigenvalue: -1.0000000000000000 real eigenvalue: -1.0000000000000000
   difference: 0.0000000000000000 +/- 1.00E-10
2 eigenvalue: -3.0000000000000000 real eigenvalue: -3.0000000000000000
   difference: 0.0000000000000000 +/- 1.00E-10
```

```
> $ ./L4-5255417-ex-1.exe
Insert matrix dimension:
10
Insert tolerance
1.0e-10
```

Figura 2: Dimensão da Matriz = 10

Com o resultado:

1	eigenvalue: -0.081014052771	real	eigenvalue: -0.081014052771
	difference: 0.000000000000	+/-	1.00E-10
2	eigenvalue: -0.317492934338	real	eigenvalue: -0.317492934338
	difference: 0.000000000000	+/-	1.00E-10
3	eigenvalue: -0.690278532109	real	eigenvalue: -0.690278532109
	difference: 0.000000000000	+/-	1.00E-10
4	eigenvalue: -1.169169973996	real	eigenvalue: -1.169169973996
	difference: 0.000000000000	+/-	1.00E-10
5	eigenvalue: -1.715370323453	real	eigenvalue: -1.715370323453
	difference: 0.000000000000	+/-	1.00E-10
6	eigenvalue: -2.284629676547	real	eigenvalue: -2.284629676547
	difference: 0.000000000000	+/-	1.00E-10
7	eigenvalue: -2.830830026004	real	eigenvalue: -2.830830026004
	difference: 0.000000000000	+/-	1.00E-10
8	eigenvalue: -3.309721467891	real	eigenvalue: -3.309721467891
	difference: 0.000000000000	+/-	1.00E-10
9	eigenvalue: -3.682507065662	real	eigenvalue: -3.682507065662
	difference: 0.000000000000	+/-	1.00E-10
10	eigenvalue: -3.918985947229	real	eigenvalue: -3.918985947229
	difference: 0.000000000000	+/-	1.00E-10

```
> $ ./L4-5255417-ex-1.exe
Insert matrix dimension:
100
Insert tolerance
1.0e-10
```

Figura 3: Dimensão da Matriz = 100

Com o resultado:

1	eigenvalue: -0.000967435416	real	eigenvalue: -0.000967435416
	difference: 0.000000000000	+/-	1.00E-10
2	eigenvalue: -0.003868805733	real	eigenvalue: -0.003868805733
	difference: 0.000000000000	+/-	1.00E-10
3	eigenvalue: -0.008701304062	real	eigenvalue: -0.008701304062
	difference: 0.000000000000	+/-	1.00E-10
4	eigenvalue: -0.015460255273	real	eigenvalue: -0.015460255273
	difference: 0.000000000000	+/-	1.00E-10
5	eigenvalue: -0.024139120518	real	eigenvalue: -0.024139120518
	difference: 0.000000000000	+/-	1.00E-10
6	eigenvalue: -0.034729503555	real	eigenvalue: -0.034729503555
	difference: 0.000000000000	+/-	1.00E-10
7	eigenvalue: -0.047221158873	real	eigenvalue: -0.047221158873
	difference: 0.000000000000	+/-	1.00E-10
8	eigenvalue: -0.061602001601	real	eigenvalue: -0.061602001601
	difference: 0.000000000000	+/-	1.00E-10
9	eigenvalue: -0.077858119203	real	eigenvalue: -0.077858119203
	difference: 0.000000000000	+/-	1.00E-10
10	eigenvalue: -0.095973784935	real	eigenvalue: -0.095973784935
	difference: 0.000000000000	+/-	1.00E-10
11	eigenvalue: -0.115931473060	real	eigenvalue: -0.115931473060
	difference: 0.000000000000	+/-	1.00E-10
12	eigenvalue: -0.137711875805	real	eigenvalue: -0.137711875805
	difference: 0.000000000000	+/-	1.00E-10

13	eigenvalue: -0.161293922036	real	eigenvalue: -0.161293922036
	difference: 0.000000000000	+/-	1.00E-10
14	eigenvalue: -0.186654797646	real	eigenvalue: -0.186654797646
	difference: 0.000000000000	+/-	1.00E-10
15	eigenvalue: -0.213769967626	real	eigenvalue: -0.213769967626
	difference: 0.000000000000	+/-	1.00E-10
16	eigenvalue: -0.242613199801	real	eigenvalue: -0.242613199801
	difference: 0.000000000000	+/-	1.00E-10
17	eigenvalue: -0.273156590207	real	eigenvalue: -0.273156590207
	difference: 0.000000000000	+/-	1.00E-10
18	eigenvalue: -0.305370590084	real	eigenvalue: -0.305370590084
	difference: 0.000000000000	+/-	1.00E-10
19	eigenvalue: -0.339224034470	real	eigenvalue: -0.339224034470
	difference: 0.000000000000	+/-	1.00E-10
20	eigenvalue: -0.374684172343	real	eigenvalue: -0.374684172343
	difference: 0.000000000000	+/-	1.00E-10
21	eigenvalue: -0.411716698310	real	eigenvalue: -0.411716698310
	difference: 0.000000000000	+/-	1.00E-10
22	eigenvalue: -0.450285785794	real	eigenvalue: -0.450285785794
	difference: 0.000000000000	+/-	1.00E-10
23	eigenvalue: -0.490354121693	real	eigenvalue: -0.490354121693
	difference: 0.000000000000	+/-	1.00E-10
24	eigenvalue: -0.531882942481	real	eigenvalue: -0.531882942481
	difference: 0.000000000000	+/-	1.00E-10
25	eigenvalue: -0.574832071705	real	eigenvalue: -0.574832071705
	difference: 0.000000000000	+/-	1.00E-10
26	eigenvalue: -0.619159958857	real	eigenvalue: -0.619159958857
	difference: 0.000000000000	+/-	1.00E-10
27	eigenvalue: -0.664823719568	real	eigenvalue: -0.664823719568
	difference: 0.000000000000	+/-	1.00E-10
28	eigenvalue: -0.711779177099	real	eigenvalue: -0.711779177099
	difference: 0.000000000000	+/-	1.00E-10
29	eigenvalue: -0.759980905078	real	eigenvalue: -0.759980905078
	difference: 0.000000000000	+/-	1.00E-10
30	eigenvalue: -0.809382271447	real	eigenvalue: -0.809382271447
	difference: 0.000000000000	+/-	1.00E-10
31	eigenvalue: -0.859935483572	real	eigenvalue: -0.859935483572
	difference: 0.000000000000	+/-	1.00E-10
32	eigenvalue: -0.911591634488	real	eigenvalue: -0.911591634488
	difference: 0.000000000000	+/-	1.00E-10
33	eigenvalue: -0.964300750203	real	eigenvalue: -0.964300750203
	difference: 0.000000000000	+/-	1.00E-10
34	eigenvalue: -1.018011838053	real	eigenvalue: -1.018011838053
	difference: 0.000000000000	+/-	1.00E-10
35	eigenvalue: -1.072672936029	real	eigenvalue: -1.072672936029
	difference: 0.000000000000	+/-	1.00E-10
36	eigenvalue: -1.128231163049	real	eigenvalue: -1.128231163049
	difference: 0.000000000000	+/-	1.00E-10
37	eigenvalue: -1.184632770116	real	eigenvalue: -1.184632770116
	difference: 0.000000000000	+/-	1.00E-10
38	eigenvalue: -1.241823192319	real	eigenvalue: -1.241823192319
	difference: 0.000000000000	+/-	1.00E-10
39	eigenvalue: -1.299747101617	real	eigenvalue: -1.299747101617
	difference: 0.000000000000	+/-	1.00E-10
40	eigenvalue: -1.358348460369	real	eigenvalue: -1.358348460369
	difference: 0.000000000000	+/-	1.00E-10
41	eigenvalue: -1.417570575545	real	eigenvalue: -1.417570575545
	difference: 0.000000000000	+/-	1.00E-10

42	eigenvalue: -1.477356153574	real	eigenvalue: -1.477356153574
	difference: 0.000000000000	+/-	1.00E-10
43	eigenvalue: -1.537647355770	real	eigenvalue: -1.537647355770
	difference: 0.000000000000	+/-	1.00E-10
44	eigenvalue: -1.598385854289	real	eigenvalue: -1.598385854289
	difference: 0.000000000000	+/-	1.00E-10
45	eigenvalue: -1.659512888553	real	eigenvalue: -1.659512888553
	difference: 0.000000000002	+/-	1.00E-10
46	eigenvalue: -1.720969322112	real	eigenvalue: -1.720969322112
	difference: 0.000000000000	+/-	1.00E-10
47	eigenvalue: -1.782695699829	real	eigenvalue: -1.782695699829
	difference: 0.000000000000	+/-	1.00E-10
48	eigenvalue: -1.844632305422	real	eigenvalue: -1.844632305422
	difference: 0.000000000000	+/-	1.00E-10
49	eigenvalue: -1.906719219225	real	eigenvalue: -1.906719219225
	difference: 0.000000000000	+/-	1.00E-10
50	eigenvalue: -1.968896376160	real	eigenvalue: -1.968896376159
	difference: 0.000000000001	+/-	1.00E-10
51	eigenvalue: -2.031103623840	real	eigenvalue: -2.031103623841
	difference: 0.000000000001	+/-	1.00E-10
52	eigenvalue: -2.093280780775	real	eigenvalue: -2.093280780775
	difference: 0.000000000000	+/-	1.00E-10
53	eigenvalue: -2.155367694578	real	eigenvalue: -2.155367694578
	difference: 0.000000000000	+/-	1.00E-10
54	eigenvalue: -2.217304300171	real	eigenvalue: -2.217304300171
	difference: 0.000000000000	+/-	1.00E-10
55	eigenvalue: -2.279030677888	real	eigenvalue: -2.279030677888
	difference: 0.000000000000	+/-	1.00E-10
56	eigenvalue: -2.340487111447	real	eigenvalue: -2.340487111445
	difference: 0.000000000002	+/-	1.00E-10
57	eigenvalue: -2.401614145711	real	eigenvalue: -2.401614145711
	difference: 0.000000000000	+/-	1.00E-10
58	eigenvalue: -2.462352644230	real	eigenvalue: -2.462352644230
	difference: 0.000000000000	+/-	1.00E-10
59	eigenvalue: -2.522643846426	real	eigenvalue: -2.522643846426
	difference: 0.000000000000	+/-	1.00E-10
60	eigenvalue: -2.582429424455	real	eigenvalue: -2.582429424455
	difference: 0.000000000000	+/-	1.00E-10
61	eigenvalue: -2.641651539631	real	eigenvalue: -2.641651539631
	difference: 0.000000000000	+/-	1.00E-10
62	eigenvalue: -2.700252898383	real	eigenvalue: -2.700252898383
	difference: 0.000000000000	+/-	1.00E-10
63	eigenvalue: -2.758176807681	real	eigenvalue: -2.758176807681
	difference: 0.000000000000	+/-	1.00E-10
64	eigenvalue: -2.815367229884	real	eigenvalue: -2.815367229883
	difference: 0.000000000000	+/-	1.00E-10
65	eigenvalue: -2.871768836951	real	eigenvalue: -2.871768836951
	difference: 0.000000000000	+/-	1.00E-10
66	eigenvalue: -2.927327063971	real	eigenvalue: -2.927327063971
	difference: 0.000000000000	+/-	1.00E-10
67	eigenvalue: -2.981988161947	real	eigenvalue: -2.981988161947
	difference: 0.000000000000	+/-	1.00E-10
68	eigenvalue: -3.035699249797	real	eigenvalue: -3.035699249797
	difference: 0.000000000000	+/-	1.00E-10
69	eigenvalue: -3.088408365512	real	eigenvalue: -3.088408365512
	difference: 0.000000000000	+/-	1.00E-10
70	eigenvalue: -3.140064516428	real	eigenvalue: -3.140064516428
	difference: 0.000000000000	+/-	1.00E-10

71	eigenvalue: -3.190617728553	real	eigenvalue: -3.190617728553
	difference: 0.000000000000	+/-	1.00E-10
72	eigenvalue: -3.240019094922	real	eigenvalue: -3.240019094922
	difference: 0.000000000000	+/-	1.00E-10
73	eigenvalue: -3.288220822901	real	eigenvalue: -3.288220822901
	difference: 0.000000000000	+/-	1.00E-10
74	eigenvalue: -3.335176280432	real	eigenvalue: -3.335176280432
	difference: 0.000000000000	+/-	1.00E-10
75	eigenvalue: -3.380840041143	real	eigenvalue: -3.380840041143
	difference: 0.000000000000	+/-	1.00E-10
76	eigenvalue: -3.425167928295	real	eigenvalue: -3.425167928295
	difference: 0.000000000000	+/-	1.00E-10
77	eigenvalue: -3.468117057519	real	eigenvalue: -3.468117057519
	difference: 0.000000000000	+/-	1.00E-10
78	eigenvalue: -3.509645878307	real	eigenvalue: -3.509645878307
	difference: 0.000000000000	+/-	1.00E-10
79	eigenvalue: -3.549714214206	real	eigenvalue: -3.549714214206
	difference: 0.000000000000	+/-	1.00E-10
80	eigenvalue: -3.588283301690	real	eigenvalue: -3.588283301690
	difference: 0.000000000000	+/-	1.00E-10
81	eigenvalue: -3.625315827657	real	eigenvalue: -3.625315827656
	difference: 0.000000000000	+/-	1.00E-10
82	eigenvalue: -3.660775965530	real	eigenvalue: -3.660775965530
	difference: 0.000000000000	+/-	1.00E-10
83	eigenvalue: -3.694629409916	real	eigenvalue: -3.694629409916
	difference: 0.000000000000	+/-	1.00E-10
84	eigenvalue: -3.726843409793	real	eigenvalue: -3.726843409793
	difference: 0.000000000000	+/-	1.00E-10
85	eigenvalue: -3.757386800199	real	eigenvalue: -3.757386800199
	difference: 0.000000000000	+/-	1.00E-10
86	eigenvalue: -3.786230032374	real	eigenvalue: -3.786230032374
	difference: 0.000000000000	+/-	1.00E-10
87	eigenvalue: -3.813345202354	real	eigenvalue: -3.813345202354
	difference: 0.000000000000	+/-	1.00E-10
88	eigenvalue: -3.838706077964	real	eigenvalue: -3.838706077964
	difference: 0.000000000000	+/-	1.00E-10
89	eigenvalue: -3.862288124195	real	eigenvalue: -3.862288124195
	difference: 0.000000000000	+/-	1.00E-10
90	eigenvalue: -3.884068526940	real	eigenvalue: -3.884068526940
	difference: 0.000000000000	+/-	1.00E-10
91	eigenvalue: -3.904026215065	real	eigenvalue: -3.904026215065
	difference: 0.000000000000	+/-	1.00E-10
92	eigenvalue: -3.922141880797	real	eigenvalue: -3.922141880797
	difference: 0.000000000000	+/-	1.00E-10
93	eigenvalue: -3.938397998399	real	eigenvalue: -3.938397998399
	difference: 0.000000000000	+/-	1.00E-10
94	eigenvalue: -3.952778841127	real	eigenvalue: -3.952778841127
	difference: 0.000000000000	+/-	1.00E-10
95	eigenvalue: -3.965270496445	real	eigenvalue: -3.965270496445
	difference: 0.000000000000	+/-	1.00E-10
96	eigenvalue: -3.975860879482	real	eigenvalue: -3.975860879482
	difference: 0.000000000000	+/-	1.00E-10
97	eigenvalue: -3.984539744727	real	eigenvalue: -3.984539744727
	difference: 0.000000000000	+/-	1.00E-10
98	eigenvalue: -3.991298695938	real	eigenvalue: -3.991298695938
	difference: 0.000000000000	+/-	1.00E-10
99	eigenvalue: -3.996131194267	real	eigenvalue: -3.996131194267
	difference: 0.000000000000	+/-	1.00E-10


```

100 eigenvalue:    -3.999032564584  real  eigenvalue:    -3.999032564584
      difference: 0.0000000000000 +/-  1.00E-10

```

```

> $ ./L4-5255417-ex-1.exe
Insert matrix dimension:
200
Insert tolerance
1.0e-10

```

Figura 4: Dimensão da Matriz = 200

Com o resultado:

```

1 eigenvalue:    -0.000244286119  real  eigenvalue:    -0.000244286119
  difference: 0.0000000000000 +/-  1.00E-10
2 eigenvalue:    -0.000977084799  real  eigenvalue:    -0.000977084799
  difference: 0.0000000000000 +/-  1.00E-10
3 eigenvalue:    -0.002198217029  real  eigenvalue:    -0.002198217029
  difference: 0.0000000000000 +/-  1.00E-10
4 eigenvalue:    -0.003907384502  real  eigenvalue:    -0.003907384502
  difference: 0.0000000000000 +/-  1.00E-10
5 eigenvalue:    -0.006104169692  real  eigenvalue:    -0.006104169692
  difference: 0.0000000000000 +/-  1.00E-10
6 eigenvalue:    -0.008788035956  real  eigenvalue:    -0.008788035956
  difference: 0.0000000000000 +/-  1.00E-10
7 eigenvalue:    -0.011958327662  real  eigenvalue:    -0.011958327662
  difference: 0.0000000000000 +/-  1.00E-10
8 eigenvalue:    -0.015614270353  real  eigenvalue:    -0.015614270353
  difference: 0.0000000000000 +/-  1.00E-10
9 eigenvalue:    -0.019754970931  real  eigenvalue:    -0.019754970931
  difference: 0.0000000000000 +/-  1.00E-10
10 eigenvalue:    -0.024379417881  real  eigenvalue:    -0.024379417881
  difference: 0.0000000000000 +/-  1.00E-10
11 eigenvalue:    -0.029486481515  real  eigenvalue:    -0.029486481515
  difference: 0.0000000000000 +/-  1.00E-10
12 eigenvalue:    -0.035074914249  real  eigenvalue:    -0.035074914249
  difference: 0.0000000000000 +/-  1.00E-10
13 eigenvalue:    -0.041143350905  real  eigenvalue:    -0.041143350905
  difference: 0.0000000000000 +/-  1.00E-10
14 eigenvalue:    -0.047690309049  real  eigenvalue:    -0.047690309049
  difference: 0.0000000000000 +/-  1.00E-10
15 eigenvalue:    -0.054714189350  real  eigenvalue:    -0.054714189350
  difference: 0.0000000000000 +/-  1.00E-10
16 eigenvalue:    -0.062213275972  real  eigenvalue:    -0.062213275972
  difference: 0.0000000000000 +/-  1.00E-10
17 eigenvalue:    -0.070185736991  real  eigenvalue:    -0.070185736991
  difference: 0.0000000000000 +/-  1.00E-10
18 eigenvalue:    -0.078629624846  real  eigenvalue:    -0.078629624846
  difference: 0.0000000000000 +/-  1.00E-10
19 eigenvalue:    -0.087542876813  real  eigenvalue:    -0.087542876813
  difference: 0.0000000000000 +/-  1.00E-10
20 eigenvalue:    -0.096923315508  real  eigenvalue:    -0.096923315508
  difference: 0.0000000000000 +/-  1.00E-10
21 eigenvalue:    -0.106768649419  real  eigenvalue:    -0.106768649419
  difference: 0.0000000000000 +/-  1.00E-10

```

22	eigenvalue: -0.117076473469	real	eigenvalue: -0.117076473469
	difference: 0.000000000000	+/-	1.00E-10
23	eigenvalue: -0.127844269599	real	eigenvalue: -0.127844269599
	difference: 0.000000000000	+/-	1.00E-10
24	eigenvalue: -0.139069407386	real	eigenvalue: -0.139069407386
	difference: 0.000000000000	+/-	1.00E-10
25	eigenvalue: -0.150749144684	real	eigenvalue: -0.150749144684
	difference: 0.000000000000	+/-	1.00E-10
26	eigenvalue: -0.162880628297	real	eigenvalue: -0.162880628297
	difference: 0.000000000000	+/-	1.00E-10
27	eigenvalue: -0.175460894670	real	eigenvalue: -0.175460894670
	difference: 0.000000000000	+/-	1.00E-10
28	eigenvalue: -0.188486870620	real	eigenvalue: -0.188486870620
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29	eigenvalue: -0.201955374081	real	eigenvalue: -0.201955374081
	difference: 0.000000000000	+/-	1.00E-10
30	eigenvalue: -0.215863114885	real	eigenvalue: -0.215863114885
	difference: 0.000000000000	+/-	1.00E-10
31	eigenvalue: -0.230206695564	real	eigenvalue: -0.230206695564
	difference: 0.000000000000	+/-	1.00E-10
32	eigenvalue: -0.244982612180	real	eigenvalue: -0.244982612180
	difference: 0.000000000000	+/-	1.00E-10
33	eigenvalue: -0.260187255182	real	eigenvalue: -0.260187255182
	difference: 0.000000000000	+/-	1.00E-10
34	eigenvalue: -0.275816910287	real	eigenvalue: -0.275816910287
	difference: 0.000000000000	+/-	1.00E-10
35	eigenvalue: -0.291867759387	real	eigenvalue: -0.291867759387
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36	eigenvalue: -0.308335881482	real	eigenvalue: -0.308335881482
	difference: 0.000000000000	+/-	1.00E-10
37	eigenvalue: -0.325217253638	real	eigenvalue: -0.325217253638
	difference: 0.000000000000	+/-	1.00E-10
38	eigenvalue: -0.342507751972	real	eigenvalue: -0.342507751972
	difference: 0.000000000000	+/-	1.00E-10
39	eigenvalue: -0.360203152653	real	eigenvalue: -0.360203152653
	difference: 0.000000000000	+/-	1.00E-10
40	eigenvalue: -0.378299132942	real	eigenvalue: -0.378299132942
	difference: 0.000000000000	+/-	1.00E-10
41	eigenvalue: -0.396791272241	real	eigenvalue: -0.396791272241
	difference: 0.000000000000	+/-	1.00E-10
42	eigenvalue: -0.415675053178	real	eigenvalue: -0.415675053178
	difference: 0.000000000000	+/-	1.00E-10
43	eigenvalue: -0.434945862706	real	eigenvalue: -0.434945862706
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44	eigenvalue: -0.454598993236	real	eigenvalue: -0.454598993236
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45	eigenvalue: -0.474629643779	real	eigenvalue: -0.474629643779
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46	eigenvalue: -0.495032921126	real	eigenvalue: -0.495032921126
	difference: 0.000000000000	+/-	1.00E-10
47	eigenvalue: -0.515803841040	real	eigenvalue: -0.515803841040
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48	eigenvalue: -0.536937329473	real	eigenvalue: -0.536937329473
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49	eigenvalue: -0.558428223807	real	eigenvalue: -0.558428223807
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50	eigenvalue: -0.580271274114	real	eigenvalue: -0.580271274114
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51	eigenvalue: -0.602461144442	real	eigenvalue: -0.602461144442
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52	eigenvalue: -0.624992414112	real	eigenvalue: -0.624992414113
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53	eigenvalue: -0.647859579050	real	eigenvalue: -0.647859579050
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54	eigenvalue: -0.671057053122	real	eigenvalue: -0.671057053122
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55	eigenvalue: -0.694579169509	real	eigenvalue: -0.694579169509
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56	eigenvalue: -0.718420182084	real	eigenvalue: -0.718420182084
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57	eigenvalue: -0.742574266818	real	eigenvalue: -0.742574266818
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58	eigenvalue: -0.767035523204	real	eigenvalue: -0.767035523204
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59	eigenvalue: -0.791797975697	real	eigenvalue: -0.791797975697
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60	eigenvalue: -0.816855575173	real	eigenvalue: -0.816855575173
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61	eigenvalue: -0.842202200408	real	eigenvalue: -0.842202200408
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62	eigenvalue: -0.867831659574	real	eigenvalue: -0.867831659574
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63	eigenvalue: -0.893737691750	real	eigenvalue: -0.893737691750
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64	eigenvalue: -0.919913968450	real	eigenvalue: -0.919913968451
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65	eigenvalue: -0.946354095176	real	eigenvalue: -0.946354095176
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66	eigenvalue: -0.973051612970	real	eigenvalue: -0.973051612970
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67	eigenvalue: -1.000000000000	real	eigenvalue: -1.000000000000
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68	eigenvalue: -1.027192673148	real	eigenvalue: -1.027192673148
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69	eigenvalue: -1.054622989623	real	eigenvalue: -1.054622989623
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70	eigenvalue: -1.082284248578	real	eigenvalue: -1.082284248578
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71	eigenvalue: -1.110169692752	real	eigenvalue: -1.110169692752
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72	eigenvalue: -1.138272510118	real	eigenvalue: -1.138272510118
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73	eigenvalue: -1.166585835548	real	eigenvalue: -1.166585835548
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74	eigenvalue: -1.195102752489	real	eigenvalue: -1.195102752489
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75	eigenvalue: -1.223816294655	real	eigenvalue: -1.223816294656
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76	eigenvalue: -1.252719447726	real	eigenvalue: -1.252719447726
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77	eigenvalue: -1.281805151063	real	eigenvalue: -1.281805151063
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78	eigenvalue: -1.311066299431	real	eigenvalue: -1.311066299431
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79	eigenvalue: -1.340495744739	real	eigenvalue: -1.340495744740
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80	eigenvalue: -1.370086297783	real	eigenvalue: -1.370086297783
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81	eigenvalue: -1.399830729999	real	eigenvalue: -1.399830729999
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82	eigenvalue: -1.429721775237	real	eigenvalue: -1.429721775237
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83	eigenvalue: -1.459752131530	real	eigenvalue: -1.459752131530
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84	eigenvalue: -1.489914462877	real	eigenvalue: -1.489914462877
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85	eigenvalue: -1.520201401040	real	eigenvalue: -1.520201401040
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86	eigenvalue: -1.550605547340	real	eigenvalue: -1.550605547340
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87	eigenvalue: -1.581119474467	real	eigenvalue: -1.581119474468
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88	eigenvalue: -1.611735728292	real	eigenvalue: -1.611735728293
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89	eigenvalue: -1.642446829690	real	eigenvalue: -1.642446829690
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90	eigenvalue: -1.673245276363	real	eigenvalue: -1.673245276363
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91	eigenvalue: -1.704123544679	real	eigenvalue: -1.704123544679
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92	eigenvalue: -1.735074091507	real	eigenvalue: -1.735074091507
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93	eigenvalue: -1.766089356056	real	eigenvalue: -1.766089356056
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94	eigenvalue: -1.797161761728	real	eigenvalue: -1.797161761728
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95	eigenvalue: -1.828283717967	real	eigenvalue: -1.828283717967
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96	eigenvalue: -1.859447622109	real	eigenvalue: -1.859447622109
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97	eigenvalue: -1.890645861246	real	eigenvalue: -1.890645861247
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98	eigenvalue: -1.921870814082	real	eigenvalue: -1.921870814082
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99	eigenvalue: -1.953114852793	real	eigenvalue: -1.953114852793
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100	eigenvalue: -1.984370344895	real	eigenvalue: -1.984370344895
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101	eigenvalue: -2.015629655105	real	eigenvalue: -2.015629655105
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102	eigenvalue: -2.046885147207	real	eigenvalue: -2.046885147207
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103	eigenvalue: -2.078129185918	real	eigenvalue: -2.078129185918
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104	eigenvalue: -2.109354138754	real	eigenvalue: -2.109354138753
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105	eigenvalue: -2.140552377891	real	eigenvalue: -2.140552377891
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106	eigenvalue: -2.171716282033	real	eigenvalue: -2.171716282033
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107	eigenvalue: -2.202838238272	real	eigenvalue: -2.202838238272
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108	eigenvalue: -2.233910643944	real	eigenvalue: -2.233910643944
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109	eigenvalue: -2.264925908493	real	eigenvalue: -2.264925908493
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110	eigenvalue: -2.295876455321	real	eigenvalue: -2.295876455321
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111	eigenvalue: -2.326754723637	real	eigenvalue: -2.326754723637
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112	eigenvalue: -2.357553170310	real	eigenvalue: -2.357553170310
	difference: 0.000000000000	+/-	1.00E-10
113	eigenvalue: -2.388264271708	real	eigenvalue: -2.388264271707
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114	eigenvalue: -2.418880525533	real	eigenvalue: -2.418880525532
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115	eigenvalue: -2.449394452660	real	eigenvalue: -2.449394452660
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116	eigenvalue: -2.479798598960	real	eigenvalue: -2.479798598960
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117	eigenvalue: -2.510085537123	real	eigenvalue: -2.510085537123
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118	eigenvalue: -2.540247868470	real	eigenvalue: -2.540247868470
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119	eigenvalue: -2.570278224763	real	eigenvalue: -2.570278224763
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120	eigenvalue: -2.600169270001	real	eigenvalue: -2.600169270001
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121	eigenvalue: -2.629913702217	real	eigenvalue: -2.629913702217
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122	eigenvalue: -2.659504255261	real	eigenvalue: -2.659504255260
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123	eigenvalue: -2.688933700569	real	eigenvalue: -2.688933700569
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124	eigenvalue: -2.718194848937	real	eigenvalue: -2.718194848937
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126	eigenvalue: -2.776183705345	real	eigenvalue: -2.776183705344
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127	eigenvalue: -2.804897247511	real	eigenvalue: -2.804897247511
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128	eigenvalue: -2.833414164452	real	eigenvalue: -2.833414164452
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129	eigenvalue: -2.861727489882	real	eigenvalue: -2.861727489882
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130	eigenvalue: -2.889830307248	real	eigenvalue: -2.889830307248
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131	eigenvalue: -2.917715751422	real	eigenvalue: -2.917715751422
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132	eigenvalue: -2.945377010377	real	eigenvalue: -2.945377010377
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133	eigenvalue: -2.972807326852	real	eigenvalue: -2.972807326852
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134	eigenvalue: -3.000000000000	real	eigenvalue: -3.000000000000
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135	eigenvalue: -3.026948387030	real	eigenvalue: -3.026948387030
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136	eigenvalue: -3.053645904824	real	eigenvalue: -3.053645904824
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137	eigenvalue: -3.080086031550	real	eigenvalue: -3.080086031549
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138	eigenvalue: -3.106262308250	real	eigenvalue: -3.106262308250
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139	eigenvalue: -3.132168340426	real	eigenvalue: -3.132168340426
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140	eigenvalue: -3.157797799592	real	eigenvalue: -3.157797799592
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141	eigenvalue: -3.183144424827	real	eigenvalue: -3.183144424827
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142	eigenvalue: -3.208202024303	real	eigenvalue: -3.208202024303
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143	eigenvalue: -3.232964476796	real	eigenvalue: -3.232964476796
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144	eigenvalue: -3.257425733182	real	eigenvalue: -3.257425733182
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145	eigenvalue: -3.281579817916	real	eigenvalue: -3.281579817916
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146	eigenvalue: -3.305420830491	real	eigenvalue: -3.305420830491
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149	eigenvalue: -3.375007585888	real	eigenvalue: -3.375007585887
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150	eigenvalue: -3.397538855558	real	eigenvalue: -3.397538855558
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154	eigenvalue: -3.484196158960	real	eigenvalue: -3.484196158960
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159	eigenvalue: -3.584324946822	real	eigenvalue: -3.584324946822
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167	eigenvalue: -3.724183089713	real	eigenvalue: -3.724183089713
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169	eigenvalue: -3.755017387820	real	eigenvalue: -3.755017387820
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170	eigenvalue: -3.769793304436	real	eigenvalue: -3.769793304436
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172	eigenvalue: -3.798044625919	real	eigenvalue: -3.798044625919
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173	eigenvalue: -3.811513129380	real	eigenvalue: -3.811513129380
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175	eigenvalue: -3.837119371703	real	eigenvalue: -3.837119371703
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176	eigenvalue: -3.849250855316	real	eigenvalue: -3.849250855316
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177	eigenvalue: -3.860930592614	real	eigenvalue: -3.860930592614
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178	eigenvalue: -3.872155730401	real	eigenvalue: -3.872155730401
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179	eigenvalue: -3.882923526531	real	eigenvalue: -3.882923526531
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181	eigenvalue: -3.903076684492	real	eigenvalue: -3.903076684492
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186	eigenvalue: -3.945285810650	real	eigenvalue: -3.945285810650
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188	eigenvalue: -3.958856649095	real	eigenvalue: -3.958856649095
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190	eigenvalue: -3.970513518485	real	eigenvalue: -3.970513518485
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191	eigenvalue: -3.975620582119	real	eigenvalue: -3.975620582119
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192	eigenvalue: -3.980245029069	real	eigenvalue: -3.980245029069
	difference: 0.000000000000	+/-	1.00E-10
193	eigenvalue: -3.984385729647	real	eigenvalue: -3.984385729647
	difference: 0.000000000000	+/-	1.00E-10
194	eigenvalue: -3.988041672338	real	eigenvalue: -3.988041672338
	difference: 0.000000000000	+/-	1.00E-10
195	eigenvalue: -3.991211964044	real	eigenvalue: -3.991211964044
	difference: 0.000000000000	+/-	1.00E-10

```

196 eigenvalue:    -3.993895830308  real  eigenvalue:    -3.993895830308
    difference:  0.00000000000000 +/-  1.00E-10
197 eigenvalue:    -3.996092615498  real  eigenvalue:    -3.996092615498
    difference:  0.00000000000000 +/-  1.00E-10
198 eigenvalue:    -3.997801782971  real  eigenvalue:    -3.997801782971
    difference:  0.00000000000000 +/-  1.00E-10
199 eigenvalue:    -3.999022915201  real  eigenvalue:    -3.999022915201
    difference:  0.00000000000000 +/-  1.00E-10
200 eigenvalue:    -3.999755713881  real  eigenvalue:    -3.999755713881
    difference:  0.00000000000000 +/-  1.00E-10

```

Percebe-se que a diferença se manteve dentro da tolerância em todos os casos mostrando a eficiência do método empregado.

1.2 Exercício 2

Tarefa: Considere a mesma matriz A do exercício anterior e o vetor \vec{d} com elementos $d_i = \delta_{i,j}$, onde j é escolhido aleatoriamente entre os valores $1, 2, \dots, n$. Deseja-se resolver numericamente o sistema de equações lineares $A\vec{x} = \vec{d}$, utilizando o **algoritmo de Thomas**, específico para matrizes tridiagonais.

O algoritmo consiste em duas fases: uma substituição direta modificada para calcular coeficientes intermediários d'_m e c'_m , e uma substituição retroativa para obter a solução final \vec{x} . Abaixo estão as fórmulas utilizadas:

$$\begin{aligned}
d'_1 &= \frac{d_1}{b_1}, & c'_1 &= \frac{c_1}{b_1}, \\
d'_m &= \frac{d_m - a_m d'_{m-1}}{b_m - a_m c'_{m-1}}, & c'_m &= \frac{c_m}{b_m - a_m c'_{m-1}}, \quad \text{para } m = 2, 3, \dots, n-1, \\
d'_n &= \frac{d_n - a_n d'_{n-1}}{b_n - a_n c'_{n-1}}.
\end{aligned}$$

A solução \vec{x} é então obtida pela substituição retroativa:

$$\begin{aligned}
x_n &= d'_n, \\
x_m &= d'_m - c'_m x_{m+1}, \quad \text{para } m = n-1, n-2, \dots, 1.
\end{aligned}$$

Considere o caso de uma matriz tridiagonal de dimensão $n \times n$, com n sendo um input do código. Após resolver o sistema, verifique a solução calculando o vetor resíduo:

$$\vec{r} = A\vec{x} - \vec{d}.$$

Esse vetor deve ser próximo de zero (em norma) se a solução numérica estiver correta.

O código foi compilado com o comando:

```
gfortran L4-5255417-ex-2.f90 -Wall -Wextra -pedantic -ffree-form -o L4-
```

Resultados:

Testou-se os seguintes casos:

```
pedro@Pedro-Lenovo ~/Documentos/GitHub/quanticacomp/lista4
> $ ./L4-5255417-ex-2.exe
Insert matrix dimension:
8
The solution x of Ax = d (with j = 1) and the residue vector are:
 1  -0.888889  0.000000
 2  -0.777778  0.000000
 3  -0.666667  0.000000
 4  -0.555556  0.000000
 5  -0.444444  0.000000
 6  -0.333333  0.000000
 7  -0.222222  0.000000
 8  -0.111111  0.000000

pedro@Pedro-Lenovo ~/Documentos/GitHub/quanticacomp/lista4
> $ ./L4-5255417-ex-2.exe
Insert matrix dimension:
8
The solution x of Ax = d (with j = 5) and the residue vector are:
 1  -0.444444  0.000000
 2  -0.888889  0.000000
 3  -1.333333  0.000000
 4  -1.777778  0.000000
 5  -2.222222  0.000000
 6  -1.666667  0.000000
 7  -1.111111  0.000000
 8  -0.555556  0.000000
```

Figura 5: Testes para matriz de dimensão 8

```

pedro@Pedro-Lenovo ~/Documentos/GitHub/quanticacomp/lista4
> $ ./L4-5255417-ex-2.exe
Insert matrix dimension:
10
The solution x of  $Ax = d$  (with  $j = 8$ ) and the residue vector are:
 1   -0.272727   0.000000
 2   -0.545455   0.000000
 3   -0.818182   0.000000
 4   -1.090909   0.000000
 5   -1.363636   0.000000
 6   -1.636364   0.000000
 7   -1.909091   0.000000
 8   -2.181818   0.000000
 9   -1.454545   0.000000
10   -0.727273   0.000000

pedro@Pedro-Lenovo ~/Documentos/GitHub/quanticacomp/lista4
> $ ./L4-5255417-ex-2.exe
Insert matrix dimension:
10
The solution x of  $Ax = d$  (with  $j = 2$ ) and the residue vector are:
 1   -0.818182   0.000000
 2   -1.636364   0.000000
 3   -1.454545   0.000000
 4   -1.272727   0.000000
 5   -1.090909   0.000000
 6   -0.909091   0.000000
 7   -0.727273   0.000000
 8   -0.545455   0.000000
 9   -0.363636   0.000000
10   -0.181818   0.000000

```

Figura 6: Testes para matriz de dimensão 10

```

pedro@Pedro-Lenovo ~/Documentos/GitHub/quanticacomp/lista4
> $ ./L4-5255417-ex-2.exe
Insert matrix dimension:
20
The solution x of  $Ax = d$  (with  $j = 3$ ) and the residue vector are:
 1  -0.857143  0.000000
 2  -1.714286  0.000000
 3  -2.571429  0.000000
 4  -2.428571  0.000000
 5  -2.285714  0.000000
 6  -2.142857  0.000000
 7  -2.000000  0.000000
 8  -1.857143  0.000000
 9  -1.714286  0.000000
10  -1.571429  0.000000
11  -1.428571  0.000000
12  -1.285714  0.000000
13  -1.142857  0.000000
14  -1.000000  0.000000
15  -0.857143  0.000000
16  -0.714286  0.000000
17  -0.571429  0.000000
18  -0.428571  0.000000
19  -0.285714  0.000000
20  -0.142857  0.000000

```

(a)

```

pedro@Pedro-Lenovo ~/Documentos/GitHub/quanticacomp/lista4
> $ ./L4-5255417-ex-2.exe
Insert matrix dimension:
20
The solution x of  $Ax = d$  (with  $j = 15$ ) and the residue vector are:
 1  -0.285714  0.000000
 2  -0.571429  0.000000
 3  -0.857143  0.000000
 4  -1.142857  0.000000
 5  -1.428571  0.000000
 6  -1.714286  0.000000
 7  -2.000000  0.000000
 8  -2.285714  0.000000
 9  -2.571429  0.000000
10  -2.857143  0.000000
11  -3.142857  0.000000
12  -3.428571  0.000000
13  -3.714286  0.000000
14  -4.000000  0.000000
15  -4.285714  0.000000
16  -3.571429  0.000000
17  -2.857143  0.000000
18  -2.142857  0.000000
19  -1.428571  0.000000
20  -0.714286  0.000000

```

(b)

Figura 7: Teste para matriz de dimensão 20

Como todos os vetores resíduo obtidos foram nulos, sabemos que o código funciona de acordo com o esperado - obtendo o autovetor x corretamente.