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Numerical Methods 1
Gaussian Elimination

Calculating the determinate of a matrix using GE and GE with complete pivoting

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1 Title of a task

29. Computing det(A) and the growth factor using GE and GECP methods, where $A \in \mathbb{R}^{n\times n}$. Perform tests for various matrices, strictly dominant (row-wise, column-wise) and other.

2 Gaussian Elimination

Gaussian elimination (GE) is a method for solving systems of linear equations. The goal is to transform the matrix into an upper triangular form where all elements below the main diagonal are zeros. Here's a detailed explanation of how GE is performed:

First Column Elimination:

Use the first row to eliminate all elements below the main diagonal in the first column. For each row i (where $i > 1$), update the row as:

$$r_i := r_i - l_{i1} r_1$$

where

$$l_{i1} = \frac{a_{i1}}{a_{11}}$$

After this step, the matrix will look like:

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} & b_2^{(1)} \\ 0 & a_{32}^{(1)} & \cdots & a_{3n}^{(1)} & b_3^{(1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nn}^{(1)} & b_n^{(1)} \end{pmatrix}$$

Second Column Elimination:

Move to the second column and use the second row to eliminate all elements below the main diagonal in this column. For each row i (where $i > 2$), update the row as:

$$r_i := r_i - l_{i2} r_2$$

where

$$l_{i2} = \frac{a_{i2}^{(1)}}{a_{22}^{(1)}}$$

After this step, the matrix will look like:

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} & b_2^{(1)} \\ 0 & 0 & \cdots & a_{3n}^{(2)} & b_3^{(2)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{nn}^{(2)} & b_n^{(2)} \end{pmatrix}$$

General Step k:

For the k-th step, focus on the k-th column. Use the k-th row to eliminate all elements below the main diagonal in this column. For each row i (where $i > k$), update the row as:

$$r_i := r_i - l_{ik} r_k$$

where

$$l_{ik} = \frac{a_{ik}^{(k-1)}}{a_{kk}^{(k-1)}}$$

After the k-th step, the matrix will have zeros below the main diagonal in the k-th column.

3 Gaussian Elimination with complete pivoting

The goal of Gaussian Elimination with complete pivoting is the same as Gaussian Elimination however each iteration includes additional steps.

Pivot Selection

At each step k of the elimination, the pivot element is chosen as the largest absolute value element in the submatrix $A_{k:n,k:n}^{(k-1)}$.

Finding the Pivot

Before the first step, the largest element in the entire matrix $A^{(0)}$ is found. Indices p and q are determined such that:

$$\left|a_{pq}^{(0)}\right| = \max_{i=1,\ldots,n;j=1,\ldots,n} \left|a_{ij}^{(0)}\right|$$

Before the k-th step, the largest element in the submatrix $A_{k:n,k:n}^{(k-1)}$ is found. Indices p and q are determined such that:

$$\left|a_{pq}^{(k-1)}\right| = \max_{i=k,\ldots,n;j=k,\ldots,n} \left|a_{ij}^{(k-1)}\right|$$

Row and Column Swapping

Once the pivot $a_{pq}^{(k-1)}$ is identified, swap the p-th row with the k-th row and the q-th column with the k-th column. This brings the pivot element to the k-th position on the main diagonal.

Elimination Phase

After selecting and positioning the pivot, perform the Gaussian elimination step as usual: For each row i (where $i > k$), update the row as:

$$r_i := r_i - l_{ik} r_k$$

where

$$l_{ik} = \frac{a_{ik}^{(k-1)}}{a_{kk}^{(k-1)}}$$

This creates zeros below the pivot in column k.

4 Calculating the determinate

After transforming the matrix into upper triangular form, the determinant can be simply calculated by multiplying the elements located on the main diagonal as:

$$\det(A) = \prod_{i=1}^{n} a_{ii}$$

where a_{ii} are the elements on the main diagonal of the upper triangular matrix.
However, in GECP we need to keep track of the number of swaps during GECP to adjust the sign. If the number of swaps is odd the determinate must be multiplied by -1. Otherwise, the determinant sign remains unchanged if the number of swaps is even.

5 Calculating the Growth Factor

The growth factor for Gaussian Elimination (GE) and Gaussian Elimination with Complete Pivoting (GECP) is a measure of the stability of these methods. It is defined as the ratio of the largest element in the matrix after applying GE or GECP to the largest element in the original matrix. To calculate the growth factor, we follow these steps:

1. Identify the largest absolute value in the original matrix A, denoted as $\max_{i,j} |a_{ij}|$.
2. Perform GE or GECP on A and after each iteration find the largest element.
3. Then the formula of growth factor can be calculated using this formula:

   $\rho_n = \frac{\max_{i,j,k} |a_{ij}^{(k)}|}{\max_{i,j} |a_{ij}|}$

   where the $a_{ij}^{(k)}$ are the elements at the start of the k-th stage of Gaussian elimination.

6 Testing

Figure 1. shows the errors in the computation for a random matrix of size n.
Figure 2. shows the errors for the specific matrices, for example, a row or a column dominate matrices.
Figure 3. shows the time the function takes to compute GE and GECP for a matrix of size n.
We are confident that our algorithm computes the determinate correctly, as it has a very low error rate. We also performed a test to see if the function return correct errors. To do that, a not-square matrix was used and matrices for which there would be division by zero during iterations.

N	error_detGE	error_detGECP	N	error_detGE	error_detGECP
1	0	0	21	4.92661467177413e-16	2.35922392732846e-16
2	2.77555756156289e-17	0	22	1.58761892521397e-14	4.85722573273506e-17
3	0	5.55111512312578e-17	23	1.70835567914196e-14	1.94289029309402e-16
4	3.46944695195361e-18	1.04083408558608e-17	24	2.77174116991574e-14	1.26634813746307e-16
5	3.46944695195361e-18	6.93889390390723e-18	25	4.01761957036229e-15	1.38777878078145e-17
6	3.05311331771918e-16	5.55111512312578e-17	26	6.81676937119846e-14	2.22044604925031e-15
7	1.04083408558608e-17	8.67361737988404e-18	27	1.1518563880486e-15	6.93889390390723e-17
8	3.81639164714898e-17	1.73472347597681e-18	28	1.34225963677181e-13	4.32986979603811e-15
9	1.12757025938492e-17	7.37257477290143e-18	29	1.04916075827077e-14	6.43929354282591e-15
10	3.46944695195361e-18	1.04083408558608e-17	30	4.66293670342566e-15	3.5527136788005e-15
11	5.55111512312578e-17	0	31	1.85185200507476e-13	1.11022302462516e-15
12	1.38777878078145e-16	6.93889390390723e-18	32	1.18571819029967e-13	5.87307980026708e-14
13	5.96311194867027e-19	3.79470760369927e-19	33	7.13384906703141e-12	7.105427357601e-15
14	3.46944695195361e-17	1.38777878078145e-17	34	1.09423581307055e-12	5.6843418860808e-14
15	1.69135538907739e-16	8.67361737988404e-18	35	9.49018641449584e-13	1.33226762955019e-15
16	4.5102810375397e-17	1.38777878078145e-17	36	2.54907206453936e-13	7.90478793533111e-14
17	4.61436444609831e-16	4.16333634234434e-17	37	5.40012479177676e-13	5.11590769747272e-13
18	7.0082828429463e-16	9.71445146547012e-17	38	3.29691829392686e-12	2.27373675443232e-13
19	1.52980926537705e-15	7.68699340292223e-17	39	1.70075509231538e-10	2.27373675443232e-12
20	2.20309881449055e-16	2.25514051876985e-17	40	6.96420698886868e-12	3.66395802586794e-12

Figure 1: Errors of a random matrix of size n

Matrix	error_detGE	error_detGECP
$\begin{pmatrix} 4 & 1 & 1 \\ 2 & 6 & 2 \\ 1 & 1 & 3 \end{pmatrix}$	0	0
$\begin{pmatrix} 2 & -1 & 0 \\ -2 & 3 & -1 \\ 1 & -1 & 4 \end{pmatrix}$	0	$1.77635683940025e-15$
$\begin{pmatrix} 1 & 1 & 2 & 3 \\ 5 & 8 & -1 & -7 \\ -10 & -10 & 2 & 4 \\ 6 & 8 & 9 & 9 \end{pmatrix}$	$2.41584530158434e-13$	$9.9475983006414e-14$

Figure 2: Errors

N	time_GE (seconds)	time_GECP (seconds)
1	0.000138	0.000129
2	8.7e-05	8e-05
3	7.6e-05	9e-05
4	8.3e-05	0.000115
5	0.000218	0.000259
6	6.1e-05	9.9e-05
7	5.2e-05	0.000112
8	6.3e-05	0.000121
9	6.8e-05	0.000142
10	8e-05	0.000158
11	8.6e-05	0.000172
12	9.8e-05	0.000199
13	0.000129	0.00022
14	0.000117	0.000241
15	0.000132	0.000303
16	0.000146	0.000282
17	0.000152	0.00031
18	0.000158	0.000312
19	0.000167	0.000345
20	0.000183	0.000371
21	0.000198	0.000443
22	0.000214	0.000435
23	0.000252	0.000436
24	0.000239	0.000464
25	0.00025	0.000485
26	0.000266	0.000534
27	0.000291	0.000549
28	0.000335	0.000587
29	0.000315	0.000574
30	0.000336	0.000682
31	0.000357	0.000684
32	0.000401	0.000722
33	0.000394	0.000745
34	0.000416	0.000801
35	0.000432	0.000853
36	0.000451	0.000856
37	0.000476	0.000897
38	0.00049	0.000649
39	0.000312	0.000563
40	0.000319	0.000574
41	0.000349	0.000614
42	0.000347	0.000684
43	0.000367	0.000645
44	0.00039	0.000681
45	0.000393	0.000723
46	0.000451	0.000744
47	0.00044	0.000775
48	0.000452	0.000813
49	0.000477	0.000853
50	0.000492	0.000851
51	0.000509	0.0011
52	0.000601	0.000939
53	0.000556	0.000961
54	0.00059	0.001019
55	0.000624	0.00105
56	0.000627	0.001091
57	0.000681	0.00113
58	0.000682	0.001175
59	0.000721	0.001201
60	0.000724	0.001269
61	0.000899	0.001292
62	0.000784	0.001365
63	0.000813	0.001394
64	0.000855	0.001453
65	0.000917	0.001604
66	0.001045	0.001511
67	0.000935	0.001589
68	0.00097	0.001712
69	0.001136	0.001903
70	0.001055	0.001848
71	0.001147	0.001998
72	0.00118	0.0021
73	0.001329	0.001932
74	0.001205	0.001962
75	0.001258	0.002209
76	0.00128	0.00228
77	0.0013	0.002176
78	0.001571	0.002251
79	0.001385	0.002277
80	0.001583	0.002308
81	0.001577	0.002507
82	0.001574	0.002703
83	0.001842	0.002534
84	0.001898	0.002573
85	0.001671	0.002639
86	0.001979	0.002703
87	0.001855	0.00288
88	0.00183	0.003083
89	0.002138	0.003143
90	0.002236	0.00334
91	0.002119	0.003483
92	0.00253	0.00339
93	0.002542	0.003275
94	0.002162	0.003764
95	0.002271	0.003447
96	0.002492	0.003799
97	0.002517	0.003853
98	0.002414	0.004015
99	0.002666	0.003804
100	0.002738	0.004149

Figure 3: Time of computing GE and GECP for a random matrix of size n