Computational Physics

Lecture-18

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Contents

Solving Linear Systems

- **Jacobi Iterative Method**

$$AX = B: \qquad \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

$$i: \quad \sum_{j=1}^{n} a_{ij} x_j = b_i$$

$$i: \quad a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{i,i-1}x_{i-1} + a_{ii}x_i + a_{i,i+1}x_{i+1} + \cdots + a_{i,n-1}x_{n-1} + a_{i,n}x_n = b_i$$

Solving Linear Systems

- **Jacobi Iterative Method**

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$$i: \quad {\color{red} a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{i,i-1}x_{i-1}} + a_{ii}x_i + {\color{blue} a_{i,i+1}x_{i+1} + \cdots + a_{i,n-1}x_{n-1} + a_{i,n}x_n} = b_i$$

$$i: \quad {\color{red} \sum_{j=1}^{i-1} a_{ij} x_j} + a_{ii}x_i + {\color{blue} \sum_{j=i+1}^{n} a_{ij} x_j} = b_i$$

Solving Linear Systems

- **Jacobi Iterative Method**

$$i: \quad \sum_{j=1}^{i-1} a_{ij}x_j + a_{ii}x_i + \sum_{j=i+1}^{n} a_{ij}x_j = b_i$$

$$i: \quad a_{ii}x_i = b_i - \sum_{j=1}^{i-1} a_{ij}x_j - \sum_{j=i+1}^{n} a_{ij}x_j$$

$$i: \quad x_i = \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j - \sum_{j=i+1}^{n} a_{ij}x_j\right)$$

Solving Linear Systems

- **Jacobi Iterative Method**

1st iteration

Initial values $\{x_1^{(0)}, x_2^{(0)}, \cdots, x_n^{(0)}\}$

$$i: \quad x_i^{(1)} = \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(0)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(0)}\right)$$

$$\{x_1^{(1)}, x_2^{(1)}, \cdots, x_n^{(1)}\}$$

Solving Linear Systems

- **Jacobi Iterative Method**

2nd iteration

$$\{x_1^{(1)}, x_2^{(1)}, \cdots, x_n^{(1)}\}$$

$$i: \quad x_i^{(2)} = \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(1)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(1)}\right)$$

$$\{x_1^{(2)}, x_2^{(2)}, \cdots, x_n^{(2)}\}$$

Solving Linear Systems

- **Jacobi Iterative Method**

3rd iteration

$$\{x_1^{(2)}, x_2^{(2)}, \cdots, x_n^{(2)}\}$$

$$i: \quad x_i^{(3)} = \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(2)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(2)}\right)$$

$$\{x_1^{(3)}, x_2^{(3)}, \cdots, x_n^{(3)}\}$$

∞

Solving Linear Systems

- **Jacobi Iterative Method**

1st iteration

$$\{x_1^{(0)}, x_2^{(0)}, \cdots, x_n^{(0)}\}$$

$$i: \quad x_i^{(1)} = \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(0)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(0)}\right)$$

$$\{x_1^{(1)}, x_2^{(1)}, \cdots, x_n^{(1)}\}$$

$$\sum_i^n \left|\frac{x_i^{(1)} - x_i^{(0)}}{x_i^{(1)}}\right| \leq \epsilon$$

No

Solving Linear Systems

- **Jacobi Iterative Method**

2nd iteration

$$\{x_1^{(1)}, x_2^{(1)}, \cdots, x_n^{(1)}\}$$

$$\sum_i^n \left| \frac{x_i^{(1)} - x_i^{(0)}}{x_i^{(1)}} \right| \leq \epsilon$$

No

$$i: \quad x_i^{(2)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(1)} \right)$$

$$\{x_1^{(2)}, x_2^{(2)}, \cdots, x_n^{(2)}\}$$

$$\sum_i^n \left| \frac{x_i^{(2)} - x_i^{(1)}}{x_i^{(2)}} \right| \leq \epsilon$$

No

Solving Linear Systems

- **Jacobi Iterative Method**

3rd iteration

$$\{x_1^{(2)}, x_2^{(2)}, \cdots, x_n^{(2)}\}$$

$$\sum_i^n \left| \frac{x_i^{(2)} - x_i^{(1)}}{x_i^{(2)}} \right| \leq \epsilon$$

No

$$i: \quad x_i^{(3)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(2)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(2)} \right)$$

$$\{x_1^{(3)}, x_2^{(3)}, \cdots, x_n^{(3)}\}$$

$$\sum_i^n \left| \frac{x_i^{(3)} - x_i^{(2)}}{x_i^{(3)}} \right| \leq \epsilon$$

No

Solving Linear Systems

- **Jacobi Iterative Method**

$$\{x_1^{(k-1)}, x_2^{(k-1)}, \cdots, x_n^{(k-1)}\}$$

$$\sum_i^n \left| \frac{x_i^{(k-1)} - x_i^{(k-2)}}{x_i^{(k-1)}} \right| \leq \epsilon$$

No

$$i: \quad x_i^{(k)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k-1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} \right)$$

$$\{x_1^{(k)}, x_2^{(k)}, \cdots, x_n^{(k)}\}$$

$$\sum_i^n \left| \frac{x_i^{(k)} - x_i^{(k-1)}}{x_i^{(k)}} \right| \leq \epsilon$$

No

Solving Linear Systems

- **Jacobi Iterative Method**

Initial values $\{x_1^{(0)}, x_2^{(0)}, \cdots, x_n^{(0)}\}$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}, \quad i : |a_{ii}| > \sum_{j=1}^{i-1} |a_{ij}| + \sum_{j=i+1}^{n} |a_{ij}|$$

When the system equations can be ordered so that such diagonal entry of the coefficient matrix is larger in magnitude than the sum of the magnitudes of the order coefficients in that row **the iteration will converge for any initial values.**

Solving Linear Systems

- **Jacobi Iterative Method**

$$\begin{cases} 6x_1 - 2x_2 + x_3 = 11 \\ x_1 + 2x_2 - 5x_3 = -1 \\ -2x_1 + 7x_2 + 2x_3 = 5 \end{cases}$$

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$$\begin{cases} \boxed{6x_1} - 2x_2 + x_3 = 11 \\ -2x_1 + \boxed{7x_2} + 2x_3 = 5 \\ x_1 + 2x_2 - \boxed{5x_3} = -1 \end{cases}$$

$$(x_1, x_2, x_3) = (0, 0, 0), \quad \epsilon = 10^{-8}$$

	Δx	x_1	x_2	x_3
1	3.000000E+00	1.83333333	0.71428571	0.20000000
2	1.260992E+00	2.03809524	1.18095238	0.85238095
3	3.546645E-01	2.08492063	1.05306122	1.08000000
4	1.320321E-01	2.00435374	1.00140590	1.03820862
5	5.305158E-02	1.99410053	0.99032718	1.00143311
6	1.532902E-02	1.99653688	0.99790498	0.99495098
7	7.873779E-03	2.00014316	1.00045311	0.99846937
8	1.896712E-03	2.00040614	1.00047823	1.00020988
9	6.256010E-04	2.00012443	1.00005608	1.00027252
10	3.991642E-04	1.99997327	0.99995769	1.00004732
11	9.311353E-05	1.99997801	0.99997884	0.99997773
12	3.997063E-05	1.99999666	1.00000008	0.99998714
13	1.761920E-05	2.00000217	1.00000272	0.99999936
14	4.654980E-06	2.00000101	1.00000080	1.00000152
15	2.445596E-06	2.00000001	0.99999985	1.00000052
16	6.534520E-07	1.99999986	0.99999985	0.99999994
17	2.008001E-07	1.99999996	0.99999998	0.99999991
18	1.273940E-07	2.00000001	1.00000001	0.99999998
19	3.035408E-08	2.00000001	1.00000001	1.00000001

Solving Linear Systems

- **Jacobi Iterative Method**

$$\begin{cases} 4x_1 + x_2 - x_3 = 3 \\ 2x_1 + 7x_2 + x_3 = 19 \\ x_1 - 3x_2 + 12x_3 = 31 \end{cases}$$

$$\begin{cases} \boxed{4x_1} + x_2 - x_3 = 3 \\ 2x_1 + \boxed{7x_2} + x_3 = 19 \\ x_1 - 3x_2 + \boxed{12x_3} = 31 \end{cases}$$

$$(x_1, x_2, x_3) = (0, 0, 0), \quad \epsilon = 10^{-8}$$

	Δx	x_1	x_2	x_3
1	3.000000E+00	0.75000000	2.71428571	2.58333333
2	5.119443E-01	0.71726190	2.13095238	3.19940476
3	3.799552E-01	1.01711310	2.05229592	3.05629960
4	6.374875E-02	1.00100092	1.98706774	3.01164789
5	1.560284E-02	1.00614504	1.99805004	2.99668353
6	7.595661E-03	0.99965837	1.99871806	2.99900042
7	1.409149E-03	1.00007059	2.00024040	2.99970798
8	4.285609E-04	0.99986689	2.00002155	3.00005422
9	1.582201E-04	1.00000817	2.00003028	3.00001648
10	3.230155E-05	0.99999655	1.99999531	3.00000689
11	1.128232E-05	1.00000289	2.00000000	2.99999912
12	3.681832E-06	0.99999978	1.99999930	2.99999976
13	7.637079E-07	1.00000011	2.00000010	2.99999984
14	2.898379E-07	0.99999994	1.99999999	3.00000001
15	8.723554E-08	1.00000001	2.00000002	3.00000000

Solving Linear Systems

- **Gauss-Seidel Method**

$$\{x_1^{(k-1)}, x_2^{(k-1)}, \cdots, x_n^{(k-1)}\}$$

$$\sum_{i}^{n} \left| \frac{x_i^{(k-1)} - x_i^{(k-2)}}{x_i^{(k-1)}} \right| \leq \epsilon$$

No

$$i: \quad x_i^{(k)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} \right)$$

$$\{x_1^{(k)}, x_2^{(k)}, \cdots, x_n^{(k)}\}$$

$$\sum_{i}^{n} \left| \frac{x_i^{(k)} - x_i^{(k-1)}}{x_i^{(k)}} \right| \leq \epsilon$$

No

Solving Linear Systems

- **Gauss-Seidel Method**

$$\begin{cases} 6x_1 - 2x_2 + x_3 = 11 \\ x_1 + 2x_2 - 5x_3 = -1 \\ -2x_1 + 7x_2 + 2x_3 = 5 \end{cases}$$

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$$(x_1, x_2, x_3) = (0, 0, 0), \quad \epsilon = 10^{-8}$$

	Δx	x_1	x_2	x_3
1	3.000000E+00	1.83333333	1.23809524	1.06190476
2	3.960951E-01	2.06904762	1.00204082	1.01462585
3	5.907422E-02	1.99824263	0.99531908	0.99777616
4	7.363301E-03	1.99881033	1.00029548	0.99988026
5	1.052073E-03	2.00011845	1.00006805	1.00005091
6	1.829373E-04	2.00001420	0.99998951	0.99999864
7	1.916007E-05	1.99999673	0.99999945	0.99999913
8	3.363795E-06	1.99999996	1.00000024	1.00000009
9	3.742545E-07	2.00000006	0.99999999	1.00000001
10	4.974403E-08	2.00000000	1.00000000	1.00000000

Solving Linear Systems

- **Gauss-Seidel Method**

$$\begin{cases} 4x_1 + x_2 - x_3 = 3 \\ 2x_1 + 7x_2 + x_3 = 19 \\ x_1 - 3x_2 + 12x_3 = 31 \end{cases}$$

$$\begin{cases} \boxed{4x_1} + x_2 - x_3 = 3 \\ 2x_1 + \boxed{7x_2} + x_3 = 19 \\ x_1 - 3x_2 + \boxed{12x_3} = 31 \end{cases}$$

$$(x_1, x_2, x_3) = (0, 0, 0), \quad \epsilon = 10^{-8}$$

	Δx	x_1	x_2	x_3
1	3.000000E+00	0.75000000	2.50000000	3.14583333
2	4.700092E-01	0.91145833	2.00446429	3.00849454
3	9.542924E-02	1.00100756	1.99849862	2.99954069
4	1.638270E-03	1.00026052	1.99999118	2.99997609
5	2.794005E-04	0.99999623	2.00000449	3.00000144
6	5.707917E-06	0.99999924	2.00000001	3.00000007
7	8.145582E-07	1.00000001	1.99999999	3.00000000
8	1.941212E-08	1.00000000	2.00000000	3.00000000