Thomas Algorithm (for Tridiagonal)

$$\begin{bmatrix} d_1 & u_1 & 0 & \bullet & 0 & 0 & x_1 \\ l_2 & d_2 & u_2 & \bullet & 0 & 0 \\ 0 & l_3 & d_3 & \bullet & 0 & 0 \\ 0 & \bullet & \bullet & \bullet & \bullet & \bullet \end{bmatrix} \begin{bmatrix} b_1 \\ x_2 \\ x_3 \\ \bullet \end{bmatrix} = \begin{bmatrix} b_2 \\ b_2 \\ x_3 \\ \bullet \end{bmatrix}$$

- No need to store $n^2 + n$ elements!
- Store only 4n elements in the form of four vectors l, d, u and b
- i^{th} equation is: $l_i x_{i-1} + d_i x_i + u_i x_{i+1} = b_i$
- Notice: $l_1 = u_n = 0$

Thomas Algorithm

- Initialize two new vectors α and β as $\alpha_1 = d_1$ and $\beta_1 = b_1$
- Take the first two equation and eliminate

$$x_1$$
: $\alpha_1 x_1 + u_1 x_2 = \beta_1$
 $l_2 x_1 + d_2 x_2 + u_2 x_3 = b_2$

• Resulting equation is: $\alpha_2 x_2 + u_2 x_3 = \beta_2$ where,

$$\alpha_2 = d_2 - \left(\frac{l_2}{\alpha_1}\right)u_1$$
 $\beta_2 = b_2 - \left(\frac{l_2}{\alpha_1}\right)\beta_1$

• Similarly, we can eliminate $x_2, x_3 \dots$

Thomas Algorithm

- At the *i*th step: $\alpha_{i-1}x_{i-1} + u_{i-1}x_i = \beta_{i-1}$ $l_ix_{i-1} + d_ix_i + u_ix_{i+1} = b_i$
- Eliminate x_{i-1} to obtain: $\alpha_i x_i + u_i x_{i+1} = \beta_i$ where, $\alpha_i = d_i - \left(\frac{l_i}{\alpha_{i-1}}\right) u_{i-1}$ $\beta_i = b_i - \left(\frac{l_i}{\alpha_{i-1}}\right) \beta_{i-1}$
- Last two equations are: $\alpha_{n-1}x_{n-1} + u_{n-1}x_n = \beta_{n-1}$ $l_nx_{n-1} + d_nx_n = b_n$
- Eliminate x_{n-1} to obtain: $\alpha_n x_n = \beta_n$

$$\alpha_n = d_n - \left(\frac{l_n}{\alpha_{n-1}}\right)u_{n-1}$$
 $\beta_n = b_n - \left(\frac{l_n}{\alpha_{n-1}}\right)\beta_{n-1}$

Thomas Algorithm

- Given: four vectors l, d, u and b
- Generate: two vectors α and β as

$$\alpha_1 = d_1$$
 and $\beta_1 = b_1$

$$\alpha_i = d_i - \left(\frac{l_i}{\alpha_{i-1}}\right) u_{i-1}$$
 $\beta_i = b_i - \left(\frac{l_i}{\alpha_{i-1}}\right) \beta_{i-1}$

$$i = 2, 3, \ldots n$$

- Solution: $x_n = \frac{\beta_n}{\alpha_n} \qquad x_i = \frac{\beta_i u_i x_{i+1}}{\alpha_i}$ $i = n-1 \dots 3, 2, 1$
- FP operations: 8(n-1) + 3(n-1) + 1 = 11n 10

Thomas Algorithm: Example

$$\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\alpha_{1} = d_{1}; \alpha_{i} = d_{i} - \frac{l_{i}}{\alpha_{i-1}} u_{i-1}; \beta_{1} = b_{1}; \beta_{i} = b_{i} - \frac{l_{i}}{\alpha_{i-1}} \beta_{i-1} \qquad x_{n} = \frac{\beta_{n}}{\alpha_{n}}; x_{i} = \frac{\beta_{i} - u_{i} x_{i+1}}{\alpha_{i}}$$

$$\alpha_{1} = 2; \alpha_{2} = d_{2} - \frac{l_{2}}{\alpha_{1}} u_{1} = 2 - \frac{-1}{2} (-1) = \frac{3}{2}; \alpha_{3} = 2 - \frac{-1}{3/2} (-1) = \frac{4}{3}; \alpha_{4} = 1 - \frac{-1}{4/3} (-1) = \frac{1}{4}$$

$$\beta_{1} = 0; \beta_{2} = b_{2} - \frac{l_{2}}{\alpha_{1}} \beta_{1} = 0 - \frac{-1}{2} 0 = 0; \beta_{3} = 1 - \frac{-1}{3/2} 0 = 1; \beta_{4} = 0 - \frac{-1}{4/3} 1 = \frac{3}{4}$$

$$x_4 = \frac{\beta_4}{\alpha_4} = 3; x_3 = \frac{\beta_3 - u_3 x_4}{\alpha_2} = \frac{1 - (-1)3}{4/3} = 3; x_2 = \frac{0 - (-1)3}{3/2} = 2; x_1 = \frac{0 - (-1)2}{2} = 1$$

$$a_{11}x_{1} + a_{12}x_{2} + a_{13}x_{3} + \cdots + a_{1n}x_{n} = b_{1}$$

$$a_{21}x_{1} + a_{22}x_{2} + a_{23}x_{3} + \cdots + a_{2n}x_{n} = b_{2}$$

$$a_{31}x_{1} + a_{32}x_{2} + a_{33}x_{3} + \cdots + a_{3n}x_{n} = b_{3}$$

$$a_{i1}x_{1} + a_{i2}x_{2} + a_{i3}x_{3} + \cdots + a_{in}x_{n} = b_{i}$$

$$a_{i1}x_{1} + a_{i2}x_{2} + a_{i3}x_{3} + \cdots + a_{in}x_{n} = b_{i}$$

$$a_{i1}x_{1} + a_{i2}x_{2} + a_{i3}x_{3} + \cdots + a_{in}x_{n} = b_{i}$$

- Assume (initialize) a solution vector x
- Compute a new solution vector x_{new}
- Iterate until $\| x x_{new} \|_{\infty} \le \varepsilon$
- We will learn two methods: Jacobi and Gauss Seidel

Jacobi and Gauss Seidel

• *Jacobi*: for the iteration index k (k = 0 for the initial guess)

$$b_{i} - \sum_{j=1, j \neq i}^{n} a_{ij} x_{j}^{(k)}$$

$$x_{i}^{(k+1)} = \frac{\sum_{j=1, j \neq i}^{n} a_{ij} x_{j}^{(k)}}{a_{ii}}, \quad i = 1, 2, \dots, n$$

• *Gauss Seidel*: for the iteration index k (k = 0 for the initial guess)

$$b_{i} - \sum_{j=1}^{i-1} a_{ij} x_{j}^{(k+1)} - \sum_{j=i+1}^{n} a_{ij} x_{j}^{(k)}$$

$$x_{i}^{(k+1)} = \frac{1}{a_{ii}} \sum_{j=i+1}^{n} a_{ij} x_{j}^{(k)}, \quad i = 1, 2, \dots, n$$

Stopping Criteria

• Generate the error vector (e) at each iteration as

$$e_i^{(k+1)} = \left| \frac{x_i^{(k+1)} - x_i^{(k)}}{x_i^{(k+1)}} \right|, \quad i = 1, 2, \dots n$$

• Stop when: $\|e\|_{\infty} \le \varepsilon$

Iterative Methods (Example)

Solve the following system of equations using Jacobi and Gauss Seidel methods and using initial guess as zero for all the variables with error less than 0.01%. Compare the number iterations required for solution using two methods:

$$x_1 + 2x_2 - x_4 = 1$$

$$x_2 + 2x_3 = 1.5$$

$$-x_3 + 2x_4 = 1.5$$

$$x_1 + 2x_3 - x_4 = 2$$

$$x_3^{(k+1)} = \frac{1.5 - 2x_4^{(k)}}{-1}$$

$$x_1^{(k+1)} = \frac{1 - 2x_2^{(k)} + x_4^{(k)}}{1} \qquad x_2^{(k+1)} = \frac{1 \cdot 5 - 2x_3^{(k)}}{1}$$
$$x_3^{(k+1)} = \frac{1 \cdot 5 - 2x_4^{(k)}}{-1} \qquad x_4^{(k+1)} = \frac{2 - x_1^{(k)} - 2x_3^{(k)}}{-1}$$

$$x_1^{(k+1)} = \frac{1 - 2x_2^{(k)} + x_4^{(k)}}{1} \qquad x_2^{(k+1)} = \frac{1.5 - 2x_3^{(k)}}{1}$$
$$x_3^{(k+1)} = \frac{1.5 - 2x_4^{(k)}}{-1} \qquad x_4^{(k+1)} = \frac{2 - x_1^{(k+1)} - 2x_3^{(k+1)}}{-1}$$

Iterative methods (Example)

If you iterate, both the methods will diverge

Jacobi					
Iter	x1	x2	х3	x4	
0	0	0	0	0	
1	1	1.5	-1.5	-2	
_	_	_	_	_	00.0
2	-4	4.5	-5.5	-4	90.9
3	-12	12.5	-9.5	-17	76.5
4	-41	20.5	-35.5	-33	70.7
5	-73	72.5	-67.5	-114	71.1
6	-258	136.5	-229.5	-210	71.7
7	-482	460.5	-421.5	-719	70.8
8	-1639	844.5	-1439.5	-1327	70.6
9	-3015	2880.5	-2655.5	-4520	70.6
10	-10280	5312.5	-9041.5	-8328	70.7
11	-18952	18084.5	-16657.5	-28365	70.6
12	-64533	33316.5	-56731.5	-52269	70.6

Gauss S	eidel				
Iter	x1	x2	х3	x4	
0	0	0	0	0	
1	1	1.5	-1.5	-4	
2	-6	4.5	-9.5	-27	85.2
3	-35	20.5	-55.5	-148	81.8
4	-188	112.5	-297.5	-785	81.1
5	-1009	596.5	-1571.5	-4154	81.1
6	-5346	3144.5	-8309.5	-21967	81.1
7	-28255	16620.5	-43935.5	-116128	81.1
8	-149368	87872.5	-232258	-613885	81.1
9	-789629	464516.5	-1227772	-3245174	81.1
10	-4174206	2455545	-6490350	-1.7E+07	81.1
11	-2.2E+07	12980701	-3.4E+07	-9.1E+07	81.1
12	-1.2E+08	68619633	-1.8E+08	-4.8E+08	81.1

Is the problem *ill conditioned*? The answer is NO!

Iterative methods (Example)

$x_1 + 2x_2 - x_4 = 1$ $x_2 + 2x_3 = 1.5$ $-x_3 + 2x_4 = 1.5$

 $x_1 + 2x_3 - x_4 = 2$

Pivoting: Columns 2 to 1, 3 to 2, 4 to 3 and 1 to 4.

This is equivalent to change of variables:

$$x_1$$
 (new) = x_2 (original)
 x_2 (new) = x_3 (original)
 x_3 (new) = x_4 (original)
 x_4 (new) = x_1 (original)

Original Problem

A=	1	2	0	-1	b =	1
	0	1	2	0		1.5
	0	0	-1	2		1.5
	1	0	2	-1		2

After Pivoting

A=	2	0	-1	1	b =	1
	1	2	0	0		1.5
	0	-1	2	0		1.5
	0	2	-1	1		2

Iterative Methods (Example)

New Iteration Equations after pivoting (variable identifiers in the subscript are for the new renamed variables):

A=	2	0	-1	1	b =	1
	1	2	0	0		1.5
	0	-1	2	0		1.5
	0	2	-1	1		2

$$x_{1}^{(k+1)} = \frac{1 + x_{3}^{(k)} - x_{4}^{(k)}}{2} \quad x_{2}^{(k+1)} = \frac{1.5 - x_{1}^{(k)}}{2}$$

$$Jacobi$$

$$x_{3}^{(k+1)} = \frac{1.5 + x_{2}^{(k)}}{2} \qquad x_{4}^{(k+1)} = \frac{2 - 2x_{2}^{(k)} + x_{3}^{(k)}}{1}$$

$$x_{1}^{(k+1)} = \frac{1 + x_{3}^{(k)} - x_{4}^{(k)}}{2} \quad x_{2}^{(k+1)} = \frac{1.5 - x_{1}^{(k+1)}}{2}$$

$$Gauss$$

Gauss

Seidel
$$x_3^{(k+1)} = \frac{1.5 + x_2^{(k+1)}}{2}$$

$$x_4^{(k+1)} = \frac{2 - 2x_2^{(k+1)} + x_3^{(k+1)}}{1}$$

Solution: Jacobi

Iter	x1	x2	х3	x4	e	32	0.148	0.656	1.089	1.721	3.529	65	0.168	0.667	1.083	1.751	0.174
0	0.000	0.000	0.000	0.000		33	0.184	0.676	1.078	1.777	3.131	66	0.166	0.666	1.084	1.749	0.159
1	0.500	0.750	0.750	2.000		34	0.151	0.658	1.088	1.726	2.940	67	0.167	0.667	1.083	1.751	0.145
2	-0.125	0.500	1.125	1.250	60.000	35	0.181	0.675	1.079	1.772	2.612	68	0.166	0.666	1.084	1.749	0.133
3	0.438	0.813	1.000	2.125	41.176	36	0.153	0.659	1.087	1.730	2.449	69	0.167	0.667	1.083	1.751	0.121
4	-0.063	0.531	1.156	1.375	54.545	37	0.179	0.673	1.080	1.768	2.186	70	0.166	0.666	1.084	1.749	0.111
5	0.391	0.781	1.016	2.094	34.328	38	0.156	0.661	1.087	1.733	2.035	71	0.167	0.667	1.083	1.751	0.101
6	-0.039	0.555	1.141	1.453	44.086	39	0.177	0.672	1.080	1.765	1.827	72	0.166	0.666	1.083	1.749	0.093
7	0.344	0.770	1.027	2.031	28.462	40	0.157	0.662	1.086	1.736	1.697	73	0.167	0.667	1.083	1.751	0.084
8	-0.002	0.578	1.135	1.488	36.483	41	0.175	0.671	1.081	1.763	1.525	74	0.166	0.666	1.083	1.749	0.077
9	0.323	0.751	1.039	1.979	24.778	42	0.159	0.662	1.086	1.738	1.413	75	0.167	0.667	1.083	1.751	0.070
10	0.030	0.588	1.125	1.537	28.717	43	0.174	0.671	1.081	1.761	1.275	76	0.166	0.666	1.083	1.749	0.064
11	0.294	0.735	1.044	1.949	21.123	44	0.160	0.663	1.085	1.740	1.177	77	0.167	0.667	1.083	1.750	0.059
12	0.048	0.603	1.117	1.574	23.771	45	0.173	0.670	1.082	1.759	1.064	78	0.166	0.667	1.083	1.750	0.054
13	0.271	0.726	1.051	1.912	17.637	46	0.161	0.664	1.085	1.742	0.982	79	0.167	0.667	1.083	1.750	0.049
14	0.070	0.614	1.113	1.599	19.537	47	0.172	0.669	1.082	1.757	0.888	80	0.166	0.667	1.083	1.750	0.045
15	0.257	0.715	1.057	1.885	15.143	48	0.162	0.664	1.085	1.743	0.818	81	0.167	0.667	1.083	1.750	0.041
16	0.086	0.622	1.108	1.627	15.827	49	0.171	0.669	1.082	1.756	0.742	82	0.166	0.667	1.083	1.750	0.037
17	0.240	0.707	1.061	1.864	12.734	50	0.163	0.665	1.084	1.744	0.682	83	0.167	0.667	1.083	1.750	0.034
18	0.098	0.630	1.103	1.647	13.200	51	0.170	0.669	1.082	1.755	0.619	84	0.166	0.667	1.083	1.750	0.031
19	0.228	0.701	1.065	1.844	10.664	52	0.164	0.665	1.084	1.745	0.569	85	0.167	0.667	1.083	1.750	0.028
20	0.111	0.636	1.100	1.663	10.858	53	0.169	0.668	1.082	1.754	0.516	86	0.167	0.667	1.083	1.750	0.026
21	0.219	0.695	1.068	1.829	9.054	54	0.164	0.665	1.084	1.746	0.474	87	0.167	0.667	1.083	1.750	0.024
22	0.120	0.641	1.097	1.679	8.940	55	0.169	0.668	1.083	1.754	0.431	88	0.167	0.667	1.083	1.750	0.022
23	0.209	0.690	1.070	1.816	7.568	56	0.165	0.665	1.084	1.747	0.395	89	0.167	0.667	1.083	1.750	0.020
24	0.127	0.645	1.095	1.690	7.458	57	0.169	0.668	1.083	1.753	0.360	90	0.167	0.667	1.083	1.750	0.018
25	0.203	0.686	1.073	1.804	6.344	58	0.165	0.666	1.084	1.747	0.330	91	0.167	0.667	1.083	1.750	0.017
26	0.134	0.649	1.093	1.700	6.157	59	0.168	0.668	1.083	1.753	0.300	92	0.167	0.667	1.083	1.750	0.015
27	0.197	0.683	1.074	1.796	5.344	60	0.165	0.666	1.084	1.748	0.275	93	0.167	0.667	1.083	1.750	0.014
28	0.139	0.652	1.091	1.708	5.110	61	0.168	0.667	1.083	1.752	0.250	94	0.167	0.667	1.083	1.750	0.013
29	0.192	0.680	1.076	1.788	4.458	62	0.165	0.666	1.084	1.748	0.229	95	0.167	0.667	1.083	1.750	0.011
30	0.144	0.654	1.090	1.715	4.260	63	0.168	0.667	1.083	1.752	0.209	96	0.167	0.667	1.083	1.750	0.010
31	0.188	0.678	1.077	1.782	3.736	64	0.166	0.666	1.084	1.748	0.191	97	0.167	0.667	1.083	1.750	0.010

Number of iteration required to achieve a relative error of < 0.01% = 97

Solution: Gauss Seidel

Iter	x1	x2	x3	x4	e
0	0.000	0.000	0.000	0.000	
1	0.500	0.500	1.000	2.000	
2	0.000	0.750	1.125	1.625	30.769
3	0.250	0.625	1.063	1.813	13.793
4	0.125	0.688	1.094	1.719	7.273
5	0.188	0.656	1.078	1.766	3.540
6	0.156	0.672	1.086	1.742	1.794
7	0.172	0.664	1.082	1.754	0.891
8	0.164	0.668	1.084	1.748	0.447
9	0.168	0.666	1.083	1.751	0.223
10	0.166	0.667	1.083	1.750	0.112
11	0.167	0.667	1.083	1.750	0.056
12	0.167	0.667	1.083	1.750	0.028
13	0.167	0.667	1.083	1.750	0.014
14	0.167	0.667	1.083	1.750	0.007

Number of iteration required to achieve a relative error of < 0.01% = 14

So, what makes the methods *diverge*? When do we need *pivoting* or *scaling* or *equilibration* for the *iterative methods*? Let's analyze for the *convergence criteria*!

$$\begin{bmatrix} a_{11} & a_{12} & \cdot & \cdot & a_{1n} \\ a_{21} & a_{22} & \cdot & \cdot & a_{2n} \\ a_{31} & a_{32} & \cdot & \cdot & a_{3n} \\ & \cdot & \cdot & \cdot & \cdot \\ a_{m1} & a_{m2} & \cdot & \cdot & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ & \cdot \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ & \cdot \\ b_m \end{bmatrix}$$

How the iteration schemes look in the matrix form?

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ a_{31} & a_{32} & \cdots & a_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} 0 & 0 & \cdots & \cdots & 0 \\ a_{21} & 0 & 0 & \cdots & \cdots & 0 \\ a_{31} & a_{32} & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & 0 \end{bmatrix} +$$

$$\begin{bmatrix} a_{11} & 0 \cdots & 0 & \cdot & 0 \\ 0 & a_{22} & 0 & 0 & \cdot 0 \\ 0 & 0 & a_{33} & 0 & \cdot 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdot & \cdot \cdot a_{nn} \end{bmatrix} + \begin{bmatrix} 0 & a_{12} & a_{13} & \cdot & a_{1n} \\ 0 & 0 & a_{23} & \cdot & a_{2n} \\ 0 & 0 & 0 & \cdot & a_{3n} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdot & \cdot & 0 \end{bmatrix}$$

- A = L + D + U
- Ax = b translates to (L + D + U)x = b
- **Jacobi:** for an iteration counter k

$$Dx^{(k+1)} = -(U+L)x^{(k)} + b$$
$$x^{(k+1)} = -D^{-1}(U+L)x^{(k)} + D^{-1}b$$

• Gauss Seidel: for an iteration counter k

$$(L+D)x^{(k+1)} = -Ux^{(k)} + b$$
$$x^{(k+1)} = -(L+D)^{-1}Ux^{(k)} + (L+D)^{-1}b$$

- All iterative methods: $x^{(k+1)} = Sx^{(k)} + c$
- *Jacobi*: $S = -D^{-1}(U+L)$ $c = D^{-1}b$
- Gauss Seidel: $S = -(L+D)^{-1}U$ $c = (L+D)^{-1}b$
- For true solution vector (x): x = Sx + c
- True error: $e^{(k)} = x x^{(k)}$
- $e^{(k+1)} = Se^{(k)}$ or $e^{(k)} = S^k e^{(0)}$
- Methods will converge if: $\lim_{k \to \infty} e^{(k)} = 0$

$$\lim_{k \to \infty} S^k = 0$$

- For the solution to exist, the matrix should have full rank (= n)
- The iteration matrix S will have n eigenvalues $\{\lambda_j\}_{j=1}^n$ and n independent eigenvectors $\{v_j\}_{j=1}^n$ that will form the basis for a n-dimensional vector space
- Initial error vector: $e^{(0)} = \sum_{j=1}^{n} C_j v_j$
- From the definition of eigenvalues: $e^{(k)} = \sum_{j=1}^{n} C_j \lambda_j^k v_j$
- Necessary condition: $\rho(S) < 1$
- Sufficient condition: ||S|| < 1 because $\rho(A) \le ||A||$

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- Necessary condition: $\rho(S) < 1$
- Sufficient condition: ||S|| < 1 because $\rho(A) \le ||A||$

Using the **definition of** *S* and using *row-sum norm* for matrix *S*, we obtain the following as the **sufficient condition for convergence** for both Jacobi and Gauss Seidel:

$$|a_{ii}| > \sum_{j=1, j\neq i}^{n} |a_{ij}|, \quad i = 1, 2, \dots n$$

If the original matrix is diagonally dominant, it will always converge!