LU factorization

$A = LU$ factorization is not unique. (Why?)

We need to specify constraints.

1. Doolittle's decomposition $L_{\mathrm{ii}} = 1, i = 1, 2, \ldots, n$
2. Crout's decomposition $U_{\mathrm{ii}} = 1, i = 1, 2, \ldots, n$
3. Choleski's decomposition $L = U^T$

Doolittle's decomposition method

$$L = \begin{bmatrix} 1 & 0 & 0 \\ L_{21} & 1 & 0 \\ L_{31} & L_{32} & 1 \end{bmatrix} U = \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix} A = \mathrm{LU}$$

$$A = \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ U_{11}L_{21} & U_{12}L_{21} + U_{22} & U_{13}L_{21} + U_{23} \\ U_{11}L_{31} & U_{12}L_{31} + U_{22}L_{32} & U_{13}L_{31} + U_{23}L_{32} + U_{33} \end{bmatrix}$$

$$R_2 \leftarrow R_2 - L_{21}\, R_1 \,(\text{eliminate}\, A_{21})$$

$$R_3 \leftarrow R_3 - L_{31}\, R_1 \,(\text{eliminate}\, A_{31})$$

Doolittle's decomposition method

$$A' = \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & U_{22}L_{32} & U_{23}L_{32} + U_{33} \end{bmatrix}$$

$$R_3 \leftarrow R_3 - L_{32}\,R_2\,(\text{eliminates } A_{32})$$

$$A'' = \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

Matrix U: same as the upper triangular matrix that results from Gauss Elimination

Off-diagonal elements of L ($L_{\mathrm{ij}}; i \neq j$): pivot equation multipliers to eliminate $A_{\mathrm{ij}}; i \neq j$.

```
function x=doolittle(A,b)        % returns A=[L\U]

n=size(A,1);
for k=1:n-1
  for i=k+1:n
    if A(i,k) ~= 0
      lambda=A(i,k)/A(k,k);
      A(i,k+1:n)=A(i,k+1:n)-lambda*A(k,k+1:n);
      A(i,k) = lambda;
    end
  end
end
for k=2:n          %forward substitution to solve Ly=b
  b(k) = b(k) - A(k,1:k-1)*b(1:k-1);
end
for k=n:-1:1        %backward substitution to solve Ux=y
  b(k) = b(k) - A(k,k+1:n)*b(k+1:n)/A(k,k);
end
```

Doolittle's decomposition method

Solve $\mathrm{Ly} = b$ by forward substitution and $\mathrm{Ux} = y$ by back substitution. $L_{\mathrm{ii}} = 1$

$$\begin{aligned} y_1 &= b_1 \\ L_{21} y_1 + y_2 &= b_2 \\ &\vdots \\ L_{k1} y_1 + L_{k2} y_2 + \cdots + L_{k,k-1} y_{k-1} + y_k &= b_k \end{aligned}$$

$$y_k = b_k - \sum_{j=1}^{k-1} L_{\mathrm{kj}} y_j \quad k = 2, 3, \ldots, n$$

```
for k=2:n                %forward substitution to solve Ly = b
   b(k) = b(k) - A(k,1:k-1)*b(1:k-1);
end
for k=n:-1:1             %backward substitution to solve Ux = y
   b(k) = b(k) - A(k,k+1:n)*b(k+1:n)/A(k,k);
end
```

Choleski's decompostion for symmetric matrices

Choleski's decomposition $A = L\,L^T$

A requires to be symmetric and positive definite.

A symmtric $n \times n$ matrix is positive definite if $x^T A\,x > 0$ for every $x \neq 0$.

$A = a_{\mathrm{ij}};\ x = [x_1, x_2, \ldots, x_n]^T$

$$x^T A\,x = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{\mathrm{ij}} x_i x_j$$

$A = \begin{pmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{pmatrix};$

$$x^T A\,x = \begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$= 3x_1^2 + (x_1 - x_2)^2 + 2x_2^2 + (x_2 - x_3)^2 + 3x_3^2 > 0 \text{ unless } x_1 = x_2 = x_3 = 0$$

Choleski's decomposition

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = \begin{bmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \begin{bmatrix} L_{11} & L_{21} & L_{31} \\ 0 & L_{22} & L_{32} \\ 0 & 0 & L_{33} \end{bmatrix}$$

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = \begin{bmatrix} L_{11}^2 & L_{11}L_{21} & L_{11}L_{31} \\ L_{11}L_{21} & L_{21}^2 + L_{22}^2 & L_{21}L_{31} + L_{22}L_{32} \\ L_{11}L_{31} & L_{21}L_{31} + L_{22}L_{32} & L_{31}^2 + L_{32}^2 + L_{33}^2 \end{bmatrix}$$

Equate the coefficients

$$A_{11} = L_{11}^2, A_{21} = L_{11}L_{21}, A_{31} = L_{11}L_{31}; \Rightarrow L_{11} = \sqrt{A_{11}}, L_{21} = A_{21} / L_{11}, L_{31} = A_{31} / L_{11}$$

$$A_{22} = L_{21}^2 + L_{22}^2, A_{32} = L_{21}L_{31} + L_{22}L_{32}; \Rightarrow L_{22} = \sqrt{A_{22} - L_{21}^2}, L_{32} = (A_{32} - L_{21}L_{31}) / L_{22}$$

$$A_{33} = L_{31}^2 + L_{32}^2 + L_{33}^2; \Rightarrow L_{33} = \sqrt{(A_{33} - L_{31}^2 - L_{32}^2)}$$

Choleski's decomposition

$(\mathrm{LL}^T)_{\mathrm{ij}} = L_{i1}L_{j1} + L_{i2}L_{j2} + \cdots + L_{\mathrm{ij}}L_{\mathrm{jj}} = \sum_{(k=1)}^{j} L_{\mathrm{ik}}\, L_{\mathrm{jk}} \quad i \geqslant j$

Equate with coefficients of A

$$A_{\mathrm{ij}} = \sum_{k=1}^{j} L_{\mathrm{ik}} L_{\mathrm{jk}},\ \ i = j, j+1, \ldots, n, j = 1, 2, \ldots, n$$

$$A_{\mathrm{ij}} = \sum_{k=1}^{j-1} L_{\mathrm{ik}} L_{\mathrm{jk}} + L_{\mathrm{ij}} L_{\mathrm{jj}}$$

When $i = j$ (diagonal terms)

$$L_{\mathrm{jj}} = \sqrt{A_{\mathrm{jj}} - \sum_{k=1}^{j-1} L_{\mathrm{jk}}^2} \qquad j = 2, 3, \ldots., n$$

For $j = 1$ $\qquad L_{11} = \sqrt{A_{11}},\ \ L_{i1} = A_{i1} / L_{11}\, (i = 2, 3, \ldots, n)$

For non-diagonal terms

$$L_{\mathrm{ij}} = \left(A_{\mathrm{ij}} - \sum_{k=1}^{j-1} L_{\mathrm{ik}} L_{\mathrm{jk}} \right) / L_{\mathrm{jj}},\ j = 2, 3, \ldots, n-1,\ i = j+1, j+2, \ldots, n$$

```
function L=myChol(A)

n=size(A,1);

for j=1:n
    tempvar = A(j,j)) - dot(A(j,1:j-1),A(j,1:j-1);

    if (tempvar < 0.0)
       error('Matrix is not positive definite');
    end

    A(j,j) = sqrt(tempvar);

    for i=j+1:n
       A(i,j)=(A(i,j) - dot(A(i,1:j-1),A(j,1:j-1)))/A(j,j);
    end
end
L = tril(A);
```

$$A = \begin{pmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{pmatrix}$$

Symmetric and banded coefficient matrices

Engineering/ Physics problems: coefficient matrics sparsely populated

Nonzero coefficients clustered about the leading diagonal.

Example: tridiagonal matrix (heat equation, diffusion equation, Poisson's equation)

The matrix $A=[a_{\rm ij}]$ is said to be tridiagonal if $a_{\rm ij}=0$ for $|i-j|>1$

$$A=\begin{bmatrix} \alpha_1 & \gamma_1 & 0 & 0 & \cdots & 0 \\ \beta_2 & \alpha_2 & \gamma_2 & 0 & \cdots & 0 \\ 0 & \beta_3 & \alpha_3 & \gamma_3 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \beta_{n-1} & \alpha_{n-1} & \gamma_{n-1} \\ 0 & \cdots & \cdots & 0 & \beta_n & \alpha_n \end{bmatrix}$$

Tridiagonal matrix

For $\mathrm{Ax} = b$, equate coefficients:

$$
\begin{aligned}
\alpha_1 x_1 + \gamma_1 x_2 &= b_1, \\
\beta_i x_{i-1} + \alpha_i x_i + \gamma_i x_{i+1} &= b_i, \quad i = 2, 3, \ldots, n-1, \\
\beta_n x_{n-1} + \alpha_n x_n &= b_n.
\end{aligned}
$$

$$
A = LU = \begin{bmatrix} l_1 & 0 & 0 & 0 & \cdots & 0 \\ \beta_2 & l_2 & 0 & 0 & \cdots & 0 \\ 0 & \beta_3 & l_3 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \beta_{n-1} & l_{n-1} & 0 \\ 0 & \cdots & \cdots & 0 & \beta_n & l_n \end{bmatrix} \begin{bmatrix} 1 & u_1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & u_2 & 0 & \cdots & 0 \\ 0 & 0 & 1 & u_3 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & 1 & u_{n-1} \\ 0 & \cdots & \cdots & 0 & 0 & 1 \end{bmatrix}
$$

Tridiagonal matrix

$$\alpha_1 = l_1,\ \alpha_i = l_i + \beta_i u_{i-1}\,(i = 2, 3, \ldots, n);\ l_i u_i = \gamma_i\,(i = 1, 2, \ldots, n-1)$$

$$l_1 = \alpha_1; u_1 = \gamma_1 / l_1; l_i = \alpha_i - \beta_i u_{i-1},\ u_i = \gamma_i / l_i\,(i = 2, 3, \ldots, n-1)$$

$$l_n = \alpha_n - \beta_n u_{n-1}$$

$$\mathrm{Ux} = y, \mathrm{Ly} = b$$

$$y_1 = b_1 / l_1,\ y_i = (b_i - \beta_i y_{i-1}) / l_i, i = 2, 3, \ldots, n$$

$$x_n = y_n, x_i = y_i - u_i x_{i+1},\ i = n-1, n-2, \ldots, 1$$

Algorithm for tridiagonal matrices

TRIDIAG(α, β, γ, n) [Solutions of tridiagonal system]

1. [get $y_1$and u_1] $y_1 \leftarrow b_1/\alpha_1; u_1 \leftarrow \gamma_1/\alpha_1$.
2. [loop on i] for $i \leftarrow 2$ to $n-1$ do through step 4.
3. [get l_i and y_i] $l_i \leftarrow \alpha_i - \beta_i u_{i-1}$; $y_i \leftarrow (b_i - \beta_i y_{i-1})/l_i$; $u_i \leftarrow \gamma_i/l_i$.
4. [get y_n] $y_n \leftarrow (b_n - \beta_n y_{n-1})/(\alpha_n - \beta_n u_{n-1})$.
5. [loop for x_i] $x_n \leftarrow y_n$; for $i \leftarrow n-1$ to 1 do through step 6.
6. [get x_i] $x_i \leftarrow y_i - u_i x_{i+1}$

Matrix norm

A matrix norm on the set of all $n \times n$ matrices A is a real-valued function $N(A)$ such that

a) $N(A) \geqslant 0$.

b) $N(A) = 0$ if and only if $A \equiv 0$, the matrix with all zero elements.

c) $N(\alpha A) = |\alpha| N(A)$ for all real α.

d) $N(A + B) \leqslant N(A) + N(B)$

e) $N(\mathrm{AB}) \leqslant N(A) N(B)$

Corresponding to a vector norm $\|\cdot\|_v$, an associated matrix norm $\|A\|_v$ is defined by

$$\|A\|_v = \max_{\boldsymbol{x} \neq 0} \frac{\|A\boldsymbol{x}\|_v}{\|\boldsymbol{x}\|_v}$$

Matrix norm

Let $A = [a_{\mathrm{ij}}]$ be an $n \times n$ matrix. Then

$$\|A\|_\infty = \max_{1 \leqslant i \leqslant n} \sum_{j=1}^{n} |a_{\mathrm{ij}}|, \|A\|_1 = \max_{1 \leqslant j \leqslant n} \sum_{i=1}^{n} |a_{\mathrm{ij}}|$$

$$A = \begin{pmatrix} 2 & -3 & 1 & 3 \\ 4 & 1 & -1 & -5 \\ 1 & 1 & 0 & 6 \\ -7 & 0 & 0 & 9 \end{pmatrix}$$

$\|A\|_\infty = \max\ (|2| + |-3| + |1| + |3|, |4| + |1| + |-1| + |-5|, |1| + |1| + |0| + |6|, |-7| + |0| + |0| + |9|) = \max(9, 11, 8, 16) = 16$

$\|A\|_1 = 23$

Matrix norm

An eigenvalue of an $n \times n$ matrix is a number (real or complex) λ for which there exists a vector $\boldsymbol{x} \neq \mathbf{0}$ such that $A\boldsymbol{x} = \lambda \boldsymbol{x}$. The nonzero vector $\boldsymbol{x}$ is called the eigenvector associated with λ.

If A is an $n \times n$ matrix, then the polynomial $p_A(\lambda) = \det(A - \lambda I)$ is the characteristic polynomial of A.

$p_A(\lambda) = 0$ is the characteristic equation. The collection of all eigenvalues is the spectrum of A denoted by $\sigma(A)$

Spectral radius $\rho(A)$ of matrix A is defined by

$$\rho(A) = \max_{\lambda \in \sigma(A)} |\lambda|$$

Matrix norm

$$A = \begin{pmatrix} -8 & 20 & 20 \\ -12 & 23 & 7 \\ -4 & 5 & 21 \end{pmatrix}$$

$$p_A(\lambda) = \det(A - \lambda I) = (\lambda - 8)(\lambda - 12)(\lambda - 16)$$

$$\lambda = 8, 12, 16$$

Eigenvector corresponding to $\lambda = 8$ by solving $(A - 8I)\boldsymbol{x} = 0$

$\boldsymbol{x} = (\ 5 \quad 4 \quad 0\ )^T$,σ(A)=(8, 12, 16), ρ(A)=max(σ(A))=16

$\|A\|_2 = \sqrt{\rho(A^T A)}$

Condition number

How much is the solution altered if the coefficients in the matrix A or the right hand side vector b (or both) are perturbed?

If $\tilde{x}$ is an approximate solution to $\mathrm{Ax} = b$,

error in $\tilde{x}$ is $e = x - \tilde{x}$.

Residual $r = b - A\tilde{x}$

If $r = 0$, $\tilde{x}$ is the exact solution.

$$
\begin{aligned}
1.99x_1 + 2.01x_2 &= 4 \\
2.01x_1 + 1.99x_2 &= 4
\end{aligned}
$$

Exact solution: $x = (\begin{array}{cc} 1 & 1 \end{array})^T$.

Approximate solution $\tilde{x} = (\ 0.99 \ \ 0.99\ )^T$

$$e = x - \tilde{x} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 0.99 \\ 0.99 \end{pmatrix} = \begin{pmatrix} 0.01 \\ 0.01 \end{pmatrix}$$

$$r = b - A\tilde{x} = \begin{pmatrix} 4 \\ 4 \end{pmatrix} - \begin{pmatrix} 1.99 & 2.01 \\ 2.01 & 1.99 \end{pmatrix}\begin{pmatrix} 0.99 \\ 0.99 \end{pmatrix} = \begin{pmatrix} 0.04 \\ 0.04 \end{pmatrix}$$

$\|e\|_\infty = 0.01, \ \|r\|_\infty = 0.04$

Let A be a nonsingular matrix and $\tilde{x}$ be an approximate solution to $\mathrm{Ax} = b$. Then for any matrix norm $\|\cdot\|, \ \|e\| \leqslant \|A^{-1}\| \, \|r\|$

and

$$\frac{1}{\|A\| \, \|A^{-1}\|} \frac{\|r\|}{\|b\|} \leqslant \frac{\|e\|}{\|x\|} \leqslant \|A\| \, \|A^{-1}\| \frac{\|r\|}{\|b\|} \, \mathrm{for} \, x \neq 0 \, \mathrm{and} \, b \neq 0$$

Condition number

$\kappa(A) = \|A\| \, \|A^{-1}\|$

Useful for analysis of rounding errors.

The unit round of a computer is defined as the smallest positive floating point number u for which

$\mathrm{float}(1+u) > 1$

If $\hat{u} < u$ then $\mathrm{float}(1+\hat{u}) = 1$

A matrix A is ill-conditioned if $\kappa(A) \approx 1/u$

If $\kappa(A) \approx 10^r \; \mathrm{for} \; r > 0, r$ digits of accuracy will be lost in computing an approximate solution by any direct method.

Iterative Methods (Jacobi method)

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\ &\vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{\mathrm{nn}}x_n &= b_n \end{aligned}$$

$$\begin{aligned} x_1 &= \frac{1}{a_{11}}(b_1 - a_{12}x_2 - a_{13}x_3 - \cdots - a_{1n}x_n) \\ x_2 &= \frac{1}{a_{22}}(b_2 - a_{21}x_1 - a_{23}x_3 - \cdots - a_{2n}x_n) \\ &\vdots \\ x_n &= \frac{1}{a_{\mathrm{nn}}}(b_n - a_{n1}x_1 - a_{n2}x_2 - \cdots - a_{n,n-1}x_{n-1}) \end{aligned}$$

Initial guess: $\boldsymbol{x}^{(0)} = \left(x_1^{(0)}, x_2^{(0)}, \ldots, x_n^{(0)}\right)$, sequence after repeated iterations

$$\boldsymbol{x}^{(\boldsymbol{k})} = \left(x_1^{(k)}, x_2^{(k)}, x_3^{(k)}, \cdots, x_n^{(k)}\right) k = 1, 2, 3, \ldots$$

Jacobi method

For $k \geqslant 1$ generate $x_i^{(k)}$ from $x_i^{(k-1)}$:

$$x_i^{(k)} = \frac{1}{a_{\mathrm{ii}}}\left[\sum_{j=1, j\neq i}^{n} (-a_{\mathrm{ij}} x_j^{(k-1)}) + b_i\right] \text{for } i = 1, 2, \ldots, n$$

$\mathrm{Ax} = b$

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, b = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}, x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$D = \begin{pmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{pmatrix}, L = \begin{pmatrix} 0 & 0 & 0 \\ -a_{21} & 0 & 0 \\ -a_{31} & -a_{32} & 0 \end{pmatrix}, U = \begin{pmatrix} 0 & -a_{12} & -a_{13} \\ 0 & 0 & -a_{23} \\ 0 & 0 & 0 \end{pmatrix}$$

$\mathrm{Ax} = b \Rightarrow (D - L - U)x = b$

$$\mathrm{Dx} = (L + U)x + b$$

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

Algorithm

Input $A, b, x^{(0)}, \text{Tolerance}, N$

Output x

N:maximum number of iterations

[Iterate] for $k = 1, 2, \ldots, N$

[get x] for $i = 1, 2, \ldots, N$

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

if $\|\boldsymbol{x} - \boldsymbol{x}^{(\mathbf{0})}\|_2 < \text{Tolerance}$ then OUTPUT$(\boldsymbol{x})$; BREAK;

for $i = 1, 2, \ldots, N \quad x_i^{(0)} = x_i$

Iterative methods

An $n \times n$ matrix is strictly diagonally dominant if

$$|a_{\mathrm{ii}}| > \sum_{j \neq i}^{n} |a_{\mathrm{ij}}|, \text{ for } i = 1, 2, \ldots, n$$

$$A = \begin{bmatrix} 12 & -7 & 1 & 2 \\ 3 & 13 & -7 & 1 \\ 1 & 2 & 7 & 1 \\ 5 & -1 & 2 & 9 \end{bmatrix}$$

Jacobi iterations converge if A is strictly diagonally dominant.

Gauss-Seidel Method

$$\sum_{j=1}^{n} A_{\mathrm{ij}} x_j = b_i,\ i = 1, 2, \ldots, n$$

$$A_{\mathrm{ii}} x_i + \sum_{j=1, j \neq i}^{n} A_{\mathrm{ij}} x_j = b_i,\ i = 1, 2, \ldots, n$$

Solve for x_i

$$x_i = \frac{1}{A_{\mathrm{ii}}}\left(b_i - \sum_{j=1, j \neq i}^{n} A_{\mathrm{ij}} x_j\right), i = 1, 2, \ldots, n$$

$$x_i^{(k)} = \frac{1}{A_{\mathrm{ii}}}\left[b_i - \sum_{j=1}^{i-1} A_{\mathrm{ij}} x_j^{(k)} - \sum_{j=i+1}^{n} A_{\mathrm{ij}} x_j^{(k-1)}\right]$$

Iterative methods

$A = M - N$, M is nonsingular

$\mathrm{Ax} = b \Rightarrow (M - N)x = b \Rightarrow \mathrm{Mx} = \mathrm{Nx} + b$

$$\boldsymbol{x} = M^{-1}N\,\boldsymbol{x} + M^{-1}b$$

Iteration matrix $T = M^{-1}N$ and $c = M^{-1}b$

$\boldsymbol{x} = T\boldsymbol{x} + \boldsymbol{c}$, For an iterative method

$\boldsymbol{x}^{(k)} = T\boldsymbol{x}^{(k-1)} + \boldsymbol{c}$, Define $\boldsymbol{e}^{(k)} = \boldsymbol{x} - \boldsymbol{x}^{(k)}$ $\therefore \boldsymbol{e}^{(k)} = T\boldsymbol{e}^{(k-1)}$

Convergence if $\|\boldsymbol{e}^{(k)}\| \leqslant \|T\|\,\|\boldsymbol{e}^{(k-1)}\|$ or $\|\boldsymbol{e}^{(k)}\| \leqslant \|T\|^k\,\|\boldsymbol{e}^{(0)}\|$

Convergence if $\|T\| < 1$

$T_J = -D^{-1}(L + U)$; $T_{\mathrm{GS}} = -(D + L)^{-1}U$

Gauss-Seidel method

Acceleration of convergence

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

$$x_i^{(k)} = x_i^{(k-1)} + \frac{1}{A_{\mathrm{ii}}}\left[b_i - \sum_{j=1}^{i-1} A_{\mathrm{ij}} x_j^{(k)} - \sum_{j=i}^{n} A_{\mathrm{ij}} x_j^{(k-1)}\right] i = 1, 2, \ldots, n$$

$w = 1$ no relaxation

$w < 1$ underrelaxation

$w > 1$ overrelaxation (extrapolation)

SOR

$$\begin{aligned}
\bar{x}_i &= \frac{1}{A_{\mathrm{ii}}}\left[b_i - \sum_{j=1}^{i-1} A_{\mathrm{ij}} x_j^{(k)} - \sum_{j=i+1}^{n} A_{\mathrm{ij}} x_j^{(k-1)}\right] \\
x_i^{(k)} &= \omega \bar{x}_i + (1-\omega) x_i^{(k-1)}
\end{aligned}$$

Fixed point iteration

$f_1(x_1, x_2) = 0$, $f_2(x_1, x_2) = 0$

Reformulate in the form

$x_1 = g_1(x_1, x_2)$, $x_2 = g_2(x_1, x_2)$

Assume a solution (α_1, α_2) to be the fixed-point of the above equations.

$\alpha_1 = g_1(\alpha_1, \alpha_2)\; \alpha_2 = g_2(\alpha_1, \alpha_2)$

Begin with initial guess $\boldsymbol{x}^{(0)} = \begin{bmatrix} x_1^{(0)} & x_2^{(0)} \end{bmatrix}$.

$$\begin{aligned} x_1^{(k)} &= g_1\big(x_1^{(k-1)}, x_2^{(k-1)}\big), \\ x_2^{(k)} &= g_2\big(x_1^{(k-1)}, x_2^{(k-1)}\big) \end{aligned}$$

$$
\begin{aligned}
f_1(x_1,x_2) &= 1+x_1-x_2^2=0 \\
f_2(x_1,x_2) &= x_2-x_1^3=0 \\
g_1(x_1,x_2) &= x_1=x_2^2-1 \\
g_2(x_1,x_2) &= x_2=x_1^3
\end{aligned}
$$

Start with $\left(x_1^{(0)}, x_2^{(0)}\right)=(1.5,1.5)$, Iterations do not converge

$0-(1.5,1.5), 1-(1.25,3.375), 2-(10.39,1.95), 3-(2.84,1121.824)$

$$
\begin{aligned}
x_1 &= x_2^{1/3}=g_1(x_1,x_2) \\
x_2 &= \sqrt{1+x_1}=g_2(x_1,x_2)
\end{aligned}
$$

$0-(1.5,1.5), 10-(1.135,1.461)$

If α is the fixed point of $\boldsymbol{G}(\boldsymbol{x})$ and the components $g_i(\boldsymbol{x})$ $(i = 1,\, 2,\, \ldots,\, n)$ are continuously differentiable in some neighborhood of $\boldsymbol{\alpha}$ and $\|J_G(\alpha)\|_\infty < 1$, then the initial guess $\boldsymbol{x}^{(0)} = \boldsymbol{\alpha}$ will converge.

The Jacobian matrix $J_G(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial g_1(\boldsymbol{x})}{\partial x_1} & \frac{\partial g_1(\boldsymbol{x})}{\partial x_2} \\ \frac{\partial g_2(\boldsymbol{x})}{\partial x_1} & \frac{\partial g_2(\boldsymbol{x})}{\partial x_2} \end{pmatrix}$ for the function $\boldsymbol{G}(\boldsymbol{x}) = \begin{bmatrix} g_1(x_1, x_2) \\ g_2(x_1, x_2) \end{bmatrix}$

$[J_G]_{\mathrm{ij}} = \frac{\partial g_i}{\partial x_j}; i = 1, 2, \ldots, n; j = 1, 2, \ldots, n$

Newton's Method

$\boldsymbol{G}(\boldsymbol{x}) = \boldsymbol{x} + \mathbf{A}\mathbf{F}(\boldsymbol{x})$

A is a nonsingular matrix of order n

$J_G(\boldsymbol{x}) = I + A\,J_F(\boldsymbol{x})$. $J_F(\boldsymbol{x})$ is the Jacobian matrix for $F(\boldsymbol{x})$.

$$J_F(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial f_1(x)}{\partial x_1} & \cdots & \frac{\partial f_1(x)}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n(x)}{\partial x_1} & \cdots & \frac{\partial f_n(x)}{\partial x_n} \end{bmatrix}$$

$A = -[J_F(\alpha)]^{-1}$

Iteration: Begin with $J_F(\boldsymbol{x}^{(0)})$, update $A = -[J_F(\boldsymbol{x}^{(k-1)})]^{-1}$

$$\boldsymbol{x}^{(k)} = \boldsymbol{x}^{(k-1)} - [J_F(\boldsymbol{x}^{(k-1)})]^{-1}\boldsymbol{F}(\boldsymbol{x}^{(k-1)})$$

$$\boldsymbol{F}(\boldsymbol{x}) = \begin{bmatrix} 1 + x_1 - x_2^2 \\ x_2 - x_1^3 \end{bmatrix}$$

$$J_F(\boldsymbol{x}) = \begin{bmatrix} 1 & -2x_2 \\ -3x_1^2 & 1 \end{bmatrix}$$

$$\begin{bmatrix} x_1^{(k)} \\ x_2^{(k)} \end{bmatrix} = \begin{bmatrix} x_1^{(k-1)} \\ x_2^{(k-1)} \end{bmatrix} - \begin{bmatrix} 1 & -2x_2 \\ -3x_1^2 & 1 \end{bmatrix} \begin{bmatrix} f_1\left(x_1^{(k-1)}, x_2^{(k-1)}\right) \\ f_2\left(x_1^{(k-1)}, x_2^{(k-1)}\right) \end{bmatrix}$$

Start with $\left(x_1^{(0)}, x_2^{(0)}\right) = (1.5, 1.5)$

4^{th} iteration: $x_1 = 1.134724, x_2 = 1.46107$