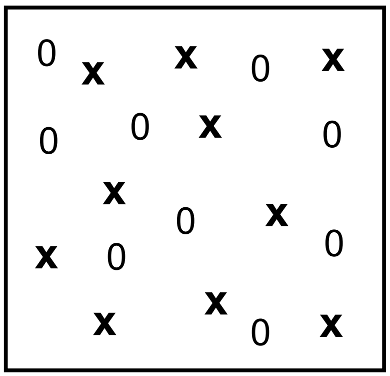
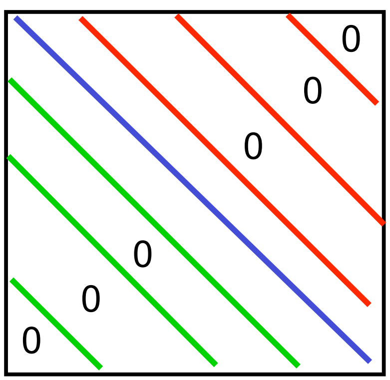
Introduction to Numerical Analysis for Engineers

- Systems of Linear Equations
  - Cramer's Rule
  - Gaussian Elimination
    - Numerical implementation
    - Numerical stability: Partial Pivoting, Equilibration, Full Pivoting
    - Multiple right hand sides
    - Computation count
    - LU factorization
    - Error Analysis for Linear Systems
      - Condition Number
    - Special Matrices
  - Iterative Methods
    - Jacobi's method
    - Gauss-Seidel iteration
    - Convergence
    - Successive Overrelaxation Method
    - Gradient Methods

Linear Systems of Equations
Iterative Methods

Sparse, Full-bandwidth Systems





Rewrite Equations

$$\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}} = \overline{\mathbf{b}} \quad \Leftrightarrow \quad \sum_{j=1}^{n} a_{ij} x_j = b_i$$

$$a_{ii} \neq 0 \Rightarrow x_i = \frac{b_i - \sum_{j=1}^{i-1} a_{ij} x_j - \sum_{j=i+1}^{n} a_{ij} x_j}{a_{ii}} \;, \; i = 1, \ldots n$$

Iterative, Recursive Methods

Jacobi's Method

$$x_i^{(k+1)} = \frac{b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)}}{a_{ii}} \;, \; i = 1, \ldots n$$

Gauss-Seidels's Method

$$x_i^{(k+1)} = \frac{b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)}}{a_{ii}} \;, \; i = 1, \ldots n$$

Linear Systems of Equations
Iterative Methods

Convergence

$$\left\|\overline{\mathbf{x}}^{(k+1)} - \overline{\mathbf{x}}\right\| \rightarrow 0 \ \text{ for } \ k \rightarrow \infty$$

Iteration – Matrix form

$$\overline{\mathbf{x}}^{(k+1)} = \overline{\overline{\mathbf{B}}}\overline{\mathbf{x}}^{(k)} + \overline{\mathbf{c}}\ , \ k = 0, \ldots$$

Decompose Coefficient Matrix

$$\overline{\overline{\mathbf{A}}} = \overline{\overline{\mathbf{D}}}\left(\overline{\overline{\mathbf{L}}} + \overline{\overline{\mathbf{I}}} + \overline{\overline{\mathbf{U}}}\right)$$

with

$$\overline{\overline{\mathbf{D}}} = \text{diag } a_{ii}$$

$$\overline{\overline{\mathbf{L}}} = \begin{cases} a_{ij}/a_{ii}\ , & i > j \\ 0, & i \leq j \end{cases}$$

Note: NOT LU-factorization

$$\overline{\overline{\mathbf{U}}} = \begin{cases} a_{ij}/a_{ii}\ , & i < j \\ 0, & i \geq j \end{cases}$$

Jacobi's Method

$$\overline{\mathbf{x}}^{(k+1)} = -\left(\overline{\overline{\mathbf{L}}} + \overline{\overline{\mathbf{U}}}\right)\overline{\mathbf{x}}^{(k)} + \overline{\overline{\mathbf{D}}}^{-1}\overline{\mathbf{b}}$$

Iteration Matrix form

$$\overline{\overline{\mathbf{B}}} = -\left(\overline{\overline{\mathbf{L}}} + \overline{\overline{\mathbf{U}}}\right)$$

$$\overline{\mathbf{c}} = \overline{\overline{\mathbf{D}}}^{-1}\overline{\mathbf{b}}$$

Convergence Analysis

$$\begin{aligned} \overline{\mathbf{x}}^{(k+1)} &= \overline{\overline{\mathbf{B}}}\overline{\mathbf{x}}^{(k)} + \overline{\mathbf{c}} \\ \overline{\mathbf{x}} &= \overline{\overline{\mathbf{B}}}\overline{\mathbf{x}} + \overline{\mathbf{c}} \\ \hline \overline{\mathbf{x}}^{(k+1)} - \overline{\mathbf{x}} &= \overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right) \\ &= \overline{\overline{\mathbf{B}}} \cdot \overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k-1)} - \overline{\mathbf{x}}\right) \\ &\ \ \cdot \\ &= \overline{\overline{\mathbf{B}}}^{k+1}\left(\overline{\mathbf{x}}^{(0)} - \overline{\mathbf{x}}\right) \end{aligned}$$

$$\left\|\overline{\mathbf{x}}^{(k+1)} - \overline{\mathbf{x}}\right\| \leq \left\|\overline{\overline{\mathbf{B}}}^{k+1}\right\| \left\|\overline{\mathbf{x}}^{(0)} - \overline{\mathbf{x}}\right\| \leq \left\|\overline{\overline{\mathbf{B}}}\right\|^{k+1} \left\|\overline{\mathbf{x}}^{(0)} - \overline{\mathbf{x}}\right\|$$

Sufficient Convergence Condition

$$\left\|\overline{\overline{\mathbf{B}}}\right\| < 1$$

Linear Systems of Equations
Iterative Methods

Sufficient Convergence Condition

$$\left\|\overline{\overline{\mathbf{B}}}\right\| < 1$$

Jacobi's Method

$$b_{ij} = -\frac{a_{ij}}{a_{ii}} \ , \ i \neq j$$

$$\left\|\overline{\overline{\mathbf{B}}}\right\|_\infty = \max_i \sum_{j=1, j\neq i}^{n} \frac{|a_{ij}|}{|a_{ii}|}$$

Sufficient Convergence Condition

$$\sum_{j=1, j\neq i}^{n} |a_{ij}| < |a_{ii}|$$

Diagonal Dominance

Stop Criterion for Iteration

$$\begin{aligned} \overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}} &= \overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k-1)} - \overline{\mathbf{x}}\right) \qquad \pm\overline{\overline{\mathbf{B}}}\,\overline{\mathbf{x}}^{(k)} \\ &= -\overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}^{(k-1)}\right) + \overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right) \end{aligned}$$

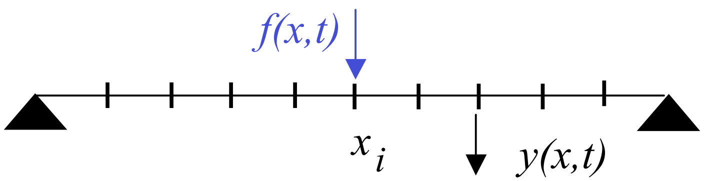
$$\left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right\| \leq \left\|\overline{\overline{\mathbf{B}}}\right\| \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}^{(k-1)}\right\| + \left\|\overline{\overline{\mathbf{B}}}\right\| \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right\|$$

$$\left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right\| \leq \frac{\left\|\overline{\overline{\mathbf{B}}}\right\|}{1 - \left\|\overline{\overline{\mathbf{B}}}\right\|} \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}^{(k-1)}\right\|$$

$$\left\|\overline{\overline{\mathbf{B}}}\right\| < 1/2 \Rightarrow \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right\| \leq \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}^{(k-1)}\right\|$$

Linear Systems of Equations
Tri-diagonal Systems

Forced Vibration of a String



Harmonic excitation

$$f(x,t) = f(x)\cos(\omega t)$$

Differential Equation

$$\frac{d^2y}{dx^2} + k^2 y = f(x)$$

Boundary Conditions

$$y(0) = 0\,, \quad y(L) = 0$$

Finite Difference

$$\left.\frac{d^2y}{dx^2}\right|_{x_i} \simeq \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2}$$

Discrete Difference Equations

$$y_{i-1} + ((kh)^2 - 2)y_i + y_{i+1} = h^2 f(x_i)$$

Matrix Form

$$\begin{bmatrix} (kh)^2-2 & 1 & \cdot & \cdot & \cdot\;\cdot & 0 \\ 1 & (kh)^2-2 & 1 & & & \cdot \\ \cdot & & \cdot & \cdot & & \cdot \\ \cdot & & 1 & (kh)^2-2 & 1 & \cdot \\ \cdot & & & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot\;\;1 & (kh)^2-2 \end{bmatrix} \bar{\mathbf{x}} = \left\{ \begin{array}{c} f(x_1)h^2 \\ \cdot \\ \cdot \\ f(x_i)h^2 \\ \cdot \\ \cdot \\ f(x_n)h^2 \end{array} \right\}$$

Tridiagonal Matrix

$kh < 1 \;\; or \;\; kh > \sqrt{3}$ Symmetric, positive definite: No pivoting needed

Linear Systems of Equations
Tri-diagonal Systems

Finite Difference

$$\left.\frac{d^2y}{dx^2}\right|_{x_i} \simeq \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2}$$

Discrete Difference Equations

$$y_{i-1} + ((kh)^2 - 2)y_i + y_{i+1} = h^2 f(x_i)$$

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Tridiagonal Matrix

$$kh > 2 \Rightarrow h > \frac{2}{k}$$

Diagonally Dominance

vib_ string.m

```
n=99;
L=1.0;
h=L/(n+1);
k=2*pi;
kh=k*h
x=[h:h:L-h]';
a=zeros(n,n);
f=zeros(n,1);
o=1
```

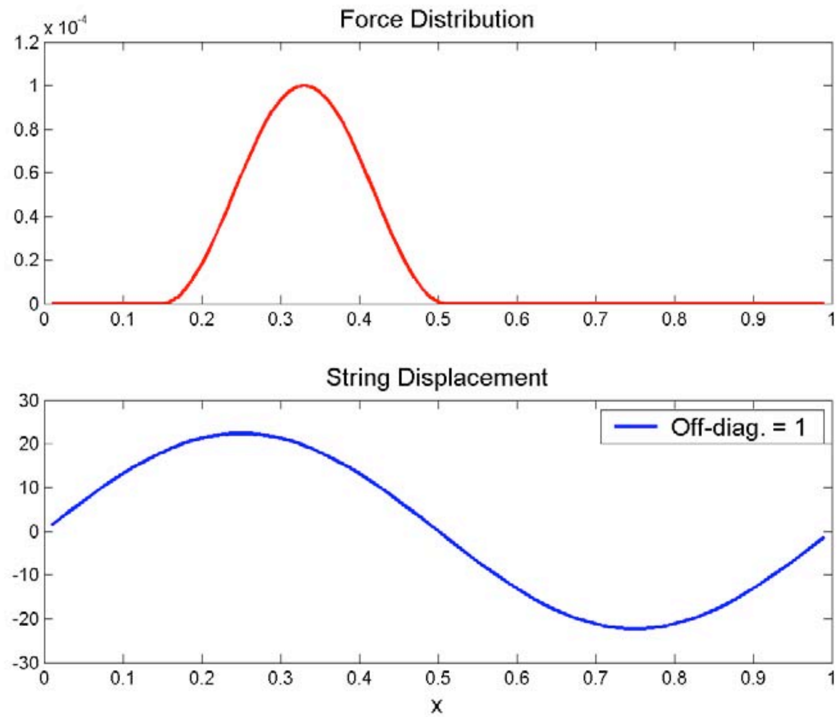
Off-diagonal values

```
a(1,1) =kh^2 - 2;
a(1,2)=o;

for i=2:n-1
    a(i,i)=a(1,1);
    a(i,i-1) = o;
    a(i,i+1) = o;
end
a(n,n)=a(1,1);
a(n,n-1)=o;
% Hanning windowed load
nf=round((n+1)/3);
nw=round((n+1)/6);
nw=min(min(nw,nf-1),n-nf);
nw1=nf-nw;
nw2=nf+nw;
f(nw1:nw2) = h^2*hanning(nw2-nw1+1);

figure(1)
hold off
subplot(2,1,1); plot(x,f,'r');
% Exact solution
y=inv(a)*f;
subplot(2,1,2); plot(x,y,'b');
```

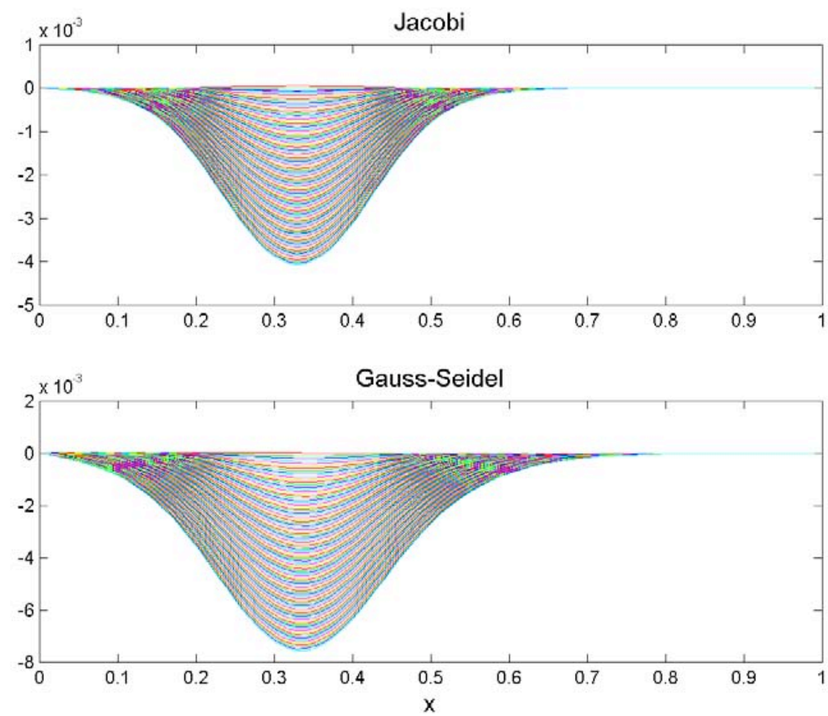
```
% Iterative solution using Jacobi and Gauss-Seidel
b=-a;
c=zeros(n,1);
for i=1:n
    b(i,i)=0;
    for j=1:n
        b(i,j)=b(i,j)/a(i,i);
        c(i)=f(i)/a(i,i);
    end
    end

nj=100;
xj=f;
xgs=f;

figure(2)
nc=6
col=['r' 'g' 'b' 'c' 'm' 'y']
hold off
for j=1:nj
    xj=b*xj+c;
    xgs(1)=b(1,2:n)*xgs(2:n) + c(1);
    for i=2:n-1
        xgs(i)=b(i,1:i-1)*xgs(1:i-1) + b(i,i+1:n)*xgs(i+1:n) +c(i);
    end
    xgs(n)= b(n,1:n-1)*xgs(1:n-1) +c(n);
    cc=col(mod(j-1,nc)+1);
    subplot(2,1,1); plot(x,xj,cc); hold on;
    subplot(2,1,2); plot(x,xgs,cc); hold on;
    hold on
end
```

vib_ string.m
o=1.0, , k=2*pi, h=.01, kh<2

Exact Solution



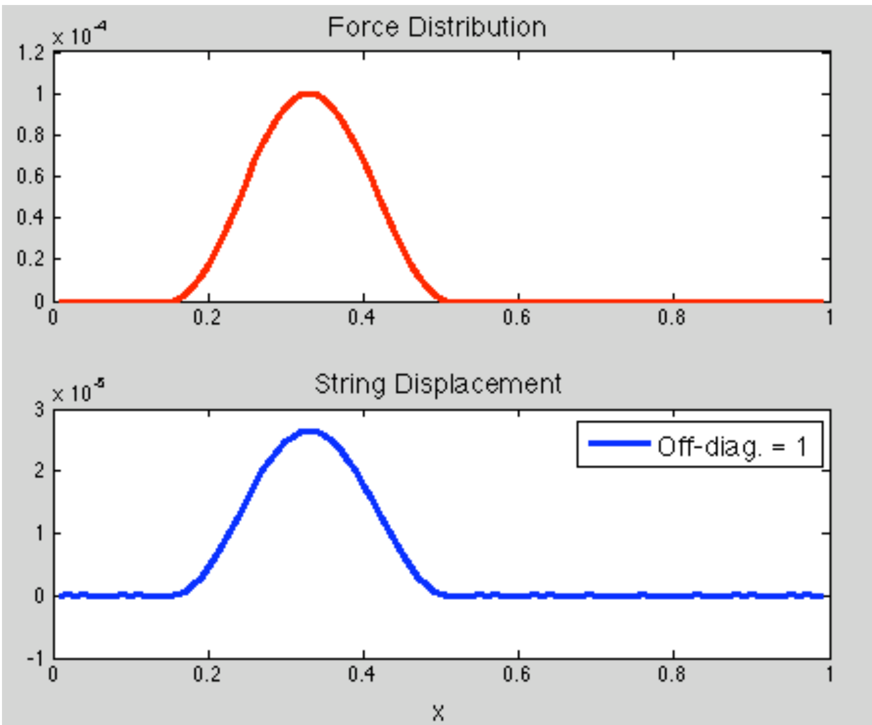
Iterative Solutions



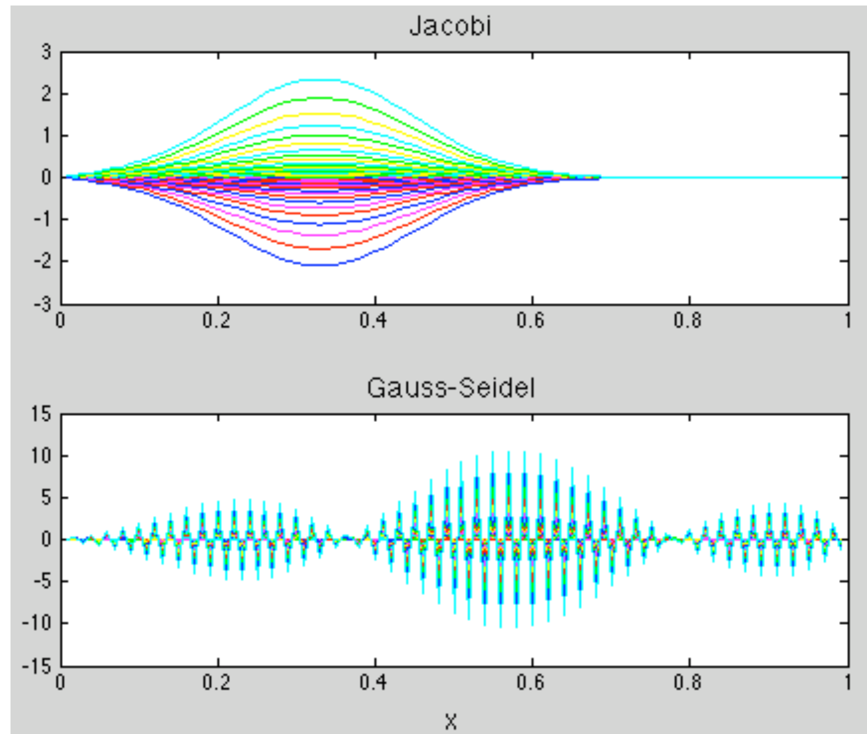
Coefficient Matrix Not Strictly Diagonally Dominant

vib_ string.m
o=1.0, , k=2*pi*31, h=.01, kh<2

Exact Solution



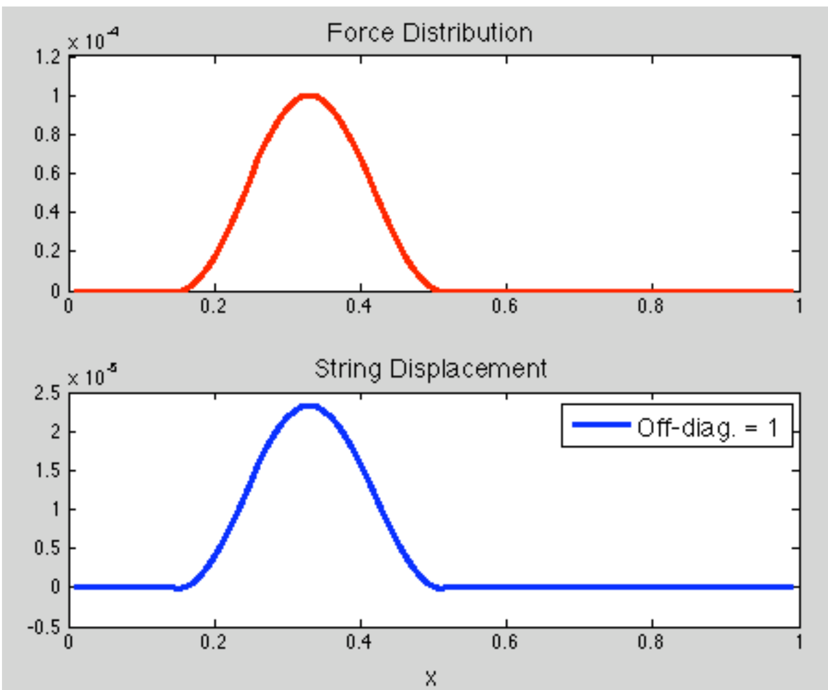
Iterative Solutions



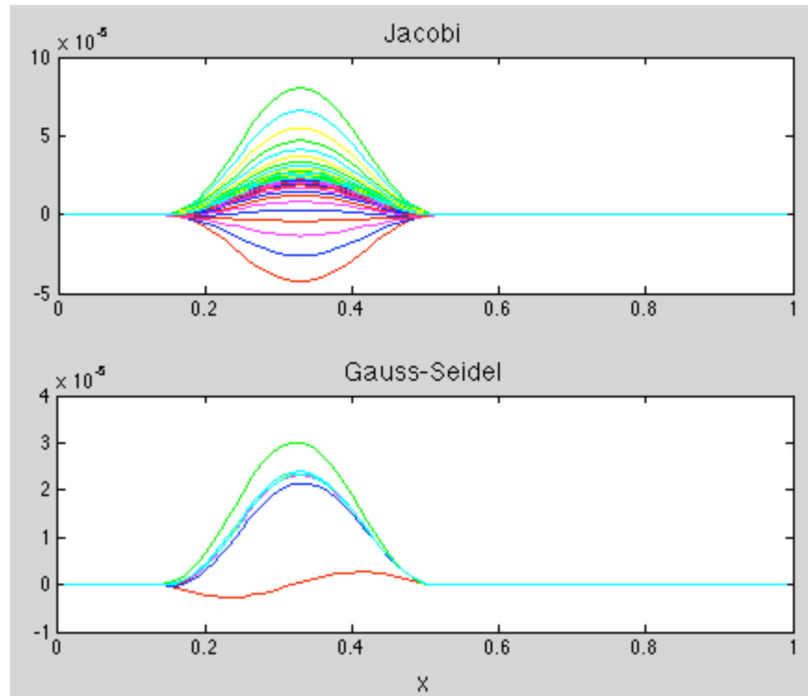
Coefficient Matrix Not Strictly Diagonally Dominant

vib_ string.m
o=1.0, k=2*pi*33, h=.01, kh>2

Exact Solution



Iterative Solutions

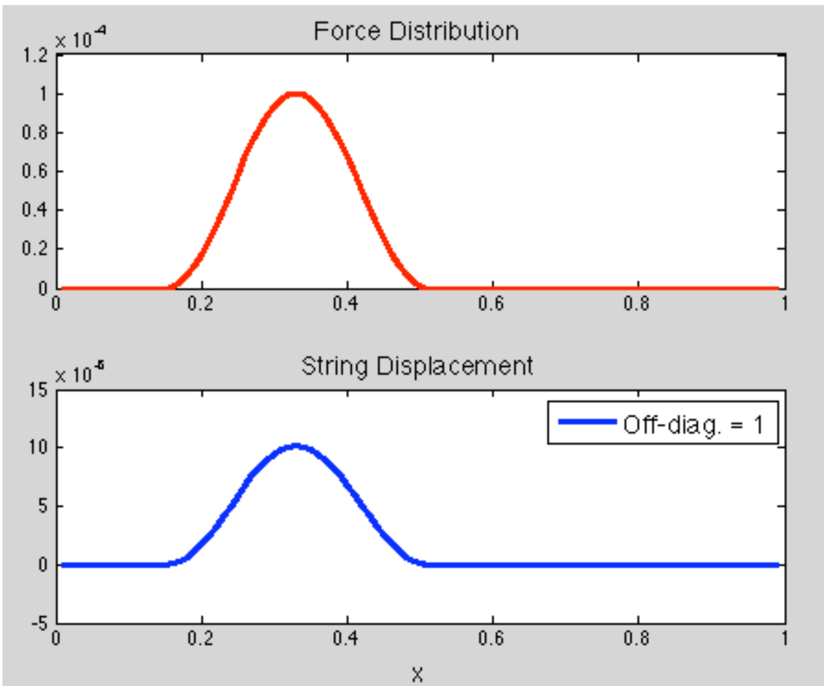


Coefficient Matrix Strictly Diagonally Dominant

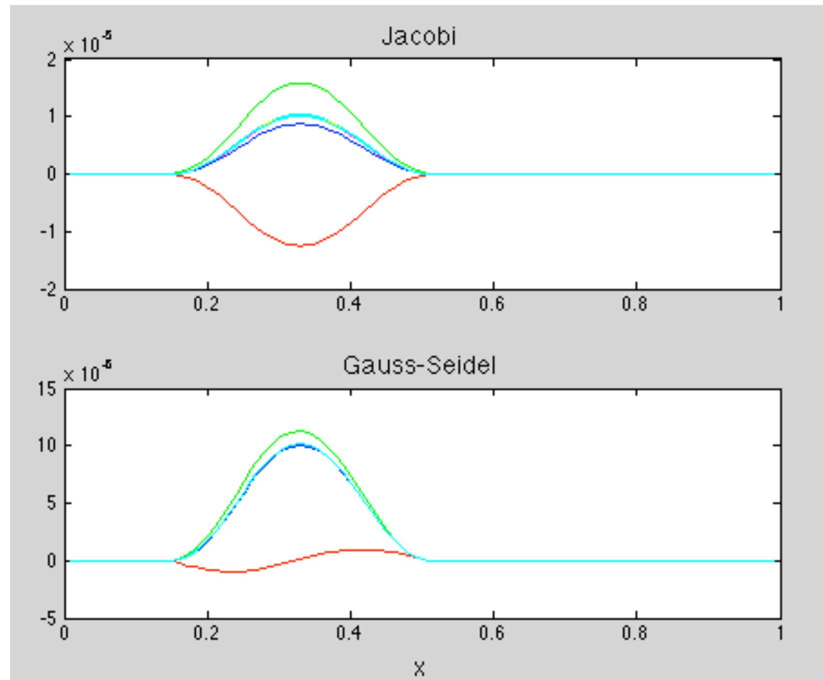
vib_ string.m

o=1.0, k=2*pi*50, h=.01, kh>2

Exact Solution



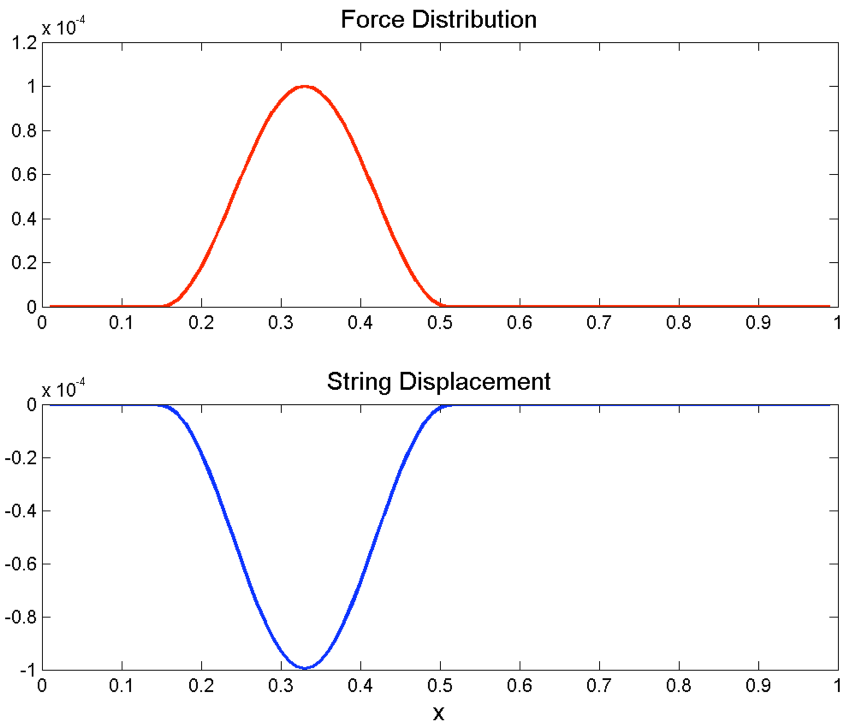
Iterative Solutions



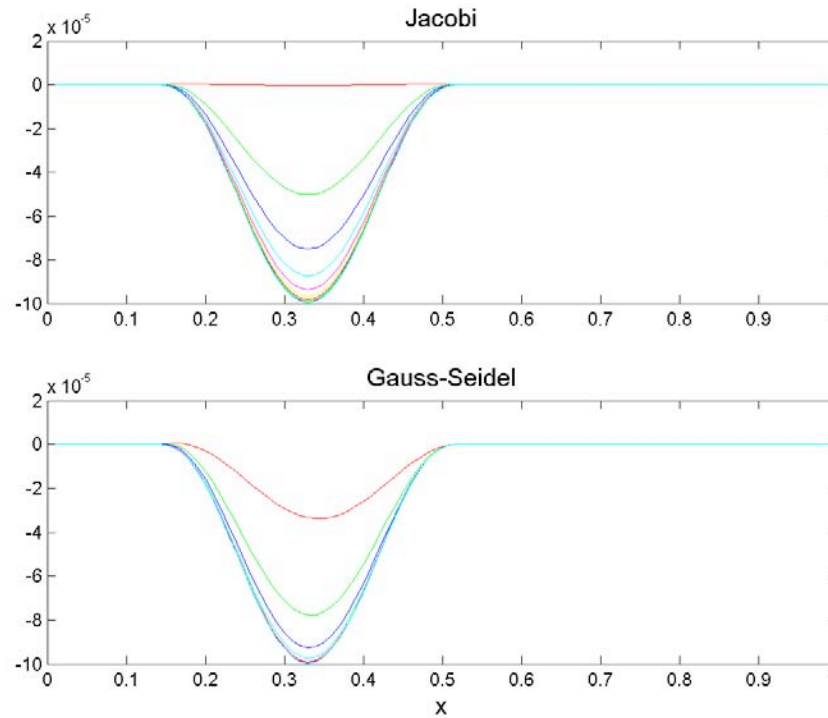
Coefficient Matrix Strictly Diagonally Dominant

vib_ string.m
o = 0.5, k=2*pi, h=.01

Exact Solution



Iterative Solutions



Coefficient Matrix Strictly Diagonally Dominant

Iterative Methods: General Principles

- Major application: sparse matrixes, unstructured mesh
- Key property: Self Correcting (avoids accumulations of errors unlike Gauss methods) $\Rightarrow$ More robust than direct methods
- Linear systems $\Rightarrow$ Usually convergence independent of initial guess
- General Formula

$$Ax_e = b$$

$$x_{i+1} = B_i x_i + C_i b \qquad i = 0,1,2,.....$$

- Numerical convergence stop:

$$i \le n_{\max}$$

$$\|x_i - x_{i-1}\| \le \varepsilon$$

$$\|r_i - r_{i-1}\| \le \varepsilon, \ \ where \ \ r_i = Ax_i - b$$

$$\|r_i\| \le \varepsilon$$

Convergence of Jacobi and Gauss-Seidel

- General criteria:

1. $x_e = B_i x_e + C_i b = B_i x_e + C_i A x_e = (B_i + C_i A) x_e \Rightarrow B_i + C_i A = I$

2. $\lim_{i\to\infty} \| B_i B_{i-1} \dots B_2 B_1 B_0 \| = 0$

- Special case of stationary iterations:

$$B_i = B,\ C_i = C \qquad i = 0,1,2,\dots$$

- Theorem: above convergent for any guess if spectral radius of "B" is smaller than one ($\rho(B) < 1$).
- Definition:

$$\rho(B) = \max_{j=1\dots n} |\lambda_j|, \quad where\ |\lambda_j| = eigenvalue(B_{n\times n})$$

- Note: $\|B\| < 1\ in\ any\ matrix\ norm \Rightarrow \rho(B) < 1$

but commonly use infinity norm due to simplicity

$$\|B\|_\infty = \max_{i=1\dots n} \left(\sum_{j=1}^{n} |b_{ij}|\right)$$

Convergence of Jacobi and Gauss-Seidel

- Jacobi:

$$Dx + (L + U)x = b$$

$$x_{i+1} = -D^{-1}(L + U)x_i + D^{-1}b$$

- Gauss-Seidel:

$$(D + L)x + Ux = b$$

$$x_{i+1} = -(D + L)^{-1}Ux_i + (D + L)^{-1}b$$

- Both converge for diagonally dominant matrixes
- Gauss-Seidel convergent for positive definite matrix
- Also Jacobi convergent for "A" if
  - "A" symmetric and {D, D+L+U, D-L-U} are all positive definite

Successive Over-relaxation (SOR) Method

- Interpolate or extrapolate the Gauss-Seidel at each sub-step:

$$x_{i+1}^{k} = \omega \bar{x}_{i+1}^{k} + (1-\omega) x_{i}^{k}, \quad where \quad \bar{x}_{i+1}^{k} \quad Gauss-Seidel \ \ guess \ for \ x_{i+1}^{k}$$

- Matrix format:

$$x_{i+1} = -(D+\omega L)^{-1}\{\omega U-(1-\omega)D\}x_i + \omega(D+\omega L)^{-1} b$$
$$\omega = 1 \Rightarrow \ SOR \equiv Gauss - Seidel$$

- For "A" symmetric and positive definite:

$$Converges \ \ for \ any \ \omega \in (0,2)$$

- Proper value of over-relaxation parameter (ω) leads to fast convergence, but hard to find:

$$\omega = \omega_{opt} = ?$$

Gradient Methods

- Applicable to physically important matrixes: "symmetric and positive definite" ones
- Construct the equivalent optimization problem

$$Q(x) = \frac{1}{2} x^T A x - x^T b$$

$$\frac{dQ(x)}{dx} = Ax - b$$

$$\frac{dQ(x_{opt})}{dx} = 0 \Rightarrow x_{opt} = x_e, \quad where \quad Ax_e = b$$

- Propose step rule

$$x_{i+1} = x_i + \alpha_{i+1} v_{i+1}$$

- Common methods
  - Gauss-Seidel
  - Steepest descent
  - Conjugate gradient

Steepest Descent Method

- Move exactly in the negative direction of Gradient

$$\frac{dQ(x)}{dx} = Ax - b = -(b - Ax) = -r$$

$$r : residual, \;\; r_i = b - Ax_i$$

- Step rule

$$x_{i+1} = x_i + \frac{r_i^T{}_i r_i}{r_i^T A r_i} r_i$$

- Q(x) reduces in each step, but not as effective as conjugate gradient method

Conjugate Gradient Method

A symmetric & positive definite:

for $i \neq j$ *we say* v_i, v_j *orthogonal with respect to A, if* $v_i^T A v_j = 0$

- Proposed in 1952 so that directions v_i are generated by the orthogonalization of residuum vectors.
- Algorithm

$$\boldsymbol{v}_0 = \boldsymbol{r}_0 = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_0$$

do

$$\begin{aligned}
\alpha_i &= (\boldsymbol{v}_i^\top \boldsymbol{r}_i)/(\boldsymbol{v}_i^\top \boldsymbol{A}\boldsymbol{v}_i) \\
\boldsymbol{x}_{i+1} &= \boldsymbol{x}_i + \alpha_i \boldsymbol{v}_i \\
\boldsymbol{r}_{i+1} &= \boldsymbol{r}_i - \alpha_i \boldsymbol{A}\boldsymbol{v}_i \\
\beta_i &= -(\boldsymbol{v}_i^\top \boldsymbol{A}\boldsymbol{r}_{i+1})/(\boldsymbol{v}_i^\top \boldsymbol{A}\boldsymbol{v}_i) \\
\boldsymbol{v}_{i+1} &= \boldsymbol{r}_{i+1} + \beta_i \boldsymbol{v}_i
\end{aligned}$$

until a stop criterion holds

Conjugate Gradient Method

- Accurate solution with "n" iterations, but decent accuracy with much fewer number of iterations
- Only matrix or vector product
- Possible variations for nonsymmetric nonsingular matrices:
  - generalized minimal residual
  - (stabilized) biconjugate gradients
  - quasi-minimal residual,