Iterative solution of Linear Equations

Introduction

Procedure – general

1) Assume initial values for the variable field

2) Use the nodal finite difference equations one at a time or in groups to obtain an improved value for the variables. Repeat the procedure until a converged solution is obtained.

Advantages

Iterative methods are used because:
Requires less computer storage.
Is reasonably computational fast.

There is, however, no guarantee that a converged solution can be obtained.

Symbols to be used

$\Phi =$ exact solution of differential equation

$\phi =$ exact solution of finite difference equations

$\hat{\phi} =$ computer solution to finite difference equations

Convergence

The solution is said to be converged when

$$\text{Limit} \quad \hat{\phi}^{(j)} = \phi$$

$$j \to \infty$$

where j is an index for the iteration number.

Procedure – details

Rearrange coefficient matrix

Solution required for $H\phi = d$

Modify H matrix by taking each equation and dividing it by the diagonal coefficient to form a "C" matrix

$$c_{ij} = \frac{h_{ij}}{h_{ii}} \quad , \quad g_i = \frac{d_i}{h_{ii}}$$

New Expression

$$C\phi = g$$

The C Matrix will have all its diagonal elements with the value 1.

One Iterative set of equations

$\phi^{(O)}$ – initial value of variable

for the calculation

$$C\hat{\phi}^{(j)} \cong g$$

residual $r^{(j)} = g - C\hat{\phi}^{(j)}$

Introduce the identity matrix,

$$\mathbf{I} = \begin{vmatrix} 1 & & & & \\ & 1 & & \text{"0"} & \\ & & 1 & & \\ & & & 1 & \\ & \text{"0"} & & & 1 \\ & & & & & 1 \end{vmatrix}$$

Define $B = I - C$ or $C = I - B$,

$$\begin{vmatrix} 1 & c_{12} & c_{13} & c_{14} \\ c_{21} & 1 & c_{23} & c_{24} \\ c_{31} & c_{32} & 1 & c_{34} \\ c_{41} & c_{42} & c_{43} & 1 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix} - \begin{vmatrix} 0 & c_{12} & c_{13} & c_{14} \\ c_{21} & 0 & c_{23} & c_{24} \\ c_{31} & c_{32} & 0 & c_{34} \\ c_{41} & c_{42} & c_{43} & 0 \end{vmatrix}$$

so an iteration can be defined as:

$$I\,\hat{\phi}^{(j+1)} = g + B\hat{\phi}^{(j)} \text{ or } \hat{\phi}^{(j+1)} = g + B\hat{\phi}^{(j)}$$

This is known as the **Jacobi** method

Error propagation

Given a starting guess at the solution $\hat{\phi}^{(O)}$

$$\hat{\phi}^{(1)} = g + B\hat{\phi}^{(O)}$$
$$\hat{\phi}^{(2)} = g + B\hat{\phi}^{(1)} = g(1+B) + B^2\hat{\phi}^{(O)}$$
$$\hat{\phi}^{(3)} = g(1+B+B^2) + B^3\hat{\phi}^{(O)}$$
$$\vdots$$
$$\hat{\phi}^{(N)} = g(1+B+B^2+\cdots B^{N-1}) + B^N\hat{\phi}^{(O)}$$

Introduce computational error

$$\in^{(j)} \equiv \phi - \phi^{(j)}$$
$$= \phi - (g + B\hat{\phi}^{(j-1)})$$
$$= (\phi - g) - B\hat{\phi}^{(j-1)}$$

Note $(I - B)\phi = g$

So $\phi - g = B\phi$

$$\in^{(j)} = B(\phi - \hat{\phi}^{(j-1)})$$
$$= B \in^{(j-1)}$$
$$\in^{(j-1)} = B \in^{(j-2)}$$
$$\in^{(j-2)} = B \in^{(j-3)}$$
$$\vdots$$
$$\in^{(2)} = B \in^{(1)}$$
$$\in^{(1)} = B \in^{(O)}$$

Back substitute to obtain

$\in^{(j)} = B^j \in^{(O)}$

Indicating that errors are propagated in an identical manner to the propagation of ϕ.

Convergence

Limit $\hat{\phi}^{(j)} = \phi$ as $j \to \infty$

residual $r^{(j)} = g - C\hat{\phi}^{(j)}$

Convergence checks

L_2 Norm $R^{(j)} \equiv \left[\sum (r^{(j)})^2\right]^{1/2} \leq \delta$

Limit $R^{(j)} = 0$ (with machine accuracy)

$j \to \infty$

Other tests (all risky for certain iteration schemes)

Maximum (Local) $\left|\hat{\phi}^{(j+1)} - \hat{\phi}^{(j)}\right| \leq \delta$

Maximum (Global) $\sum \left|(\hat{\phi}^{(j+1)} - \hat{\phi}^{(j)})\right| \leq \delta$

or $\left[\sum (\hat{\phi}^{(j+1)} - \hat{\phi}^{(j)})^2\right]^{1/2} \leq \delta$

Will the iterative solution selected converge?

Error propagation

$\in^{(j)} = B^j \in^{(O)}$

To answer this question we look at the characteristics roots (eigenvalues) of the B matrix.

$$B\gamma = \lambda\gamma$$
$$\uparrow \quad \uparrow$$

Latent root of "B" matrix

γ is the eigenvector satisfying the equality

Re-arranging

$$(B - \lambda)\gamma = O$$

we want a non-trivial solution which only occurs if $\left|B - |\lambda|\right| = O$

$$\begin{vmatrix} b_{11}-\lambda & b_{12} & b_{13} & \bullet & \bullet & \bullet & b_{1N} \\ b_{21} & b_{11}-\lambda & b_{23} & \bullet & \bullet & \bullet & b_{2N} \\ b_{31} & b_{32} & b_{33}-\lambda & b_{34} & \bullet & \bullet & b_{3N} \end{vmatrix}$$

Expand as a polynomial

$$\ell_O - \ell_1\lambda + \ell_2\lambda^2 + \cdots(-1)^N \ell_N \lambda^N = 0$$

The eigenvalues are the λ's

The eigenvalues with the largest absolute value (λ_{MAX}) is called the **spectral radius** of the matrix $\lambda_{SR.}$ The above error vector will converge to zero if:

$$|\lambda_{SR}| < 1$$

We reach that conclusion by writing the original error vector as a linear combination of the eigenvectors and noting that $\mathbf{B}^n\gamma = \lambda^n\gamma$

Gauss-Siedel Iteration Method

Introduce a lower (L) and upper (U) matrix to the Jacobi B matrix such that

$$B = L + U$$

$$\begin{vmatrix} 0 & c_{12} & c_{13} & c_{14} \\ c_{21} & 0 & c_{23} & c_{24} \\ c_{31} & c_{32} & 0 & c_{34} \\ c_{41} & c_{42} & c_{43} & 0 \end{vmatrix} = \begin{vmatrix} 0 & & & \\ c_{21} & 0 & & \\ c_{31} & c_{32} & 0 & \\ c_{41} & c_{42} & c_{43} & 0 \end{vmatrix} + \begin{vmatrix} 0 & c_{12} & c_{13} & c_{14} \\ & 0 & c_{23} & c_{24} \\ & & 0 & c_{34} \\ & & & 0 \end{vmatrix}$$

Jacobi becomes:

$$\hat{\phi}^{(j+1)} = g + (L + U)\hat{\phi}^{(j)}$$

Alter this so that the new values of $\hat{\phi}^{(j+1)} = L\hat{\phi}^{(j+1)} + U\hat{\phi}^{(j)} + g$

Rewrite the expression as:

$$(I - L)\hat{\phi}^{(j+1)} = U\hat{\phi}^{(j)} + g$$

$$\hat{\phi}^{(j+1)} = (I - L)^{-1} U\hat{\phi}^{(j)} + (I - L)^{-1} g$$

Recall the Jacobi equation $\hat{\phi}^{(j+1)} = g + B\hat{\phi}^{(j)}$

So $(I - L)^{-1}$ U is analogous to the "B" matrix the Jacobi iteration, implying that the eigenvalues of $(I - L)^{-1}$ U must be less than 1 for convergence.

Also the error propagation is

$$\in^{(j)} = \left[(I - L)^{-1} U\right]^j \in^{(O)}$$

Example assume $\Delta x = \Delta y = 1$ in a 2-D Cartisian Laplace equation for a problem defined with boundary conditions:

$\phi(0,y) = 100$
$\phi(x,3) = 100$
$\phi(x,0) = 0$
$\phi(4,y) = 0$

Locate mesh points at (x,y) = (1,1), (1,2), (2,1), (2,2), (3,1), (3,2)

If we set the order of equations in the system corresponding to the sequence of points: {(1,2), (2,2), (3,2), (1,1), (2,1), (3,1)}The finite difference equation is:

$$\begin{vmatrix} 1 & -\frac{1}{4} & 0 & -\frac{1}{4} & 0 & 0 \\ -\frac{1}{4} & 1 & -\frac{1}{4} & 0 & -\frac{1}{4} & 0 \\ 0 & -\frac{1}{4} & 1 & 0 & 0 & -\frac{1}{4} \\ -\frac{1}{4} & 0 & 0 & 1 & -\frac{1}{4} & \end{vmatrix} \begin{vmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{vmatrix} = \begin{vmatrix} \frac{200}{4} \\ \frac{100}{4} \\ \frac{100}{4} \\ \frac{100}{4} \\ 0 \\ 0 \end{vmatrix}$$

$C = I - B$

$= I - L - U$

$$\begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 & 0 & 0 \\ \frac{1}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 \end{vmatrix} \quad \begin{vmatrix} 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix}$$

L U

Equations for Gauss Seidel $\hat{\phi}^{(j+1)} = L\hat{\phi}^{(j+1)} + U\hat{\phi}^{(j)} + g$

Node 1 $$\hat{\phi}_1^{(j+1)} = \frac{\hat{\phi}_2^{(j)}}{4} + \frac{\hat{\phi}_4^{(j)}}{4} + 50$$

Node 5 $$\hat{\phi}_5^{(j+1)} = \frac{\hat{\phi}_2^{(j+1)}}{4} + \frac{\hat{\phi}_4^{(j+1)}}{4} + \frac{\phi_6^{(j)}}{4} + 0$$

Change the equation sequence to: {(1,2), (1,1),(2,1),(2,2), (3,2), (3,1)}, and the equations shift in form, changing the results of the iteration.

Node 1 $$\hat{\phi}_1^{(j+1)} = \frac{\hat{\phi}_2^{(j)}}{4} + \frac{\hat{\phi}_4^{(j)}}{4} + 50$$

Node 5 $$\hat{\phi}_5^{(j+1)} = \frac{\hat{\phi}_2^{(j)}}{4} + \frac{\hat{\phi}_4^{(j+1)}}{4} + \frac{\hat{\phi}_6^{(j)}}{4} + 0$$

Extrapolated Liebmann method or Successive Over-Relaxation (SOR):

Start with a basic Gauss-Seidel method (we can also apply this to other methods):

$$\hat{\phi}^{(j+1)} = L\hat{\phi}^{(j+1)} + U\hat{\phi}^{(j)} + g$$

Subtract $$\hat{\phi}^{(j+1)} - \phi^{(j)} = \overbrace{L\hat{\phi}^{(j+1)} + U\hat{\phi}^{(j)} + g - \hat{\phi}^{(j)}}$$

These terms represent the change in $\hat{\phi}$ as we go from the j^{th} iteration to the $j+1^{th}$ iteration.

Multiply that change by ω (over-under relaxation factor). Generally $0 < \omega < 2$

$$\hat{\phi}^{(j+1)} - \hat{\phi}^{(j)} = \omega\left[L\hat{\phi}^{(j+1)} + U\phi^{(j)} + g - \hat{\phi}^{(j)}\right]$$
$$\hat{\phi}^{(j+1)} = (1-\omega)\hat{\phi}^{(j)} + \omega\left[L\hat{\phi}^{(j+1)} + U\hat{\phi}^{(j)} + g\right]$$

$$(I - \omega L)\hat{\phi}^{(j+1)} = (1-\omega)I\hat{\phi}^{(j)} + \omega U\hat{\phi}^{(j)} + \omega g$$
$$\hat{\phi}^{(j+1)} = \underbrace{\left[(1-\omega L)^{-1}\left[(1-\omega)I + \omega U\right]\right]}_{\text{B Matrix}}\hat{\phi}^{(j)} + (1-\omega L)^{-1}\omega g$$

Error can be written as:

$$\in^{(j+1)} = \left[(1-\omega l)^{-1}[(1-\omega)I + \omega U]\right]^{(j+1)} \in^{(O)}$$

Require that $\left|\lambda_{SR|B}\right| < 1$, for convergence

Note: If $\omega = 1$ we have the Gauss Seidel method.

Example:

Use previous example problem with the original variable ordering.

$$(I - \omega L)\hat{\phi}^{(j+1)} = (1-\omega)I\hat{\phi}^{(j)} + \omega U\hat{\phi}^{(j)} + \omega g$$

Node 3 $$\hat{\phi}_3^{(j+1)} - \frac{\omega\hat{\phi}_2^{(j+1)}}{4} = (1-\omega)\hat{\phi}_3^{(j)} + \frac{\omega\hat{\phi}_6^{(j)}}{4} + 25\omega$$

Node 6 $$\hat{\phi}_6^{(j+1)} - \frac{\omega\hat{\phi}_3^{(j+1)}}{4} - \frac{\omega\hat{\phi}_5^{(j+1)}}{4} = (1-\omega)\hat{\phi}_6^{(j)} + 0$$

Some important characteristics of the "C" Matrix

The "C" Matrix has Property "A" if

- Differential equation does not have mixed derivative terms.
  - The region is subdivided using a rectangular grid pattern, and the nodes are labeled in an alternating fashion.
    - Black Nodes
    - White Nodes

● ○ ● ○ ● ○

○ ● ○ ● ○ ●

● ○ ● ○ ● ○

Values at iteration j+1 for black points determined from the iteration equation depend only on values at white points at iteration j. Values at iteration j+1 for black points determined from the iteration equation depend only on values at white points at iteration j.

$$\phi_{WHITE} = f(\phi_{BLACK})$$

and

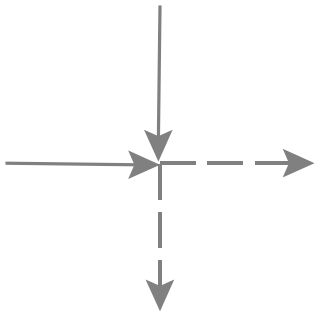
$$\phi_{BLACK} = f(\phi_{WHITE})$$

Consistent ordering

If one has consistent ordering the values of the variable field at iteration (j+1) is independent of the order in which equations are entered in the C matrix.

Simple test: Five point approximation of $\nabla^2 T$ -

- Matrix ("C") has property A.
- Select a search pattern.
- Move node by node through the grid following the order of equations in the C matrix. Look at the four surrounding nodes. If an adjacent node is not already connected to the selected node, draw an arrow from it with the head of the arrow located at the surrounding node.



- Move around a rectangle created by the grid lines. If you find two arrows going with you and two arrows going against you, the search pattern has consistent ordering.
- If three arrows are with you and one against (or 3 against and 1 with you) you do not have consistent ordering.

Why do I care about "property A" and consistent ordering? Mathematicians have shown that when matrices have these properties I have some hope of picking a good value for the over-relaxation factor for an SOR method.

Example
Poisson Equation

$$\nabla^2 \phi = f(x, y)$$

Evaluated on a rectangular grid with $\Delta x = \Delta y = h$, P nodes in the x direction and q nodes in the y direction.

ϕ known on all boundaries

Spectral radius for Jacobi method

$$\lambda_{SR} = \frac{1}{2}\left[\cos\frac{\pi}{P} + \cos\frac{\pi}{q}\right]$$

for $P = 4 \qquad q = 4$

$$\lambda_{SR} = \frac{1}{2}\left[\cos\frac{\Pi}{4} + \cos\frac{\Pi}{4}\right] = 0.707$$

If 10 x 10 mesh P = 10 q = 10

$$\lambda_{SR} = \cos\frac{\Pi}{10} = 0.95$$

For the Gauss Seidel method

$$\lambda_{SR}\big|_{GS} = \left[\lambda_{SR}\big|_{Jacobi}\right]^2$$

thus

4 x 4 $\lambda_{SR}\big|_{GS} = (0.707)^2 = 0.499$

and

10 x 10 $\lambda_{SR}\big|_{GS} = (0.95)^2 = 0.90$

Asymptotic rate of convergence

$$\in^{(j+1)} = B \in^{(j)}$$

$$\in^{(j+1)} = B^{j+1} \in^{(O)}$$

[A] $B \propto \lambda_{SR}$

so $\in^{(j+1)} \propto \lambda_{SR} \in^{(j)}$

and $\in^{(j+1)} \propto \lambda_{SR}^{j+1} \in^{(O)}$

For normal convergence using expression [A]

$$\lambda_{SR} \propto \frac{\in^{(j+1)}}{\in^{(j)}}$$

Larger λ_{SR} slower convergence

Smaller λ_{SR} faster convergence

Note It is assumed that j is very large.

Asympototic rate of convergence

$$C_R \equiv -\mathrm{Ln}(\lambda_{SR})$$

Look at examples

	C_R	
	4 x 4	10 x 10
Jacobi	0.346	0.051
Gauss-Seidel	0.695	0.105

Gauss-Seidel method converges twice as fast as the Jacobi method.

Note The smaller λ_{SR} the larger C_R i.e. the faster the convergence

Optimum over-under relaxation factor

It has been shown that for an interior node

$\omega_{OPT} = 4\alpha$ with α the smallest root of

$\alpha^2 a^2 - 4\alpha + 1 = 0$

where $a = \cos\frac{\Pi}{P} + \cos\frac{\Pi}{q}$

Example

4 x 4

$a = 2\cos\frac{\Pi}{4} = 1.4142$

$(1.4142)^2\alpha^2 - 4\alpha + 1 = 0$

$\alpha = \frac{4 \pm \sqrt{16 - 4(1.4142)^2}}{2(1.4142)^2} = \text{or } \begin{matrix} 1.707 \\ 0.293 \end{matrix}$ $\therefore \omega_{OPT} = 4(0.293) = 1.17$

10 x 10

$a = 2\cos\frac{\Pi}{10} = 1.902$

$(1.902)^2\alpha^2 - 4\alpha + 1 = 0$

$\alpha = 0.7236$

or 0.3819

$\omega_{OPT} = 4\alpha = 1.528$

For large values of P and q

$$\alpha \to \frac{1}{2} - \frac{\Pi}{2\sqrt{2}}\left(\frac{1}{P^2} + \frac{1}{q^2}\right)^{\frac{1}{2}}$$

100 x 100 $\omega = 1.937$

General Estimation Procedure:

Use $\omega = \dfrac{2}{1+\sqrt{1-\lambda_{SR}{}^2\big|_{Jacobi}}}$

To estimate the over-relaxation factor with this formula either make an experimental run with a straight Jacobi iteration or use a straight (ω=1) Gauss Seidel and assume:

$$\lambda_{SR}\Big|_{Jacobi} \cong \left[\lambda_{SR}\big|_{GS}\right]^{\frac{1}{2}}$$

i.e. $\omega = \dfrac{2}{1+\sqrt{1-\lambda_{SR}\big|_{GS}}}$

Estimate $\lambda_{SR}\big|_{GS}$ from a ratio of convergence norms.

$$\lambda_{SR} = \text{Limit}_{j \to \infty} \frac{\left\|N_O{}^{(j+1)}\right\|}{\left\|N_O{}^{(j)}\right\|}$$

where $\left\|N_O{}^{(j)}\right\| = \sum_{k=1}^{N}\left|\hat{\phi}_k{}^{(j)} - \hat{\phi}_k{}^{(j-1)}\right|$

or $= \text{MAX}\left|\hat{\phi}_k{}^{(j)} - \hat{\phi}_k{}^{(j-1)}\right|$

or $= \left[\sum_{k=1}^{N}\left[\hat{\phi}_k{}^{(j)} - \hat{\phi}_k{}^{(j-1)}\right]^2\right]^{\frac{1}{2}}$

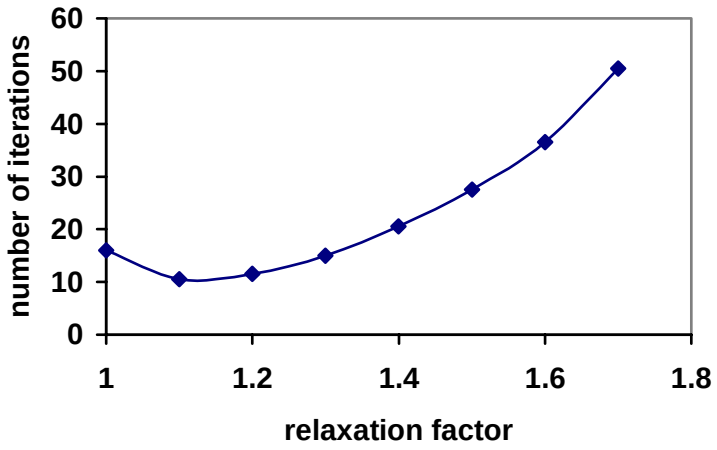


Figure 1 Influence of relaxation factor on number iterations to converge