FDM for Second-Order Elliptic Equations

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Let Ω be a bounded domain in $\mathbb{R}^2$ with boundary $\partial\Omega$. Consider

$$a(x,y)U_{xx} + b(x,y)U_{xy} + c(x,y)U_{yy} + d(x,y,U,U_x,U_y) = 0 \quad (x,y) \in \Omega. \quad (1)$$

If $b^2 - 4ac < 0$ then (1) is called an elliptic PDE.
Example.

- $U_{xx} + U_{yy} = 0$ (Laplace Equation)
- $U_{xx} + U_{yy} = f(x,y)$ (Poisson Equation)

This class of PDEs is calssified as purely boundary value problems (BVPs).
Types of Boundary Conditions.

$$\begin{aligned}
U(x,y) &= g(x,y) \quad (x,y) \in \partial\Omega \ \ (\text{Dirichlet BC (DBC)}) \\
\text{Elliptic PDE} + \text{DBC} &\Longrightarrow \text{Dirichlet BVP} \\
\frac{\partial U}{\partial n} &= h(x,y), \ \ (x,y) \in \partial\Omega \ \ (\text{Neumann BC (NBC)}) \\
\text{Elliptic PDE} + \text{NBC} &\Longrightarrow \text{Neumann BVP} \\
\alpha U(x,y) + \beta \frac{\partial U}{\partial n} &= \tilde{h}(x,y), \ (x,y) \in \partial\Omega, \ \ \alpha, \beta > 0 \\
& \quad (\text{Mixed BC (MBC)}) \\
\text{Elliptic PDE} + \text{MBC} &\Longrightarrow \text{Mixed BVP}
\end{aligned}$$

Finite Difference Approximation. Let Ω be rectangle domain in $\mathbb{R}^2$. Consider the following model problem:

$$\begin{aligned} U_{xx} + U_{yy} &= f(x,y), \quad (x,y) \in \Omega, \\ U(x,y) &= g(x,y), \quad (x,y) \in \partial\Omega. \end{aligned}$$

Let h and k be the mesh parameters along x and y directions, respectively, such that

$$\begin{aligned} x_i &= ih, \quad i = 0,1,2,\ldots \\ y_j &= jk, \quad 0,1,2,\ldots \end{aligned}$$

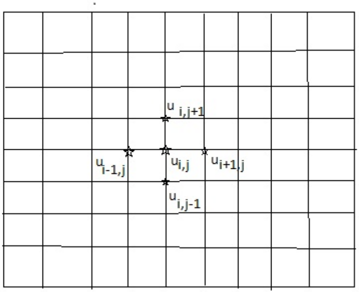
Use of central difference approximation to the partial derivatives at $(x_i, y_j) = (ih, jk)$ mesh point leads to

$$\frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} + \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{k^2} = f_{ij}.$$

With $h = k$, one obtains

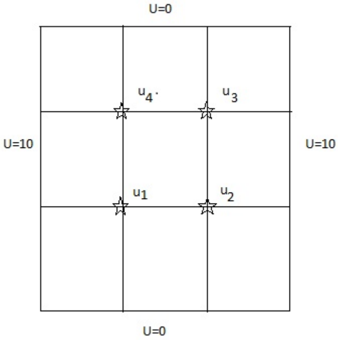
$$u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j} = h^2 f_{ij}.$$

This is known as five-point formula. The local truncation error is of $O(h^2)$ (with $h = k$).



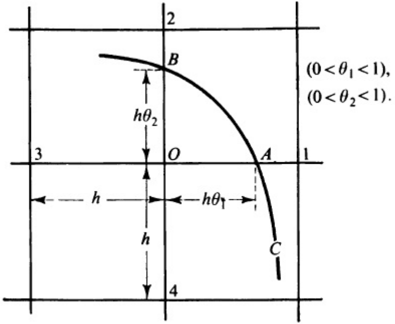
u i,j+1
u i-1,j
u i,j
u i+1,j
u i,j-1

Example. Consider $U_{xx} + U_{yy} = 2, \ \ (x,y) \in \Omega$ with $U(x,y)$ is prescribed on the boundary as shown in figure.



$$
\begin{aligned}
10 + u_2 + u_4 + 0 - 4u_1 &= 2h^2 &\implies&& u_2 + u_4 - 4u_1 &= 2h^2 - 10\\
u_1 + 10 + u_3 + 0 - 4u_2 &= 2h^2 &\implies&& u_1 + u_3 - 4u_2 &= 2h^2 - 10\\
u_2 + 0 + u_4 + 10 - 4u_3 &= 2h^2 &\implies&& u_2 + u_4 - 4u_3 &= 2h^2 - 10\\
u_3 + 10 + u_1 + 0 - 4u_4 &= 2h^2 &\implies&& u_1 + u_3 - 4u_4 &= 2h^2 - 10
\end{aligned}
$$

Formulae for derivatives near curve boundary: We are concerned with the finite difference approximations to the derivatives at a point O, close to the boundary curve C. Let the mesh be square of side h as shown in Figure below.



By Taylor's theorem,

$$U_A = U_0 + h\theta_1 \frac{\partial U_0}{\partial x} + \frac{1}{2} h^2 \theta_1^2 \frac{\partial^2 U_0}{\partial x^2} + O(h^3) \qquad (2)$$

$$U_3 = U_0 - h \frac{\partial U_0}{\partial x} + \frac{1}{2} h^2 \frac{\partial^2 U_0}{\partial x^2} + O(h^3) \qquad (3)$$

Formulae for first-order derivatives: Elimination of the term $\frac{\partial^2 U_0}{\partial x^2}$ from (2)-(3) gives

$$\frac{\partial U_0}{\partial x} = \frac{1}{h}\left\{\frac{1}{\theta_1(1+\theta_1)}U_A - \frac{1-\theta_1}{\theta_1}U_0 - \frac{\theta_1}{(1+\theta_1)}U_3\right\} + O(h^2)$$

Similarly, along y-direction:

$$\frac{\partial U_0}{\partial y} = \frac{1}{h}\left\{\frac{1}{\theta_2(1+\theta_2)}U_B - \frac{1-\theta_2}{\theta_2}U_0 - \frac{\theta_2}{(1+\theta_2)}U_4\right\} + O(h^2)$$

Formulae for second-order derivatives: Elimination of $\frac{\partial U_0}{\partial x}$ from (2) and (3) gives

$$\frac{\partial^2 U_0}{\partial x^2} = \frac{1}{h^2}\left\{\frac{2}{\theta_1(1+\theta_1)}U_A - \frac{2}{\theta_1}U_0 + \frac{2}{(1+\theta_1)}U_3\right\} + O(h)$$

Similarly, along y-direction, one obtains

$$\frac{\partial^2 U_0}{\partial y^2} = \frac{1}{h^2}\left\{\frac{2}{\theta_2(1+\theta_2)}U_B - \frac{2}{\theta_2}U_0 + \frac{2}{(1+\theta_2)}U_4\right\} + O(h)$$

Hence the Poisson equation $U_{xx} + U_{yy} = f(x, y)$ at the point O is approximated by

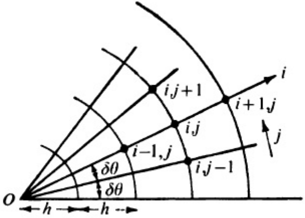
$$\frac{1}{h^2}\left\{ \frac{2u_A}{\theta_1(1+\theta_1)} + \frac{2u_B}{\theta_2(1+\theta_2)} + \frac{2u_3}{(1+\theta_1)} + \frac{2u_4}{(1+\theta_2)} - 2\left(\frac{1}{\theta_1} + \frac{1}{\theta_2}\right) u_0 \right\} = f_0$$

Finite Differences in Polar Co-ordinates.

- Problems involving circular boundaries can usually be solved more conveniently in polar coordinates than cartesian coordinates.
- One can avoid the use of awkward difference formulae near the curved boundary.

Consider Laplace equation in polar coordinates:

$$U_{rr} + \frac{1}{r} U_r + \frac{1}{r^2} U_{\theta\theta} = 0.$$



Define the mesh-point in r-θ plane by the points of intersection of circles $r = ih,\ (i = 1, 2, \ldots)$ and the starightline $\theta = j\delta\theta,\ (j = 0, 1, 2, \ldots)$. Approximating Laplace equation at (i, j) point by

$$\frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} + \frac{1}{ih}\frac{(u_{i+1,j} - u_{i-1,j})}{2h} + \frac{1}{(ih)^2}\frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{(\delta\theta)^2} = 0$$

$$\implies \quad \left(1 - \frac{1}{2i}\right)u_{i-1,j} + \left(1 + \frac{1}{2i}\right)u_{i+1,j} - 2\left(1 + \frac{1}{(i\delta\theta)^2}\right)u_{i,j} + \frac{1}{(i\delta\theta)^2}u_{i,j-1} + \frac{1}{(i\delta\theta)^2}u_{i,j+1} = 0$$

Writing out these equations for $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, m$ and assuming the boundary values for $i = 0$, $i = n + 1$, $j = 0$, and $j = m + 1$ are prescribed, one arrives at the linear system $\mathbf{A}\,\mathbf{u} = \mathbf{b}$. This system needs to be solved for the unknown

$$\mathbf{u} = (u_{1,1}, u_{1,2}, \ldots, u_{1,m}, u_{2,1}, \ldots, u_{2,m}, \ldots, u_{n,1}, u_{n,2}, \ldots, u_{n,m})^t.$$

Iterative Methods for Solving Large Linear Systems

For simplicity, consider the four equations

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

where $a_{ii} \neq 0$, $i = 1(1)4$. Rewriting the above equations as

$$\begin{aligned}
x_1 &= \frac{1}{a_{11}}(b_1 - a_{12}x_2 - a_{13}x_3 - a_{14}x_4) \\
x_2 &= \frac{1}{a_{22}}(b_2 - a_{21}x_1 - a_{23}x_3 - a_{24}x_4) \\
x_3 &= \frac{1}{a_{33}}(b_3 - a_{31}x_1 - a_{32}x_2 - a_{34}x_4) \\
x_4 &= \frac{1}{a_{44}}(b_4 - a_{41}x_1 - a_{42}x_2 - a_{43}x_3)
\end{aligned}$$

Jacobi Method

Let $x_i^{(n)}$ denote the n^{th} approximation to x_i for $i = 1(1)4$. The Jacobi iterative method expresses the $(n+1)$th iterative values exclusively in terms of the nth iterative values, and the iteration is defined by

$$\begin{aligned}
x_1^{(n+1)} &= \frac{1}{a_{11}}(b_1 - a_{12}x_2^{(n)} - a_{13}x_3^{(n)} - a_{14}x_4^{(n)}) \\
x_2^{(n+1)} &= \frac{1}{a_{22}}(b_2 - a_{21}x_1^{(n)} - a_{23}x_3^{(n)} - a_{24}x_4^{(n)}) \\
x_3^{(n+1)} &= \frac{1}{a_{33}}(b_3 - a_{31}x_1^{(n)} - a_{32}x_2^{(n)} - a_{34}x_4^{(n)}) \\
x_4^{(n+1)} &= \frac{1}{a_{44}}(b_4 - a_{41}x_1^{(n)} - a_{42}x_2^{(n)} - a_{43}x_3^{(n)})
\end{aligned} \tag{4}$$

In general, for m equations

$$x_i^{(n+1)} = \frac{1}{a_{ii}}\{b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(n)} - \sum_{j=i+1}^{m} a_{ij}x_j^{(n)}\}, \quad i = 1(1)m.$$

Let's put the linear system in matrix and vector form

$$A\mathbf{x} = \mathbf{b}.$$

Decomposing A as

$$A = D - L - U,$$

where D is the diagonal matrix, L is the strictly lower triangular matrix and U is the strictly upper triangular matrix. Thus,

$$D\mathbf{x} = (L + U)\mathbf{x} + \mathbf{b}.$$

The Jacobi iteration (4) can be expressed as

$$\begin{aligned} & D\mathbf{x}^{(n+1)} = (L + D)\mathbf{x}^{(n)} + \mathbf{b} \\ \Longrightarrow \qquad & \mathbf{x}^{(n+1)} = \underbrace{D^{-1}(L + U)}_{H_J}\mathbf{x}^{(n)} + D^{-1}\mathbf{b} \end{aligned}$$

The matrix $H_J = D^{-1}(L + U)$ is called the Jacobi iteration matrix.

Gauss-Seidel Method

In this method, the $(n+1)$th iterative values are used as soon as they are available. The iteration (for system of four equations) is given by

$$\begin{aligned}
x_1^{(n+1)} &= \frac{1}{a_{11}}(b_1 - a_{12}x_2^{(n)} - a_{13}x_3^{(n)} - a_{14}x_4^{(n)}) \\
x_2^{(n+1)} &= \frac{1}{a_{22}}(b_2 - a_{21}x_1^{(n+1)} - a_{23}x_3^{(n)} - a_{24}x_4^{(n)}) \\
x_3^{(n+1)} &= \frac{1}{a_{33}}(b_3 - a_{31}x_1^{(n+1)} - a_{32}x_2^{(n+1)} - a_{34}x_4^{(n)}) \\
x_4^{(n+1)} &= \frac{1}{a_{44}}(b_4 - a_{41}x_1^{(n+1)} - a_{42}x_2^{(n+1)} - a_{43}x_3^{(n+1)})
\end{aligned} \tag{5}$$

In general, for m equations

$$x_i^{(n+1)} = \frac{1}{a_{ii}}\{b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(n+1)} - \sum_{j=i+1}^{m} a_{ij}x_j^{(n)}\}, \quad i = 1(1)m.$$

As before, the Gauss-Seidel iteration in matrix form

$$
\begin{aligned}
& D\mathbf{x}^{(n+1)} = L\mathbf{x}^{(n+1)} + U\mathbf{x}^{(n)} + \mathbf{b} \\
\implies \quad & (D-L)\mathbf{x}^{(n+1)} = U\mathbf{x}^{(n)} + \mathbf{b}, \\
\implies \quad & \mathbf{x}^{(n+1)} = \underbrace{(D-L)^{-1}U}_{H_{GS}}\mathbf{x}^{(n)} + (D-L)^{-1}\mathbf{b}.
\end{aligned}
$$

The matrix $H_{GS} = (D-L)^{-1}U$ is called the Gauss-Seidel iteration matrix.

Successive Over-relaxation Method

Add and subtract $x_i^{(n)}$ to the right-hand side of the ith Gauss-Seidel equation (5), $i = 1(1)4$ and write

$$\begin{aligned}
x_1^{(n+1)} &= x_1^{(n)} + \left[\frac{1}{a_{11}}(b_1 - a_{11}x_1^{(n)} - a_{12}x_2^{(n)} - a_{13}x_3^{(n)} - a_{14}x_4^{(n)})\right] \\
x_2^{(n+1)} &= x_2^{(n)} + \left[\frac{1}{a_{22}}(b_2 - a_{21}x_1^{(n+1)} - a_{22}x_2^{(n)} - a_{23}x_3^{(n)} - a_{24}x_4^{(n)})\right] \\
x_3^{(n+1)} &= x_3^{(n)} + \left[\frac{1}{a_{33}}(b_3 - a_{31}x_1^{(n+1)} - a_{32}x_2^{(n+1)} - a_{33}x_3^{(n)} - a_{34}x_4^{(n)})\right] \\
x_4^{(n+1)} &= x_4^{(n)} + \left[\frac{1}{a_{44}}(b_4 - a_{41}x_1^{(n+1)} - a_{42}x_2^{(n+1)} - a_{43}x_3^{(n+1)} - a_{44}x_4^{(n)})\right]
\end{aligned}$$

Observe that the expressions in the square brackets are the corrections or changes made to $x_i^{(n)}$, $i = 1(1)4$. If successive corrections are all one-signed, it would be reasonable to expect convergence to be accelerated. This idea leads to the successive over-relaxation or SOR iteration.

The SOR iteration is defined by

$$
\begin{aligned}
x_1^{(n+1)} &= x_1^{(n)} + \frac{\omega}{a_{11}}(b_1 - a_{11}x_1^{(n)} - a_{12}x_2^{(n)} - a_{13}x_3^{(n)} - a_{14}x_4^{(n)}) \\
\vdots \quad &\quad \vdots \\
x_4^{(n+1)} &= x_4^{(n)} + \frac{\omega}{a_{44}}(b_4 - a_{41}x_1^{(n+1)} - a_{42}x_2^{(n+1)} - a_{43}x_3^{(n+1)} - a_{44}x_4^{(n)})
\end{aligned}
$$

The factor ω is called the acceleration parameter or relaxation factor. It lies in the range $1 < \omega < 2$. The value $\omega = 1$ gives the Gauss-Seidel iteration.

In general, for m equations, the SOR iteration is defined by

$$
x_i^{(n+1)} = x_i^{(n)} + \frac{\omega}{a_{ii}}\Big\{b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(n+1)} - \sum_{j=i}^{m} a_{ij}x_j^{(n)}\Big\}, \quad i = 1(1)m.
$$

This scheme can easily be remembered by writing as

$$\begin{aligned} x_i^{(n+1)} &= \frac{\omega}{a_{ii}}\{b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(n+1)} - \sum_{j=i+1}^{m} a_{ij}x_j^{(n)}\} - (\omega-1)x_i^{(n)}, \quad i = 1(1)m \\ &= \omega\{\text{ R.H.S. of the Gauss-Seidel iteration}\} - (\omega-1)x_i^{(n)}. \end{aligned}$$

To write it in matrix and vector form, we first observe that the correction or displacement vector for the Gauss-Seidel iteration is

$$\begin{aligned} \mathbf{x}^{(n+1)} - \mathbf{x}^{(n)} &= D^{-1}(L\mathbf{x}^{(n+1)} + U\mathbf{x}^{(n)} + \mathbf{b}) - \mathbf{x}^{(n)} \\ &= D^{-1}(L\mathbf{x}^{(n+1)} + U\mathbf{x}^{(n)} + \mathbf{b} - D\mathbf{x}^{(n)}). \end{aligned}$$

Hence the SOR iteration is defined by

$$\mathbf{x}^{(n+1)} - \mathbf{x}^{(n)} = \omega D^{-1}(L\mathbf{x}^{(n+1)} + U\mathbf{x}^{(n)} + \mathbf{b} - D\mathbf{x}^{(n)}).$$

Thus,

$$(I - \omega D^{-1}L)\mathbf{x}^{(n+1)} = \{(1-\omega)I + \omega D^{-1}U\}\mathbf{x}^{(n)} + \omega D^{-1}\mathbf{b}.$$

Therefore,

$$\mathbf{x}^{(n+1)} = \underbrace{(I - \omega D^{-1}L)^{-1}\{(1-\omega)I + \omega D^{-1}U\}}_{H_{SOR}(\omega)}\mathbf{x}^{(n)} + (I - \omega D^{-1}L)^{-1}\omega D^{-1}\mathbf{b}.$$

The SOR iteration matrix $H_{SOR}(\omega)$ is given by

$$H_{SOR}(\omega) = (I - \omega D^{-1}L)^{-1}\{(1-\omega)I + \omega D^{-1}U\}.$$

Theorem. A necessary and sufficient condition for the convergence of iterative methods for any starting value $\mathbf{x}^{(0)}$ is the spectral radius of the iteration matrix (H) is less than one i.e., $\rho(H) < 1$.

Finding eigenvalues of the iteration matrices.

Suppose that m linear equations

$$A\mathbf{x} = \mathbf{b}$$

are such that matrix $A = D - L - U$ is non-singular and has nonzero diagonal elements i.e., $a_{ii} \neq 0$, $i = 1(1)m$.
The eigenvalues (λ) of the Jacobi iteration matrix $H_J = D^{-1}(L + U)$ are the roots of $\det(\lambda I - H_J) = 0$. That is,

$$\begin{aligned}
\det\{\lambda I - D^{-1}(L + U)\} &= \det\{D^{-1}(\lambda D - L - U)\} \\
&= \det(D^{-1}) \det(\lambda D - L - U) = 0 \\
&= \det(\lambda D - L - U) = 0,
\end{aligned}$$

as

$$\det D^{-1} = \frac{1}{\det D} = \frac{1}{a_{11} a_{22} \dots a_{mm}} \neq 0.$$

The eigenvalues λ of SOR iteration matrix

$$H_{SOR}(\omega) = (I - \omega D^{-1}L)^{-1}\{(1-\omega)I + \omega D^{-1}U\}$$

are the roots of $\det(\lambda I - H_{SOR}) = 0$. Now,

$$\begin{aligned}
\lambda I - H_{SOR} &= \lambda(I - \omega D^{-1}L)^{-1}(I - \omega D^{-1}L) \\
&\quad -(I - \omega D^{-1}L)^{-1}\{(1-\omega)I + \omega D^{-1}U\} \\
&= (I - \omega D^{-1}L)^{-1}\{\lambda(I - \omega D^{-1}L) - (1-\omega)I - \omega D^{-1}U\} \\
&= (I - \omega D^{-1}L)^{-1}D^{-1}\{(\lambda + \omega - 1)D - \lambda\omega L - \omega U\}.
\end{aligned}$$

Therefore,

$$\det(\lambda I - H_{SOR}) = \frac{\det\{(\lambda + \omega - 1)D - \lambda\omega L - \omega U\}}{\det(I - \omega D^{-1}L)\ \det D}.$$

$\det(I - \omega D^{-1}L) = 1$ (being determinant of a unit lower triangular matrix).

and

$$\det D = a_{11}a_{22}\dots a_{mm} \neq 0.$$

Hence the eigenvalues of λ are the roots of

$$\det\{(\lambda + \omega - 1)D - \lambda\omega L - \omega U\} = 0.$$

Putting $\omega = 1$ in the above the eigenvalues λ of the Gauss-Seidel iteration matrix (H_{GS}) are the roots λ of

$$\det(\lambda D - \lambda L - U) = 0.$$

***** Ends *****