Advanced Numerical Mathematics

Finite difference method for solving boundary value problems

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The problem

Differential equation:

$$y''(x) + y(x) = 3\sin x$$

Boundary conditions:

$$y(0) + y'(0) = 0$$
$$y(\frac{\pi}{2}) + y'(\frac{\pi}{2}) = 0$$

Find solutions x to the differential equation which satisfy the boundary conditions.

Finite difference method

Solve differential equations with the help of finite differences to approximate derivatives.

Introduce discretization on a grid

Given: boundary values a, b, the number of steps N

$$h = \frac{b-a}{N-1}$$

$$x_i = a + (i-1)h \quad \text{with } i \in [1, N]$$

Finite difference method

Discretization of problem

$$a = 0,\ \ b = \frac{\pi}{2},\ \ N = 10$$

$$h = \frac{\frac{\pi}{2} - 0}{10 - 1} = \frac{\pi}{18}$$

$$x = \{0 \cdot \frac{\pi}{18}, 1 \cdot \frac{\pi}{18}, \ldots, 9 \cdot \frac{\pi}{18}\}$$

Finite difference operators

First-order

$$\text{Forward: } y'(x_i) \approx \frac{y(x_{i+1}) - y(x_i)}{h}$$
$$\text{Backward: } y'(x_i) \approx \frac{y(x_i) - y(x_{i-1})}{h}$$
$$\text{Central: } y'(x_i) \approx \frac{y(x_{i+1}) - y(x_{i-1})}{2h}$$

Second-order

$$y''(x_i) \approx \frac{y(x_{i-1}) - 2y(x_i) + y(x_{i+1})}{h^2}$$

Finite difference operators

Approximate derivatives in the differential equation with finite difference operators:

$$
\begin{aligned}
y''(x_i) + y(x_i) &= 3\sin x_i \\
\frac{y(x_{i-1}) - 2y(x_i) + y(x_{i+1})}{h^2} + y(x_i) &= 3\sin x_i \\
\frac{y(x_{i-1}) + (h^2 - 2)y(x_i) + y(x_{i+1})}{h^2} &= 3\sin x_i \\
y(x_{i-1}) + (h^2 - 2)y(x_i) + y(x_{i+1}) &= 3h^2 \sin x_i
\end{aligned}
$$

Finite difference method

Build linear equation system for *interior points* of discretization

$$
\begin{aligned}
\text{for } i = 2: &\; y(x_1) + (h^2 - 2)y(x_2) + y(x_3) = 3h^2 \sin x_2 \\
\text{for } i = 3: &\; y(x_2) + (h^2 - 2)y(x_3) + y(x_4) = 3h^2 \sin x_3 \\
\text{for } i = 4: &\; y(x_3) + (h^2 - 2)y(x_4) + y(x_5) = 3h^2 \sin x_4 \\
&\vdots \\
\text{for } i = 9: &\; y(x_8) + (h^2 - 2)y(x_9) + y(x_{10}) = 3h^2 \sin x_9
\end{aligned}
$$

Boundary conditions

$$y(x_1) + y'(x_1) = 0$$
$$y(x_{10}) + y'(x_{10}) = 0$$

Approximate derivatives in boundary conditions with finite differences.

$$y(x_1) + \frac{y(x_2) - y(x_1)}{h} = 0$$
$$(h-1)y(x_1) + y(x_2) = 0$$

$$y(x_{10}) + \frac{y(x_{10}) - y(x_9)}{h} = 0$$
$$-y(x_9) + (h+1)y(x_{10}) = 0$$

Linear equation system

The final linear equation system:

$$
\begin{pmatrix}
h-1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & h^2-2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & h^2-2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & h^2-2 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & h^2-2 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & h^2-2 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & h^2-2 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & h^2-2 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & h^2-2 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & h+1
\end{pmatrix}
\begin{pmatrix}
y(x_0) \\ y(x_1) \\ y(x_2) \\ y(x_3) \\ y(x_4) \\ y(x_5) \\ y(x_6) \\ y(x_7) \\ y(x_8) \\ y(x_9) \\ y(x_{10})
\end{pmatrix}
=
\begin{pmatrix}
0 \\ 3h^2 \sin x_2 \\ 3h^2 \sin x_3 \\ 3h^2 \sin x_4 \\ 3h^2 \sin x_5 \\ 3h^2 \sin x_6 \\ 3h^2 \sin x_7 \\ 3h^2 \sin x_8 \\ 3h^2 \sin x_9 \\ 0
\end{pmatrix}
$$

Solvers

Solving of the linear equation system is implemented with the following methods:

Direct methods:

- Classical Gaussian Elimination
- Gaussian Elimination with pivot selection

Iterative methods:

- Jacobi method
- Successive over-relaxation (SOR)

Classical Gaussian Elimination

Let us consider a linear equation system $Ax = b$ with

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,m} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,m} \\ \vdots & & & \\ a_{m,1} & a_{m,2} & \cdots & a_{m,m} \end{pmatrix} \quad b = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}$$

We compute factors in the k-th step $\mu_{i,k}$ with $k = 1, ..., m-1$ and $i = k+1, ..., m$.

$$\mu_{i,k} = \frac{a_{i,k}^{(k-1)}}{a_{k,k}^{(k-1)}}$$

Multiply the k-th row with factor and subtract from $k+1, ..., m$ row to obtain *row echelon form* (Stufenform). Back-substitution yields result x.

Gaussian Elimination with pivot selection

Search for the maximum pivot in k-th step $a_{i,j}^{(k-1)}$ with $k = 1, ..., m-1$ $i = k, ..., m$ and $j = k, ..., m$.

$$(i_{max}, j_{max}) = \underset{i,j}{\operatorname{argmax}}\, a_{i,j}^{(k-1)}$$

Swap k-th row with i_{max} row and compute factors.

$$\mu_{i,j_{max}} = \frac{a_{i,j_{max}}^{(k-1)}}{a_{i_{max},j_{max}}^{(k-1)}}$$

Multiply the k-th row with factor and subtract from $k+1, ..., m$ row to obtain *row echelon form* (Stufenform). Back-substitution yields result x.

Jacobi method

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

Iteration:

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

with an initial guess x_0.
Convergence:

$$\sum_{j=1, j\neq i}^{m} |a_{i,j}| < |a_{j,j}|$$

$\Rightarrow$ A must be *diagonally dominant*!

Successive over-relaxation (SOR)

$$Lx + Dx + Ux = b$$

$$x = x + D^{-1}(b - Lx - Rx - Dx)$$

Introducing a relaxation factor ω with $0 < \omega < 2$
Iteration:

$$x^{(k+1)} = x^{(k)} + \omega D^{-1}(b - Lx^{(k+1)} - Rx^{(k)} - Dx^{(k)})$$

Evaluation

Exact solutions of the problem described by:

$$\hat{y}(x) = \frac{3}{8}\left((\pi + 2)\cos x - (\pi - 2)\sin x\right) - \frac{3}{2}x\cos x$$

Error calculations:

$$\text{Absolute error}: \quad ||\hat{y} - y||$$

$$\text{Relative error}: \quad \frac{||\hat{y} - y||}{||\hat{y}||}$$

Evaluation

n	Gauss		Gauss with PS		SOR	
	Abs	Rel	Abs	Rel	Abs	Rel
10	0.3962	0.1330	0.3962	0.1330	0.4102	0.1377
50	0.1785	0.0285	0.1785	0.0285	2.6691	0.4268
100	0.1263	0.0144	0.1263	0.0144	4.7574	0.5422

Jacobi method: The equation system obtained by finite difference method is not diagonally dominant and thus achieves no convergence towards the solution.

Evaluation

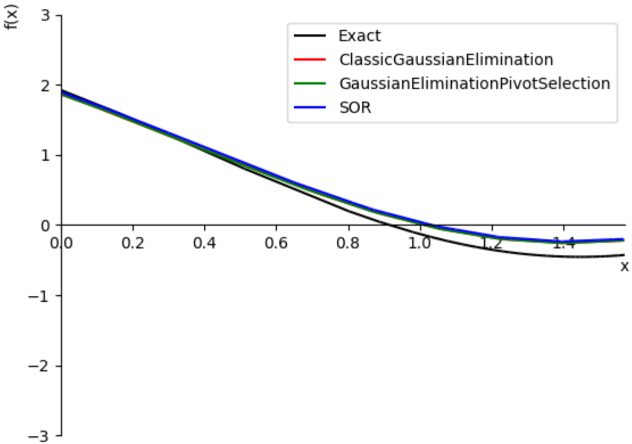

Figure: Plot of the solution with $n = 10$