Finite Difference Methods for Two-Point Boundary Value Problems

The shooting method for a two-point boundary value problem of the form

\[ y'' = f(x, y, y'), \quad a < x < b, \quad y(a) = \alpha, \quad y(b) = \beta, \]

while taking advantage of effective methods for initial value problems, can not readily be generalized to boundary value problems in higher spatial dimensions. We therefore consider an alternative approach, in which the first and second derivatives of the solution \( y(x) \) are approximated by finite differences.

We discretize the problem by dividing the interval \([a, b]\) into \(N + 1\) subintervals of equal width \(h = (b - a)/(N + 1)\). Each subinterval is of the form \([x_{i-1}, x_i]\), for \(i = 1, 2, \ldots, N\), where \(x_i = a + ih\). We denote by \(y_i\) an approximation of the solution at \(x_i\); that is, \(y_i \approx y(x_i)\). Then, assuming \(y(x)\) is at least four times continuously differentiable, we approximate \(y'\) and \(y''\) at each \(x_i\), \(i = 1, 2, \ldots, N\), by the finite differences

\[
y'(x_i) = \frac{y(x_{i+1}) - y(x_i)}{2h} - \frac{h^2}{6} y'''(\eta_i),
\]

\[
y''(x_i) = \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} - \frac{h^2}{12} y^{(4)}(\xi_i),
\]

where \(\eta_i\) and \(\xi_i\) lie in \([x_{i-1}, x_{i+1}]\).

If we substitute these finite differences into the boundary value problem, and apply the boundary conditions to impose

\[ y_0 = \alpha, \quad y_{N+1} = \beta, \]

then we obtain a system of equations

\[
\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = f\left(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right), \quad i = 1, 2, \ldots, N,
\]

for the values of the solution at each \(x_i\), in which the local truncation error is \(O(h^2)\).

We first consider the case in which the boundary value problem includes a linear ODE of the form

\[ y'' = p(x)y' + q(x)y + r(x). \]
Then, the above system of equations is also linear, and can therefore be expressed in matrix-vector form

$$A y = r,$$

where $A$ is a tridiagonal matrix, since the approximations of $y'$ and $y''$ at $x_i$ only use $y_{i-1}$, $y_i$ and $y_{i+1}$, and $r$ is a vector that includes the values of $r(x)$ at the grid points, as well as additional terms that account for the boundary conditions.

Specifically,

$$a_{ii} = 2 + h^2 q(x_i), \quad i = 1, 2, \ldots, N,$$

$$a_{i,i+1} = -1 + \frac{h}{2} p(x_i), \quad i = 1, 2, \ldots, N - 1,$$

$$a_{i+1,i} = -1 - \frac{h}{2} p(x_{i+1}), \quad i = 1, 2, \ldots, N - 1,$$

$$r_1 = -h^2 r(x_1) + \left(1 + \frac{h}{2} p(x_1)\right) \alpha,$$

$$r_i = -h^2 r(x_i), \quad i = 2, 3, \ldots, N - 1,$$

$$r_N = -h^2 r(x_N) + \left(1 - \frac{h}{2} p(x_N)\right) \beta.$$

This system of equations is guaranteed to have a unique solution if $A$ is diagonally dominant, which is the case if $q(x) \geq 0$ and $h < 2/L$, where $L$ is an upper bound on $|p(x)|$.

If the ODE is nonlinear, then we must solve a system of nonlinear equations of the form

$$F(y) = 0,$$

where $F(y)$ is a vector-valued function with coordinate functions $f_i(y)$, for $i = 1, 2, \ldots, N$. These coordinate functions are defined as follows:

$$f_1(y) = y_2 - 2y_1 + \alpha - h^2 f \left(x_1, y_1, \frac{y_2 - \alpha}{2h}\right),$$

$$f_2(y) = y_3 - 2y_2 + y_1 - h^2 f \left(x_2, y_2, \frac{y_3 - y_1}{2h}\right),$$

$$\vdots$$

$$f_{N-1}(y) = y_N - 2y_{N-1} + y_{N-2} - h^2 \left(x_{N-1}, y_{N-1}, \frac{y_N - y_{N-2}}{2h}\right),$$

$$f_N(y) = \beta - 2y_N - y_{N-1} - h^2 \left(x_N, y_N, \frac{\beta - y_{N-1}}{2h}\right).$$

This system of equations can be solved approximately using an iterative method such as Fixed-point Iteration, Newton’s Method, or the Secant Method.
For example, if Newton’s Method is used, then, by the Chain Rule, the entries of the Jacobian matrix $J_F(y)$, a tridiagonal matrix, are defined as follows:

$$J_F(y)_{ii} = \frac{\partial f_i}{\partial y_i}(y) = -2 - h^2 f_y\left(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right), \quad i = 1, 2, \ldots, N,$$

$$J_F(y)_{i,i+1} = \frac{\partial f_i}{\partial y_{i+1}}(y) = 1 - \frac{h}{2} f_y\left(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right), \quad i = 1, 2, \ldots, N - 1,$$

$$J_F(y)_{i,i-1} = \frac{\partial f_i}{\partial y_{i-1}}(y) = 1 + \frac{h}{2} f_y\left(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right), \quad i = 2, 3, \ldots, N.$$

Then, during each iteration of Newton’s Method, the system of equations

$$J_F(y^{(k)})s_{k+1} = -F(y^{(k)})$$

is solved in order to obtain the next iterate

$$y^{(k+1)} = y^{(k)} + s_{k+1}$$

from the previous iterate. An appropriate initial guess is the unique linear function that satisfies the boundary conditions,

$$y^{(0)} = \alpha + \frac{\beta - \alpha}{b - a} (x - a),$$

where $x$ is the vector with coordinates $x_1, x_2, \ldots, x_N$.

It is worth noting that for two-point boundary value problems that are discretized by finite differences, it is much more practical to use Newton’s Method, as opposed to a quasi-Newton Method such as the Secant Method or Broyden’s Method, than for a general system of nonlinear equations because the Jacobian matrix is tridiagonal. This reduces the expense of the computation of $s_{k+1}$ from $O(N^3)$ operations in the general case to only $O(N)$ for two-point boundary value problems. It can be shown that regardless of the choice of iterative method used to solve the system of equations arising from discretization, the local truncation error of the finite difference method for nonlinear problems is $O(h^2)$, as in the linear case. The order of accuracy can be increased by applying Richardson extrapolation.