Difference method for second order nonlinear two-point boundary problem on the interval

Let us consider the following Dirichlet boundary value condition problem on an interval

$$\begin{cases} u'' = f(x,u,u'), \\ u(a) = d_0,\ u(b) = d_1, \end{cases} \tag{1}$$

where the function $f = f(x,u,u')$ is given. The solution to (1) is any function $u:[a,\,b]\to\mathbb{R}$ twice differentiable which satisfies identity $u''(x) = f(x,u(x),u'(x))$ for all $x\in[a,\,b]$ and boundary conditions, i.e. $u(a)=d_0,\ u(b)=d_1$. We also assume that the function $f = f(x)$ has properties that guarantee the unique solvability of the problem (1).[1]

To solve the stated problem by the finite difference method we follow the standard procedure, i.e. we introduce the grid $a = x_0 < x_1 < \ldots < x_n < x_{n+1} = b$ of $n+2$ points on the interval $[a,\,b]$ and replace derivative with proper finite differences. As we deal here with the Dirichlet boundary conditions, the discretization on the boundary points will be straight forward. Thus, let us write the equation at the internal mesh point $x = x_i$ (so $i = 1,\ldots,n$)

$$u''(x_i) = f(x_i, u(x_i), u'(x_i)),$$

and substitute $u''(x_i),\ u'(x_i)$ with second order approximations

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = f\left(x_i,\, u_i,\, \frac{u_{i+1} - u_{i-1}}{2h}\right) \qquad (1 \le i \le n). \tag{2}$$

Taking also into account the boundary conditions $u_0 = d_0,\ u_{n+1} = d_1$ we arrive at the following nonlinear system of equations for unknowns $(u_1,\ldots,u_n)\in\mathbb{R}^n$

$$\begin{cases} -2u_1 + u_2 = h^2 f\left(x_1,\, u_1,\, \dfrac{u_2 - d_0}{2h}\right) - d_0 & (i=1), \\ \ldots & \\ u_{i-1} - 2u_i + u_{i+1} = h^2 f\left(x_i,\, u_i,\, \dfrac{u_{i+1} - u_{i-1}}{2h}\right) & (2 \le i \le n-1), \\ \ldots & \\ u_{n-1} - 2u_n = h^2 f\left(x_n,\, u_n,\, \dfrac{d_1 - u_{n-1}}{2h}\right) - d_1 & (i=n). \end{cases} \tag{3}$$

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[1] For example: (i) $f,\ \frac{\partial f}{\partial u},\ \frac{\partial f}{\partial u'} : [0,1]\times\mathbb{R}^2 \to \mathbb{R}$ are continuous; (ii) $\frac{\partial f}{\partial u} > 0$ in whole domain; (iii) $\frac{\partial f}{\partial u'}$ is lower and upper bounded. For instance the function $f(x,u,u') = xu^3 + u + \sin(xu')$ meets these criteria. The equation reads: $u'' = xu^3 + u + \sin(xu')$.

To obtain the standard form of a nonlinear system of equations we arrange all terms (3) on one side and equalize it zero

$$\begin{cases} 2u_1 - u_2 + h^2 f\left(x_1,\, u_1,\, \dfrac{u_2 - d_0}{2h}\right) - d_0 = 0 & (i=1), \\ \dots & \\ -u_{i-1} + 2u_i - u_{i+1} + h^2 f\left(x_i,\, u_i,\, \dfrac{u_{i+1} - u_{i-1}}{2h}\right) = 0 & (2 \le i \le n-1), \\ \dots & \\ -u_{n-1} + 2u_n + h^2 f\left(x_n,\, u_n,\, \dfrac{d_1 - u_{n-1}}{2h}\right) - d_1 = 0 & (i=n). \end{cases} \tag{4}$$

The resulting system (4) can be solved numerically – basically – by two methods: (i) simple iterations; (ii) Newton-Raphson multidimensional method. In what follows we present the second method.

The Newton-Raphson method

The Newton-Raphson method for solving an equation

$$f(x) = 0, \tag{5}$$

is based upon the convergence of the sequence

$$x_{j+1} = x_j - \frac{f(x_j)}{f'(x_j)} \qquad (j = 0, 1, 2, \dots). \tag{6}$$

This method may be used for differentiable functions and has a simple geometric interpretation: a new value x_{j+1} is obtained as the intersection of the tangent line to the graph of f at the point $x = x_j$, with the Ox axis. The process is repeated until a sufficient accuracy is reached.

To start the iterative process (6) we have to chose "the initial guess" x_0. The method will converge to solution, provided that x_0 is close enough to the unknown zero x_* and $f'(x_*) \neq 0$. The condition $f'(x_*) \neq 0$ is fairly obvious as it is necessary to have $f' \neq 0$ in the vicinity of x_* if we want the expression $\frac{f(x_j)}{f'(x_j)}$ to be correctly defined. On the other hand there are many functions for which the process (6) converges virtually from every starting point. For example, if we seek the solution to the equation

$$x^2 = c,$$

for some positive number $c \in \mathbb{R}_+$, the iterations for the function $f(x) = x^2 - c$ are

$$x_{j+1} = x_j - \frac{x_j^2 - c}{2x_j} = \frac{x_j^2 + c}{2x_j} = \frac{1}{2}\left(x_j + \frac{c}{x_j}\right),$$

and the sequence $(x_j)_{j=0}^{\infty}$ is convergent to $\sqrt{c}$ for *any* starting point $x_0 > 0!$

The one-dimensional Newton method may be easily extended to multi-dimensional case, i.e. to the system of nonlinear equations

$$\begin{cases} f_1(x_1,\dots,x_m) = 0, \\ \vdots \\ f_m(x_1,\dots,x_m) = 0, \end{cases} \tag{7}$$

where differentiable functions (of several variables) $f_1,\dots, f_m : \mathbb{R}^m \to \mathbb{R}$ are given. This may be written in a compact from as the solution of the following vector equation

$$F(x) = 0, \tag{8}$$

where $x = (x_1,\dots,x_m) \in \mathbb{R}^m$ and $F(x) = (f_1(x),\dots, f_m(x)) \in \mathbb{R}^m$, thus $F : \mathbb{R}^m \to \mathbb{R}^m$. In the multidimensional case, however, we cannot simply divide by $F'(x^j)$ as in the formula (6) because now the derivative $F'(x)$ is a linear operator, $F'(x) \in L(\mathbb{R}^m, \mathbb{R}^m)$, which in the standard canonical basis of $\mathbb{R}^m$ is represented by the Jacobi matrix

$$DF(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x) & \dots & \frac{\partial f_1}{\partial x_m}(x) \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1}(x) & \dots & \frac{\partial f_m}{\partial x_m}(x) \end{bmatrix}. \tag{9}$$

In this case the formula for the iteration step will involve the inverse of the Jacobi matrix $DF(x)$ instead division by $f'(x)$, thus is given by

$$x^{(j+1)} = x^{(j)} - \left[DF(x^{(j)})\right]^{-1} F(x^{(j)}) \qquad (j = 0,1,2,\dots). \tag{10}$$

It seems that each step involves the inversion of the matrix $DF(x^{(j)})$, but in fact this can be rewritten as

$$DF(x^{(j)})(x^{(j+1)} - x^{(j)}) = -F(x^{(j)}) \qquad (j = 0,1,2,\dots), \tag{11}$$

what in fact is a system of linear equations of the form $A\xi = b$, where matrix $A = DF(x^{(j)})$ and the column $b = -F(x^{(j)})$. It means that at each step we have to solve the following linear system of equations, and next change the matrix A and column b,

$$\begin{cases} DF(x^{(j)})\delta x^j = -F(x^{(j)}), \\ x^{(j+1)} = x^{(j)} + \delta x^j, \\ \text{for } j = 0,1,2,\dots \end{cases} \tag{12}$$

Thus the Newton-Raphson method to be employed operates as follows. Given an initial guess $x^{(0)}$ for the solution of (7) (or (8)), the system of linear equations $DF(x^{(0)})\delta x^0 = -F(x^{(0)})$ is solved. A new approximation to the solution is obtained by adding the solution vector to the previous approximation, hence $x^{(1)} = x^{(0)} + \delta x^0$. The matrix $A = DF(x)$ and column $b = -F(x)$ are reevaluated using the new solution vector $x^{(1)}$, i.e. we insert there $x = x^{(1)}$, and the entire process is repeated until convergence is obtained. In practice, the phrase "*until convergence is obtained*" means the we perform several iterations and check the consecutive updates δx^j. If they are small enough we stop iterations.

The Newton-Raphson method requires the knowledge of the Jacobi matrix what is equivalent to knowledge of all the partial derivatives for each equation. If the system (7) is given in the analytical from, e.g.

$$\begin{cases} 2x_1^2 + x_2^2 + 4x_2^2 - 3 = 0, \\ x_1 x_3 + 2x_2 - 7\ln x_3 = 0, \\ \frac{2}{5} x_1 - 3x_2 \cos x_1 + x_3^5 = 0, \end{cases}$$

then the Jacobi matrix can be easily expressed in the analytical form as well, here

$$DF(x_1, x_2, x_3) = \begin{bmatrix} 4x_1 & 2x_2 & 8x_2 \\ x_3 & 2 & x_1 - \frac{7}{x_3} \\ \frac{2}{5} + 3x_2 \sin x_1 & -3\cos x_1 & 5x_3^4 \end{bmatrix},$$

and the method runs smoothly. On the other hand, if for some reasons, the analytical form is not possible, or it is, but is too complicated, or too large for efficient use of the analytical differentiation, we can resort to the finite differences to approximate the Jacobi matrix.

For the case of the boundary value problem (1), which leads to the nonlinear system (4), the analytical form of the Jacobi matrix $DF(u)$ (remember, that now the unknowns are denoted by $u_1, \dots, u_m$ and $m = n$) is available as long as the function $f(x, u, u')$ is provided in the analytical form. The computation of the Jacobi matrix $DF(u)$ gives

$$\begin{bmatrix} 2+h^2 \frac{\partial f}{\partial u}\left(x_1, u_1, \frac{u_2 - d_0}{2h}\right) & -1+\frac{h}{2}\frac{\partial f}{\partial u'}\left(x_1, u_1, \frac{u_2 - d_0}{2h}\right) & 0 & \cdots & 0 \\ -1-\frac{h}{2}\frac{\partial f}{\partial u'}\left(x_2, u_2, \frac{u_3 - u_1}{2h}\right) & 2+h^2 \frac{\partial f}{\partial u}\left(x_2, u_2, \frac{u_3 - u_1}{2h}\right) & -1+\frac{h}{2}\frac{\partial f}{\partial u'}\left(x_2, u_2, \frac{u_3 - u_1}{2h}\right) & & \\ & & & & \\ 0 & \cdots & 0 & -1-\frac{h}{2}\frac{\partial f}{\partial u'}\left(x_{n-1}, u_{n-1}, \frac{d_1 - u_{n-2}}{2h}\right) & 2+h^2 \frac{\partial f}{\partial u}\left(x_{n-1}, u_{n-1}, \frac{d_1 - u_{n-2}}{2h}\right) \end{bmatrix}.$$

As we can see the matrix is tridiagonal, so solving the linear system (12), which in the current notation reads

$$\begin{cases} DF(u^{(j)})\delta u^j = -F(u^{(j)}), \\ u^{(j+1)} = u^{(j)} + \delta u^j, \\ \text{for } j = 0,1,2,\ldots \end{cases} \quad (13)$$

can be quickly carried out by the reduced Gaussian elimination. Here components of $F(u)$ are the functions that on the left-hand side of the system (4).

To start the iterations (13) we have to select some initial guess $u^{(0)} = (u_1^{(0)},\ldots,u_n^{(0)})$. It seems that the best choice here is the linear interpolation between the boundary values $u(a) = d_0$, $u(b) = d_1$

$$u_i^{(0)} = d_0 + (d_1 - d_0)\frac{i}{n+1} \qquad (1 \le i \le n). \quad (14)$$