Mathematics for chemical engineers

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6. Numerical solution of ordinary differential equations

Boundary value problem

Outline

Boundary value problems

Example Let us solve the equation

$$y'' + y = 0, \quad y(0) = 1,\ y'(0) = A \quad \ldots \text{initial value problem}$$

Characteristic equation: $\lambda^2 + 1 = 0 \quad \Longrightarrow$

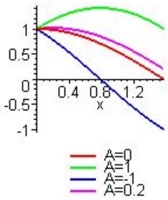
$$y_H(x) = C_1 \cos x + C_2 \sin x\,, \quad y_H'(x) = -C_1 \sin x + C_2 \cos x$$

initial condition $\Longrightarrow 1 = C_1,\ A = C_2 \quad \Longrightarrow$

$$y_P(x) = \cos x + A \sin x\,, \quad x \in \mathbb{R}\,.$$

Let us investigate the value of the solution at the point $\frac{\pi}{2}$ for different A, $y_P(\frac{\pi}{2}) = A$

$A = 0 \quad \Rightarrow \quad y_P(x) = \cos x$
$A = 1 \quad \Rightarrow \quad y_P(x) = \cos x + \sin x$
$A = -1 \quad \Rightarrow \quad y_P(x) = \cos x - \sin x$
$A = 0,2 \quad \Rightarrow \quad y_P(x) = \cos x + 0,2 \sin x$



Different $A \Longrightarrow$ different values of the solution at the point $\frac{\pi}{2}$

Our boundary value problem is

$$y'' + y = 0, \quad y(0) = 1,\ y\left(\frac{\pi}{2}\right) = A\,.$$

If we know the "correct" A we could solve our boundary value problem as an initial value problem.

Remark The differential equations for a boundary value problem have to be at least of the order 2 (2 conditions in different points) .

Basic techniques for solution of boundary value problems are:

1. Shooting method: An iterative technique that exploits classical methods for solving initial value problems, i.e., Runge–Kutta methods.
2. Direct methods: Difference methods, based on a replacement of derivatives by differences. The resulting system of linear algebraic equations is solved by standard techniques.

Shooting Method

We first consider the single linear second-order equation

$$Ly \equiv -y'' + p(x)y' + q(x)y = r(x), \quad a < x < b \tag{1}$$

with the general linear two-point boundary conditions

$$\begin{aligned} a_0 y(a) - a_1 y'(a) &= \alpha \\ b_0 y(b) + b_1 y'(b) &= \beta \end{aligned} \tag{2}$$

where $a_0, a_l, \alpha, b_0, b_l$ and β are constants, such that

$$|a_0| + |b_0| \neq 0\,,$$

$$\begin{aligned} a_0 a_1 \geq 0, \qquad |a_0| + |a_1| \neq 0 \\ b_0 b_1 \geq 0, \qquad |b_0| = |b_1| \neq 0 \end{aligned} \tag{3}$$

We assume that the functions $p(x), q(x)$, and $r(x)$ are continuous on $\langle a, b\rangle$ and that $q(x) > 0$. With these assumptions, the solution of (1) is unique.

To solve (1), we first define two functions, $y^{(1)}(x)$ and $y^{(2)}(x)$, on $\langle a, b\rangle$ as solutions of the respective initial-value problems

$$Ly^{(1)} = r(x)\,, \quad y^{(1)}(a) = -\alpha C_1\,, \quad (y^{(1)})'(a) = -\alpha C_0\,, \tag{4}$$

$$Ly^{(2)} = 0\,, \quad y^{(2)}(a) = a_1\,, \quad (y^{(2)})'(a) = a_0\,, \tag{5}$$

where C_0 and C_1 are any constants such that

$$a_1 C_0 - a_0 C_1 = 1\,. \tag{6}$$

The function $y(x)$ defined by

$$y(x) \equiv y(x,s) = y^{(1)}(x) + sy^{(2)}(x), \quad a \le x \le b\,, \tag{7}$$

satisfies $a_0 y(a) - a_1 y'(a) = \alpha(a_1 C_0 - a_0 C_1) = \alpha$, and will be the solution of (1) if s is chosen such that

$$\phi(s) = b_0 y(b,s) + b_1 y'(b,s) - \beta = 0\,. \tag{8}$$

This equation is linear in s and has the single root

$$s = \frac{\beta - \left(b_0 y^{(1)}(b) + b_1 {y^{(1)}}'(b)\right)}{b_0 y^{(2)}(b) + b_1 {y^{(2)}}'(b)}\,. \tag{9}$$

Steps of the shooting method

The presented shooting method involves:

1. Converting the BVP into an IVP by specifying extra initial conditions, i.e. equations (1), (2)
2. Guessing the initial conditions and solving the IVP over the entire interval, i.e. guess C_0, evaluate C_1 from (6) and solve (5)
3. Solving for s and constructing y, i.e., evaluate (9) for s; use s in (7) .

Shooting method for a second-order nonlinear equation

Let us consider a differential equation of the second order

$$y'' = f(t, y, y'), \quad y(a) = A,\ y(b) = B, \quad a < b, \quad t \in \langle a, b\rangle\,. \tag{10}$$

Let us suppose that the problem has just one solution. We guess $y'(a)$ and denote by $y(t, s)$ the solution of the initial value problem

$$y'' = f(t, y, y'), \quad y(a) = A,\ y'(a) = s\,. \tag{11}$$

Now, we will rewrite this initial value problem as a system of two differential equations of the first order.

Remark The direct solution of the boundary value problem (10) may lead to a system of two, in general, nonlinear equations for A and B and their solution might be a problem.

Let us denote

$$u(t,s) = y(t,s)\,, \quad v(t,s) = \frac{\partial}{\partial t} y(t,s)\,. \tag{12}$$

From the equation (11), we obtain an initial value problem

$$\begin{aligned} \frac{\partial}{\partial t} u(t,s) &= v(t,s)\,, \quad u(a,s) = A \\ \frac{\partial}{\partial t} v(t,s) &= f(t; u(t,s); v(t,s))\,, \quad v(a,s) = s\,. \end{aligned} \tag{13}$$

The solution $u(t,s)$ of the initial value problem (13) will be the same as the solution $y(t)$ of the boundary value problem (10), if we will find such a value of s that

$$\varphi(s) \equiv \underbrace{u(b,s) - B = 0}\quad \Longrightarrow \quad y(b) = B\,.$$

the solution of this equation has to be computed numerically: Newton's method, bisection method, etc.

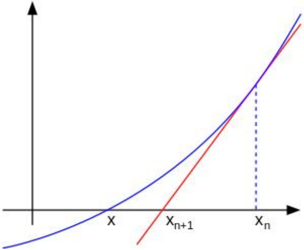
Newton's–Raphson's method

We will solve the equation

$$? \ s \in \mathbb{R} \ : \quad \varphi(s) \ \equiv \ u(b; s) - B = 0 \tag{14}$$

Let s_0 is any initial condition in a neighborhood of the root and let

$$s_{n+1} := s_n - \frac{\varphi(s_n)}{\varphi'(s_n)}, \quad n = 0, 1, 1, \ldots$$



Then $\{s_n\} \longrightarrow s$ quadratically, if

1. $\varphi'(s) \neq 0 \ \forall s \in I$ where I is a separation interval
2. $\varphi''(s) \in \mathbb{R}$ on I
3. the initial approximation s_0 is closed enough to the root

How we can compute the derivative $\varphi'(s_n)$ when we even don't know the function φ?

Let us go back to our equation (11), i.e., we consider the equation

$$y''(t,s) = f(t, y(t,s), y'(t,s))\,, \quad y(a,s) = A, \quad y'(a,s) = s\,.$$

$y'(a,s) = s$ ... our guess of the initial condition – we will change slopes in such a way that we will "shoot" exactly into B.

Now, we will study the changes of the solution y in dependence of changes of the initial slope s:

$$\frac{\partial y''(t,s)}{\partial s} = \frac{\partial}{\partial s} f(t, y(t,s), y'(t,s)) = \frac{\partial f}{\partial y} \cdot \frac{\partial y}{\partial s} + \frac{\partial f}{\partial y'} \cdot \frac{\partial y'}{\partial s}\,.$$

From initial conditions we have $\dfrac{\partial y}{\partial s}(a,s) = 0\,,\ \dfrac{\partial y'}{\partial s}(a,s) = 1$ and $v(t) = \dfrac{\partial y}{\partial s}(t,s)$ we obtain from the equation (12).

The initial value problem for the function v:

$$v''(t) = \frac{\partial f}{\partial y}(t, y(t), y'(t)) \cdot v(t) + \frac{\partial f}{\partial y'}(t, y(t), y'(t)) \cdot v'(t)\,, \ v(a) = 0, \ v'(a) = 1\,. \tag{15}$$

and from the equation (12) we have $u(b, s) = y(b, s)$. We obtain

$$\varphi(s) = y(b, s) - B \implies \varphi'(s) = \frac{\partial y}{\partial s}(b, s) = v(b)\,.$$

So the needed derivative in Newton's method $\varphi'(s_n)$ we obtain by solution of the equation (15) up to the point $t = b$.

Remark The equation (15) is very sensitive to perturbations of the initial guess s_0. The consequence of the wrong guess s_0 is that Newton's method doesn't converge to s.

Remedy Multiple shooting method: We divide the interval $\langle a, b\rangle$ to subintervals $a = t_0 < t_1 < \cdots < t_k = b$ and, roughly speaking, we repeat the shooting method on each of these subintervals.

★ Solution of the adiabatic tubular reactor with an axial dispersion

Axial heat and mass transfer in a tubular reactor can be described, on the basis of the diffusion model, by the system of two nonlinear differential equations of the 2nd order.
After some adjustment and a suitable substitution we get one dimensionless equation of the second order:

$$\frac{1}{Pe}\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - \frac{\mathrm{d}y}{\mathrm{d}x} - p y^m \Theta^{-m} \exp\left(K - \frac{R}{\Theta}\right) = 0\,, \tag{16}$$

where $\Theta = 1 - H(1-y)$, with boundary equations

$$y(0) = 1 + \frac{y'(0)}{Pe}\,, \tag{17}$$

$$y'(1) = 0\,. \tag{18}$$

Here, Pe, p, m, K, R, and H are parameters of the mathematical model, x is the axial coordinate, y dimensionless concentration and Θ stands for temperature.

We convert our boundary value problem into the initial one at point $x = 1$. Let us choose

$$y(1) = \eta_1 \,. \tag{19}$$

Then we can integrate equation (16) (rewritten as a system of two differential equations of the first order) from $x = 1$ with initial conditions (18) and (19) to $x = 0$, and we calculate $y(0)$ and $y'(0)$. Let us denote

$$\varphi(\eta_1) = y(0) - \frac{y'(0)}{Pe} - 1 \,. \tag{20}$$

Integration of the initial value problem was performed by Runge–Kutta method.

Finite differences

Let us solve the following boundary value problem:

$$y''(t) = f(t, y(t), y'(t)), \quad y(a) = \alpha, \quad y(b) = \beta.$$

We divide the interval $\langle a, b\rangle$ to $m+1$ subinervals $\langle t_k, t_{k+1}\rangle$, $k = 0, 1, \ldots, m$, where

$$t_k = a + kh,\ k = 0, 1, \ldots, m+1; \quad h = \frac{b-a}{m+1}$$

Basic idea: Numerical derivative

We discretize the given equation for the given dividing of the interval $\langle a, b\rangle$. How we will approximate the derivative? Taylor's expansion:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\eta), \quad \eta \text{ mezi } x \text{ a } x+h \quad \Longrightarrow$$

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \underbrace{\frac{h^2}{2h} f''(\eta)}_{\text{discretization error is of order } h^1}.$$

i.e.. we approximate the first derivative with the error $\mathcal{O}(h)$

$$\Longrightarrow \quad f'(x) \approx \frac{f(x+h) - f(x)}{h}, \quad h \text{ small}$$

In order to obtain better approximation we compute two Taylor's expansions:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(\eta_1)\,, \tag{21}$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(\eta_2)\,. \tag{22}$$

We subtract equations (21) and (22) $\Longrightarrow$

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{6}\left(f'''(\eta_1) + f'''(\eta_2)\right) \quad \Longrightarrow$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2)\,, \tag{23}$$

Now we add the equations (21) and (22) and obtain

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^3}{6}\left(f'''(\eta_1) - f'''(\eta_2)\right) \quad \Longrightarrow$$

$$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} + \mathcal{O}(h)\,. \tag{24}$$

Linear finite differences

Let f be a linear function of y and y', i.e.,

$$f(t, y(t), y'(t)) = u(t) + v(t)y(t) + w(t)y'(t)\,,$$

$$y_0 = \alpha\,, \quad y'(t) = \frac{y(t+h) - y(t-h)}{2h} + \frac{h^3}{6}y'''(\eta)\,.$$

$$y''(t) = \frac{y(t+h) - 2y(t) + y(t-h)}{h^2} + \frac{h^2}{12}y^{(4)}(\tau)\,, \quad y_{m+1} = \beta\,.$$

We denote

$$y_k := y(t_k)\,,\; u_k := u(t_k)\,,\; v_k := v(t_k)\,,\; w_k := w(t_k)\,,$$

and put everything into the equation

$$y''(t) = f(t, y(t), y'(t))\,, \quad y(a) = \alpha\,,\; y(b) = \beta\,.$$

We obtain the system of m linear algebraic equations for m unknowns:

$$y_0 = \alpha$$

$$\frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} = u_k + v_k y_k + w_k \frac{y_{k+1} - y_{k-1}}{2h}, \quad k = 1, \dots, m$$

$$y_{m+1} = \beta\,.$$

We rewrite this system as:

$$y_0 = \alpha\,,$$

$$(-1 + \frac{1}{2}hw_k)y_{k+1} + (2 + h^2 v_k)y_k + (-1 - \frac{1}{2}hw_k)y_{k-1} = -h^2 u_k\,,\ k = 1 \dots, m\,,$$

$$y_{m+1} = \beta\,.$$

This system has a tridiagonal diagonally dominant matrix. It can be advantageously solved in Matlab (tridiag.m) .

In the matrix form $\mathbf{A}\,\overrightarrow{\mathbf{y}} = \overrightarrow{\mathbf{b}}$ where

$$\mathbf{A} = \begin{pmatrix} 2+h^2v_1 & -1+\frac{1}{2}hw_1 & 0 & \dots & 0 \\ -1-\frac{1}{2}hw_2 & 2+h^2v_2 & -1+\frac{1}{2}hw_2 & \dots & 0 \\ \ddots & \ddots & \ddots & & \\ & & -1-\frac{1}{2}hw_{m-1} & 2+h^2v_{m+1} & -1+\frac{1}{2}hw_{m-1} \\ & & 0 & -1-\frac{1}{2}hw_m & 2h^2v_m \end{pmatrix}$$

$$\overrightarrow{\mathbf{y}} = (y_1, y_2, \dots, y_{m-1}, y_m)^{\mathrm{T}}$$

$$\overrightarrow{\mathbf{b}} = \begin{pmatrix} -h^2u_1 + (1+\frac{1}{2}hw_1)\alpha \\ -h^2u_2 \\ \vdots \\ -h^2u_m - \beta(-1+\frac{1}{2}hw_m) \end{pmatrix}, \quad \begin{matrix} (1+\frac{1}{2}hw_1)\alpha \quad \text{from b.c.} \\ \\ \\ -\beta(-1+\frac{1}{2}hw_m) \quad \text{from b.c.} \end{matrix}$$

We solve the system and obtain $y_k,\ k = 1, \dots, m$, the discrete approximation of the solution $\overrightarrow{y}$ at points $t_1, t_2, \dots, t_m$.

★ Error estimation

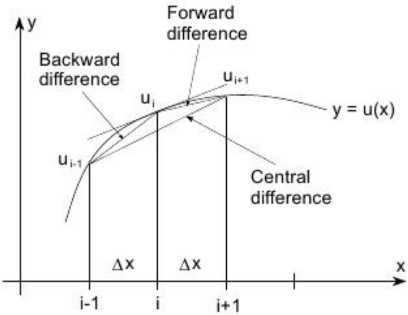
For the maximal error of linear finite difference method we have:

$$\max_{k=1,\ldots,m} |y(t_k) - y_k| \leq Ch^2 \quad \text{for} \quad h \longrightarrow 0\,,$$

where $y(t_k)$ is the exact solution in the point t_k and y_k is the corresponding approximation obtained by the finite difference method.

Remark If f is not linear, we can apply the method of nonlinear differences (we will not study here).

Difference formulas derived from Taylor's polynomial:



Graphic illustration of the approximation of the derivative by difference formulas.

1. Forward difference of the first order:

$$u_j' = \frac{u_{j+1} - u_j}{h} + \mathcal{O}(h^1)$$

2. Backward difference of the first order:

$$u_j' = \frac{u_j - u_{j-1}}{h} + \mathcal{O}(h^1)$$

3. Central difference of the second order:

$$u_j' = \frac{u_{j+1} - u_{j-1}}{2h} + \mathcal{O}(h^2)$$

Solution of the boundary value problem by finite differences

Two points boundary problem for one differential equation of the second order:

$$y'' = f(t, y(t), y'(t)) \tag{25}$$

with linear boundary conditions

$$\begin{array}{rcrcl} \alpha_0 y(a) & + & \beta_0 y'(a) & = & \gamma_0 \,, \\ \alpha_1 y(b) & + & \beta_1 y'(b) & = & \gamma_1 \,. \end{array} \tag{26}$$

Let us choose an equidistant division of the interval $\langle a, b \rangle$:

$$t_0 = a < t_1 < \ \ldots \ < t_N = b \,, \quad h = \frac{b-a}{N} \,, \ t_k = a + kh \,, \ k = 0, \ldots, N \,.$$

We approximate the solution in nodes by values of a discrete function $y(x_i) \sim y_i$. We replace the derivative in the equation by central difference formula with error $\mathcal{O}(h^2)$:

$$\frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} = f\left(t_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right) \,, \quad i = 1, \ldots, N-1 \,.$$

We replace also the boundary conditions for example by forward differences (error $\mathcal{O}(h)$):

$$\begin{aligned} \alpha_0 y_0 &+ \beta_0 \frac{y_1 - y_0}{h} = \gamma_0 \\ \alpha_1 y_N &+ \beta_1 \frac{y_N - y_{N-1}}{h} = \gamma_1 \end{aligned}$$

We obtain the system of $N+1$ nonlinear equations for $N+1$ unknowns $y_0, y_1, \ldots, y_N$. The resulting system of nonlinear equations is usually solved by Newton's method.

We approximated the equation with the error $\mathcal{O}(h^2)$, but the error is corrupted by difference formulas for boundary condition with error $\mathcal{O}(h)$. Then the resulting error is only of order $\mathcal{O}(h)$. Let us try to replace boundary conditions by a difference formula of order $\mathcal{O}(h^2)$, too.

$$\begin{aligned} \alpha_0 y_0 &+ \beta_0 \frac{-3y_0 + 4y_1 - y_2}{2h} = \gamma_0 \\ \alpha_1 y_N &+ \beta_1 \frac{3y_N - 4y_{N-1} + y_{N-2}}{2h} = \gamma_1 \end{aligned}$$

Then the resulting error will be of order $O(h^2)$.

★

Remark It is also possible to apply so called method of fictitious node. For example we can approximate the boundary condition at the point $t = a$ by

$$\alpha_0 y_0 + \beta_0 \frac{y_1 - y_{-1}}{2h} = \gamma_0$$

and we consider the approximation of the differential equation also for $i = 0$.

Remark If we write the equations for the solution in the matrix form, in the case with the error $\mathcal{O}(h)$ in approximation of boundary conditions we obtain also the system with tridiagonal matrix. In all other cases we have to transform the resulting matrix into the tridiagonal form.

Example Let $N = 3,\; a = 0,\; b = 1$. We approximate the equation (25) with the error $\mathcal{O}(h^2)$, boundary conditions (26) with the error $\mathcal{O}(h)$, i.e., $h = \frac{1}{3},\; i = 1, 2$.

$$
\begin{aligned}
i = 1 \qquad & \frac{y_0 - 2y_1 + y_2}{h^2} &=& \; f\left(t_1, y_1, \frac{y_2 - y_0}{2h}\right) \\
i = 2 \qquad & \frac{y_1 - 2y_2 + y_3}{h^2} &=& \; f\left(t_2, y_2, \frac{y_3 - y_1}{2h}\right) \\
\text{bc conditions} \qquad & \alpha_0 y_0 + \beta_0 \frac{y_1 - y_0}{h} &=& \; \gamma_0 \\
& \alpha_1 y_3 + \beta_1 \frac{y_3 - y_2}{h} &=& \; \gamma_1 .
\end{aligned}
$$

In the matrix form

$$
\frac{1}{h^2}\begin{pmatrix} h^2(\alpha_0 - \frac{\beta_0}{h}) & h\beta_0 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & -h\beta_1 & h^2(\alpha_1 + \frac{\beta_1}{h}) \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} \gamma_0 \\ f(t_1, y_1, \frac{y_2 - y_1}{2h}) \\ f(t_2, y_2, \frac{y_3 - y_1}{2h}) \\ \gamma_1 \end{pmatrix} .
$$

The first and last equations result from boundary conditions.

The matrix is tridiagonal.

Recommended literature

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