0.1 Conversion to initial value problem

The methods we are going to describe in this section are called shooting methods. Let us remind the difference between an initial value problem and an boundary value problem. In initial value problem the initial conditions specified in one value of the independent variable x contain enough information to start the numerical integration. In the boundary value problem, however, this information is divided into two (or more) pieces, each of them specified in different x. The main idea of the shooting method is to choose the remaining information in one x value so that we can start the integration (to shoot) and to observe, how the boundary condition in the other x value is satisfied (how the target is hit). Let us explain it more precisely. Consider the system of differential equations

$$\frac{\mathrm{d}y_i}{\mathrm{d}x} = f_i(x, y_1, \ldots, y_n) \;, \qquad i = 1, 2, \ldots, n \tag{1}$$

with 2-point boundary conditions

$$g_i\Big(y_1(a), \ldots, y_n(a), y_1(b), \ldots, y_n(b)\Big) = 0 \;, \qquad i = 1, 2, \ldots, n \;. \tag{2}$$

The problem (1), (2) can be written in a vector form

$$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}x} = \boldsymbol{f}(x, \boldsymbol{y}) \;, \quad \boldsymbol{g}(\boldsymbol{y}(a), \boldsymbol{y}(b)) = \boldsymbol{0} \,.$$

Assume $\boldsymbol{f}$ and $\boldsymbol{g}$ have continuous derivatives according to all the arguments. If the appearance scheme of (2), (n equations in $2n$ unknowns) is in the form

$$\text{a)}\ \begin{array}{cccccccccc} \times & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \times & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \times & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \times & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \times & 0 & 0 & 0 & 0 & 0 \end{array} \quad \text{resp. b)}\ \begin{array}{cccccccccc} \times & \times & \times & \times & \times & 0 & 0 & 0 & 0 & 0 \\ \times & \times & \times & \times & \times & 0 & 0 & 0 & 0 & 0 \\ \times & \times & \times & \times & \times & 0 & 0 & 0 & 0 & 0 \\ \times & \times & \times & \times & \times & 0 & 0 & 0 & 0 & 0 \\ \times & \times & \times & \times & \times & 0 & 0 & 0 & 0 & 0 \end{array}$$

(here $n = 5$), then it is an initial value problem (a Cauchy problem) in $x = a$ in a standard form or a Cauchy problem where the initial condition can be found by solving n equations (2) in n unknowns. After solving this system we again have all the n conditions in $x = a$ necessary to start the integration.

Now, suppose that the complete initial conditions cannot be found from (2). Instead, consider some other initial condition

$$y_1(a) = \eta_1, \ldots, y_n(a) = \eta_n \tag{3}$$

and suppose the Cauchy problem (1) with this initial condition has a unique solution for any $\boldsymbol{\eta} = (\eta_1, \eta_2, \ldots, \eta_n)$ in some domain $M \subset R^n$. Then the solution of (1), (3) for any fixed $x \in [a, b]$ defines in this domain M a unique vector-valued function depending on n variables - the components of the vector $\boldsymbol{\eta}$:

$$\boldsymbol{y}(x) = \boldsymbol{w}(x, \boldsymbol{\eta}) \;. \tag{4}$$

For $x = b$ we have $\boldsymbol{y}(b) = \boldsymbol{w}(b, \boldsymbol{\eta})$. Substituting into boundary condition (2) we have

$$\boldsymbol{g}(\boldsymbol{\eta}, \boldsymbol{w}(b, \boldsymbol{\eta})) = 0 \;, \tag{5}$$

or

$$G(\boldsymbol{\eta}) = \mathbf{0} \ . \tag{6}$$

Now (6) is a system of n nonlinear algebraic equations for n unknowns $\eta_1, \eta_2, \ldots, \eta_n$ (of course it is not written by elementary functions if the system of differential equations (1) cannot be solved analytically).

We have the following result: If for any $\boldsymbol{\eta}$ there exists a solution of the Cauchy problem (1) with the initial condition (3) on the interval $[a, b]$ then the number of solutions of the boundary value problem is the same as the number of solutions of the equation (6) in the corresponding domain. If the equation (6) has no solution, then the boundary value problem (1), (2) has no solution either.

The main task is to find $\boldsymbol{\eta}$ satisfying $G(\boldsymbol{\eta}) = \mathbf{0}$. In other words we want to find an initial condition for (1) in $x = a$ satisfying the boundary condition (2). This can be achieved by various methods for nonlinear algebraic equations.

Boundary conditions have been formulated in a rather general way, including also so-called mixed boundary conditions, meaning values of $\boldsymbol{y}$ both in $x = a$ and in $x = b$ appear in the function g_i. Many practical problems involve separated boundary conditions, meaning values of $\boldsymbol{y}$ either in $x = a$ or in $x = b$ appear in each function g_i. Then in the appearance scheme for (2) in each row either the first n entries are zeroes or the last n entries are zeroes which may (for $n = 5$) look like this

$$\begin{array}{cccccccccc} \times & \times & \times & \times & \times & 0 & 0 & 0 & 0 & 0 \\ \times & \times & 0 & 0 & \times & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & 0 & 0 & \times & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \times & \times & 0 \end{array} \ . \tag{7}$$

Let us introduce the term problem of order p in the point $x = a$ (or $x = b$ resp.). We say that a boundary value problem with separated boundary conditions is of order p in $x = a$ (or in $x = b$ resp.) if $p = n - r$ where r is the number of functions g_i in (2) depending on $\boldsymbol{y}(a)$ (or on $\boldsymbol{y}(b)$ resp.). E.g. the problem described by the scheme (7) is of order 3 in $x = a$ and it is of order 2 in $x = b$. It is obvious that if a given problem with separated boundary conditions is of order p in $x = a$ then it is of order $(n - p)$ in $x = b$.

In simple words in a point where the problem is of order p we must choose p initial conditions and to compute the remaining $n - p$ ones from the boundary conditions. The problem can be converted into an initial value problem either in $x = a$ or in $x = b$ and it is convenient to choose $x = a$ or $x = b$ according to where the order is lower.

0.1.1 Problem of order 1

To start with consider the differential equation (**??**) written as a system of differential equations of the first order

$$\begin{aligned} y_1' &= y_2, \\ y_2' &= f(x, y_1, y_2). \end{aligned} \tag{8}$$

Boundary conditions (**??**), (**??**) are then

$$\begin{aligned} \alpha_0 y_1(a) &+ \beta_0 y_2(a) = \gamma_0, \\ \alpha_1 y_1(b) &+ \beta_1 y_2(b) = \gamma_1. \end{aligned} \tag{9}$$

The appearance scheme for (9) is for nonzero α_i, β_i, $i = 0, 1$, in the form

$$\begin{matrix} \times & \times & 0 & 0 \\ 0 & 0 & \times & \times \end{matrix} .$$

Thus it is a problem with separated boundary conditions. As this is a problem of order 1 in $x = a$ (and also in $x = b$) we must choose one condition in $x = a$ (or in $x = b$). Assuming $\beta_0 \neq 0$ we choose the initial condition

$$y_1(a) = \eta_1 \tag{10}$$

and we compute

$$y_2(a) = \eta_2 = \frac{\gamma_0 - \alpha_0 \eta_1}{\beta_0} \tag{11}$$

from the first equation (9). When integrating (8) with the initial conditions (10) and (11) we get $y_1(b) = y_1(b, \eta_1)$ and $y_2(b) = y_2(b, \eta_1)$, dependent on the choice of η_1. These values must satisfy the boundary conditions (9). The first of them is automatically satisfied by the choice of (11), the second one can be written as

$$\alpha_1 y_1(b, \eta_1) + \beta_1 y_2(b, \eta_1) - \gamma_1 = \varphi(\eta_1) = 0 . \tag{12}$$

Now, after choosing η_1, we can compute the value of $\varphi(\eta_1)$ according to (12) using some method for numerical integration of initial value problem. To solve the equation $\varphi(\eta_1) = 0$ we use some method from chapter **??**. Efficient methods use derivatives, an example being the Newton's method or the Richmond's method. The derivative can be found using some difference formula, but this is not very precise, since the numerical integration itself introduces certain error. A better choice is to consider variation

$$\Omega_1 = \frac{\partial y_1}{\partial y_1(a)} = \frac{\partial y_1}{\partial \eta_1} , \qquad \Omega_2 = \frac{\partial y_2}{\partial y_1(a)} = \frac{\partial y_2}{\partial \eta_1} . \tag{13}$$

The equations for Ω_1 and Ω_2 can be derived by differentiating (8) with respect to η_1 and interchanging the differentiation with respect to x and η_1

$$\begin{aligned} \Omega_1' &= \Omega_2 , \\ \Omega_2' &= \tfrac{\partial f}{\partial y_1} \Omega_1 + \tfrac{\partial f}{\partial y_2} \Omega_2 \end{aligned} \tag{14}$$

with the initial conditions

$$\Omega_1(a) = 1 , \qquad \Omega_2(a) = -\frac{\alpha_0}{\beta_0} \tag{15}$$

derived from (10) and (11). From (12) we have

$$\frac{\mathrm{d}\varphi(\eta_1)}{\mathrm{d}\eta_1} = \alpha_1 \Omega_1(b) + \beta_1 \Omega_2(b) . \tag{16}$$

Then the Newton's method can be written as

$$\eta_1^{k+1} = \eta_1^k - \frac{\varphi(\eta_1^k)}{\varphi'(\eta_1^k)} = \eta_1^k - \frac{\alpha_1 y_1(b) + \beta_1 y_2(b) - \gamma_1}{\alpha_1 \Omega_1(b) + \beta_1 \Omega_2(b)} , \tag{17}$$

where $y_1(b), y_2(b), \Omega_1(b), \Omega_2(b)$ are evaluated for $\eta_1 = \eta_1^k$.

The following example illustrates this method.

Example 0.1.1 *Consider the equation describing non-isothermal inner diffusion in a slab catalyst with the concentration $y \in [0,1]$*

$$y'' = \Phi^2 \; y \; \exp\left(\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right) \tag{18}$$

with boundary conditions

$$y'(0) = 0\,, \qquad y(1) = 1. \tag{19}$$

Introducing $y_1 = y$, $y_2 = y'$ the equation (18) can be written as

$$y_1' = y_2\,, \qquad y_2' = \Phi^2 \; y_1 \; \exp\left(\frac{\gamma\beta(1-y_1)}{1+\beta(1-y_1)}\right)\,. \tag{20}$$

We choose

$$y_1(0) = \eta_1 \tag{21}$$

and from (19) using $y_2 = y'$ we have

$$y_2(0) = 0\,. \tag{22}$$

The function φ is then defined by the expression

$$\varphi(\eta_1) = y_1(1) - 1\,. \tag{23}$$

The variational equations corresponding to (20) are

$$\begin{aligned} \Omega_1' &= \Omega_2\,, \\ \Omega_2' &= \Phi^2 \exp\left(\frac{\gamma\beta(1-y_1)}{1+\beta(1-y_1)}\right)\cdot\left(1 - \frac{\gamma\beta y_1}{(1+\beta(1-y_1))^2}\right)\,\Omega_1 \end{aligned} \tag{24}$$

and the initial conditions are

$$\Omega_1(0) = 1\,, \qquad \Omega_2(0) = 0\,. \tag{25}$$

The numerical integration of the initial value problem (20), (24) with initial conditions (21), (22) and (25) was done using the Merson modification of the Runge-Kutta method. The results are shown in Table 1. The convergence is very fast.

0.1.2 Problem of higher order

Boundary conditions (2) for the system of equations (1) are for the problem with separated boundaries in the form of

$$\begin{aligned} g_i\big(y_1(a), \ldots, y_n(a)\big) &= 0\,, \qquad i = 1, 2, \ldots, r \qquad (26) \\ g_i\big(y_1(b), \ldots, y_n(b)\big) &= 0\,, \qquad i = r+1, \ldots, n\,. \qquad (27) \end{aligned}$$

Problem (1), (26), (27) is thus of order $n - r$ in $x = a$ and of order r in $x = b$. After choosing $n - r$ "missing" values of initial conditions in $x = a$

$$y_1(a) = \eta_1, \quad y_2(a) = \eta_2, \ldots, y_{n-r}(a) = \eta_{n-r}\,, \tag{28}$$

Table 1: Newton method for Example 0.1.1 ($\gamma = 20$; $\beta = 0.1$; $\Phi = 1$)

$y(0) = \eta_1$	$y(1)$	$y'(1)$	$\Omega_1(1)$	$\varphi(\eta_1)$	$\varphi'(\eta_1)$
1.00000	1.45949	0.84223	0.53898	0.45949	0.53898
0.14747	0.58712	1.00124	2.68144	−0.41288	2.68144
0.30145	0.89906	1.21398	1.53643	−0.10094	1.53643
0.36715	0.99073	1.23051	1.26792	−0.00927	1.26792
0.37446	0.99991	1.23081	1.24276	−0.00009	1.24276
0.37453	1.00000	1.23081	1.24251	0.00000	1.24251
0.50000	1.13356	1.20276	0.91577	0.13356	0.91577
0.35416	0.97396	1.22931	1.31470	−0.02604	1.31470
0.37396	0.99929	1.23080	1.24444	−0.00071	1.24444
0.37453	1.00000	1.23081	1.24251	0.00000	1.24251
0.10000	0.44534	0.83312	3.32963	−0.55466	3.32963
0.26658	0.84243	1.19239	1.71764	−0.15757	1.71764
0.35832	0.97940	1.22979	1.29940	−0.02060	1.29940
0.37417	0.99955	1.23080	1.24373	−0.00045	1.24373
0.37453	1.00000	1.23081	1.24251	0.00000	1.24251

it is possible to solve r values

$$y_{n-r+1}(a) = \eta_{n-r+1}, \ldots, y_n(a) = \eta_n \tag{29}$$

from (26), possibly after a suitable rearrangement of $(y_1, ..., y_n)$. As a result we have n conditions (28) and (29) in $x = a$, this presenting a Cauchy (initial value) problem. After integrating this initial value problem in the interval $[a, b]$ we get the values $y_1(b), \ldots, y_n(b)$, dependent on the chosen initial conditions (28). These values must also satisfy the conditions (27) (so far unused)

$$g_i\Big(y_1(b, \eta_1, \ldots, \eta_{n-r}), \ldots, y_n(b, \eta_1, \ldots, \eta_{n-r})\Big) = 0 \,, \qquad i = r+1, \ldots, n \,. \tag{30}$$

The equations (30) can be written as

$$G_i(\eta_1, \ldots, \eta_{n-r}) = 0 \,, \qquad i = 1, \ldots, n-r \,. \tag{31}$$

To solve this system we can use some method from chapter **??**. So we are able to evaluate $G_1, \ldots, G_{n-r}$ for given $\eta_1, \ldots, \eta_{n-r}$. Without the knowledge of derivatives of G_i Warner scheme can be applied (see section **??**). To do this we have to evaluate the functions G_i for $n-r+1$ different values $\eta_1^k, \ldots, \eta_{n-r}^k$, $k = 1, 2, \ldots, n-r+1$, meaning we have to solve the initial value problem (1), (28), (29) with $(n-r+1)$ different initial conditions (28) (thus $(n-r+1)$ times).

The system (31) can also be solved by some method from chapter **??** that uses derivatives if the derivatives of the functions G_i are known. Let us try to derive the Newton's method for system (31), thus for the boundary value problem of order $n-r$ in $x = a$. To find the Jacobi matrix we must compute the partial derivatives $\frac{\partial G_i}{\partial \eta_j}, i, j = 1, 2, \dots, n-r$. Considering (30) we have

$$\frac{\partial G_i}{\eta_j} = \sum_{k=1}^{n} \frac{\partial g_{i+r}}{\partial y_k(b)} \frac{\partial y_k(b)}{\partial \eta_j} , \qquad i, j = 1, 2, \dots, n-r . \tag{32}$$

After differentiating the system (1) with respect to η_j and denoting

$$\Omega_{kj} = \frac{\partial y_k}{\partial \eta_j} , \qquad k = 1, 2, \dots, n , \quad j = 1, 2, \dots, n-r , \tag{33}$$

and changing the order of differentiation we get a system of variational differential equations

$$\frac{\mathrm{d}\Omega_{kj}}{\mathrm{d}x} = \sum_{m=1}^{n} \frac{\partial f_k}{\partial y_m} \Omega_{mj} , \qquad k = 1, 2, \dots, n , \quad j = 1, 2, \dots, n-r . \tag{34}$$

In view of the initial condition (28) the variational variables Ω_{kj} satisfy the initial conditions

$$\Omega_{kj}(a) = \begin{cases} 0 & \text{pro} \quad k \neq j \\ 1 & \text{pro} \quad k = j \end{cases} \qquad k, j = 1, 2, \dots, n-r . \tag{35}$$

The remaining initial conditions can be found from the conditions (26) assuming the system of r equations (26) is solvable in r variables $y_{n-r+1}(a), y_{n-r+2}(a), \dots$ $\dots, y_n(a)$, thus

$$y_k(a) = \Phi_k\Big(y_1(a), y_2(a), \dots, y_{n-r}(a)\Big) , \qquad k = n-r+1, \dots, n . \tag{36}$$

Then

$$\frac{\partial y_k(a)}{\partial \eta_j} = \Omega_{kj}(a) = \frac{\partial \Phi_k(\eta_1, \dots, \eta_{n-r})}{\partial \eta_j}, \quad k = n-r+1, \dots, n, \; j = 1, 2, \dots, n-r . \tag{37}$$

Even in case the equations (36) cannot be solved explicitly, we still can get (37) as a solution of some system of linear algebraic equations using the Implicit function theorem. The relations (35) and (37) present a complete set of $n(n-r)$ initial conditions for $n(n-r)$ functions Ω_{kj} and $n(n-r)$ differential equations (34).

To conclude we integrate the system of equations (1) with initial conditions (28) and

$$y_k(a) = \Phi_k(\eta_1, \eta_2, \dots, \eta_{n-r}) , \qquad k = n-r+1, \dots, n , \tag{38}$$

and the system of equations (34) with initial conditions (35) and (37) simultaneously, this is an initial value problem of $n + n(n-r)$ differential equations with the same number of initial conditions. For chosen $\eta_1, \eta_2, \dots, \eta_{n-r}$ we have in $x = b$

$$\begin{array}{l} y_1(b), \quad y_2(b), \dots, y_n(b) \\ \Omega_{11}(b), \quad \Omega_{12}(b), \dots, \Omega_{1,n-r}(b) \\ \vdots \\ \Omega_{n1}(b), \quad \Omega_{n2}(b), \dots, \Omega_{n,n-r}(b). \end{array}$$

We can evaluate G_i from (31) and (30) and we can find the Jacobi matrix of the functions G_i from (32), where $\partial y_k(b)/\partial \eta_j$ is replaced by $\Omega_{kj}(b)$. We have all we need for the Newton's method.

This shooting method for boundary value problems is a reliable algorithm. The method is widely applicable if initial value problem can be integrated. In some problems the numerical integration can be done from one side only or it cannot be integrated from either side. For these problems the shooting method must be modified (the multiple shooting method) or it cannot be applied at all.

The following example illustrates the use of variational equations once again.

Example 0.1.2 *The stationary regime of a homogeneous exothermic reaction of the first order in a tube non-isothermal non-adiabatic flow-through system can be described by the equations* ($' = \frac{d}{dx}$):

$$\frac{1}{\mathrm{Pe}}\,\theta'' - \theta' - \beta(\theta - \theta_c) + \mathrm{B}\,\mathrm{Da}\,(1-y)\,\exp\left(\frac{\theta}{1+\varepsilon\theta}\right) = 0\,, \tag{39}$$

$$\frac{1}{\mathrm{Pe}}\,y'' - y' + \mathrm{Da}\,(1-y)\,\exp\left(\frac{\theta}{1+\varepsilon\theta}\right) = 0 \tag{40}$$

with boundary conditions

$$x = 0: \qquad \theta' = \mathrm{Pe}\,\theta\,; \quad y' = \mathrm{Pe}\,y \tag{41}$$

$$x = 1: \qquad \theta' = 0\,; \quad y' = 0 \quad . \tag{42}$$

Here y is the dimensionless conversion, θ is the dimensionless temperature, Pe *is the Peclet criterion, x is the dimensionless space coordinate,* B *is the dimensionless adiabatic thermal increase,* Da *is the Damköhler criterion, ε is the dimensionless activation energy, β is the dimensionless thermal throughput coefficient, θ_c is the dimensionless cooling medium temperature.*

We convert the problem to the initial value problem in $x = 1$ (this is better from the numerical point of view, for higher Pe it is not possible to convert it to the initial value problem in $x = 0$ at all due to instability of the integration of the corresponding initial value problem) and we use the Newton's method. Thus we choose

$$\theta(1) = \eta_1; \qquad y(1) = \eta_2 \tag{43}$$

and the conditions (42) give the remaining two initial values necessary for the integration. Let us denote the variation variables

$$\Omega_{11} = \frac{\partial\theta}{\partial\eta_1}\,; \quad \Omega_{12} = \frac{\partial\theta}{\partial\eta_2}\,; \quad \Omega_{21} = \frac{\partial y}{\partial\eta_1}\,; \quad \Omega_{22} = \frac{\partial y}{\partial\eta_2}\,. \tag{44}$$

For these functions we get the equations

$$\frac{1}{\mathrm{Pe}}\Omega_{11}'' - \Omega_{11}' - \beta\Omega_{11} + \mathrm{B}\ \mathrm{Da}\ \exp\left(\frac{\theta}{1+\varepsilon\theta}\right)\cdot\left(-\Omega_{21} + \frac{1-y}{(1+\varepsilon\theta)^2}\Omega_{11}\right) = 0 \tag{45}$$

$$\frac{1}{\mathrm{Pe}}\Omega_{12}'' - \Omega_{12}' - \beta\Omega_{12} + \mathrm{B}\ \mathrm{Da}\ \exp\left(\frac{\theta}{1+\varepsilon\theta}\right)\cdot\left(-\Omega_{22} + \frac{1-y}{(1+\varepsilon\theta)^2}\Omega_{12}\right) = 0 \tag{46}$$

$$\frac{1}{\mathrm{Pe}}\Omega_{21}'' - \Omega_{21}' + \mathrm{Da}\ \exp\left(\frac{\theta}{1+\varepsilon\theta}\right)\cdot\left(-\Omega_{21} + \frac{1-y}{(1+\varepsilon\theta)^2}\Omega_{11}\right) = 0 \tag{47}$$

$$\frac{1}{\mathrm{Pe}}\Omega_{22}'' - \Omega_{22}' + \mathrm{Da}\ \exp\left(\frac{\theta}{1+\varepsilon\theta}\right)\cdot\left(-\Omega_{22} + \frac{1-y}{(1+\varepsilon\theta)^2}\Omega_{12}\right) = 0 \tag{48}$$

The equations (45) and (47) come from differentiation of (39) and (40) with respect to η_1*, the equations (46) and (48) come from differentiation with respect to* η_2*. We let the equations of the second order and we do not convert them into a system of 1-st order equations for clear arrangement. The initial conditions for (45) - (48) are*

$$\Omega_{11}(1) = 1\,; \quad \Omega_{12}(1) = 0\,; \quad \Omega_{21}(1) = 0\,; \quad \Omega_{22}(1) = 1\,; \tag{49}$$

$$\Omega'_{11}(1) = \Omega'_{12}(1) = \Omega'_{21}(1) = \Omega'_{22}(1) = 0\,. \tag{50}$$

To satisfy the boundary conditions (41) we must solve

$$G_1(\eta_1, \eta_2) = \mathrm{Pe}\ \theta(0) - \theta'(0) = 0 \tag{51}$$

$$G_2(\eta_1, \eta_2) = \mathrm{Pe}\ y(0) - y'(0) = 0\,. \tag{52}$$

Partial derivatives for the Jacobi matrix are

$$\frac{\partial G_1}{\partial \eta_1} = \mathrm{Pe}\ \Omega_{11}(0) - \Omega'_{11}(0) = a_{11}\,, \quad \frac{\partial G_1}{\partial \eta_2} = \mathrm{Pe}\ \Omega_{12}(0) - \Omega'_{12}(0) = a_{12}\,,$$

$$\frac{\partial G_2}{\partial \eta_1} = \mathrm{Pe}\ \Omega_{21}(0) - \Omega'_{21}(0) = a_{21}\,, \quad \frac{\partial G_2}{\partial \eta_2} = \mathrm{Pe}\ \Omega_{22}(0) - \Omega'_{22}(0) = a_{22}\,. \tag{53}$$

For a given $\boldsymbol{\eta} = (\eta_1, \eta_2)$ *we can integrate the equations (39), (40), (45)-(48) with the initial conditions (42), (43), (49), (50) from* $x = 1$ *to* $x = 0$*. In this way we get the values of all the functions* y, θ, Ω_{ij} *along with their derivatives in* $x = 0$*. Then we can evaluate* G_1 *and* G_2 *using (51), (51) and the Jacobi matrix using (53). Table 2 gives the results of the Newton's method for one initial approximation* $\eta = (0; 0)$ *for the following parameter values*

$$\mathrm{Pe} = 2\,; \quad \beta = 2\,; \quad \theta_c = 0\,; \quad \mathrm{B} = 12\,; \quad \mathrm{Da} = 0.12\,; \quad \varepsilon = 0\,. \tag{54}$$

Table 3. shows the iterations for four other initial approximations $\boldsymbol{\eta}$*. These two tables show that we have found five different solutions of the boundary value problem (39), (42). The solutions* $\theta(x)$ *and* $y(x)$ *are plotted in Fig. 1. The solution from Table 2 is denoted* `e`*, other solutions are denoted* `a`, `b`, `c`, `d` *in agreement with Table 3. This example illustrates that a boundary value problem (especially a nonlinear one) can have more than one solution. On the other hand, such a problem can have no solution.*

* * *

For further study the reader is invited to check the following literature [?], [?], [?], [?], [?], [?], [?], [?].

Table 2: Newton method for Example 0.1.2

	iteration					
	0	1	2	3	4	5
η_1	0.0000	0.7395	1.0299	1.0932	1.0963	1.0963
η_2	0.0000	0.1570	0.2206	0.2340	0.2346	0.2346
$\theta(0)$	-0.9236	0.1165	0.4170	0.4732	0.4759	0.4759
$\theta'(0)$	1.6624	1.0066	0.9499	0.9516	0.9518	0.9518
$y(0)$	-0.0568	0.0496	0.0866	0.0936	0.0940	0.0940
$y'(0)$	0.0680	0.1416	0.1790	0.1857	0.1880	0.1880
G_1	-3.5150	-0.7736	-0.1160	-0.0051	0.0000	0.0000
G_2	-0.1816	-0.0424	-0.0057	-0.0002	0.0000	0.0000
$\Omega_{11}(0)$	1.5021	0.8118	0.5151	0.4503	0.4471	
$\Omega'_{11}(0)$	-1.1431	0.0906	0.5023	0.5789	0.5825	
$\Omega_{12}(0)$	0.7947	1.5142	1.8810	1.9658	1.9700	
$\Omega'_{12}(0)$	-1.2645	-2.1345	-2.4099	-2.4557	-2.4578	
$\Omega_{21}(0)$	-0.0621	-0.1043	-0.1215	-0.1251	-0.1253	
$\Omega'_{21}(0)$	0.0838	0.1339	0.1438	0.1447	0.1447	
$\Omega_{22}(0)$	1.0473	1.0881	1.1075	1.1118	1.1120	
$\Omega'_{22}(0)$	-0.0424	-0.0540	-0.0434	-0.0391	-0.0389	
a_{11}	4.1474	1.5330	0.5279	0.3218	0.3118	
a_{12}	2.8539	5.1630	6.1718	6.3873	6.3977	
a_{21}	-0.2081	-0.3425	-0.3868	-0.3950	-0.3953	
a_{22}	2.1370	2.2303	2.2583	2.2627	2.2628	
$\triangle\eta_1$	0.7395	0.2904	0.0633	0.0031	0.0000	
$\triangle\eta_2$	0.1570	0.0636	0.0134	0.0006	0.0000	

Table 3: Newton method for Example 0.1.2

a		b		c		d	
η_1	η_2	η_1	η_2	η_1	η_2	η_1	η_2
2.0000	0.0000	4.0000	0.7500	2.9000	0.9800	3.6000	0.9500
2.1644	0.4378	3.1441	0.6149	3.2155	0.9815	3.6781	0.9396
4.4148	0.8706	3.1447	0.6189	3.2114	0.9853	3.6919	0.9374
4.1768	0.8817	3.1448	0.6189	3.2132	0.9848	3.6926	0.9373
4.1098	0.8949			3.2133	0.9848	3.6926	0.9373
4.0792	0.8971						
4.0775	0.8973						
4.0774	0.8973						

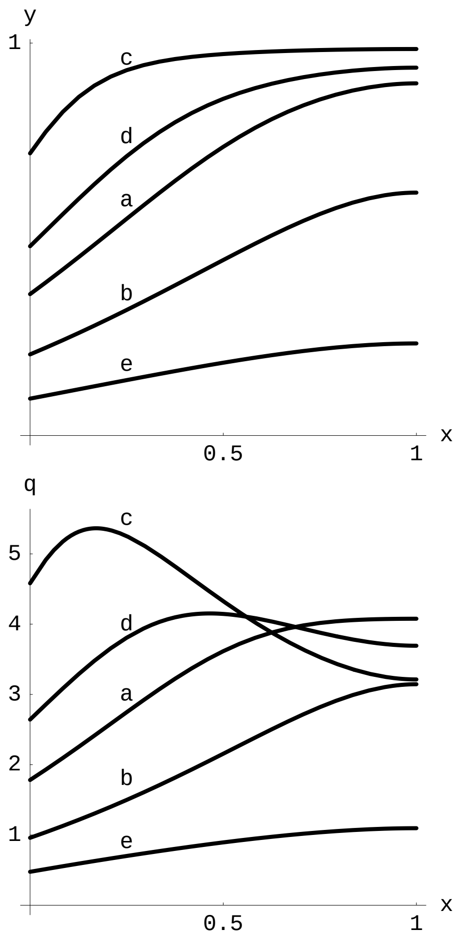

Figure 1: Five different solutions of the boundary value problem from Example 0.1.2