Dirichlet-type Boundary Value Problem

Using the shooting method and Newton's algorithm

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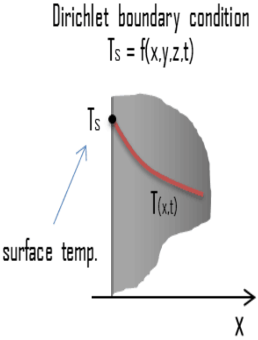
Outline

- Brief overview of the theory and applications of the boundary value problem (BVP).
- Formulation of the general Dirichlet BVP. Discussion of the selected numerical methods to solve this problem.
- Present a computational approach to solve two selected BVPs by means of numerical methods using Octave.
- Discuss findings and future improvements.

What is the BVP?

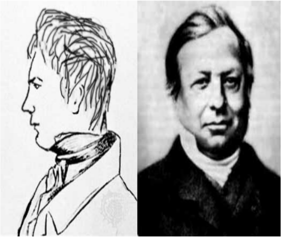


- BVPs are extremely important as they are vital in the study of many multidisciplinary applications such as:
  - fluid mechanics
  - solid mechanics to heat transfer
  - electromagnetic potential

What is the BVP?

- A BVP consists of a system of differential equations where a set of conditions is known, and whose solutions are to be found in a specified domain.
- It is opposed to the initial value problem, in which only the conditions on one extreme of the interval are known.
- Thus, the choice of the boundary condition is fundamental for the resolution of the given system since it will determine its accuracy, and in some cases, its convergence.

What is the BVP?

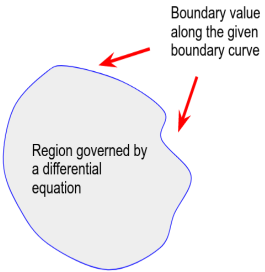


J.C Francois Sturm and J. Liouville

J.C Francois Sturm and J. Liouville studied the conditions which guarantee the existence and uniqueness of BVP solutions and how boundary conditions influence them, specially on well-posed systems.

In this work, we study the Dirichlet BVP problem for given conditions along the boundary of the domain in the x-y plane.

What is the BVP?



- The Dirichlet problem was initially intended to particularly find solutions to the Laplace's equation.
- Its main purpose is to find the solution of a second-order elliptic equation which is regular in the domain.
- Note: the Dirichlet problem for harmonic functions always has a solution, and that solution is unique, when the boundary is sufficiently smooth and *f(s)* is continuous.

Objectives

- Discuss the general formulation of the Dirichlet problem and its applicability to specific problems.
- Develop a set of Octave scripts to solve two given Dirichlet BVPs.
- Apply the shooting and Newton's numerical methods to approximate the solutions of the given systems.

Dirichlet Boundary Value Problem Formulation

The general Dirichlet-type BVP for a function $y(t)$ in an interval [a,b] is given by:

$$\begin{cases} y''(t) = f(t, y(t), y'(t)), & a < t < b, \\ y(a) = \alpha, \quad y(b) = \beta, \end{cases} \tag{1}$$

where α, β are given numbers.This linear two-point BVP can be solved by forming a combination of the solutions to two initial value problems, the so called shooting method.

Dirichlet Boundary Value Problem Formulation

Let $y(t,\gamma)$ be the solution of the initial value problem:

$$\begin{cases} y''(t) = f(t, y(t), y'(t)), & a < t < b, \\ y(a) = \alpha, \quad y'(a) = \gamma \end{cases} \tag{2}$$

We can now find a value for γ such that $y(b,\gamma) = \beta$. Thereby, we can find a root $\gamma*$ for the equation $y(b,\gamma) - \beta = 0$.

If we define

$$g(\gamma) \equiv y(b, \gamma) - \beta \tag{3}$$

we can find a root $\gamma*$ of function g with Newton's Method. Each evaluation of function g requires finding the solution of initial value problem (2). Also, $g'(\gamma)$ must be found in order to use Newton's Method. Taking the derivative in (3), we have that $g'(\gamma) = u(b)$, where:

$$u(t) = \frac{\partial y}{\partial \gamma}(t, \gamma)$$

(We are omitting the dependency of u in γ for simplification purposes).

Dirichlet Boundary Value Problem Formulation

By finding the derivative of the initial value problem (2) with respect to γ, it can be concluded that $u(t)$ is the solution of the following initial value problem:

$$\begin{cases} u''(t) = \frac{\partial f}{\partial y}(t, y(t,\gamma), y'(t,\gamma))u(t) + \frac{\partial f}{\partial z}(t, y(t,\gamma), y'(t,\gamma))u'(t), \\ u(a) = 0, \qquad u'(a) = 1, \quad a < t < b. \end{cases} \tag{4}$$

Given the function $y(t,\gamma)$, this is a linear problem for $u(t)$; thus the initial value problems (2) and (4) can be numerically solved in parallel.

Consider the first problem defined by:

$$\begin{cases} y''(t) = \frac{1}{8}(32 + 2t^3 - y(t)y'(t)), & 1 < t < 3, \\ y(1) = 17, \quad y(3) = \frac{43}{3}. \end{cases} \tag{5}$$

Let $y(t, \gamma)$ be the solution of the initial value problem

$$\begin{cases} y''(t) = \frac{1}{8}(32 + 2t^3 - y(t)y'(t)), & 1 < t < 3, \\ y(1) = 17, \quad y'(1) = \gamma, \end{cases} \tag{6}$$

Let $u(t) = \frac{\partial y}{\partial \gamma}(t,\gamma)$ be the solution of the following initial value problem:

$$\begin{cases} u''(t) = -\frac{1}{8}y'(t)u(t) - \frac{1}{8}y(t)u'(t), \qquad 1 < t < 3, \\ u(0) = 0, \qquad u'(0) = 1. \end{cases} \tag{7}$$

Thus we proceed to calculate the root of the following equation:

$$g(\gamma) \equiv y(1,\gamma) - \frac{43}{3} = 0. \tag{8}$$

Using the substitutions $u_1(t) = y(t)$, $u_2(t) = y'(t)$, $u_3(t) = u(t)$ and $u_4(t) = u'(t)$ we can transform (6) to a first-order system:

$$\begin{cases} u_1'(t) = u_2(t) \\ u_2'(t) = \frac{1}{8}(32 + 2t^3 - u_1(t)u_2(t)) \\ u_3'(t) = u_4(t) \\ u_4'(t) = -\frac{1}{8}u_2(t)u_3(t) - \frac{1}{8}u_1(t)u_4(t), \end{cases} \tag{9}$$

where $u_1(1) = 17$, $u_2(1) = \gamma$, $u_3(1) = 0$, and $u_4(1) = 1$. By solving this system, we find the value of $g(\gamma)$. Now that we know the values of $g(\gamma)$ and $g'(\gamma)$, which is u(3), we proceed to calculate $\gamma *$ with Newton's Method.

Selected Boundary Value Problems Formulation

Consider the second problem defined by:

$$\begin{cases} y''(t) = \frac{1+(y'(t))^2}{1+y(t)}, & 0 < t < 5, \\ y(0) = 1, & y(5) = 10. \end{cases} \tag{10}$$

Let $y(t,\gamma)$ be the solution of the initial value problem

$$\begin{cases} y''(t) = \frac{1+(y'(t))^2}{1+y(t)}, & 0 < t < 5, \\ y(0) = 1, & y'(0) = \gamma. \end{cases} \tag{11}$$

Let $u(t) = \frac{\partial y}{\partial \gamma}(t, \gamma)$ be the solution of the following initial value problem:

$$\begin{cases} u''(t) = -\frac{1+(y'(t))^2}{(1+y(t))^2} u(t) + \frac{2y'(t)}{1+y(t)} u'(t), & 0 < t < 5, \\ u(0) = 0, \quad u'(0) = 1. \end{cases} \tag{12}$$

Thus we proceed to calculate the root of the following equation:

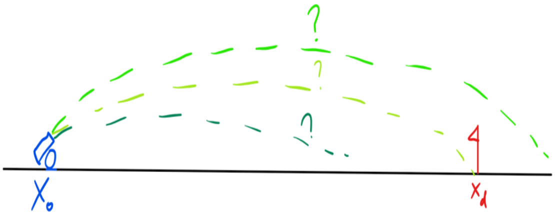
$$g(\gamma) \equiv y(0, \gamma) - 10 = 0. \tag{13}$$

Using the substitutions $u_1(t) = y(t)$, $u_2(t) = y'(t)$, $u_3(t) = u(t)$ and $u_4(t) = u'(t)$ we can transform (11) to a first-order system:

$$\begin{cases} u_1'(t) = u_2(t) \\ u_2'(t) = \frac{1+(u_2(t))^2}{1+u_1(t)} \\ u_3'(t) = u_4(t) \\ u_4'(t) = -\frac{1+(u_2(t))^2}{(1+u_1(t))^2} u_3(t) + \frac{2u_2(t)}{1+u_1(t)} u_4(t), \end{cases} \tag{14}$$

where $u_1(0) = 1$, $u_2(0) = \gamma$, $u_3(0) = 0$, and $u_4(0) = 1$. By solving this system, we find the value of $g(\gamma)$. Now that we know the values of $g(\gamma)$ and $g'(\gamma)$, which is u(5), we proceed to calculate $\gamma*$ with Newton's Method.

- The shooting method was selected to find the solutions of the given BVPs. This method transforms the BVP into a combination of two initial value problems and proceeds to calculate the root of the equation given by (3).
- In the previous section, the original systems were transformed into first-order systems to find their numerical solutions, particularly to find the value of $g(\gamma)$.



Numerical Methods: Newton Method

- These solutions were found using an ODE45 solver, which implements a combination of order four and order five Runge-Kutta methods to evaluate given differential equations systems.
- Once the systems were solved and the solution of $g(\gamma)$ was found, the Newton method was applied to approximate a numerical root of $\gamma*$.
- This method was selected over the bisection and secant methods due to its superior order of convergence and computational speed. The availability of a continuous derivative of f reaffirmed this selection.

Newton's method supposes that the given function f, which in this problem is represented by $g(\gamma)$, is differentiable. Then, the tangent line to f in the point $(x_0, f(x_0))$ is given by the equation

$$y = f(x_0) + f'(x_0)(x - x_0) \tag{15}$$

which is also the first degree Taylor polynomial. Therefore, an approximation of f can be found using this tangent line and defining x_1 as the x-intercept of the line. That is:

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}, \qquad f'(x_0) \neq 0. \tag{16}$$

Thus, this process can be repeated as long as it is needed, obtaining the following recursion:

$$\begin{cases} x_{n+1} = x + n - \frac{f(x_n)}{f'(x_n)} & n \geq 0, \\ x_0 \ \ given, \end{cases} \tag{17}$$

which is generally described as a fixed point iteration. Newton's method convergence is covered by *Theorem 1* (next slide).

In order to analyze the order of convergence of the Newton method we need to define the following theorems:

Theorem 1. Suppose that $f : \mathbb{R} \to \mathbb{R}$ is a function C^2 in a neighborhood of the scalar α, where $f(\alpha) = 0, f'(\alpha) \neq 0$. Then, if x_0 is selected close enough to α, the interations from (17) converge to α. Furthermore,

$$\lim_{n \to \infty} \frac{\alpha - x_{n+1}}{(\alpha - x_n)^2} = -\frac{f''(\alpha)}{2f'(\alpha)} \tag{18}$$

that is, (x_n) converges to α with convergence order of $p = 2$. The proof of this theorem is discussed in detail on professor's P. Negrón book.

Theorem 2. Suppose $f \in C^{n+1}(\alpha,\beta)$ and $a \in (\alpha,\beta)$. Let $R_n(x) = f(x) - p_n(x)$ the error of approximating f with p_n. Then:

$$R_n(x) = \frac{1}{n!}\int_a^x f^(n+1)(\xi)(x-\xi)^n d\xi = \frac{f^(n+1)(c_x)}{(n+1)!}(x-a)^{n+1}, x \in (\alpha,\beta), \tag{19}$$

where c_x is a number between a and x.

Therefore, using the Taylor Theorem (*Theorem 2*) we can write:

$$f(\alpha) = f(x_n) + f'(x_n)(\alpha - x_n) + \frac{1}{2}f''(\xi_n)(\alpha - x_n)^2 \ , \tag{20}$$

where ξ_n is between α and x_n. Since $f'(\alpha) \neq 0$ and f' is continuous, there exists a closed interval I around $x = \alpha$ such that $f'(\alpha) \neq 0$ for $x \in I$.

Therefore we can define the number M as

$$M = \frac{1}{2}\frac{max_{x\in I}|f''(x)|}{min_{x\in I}(f'(x))} \tag{21}$$

which is finite and exists. Note that the selection of the initial value x_0 is extremely important to guarantee convergence.

From *Theorem 1* and (21), it can be observed that if $M|\alpha - x_0| < 1$, then the iterations of this method converge to the root. Unfortunately, this estimate is not practical since M, which is given by (21), is in general hard or impossible to calculate.

Lastly, a heuristic criterion to stop the iterations of this method, supposing iterations (x_n) are close to the root α, could be given by:

$$Rel(x_n) = \frac{\alpha - x_n}{\alpha} \approx \frac{x_{n+1} - x_n}{x_n}. \tag{22}$$

Thus, if $|x_{n+1} - x_n| \leq |x_n| 10^{-t}$ there are approximately t significant numbers in x_n as an approximation of α.

The main possible sources of errors of this work reside on the ODE solvers and the Newton method. The parameters of absolute tolerance and max step-size were set to 10^{-6} and 10^{-3} respectively. Similarly, the tolerance of the Newton method was set to 10^{-5}, in order to control the accuracy of the calculated root value.

Computational Analysis

- Using the Octave interpreter, we programmed:
  - Systems of equations
  - Newton method algorithm
  - g function calculator
  - Driver for finding the solutions of the given systems

Computational Analysis: Newthon Method

The function for the Newton method was provided by P. Negrón.

```
    function [x,iter]=newton(f,x0,tol,itermax)
        if nargin<3
           tol=1.0e-4;
        end
        if nargin<4
           itermax=20;
        end
        x=x0;
        normx=0;
        normz=inf;
        iter=0;
        while (normz>tol*normx)&(iter<=itermax)
            [f0,fp0]=feval(f,x);
            z=-fp0\f0;
            normz=norm(z,2);
            normx=norm(x,2);
            x=x+z;
            iter=iter+1;
        end
```

Computational Analysis: g function

Then, the g function is calculated by:

```
function [g,gp]= gfunc(gam,a,b,alf,bet)
  y0=[alf,gam,0,1]';
  [t,u]=ode45(@sistyu,[a,b],y0);
  m=size(u,1);
  g=u(m,1)-bet;
  gp=u(m,3);
end
```

This function returns an approximation of the $g(\gamma)$ and $g'(\gamma)$ values when given the boundaries of the interval, and the α and β constants.

Functions for the first BVP are given by:

```
function w=sistyu(t,u)
  w=zeros(4,1);
  w(1)=u(2);
  w(2)=f(t,u(1),u(2));
  w(3)=u(4);
  w(4)=fy(t,u(1),u(2))*u(3) + fz(t,u(1),u(2))*u(4);
end
function w=f(t,y,z)
  w=(32+2*t^3-y*z)/8;
end
function w=fy(t,y,z)
  w=-z/8;
end
function w=fz(t,y,z)
  w=-y/8;
end
```

The driver program for the first BVP is given by:

```
a=1.0;
b=3.0;
alf=17.0;
bet=43/3;

x=1:.1:3;
yexacta=x.^2+16./x;
tm=newton(@(x)gfunc(x,a,b,alf,bet),a)
y0=[alf,tm, 0,1]';
[t,u]= ode45(@sistyu, [a,b],y0);

plot(t,u(:,1),'k',x,yexacta,'k+')
xlabel('t'); ylabel('y');
legend('Numerical Solution', 'Exact Solution');
```

Functions for the second BVP are given by:

```
function w=sistyu(t,u)
  w=zeros(4,1);
  w(1)=u(2);
  w(2)=f(t,u(1),u(2));
  w(3)=u(4);
  w(4)=fy(t,u(1),u(2))*u(3) + fz(t,u(1),u(2))*u(4);
end
function w=f(t,y,z)
  w=(1+z^2)/(1+y);
end
function w=fy(t,y,z)
  w=-(1+z^2)/((1+y)^2);
end
function w=fz(t,y,z)
  w= (2*z)/(1+y);
end
```

The driver program for the second BVP is given by:

```
a=0.0;
b=5.0;
alf=1.0;
bet=10.0;

tm=newton(@(x)gfunc(x,a,b,alf,bet),a)
y0=[alf,tm, 0,1]';
[t,u]= ode45(@sistyu, [a,b],y0);
plot(t,u(:,1))
xlabel('t'); ylabel('y')
```

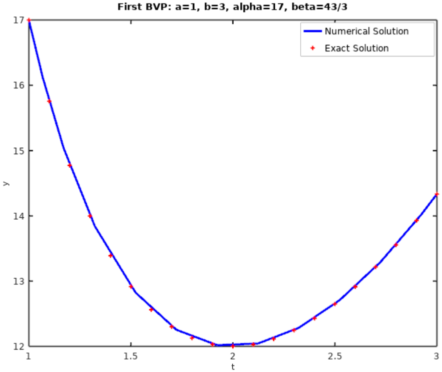


Figure: *Exact (red) and approximated solutions (blue) of the first BVP. The shooting method with initial parameters given by $a = 1.0, b = 3.0$, $\alpha = 17.0$, and $\beta = \frac{43}{3}$ was used for the approximation of the numerical solutions. The value of $\gamma*$ obtained was -14.000.*

Results: Second BVP

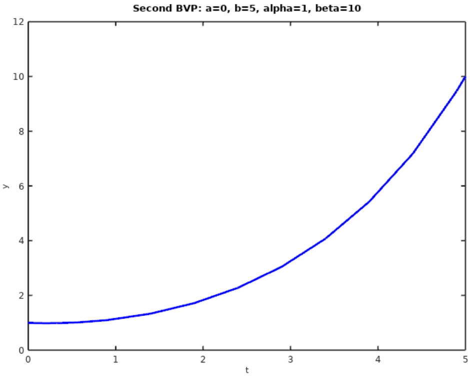


Figure: *Approximated solutions of the second BVP. The shooting method with initial parameters given by* $a = 0.0, b = 5.0, \alpha = 1.0,$ *and* $\beta = 10.0$ *was used for the approximation of the numerical solutions. The value of* $\gamma*$ *obtained was -0.12175.*

Conclusions

- The BVP has a wide range of multidisciplinary applications and can be approached using numerical methods.
- We have successfully developed a computational method for calculating the approximate solutions of two boundary value problems.
- It was proven that the proposed method could accurately find solutions for given systems when compared to exact solutions.
- The Newton method has proven to be fast and accurate when the continuous derivative of f is present. Approximation errors can in fact be restricted with the parameters of absolute tolerance and max step size.

Future Work

- Automation of the proposed set of scripts in order to calculate the derivatives using Matlab's symbolic libraries.
- Further analysis of the Dirichlet problem using additional numerical methods such as the bisection and the secant algorithms to compare their accuracy against the Newton method.
- Study the Neumann and Robin BVPs to validate the use of the proposed numerical methods.

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