Rigorous and non-rigorous error estimates for numerical solutions of initial value problems

Elena Ferreira Pires

July 4, 2022

Supervisor: M. Schlottbom

1 Introduction

Differential equations are used for a wide variety of mathematical models. When these differential equations have some initial condition that that has to be satisfied they become initial value problems. When such a problem cannot be solved exactly then the solution used be approximated using a numerical method.
Error estimation is an important issue when it comes to numerically solving initial value problems, since it can be used to make sure that a certain outcome is accurate enough for its purpose. Also it can be used to better inform the trade-off between a more accurate solution and the computing power needed.
The aim of this report is to look into two types of error estimation. First we will see some heuristic error estimates. We look into the explicit Euler method and general Runge-Kutta methods in sections 2 and 3 respectively, as well as Richardson extrapolation in section 4.
Second we look into finding a rigorous error estimate for Euler's method and the Crank-Nicolson method by using a reconstruction method in section 5.
At the end we will have a guaranteed error bound for the starting initial value problem.
For sections 2 and 3 the lecture notes by Kanschat [4] and the book by Griffiths [2] were used. For section 4 the book by Strehmel [5] was used. For section 5 the article by G. Akrivis, et al. [1] and the book by Hairer [3] was used.

2 Euler's method

Most standard numerical scheme for solving initial value problem

$$y'(x) = f(x, y),\ y(x_0) = y_0 \tag{1}$$

is the explicit Euler method. This method is of the form

$$y_{n+1} = y_n + hf(x_n, y_n), \tag{2}$$

where h is the step size and $x_n = x_0 + nh$.

The Euler scheme is of first order, which means that the global error e is given by $e \leq Ch^2$, where C is a constant. We can show this using Taylor expansion. We start with a general definition of this Taylor polynomial. A kth order Taylor polynomial of $g(x)$ around a is given by

$$f(x) = f(a) + (x-a)f'(a) + \frac{1}{2}(x-a)^2 f''(a) + ... + \frac{1}{k!}(x-a)^k f^{(k)}(a) + R,$$

where $k \geq 1$ and g is k times differentiable at a. For the remainder term R we have in general that

$$R = \mathcal{O}((x-a)^{k+1}) = C(x-a)^{k+1},$$

where C is a constant. An explicit expression for the remainder is given by

$$R = \frac{1}{(k+1)!}(x-a)^{k+1} f^{(k+1)}(s),$$

where s is between x and a.

We try to find an expression for the error $e_{n+1} = y(x_{n+1}) - y_{n-1}$. Here $y(x_{n+1})$ is the actual solution at x_{n+1} and y_{n+1} is the approximation, which is in this case obtained by using the Euler scheme.
For $y(x_{n+1})$ we have the Taylor expansion

$$y(x_{n+1}) = y(x_n + h) = y(x_n) + hy'(x_n) + O(h^2).$$

The original initial value problem (1) gives

$$y(x_{n+1}) = y(x_n + h) = y(x_n) + hf(x_n, y(x_n)) + O(h^2)$$

Now by the Euler method (2), we have local error

$$\begin{aligned} y(x_{n+1}) - y_{n+1} &= y(x_n) + hf(x_n, y(x_n)) + O(h^2) - (y_n + hf(x_n, y_n)) \\ &= (y(x_n) - y_n) + h(f(x_n, y(x_n)) - f(x_n, y_n)) + O(h^2) \end{aligned}$$

We have $e_n = y(x_n) - y_n$, and for $f(x_n, y(x_,n)) - f(x_n, y_n)$ we again use a Taylor expansion. Namely, the expansion of $f(x, y)$ around (x_n, y_n) which looks as follows

$$\begin{aligned} f(x_n, y(x_n)) = f(x_n, y_n) &+ (x_n - x_n)f_x(x_n, y_n) + (y(x_n) - y_n)f_y(x_n, y_n) \\ &+ \mathcal{O}((y(x_n) - y_n)^2). \end{aligned}$$

This gives

$$f(x_n, y(x_n)) - f(x_n, y_n) = e_n f_y(x_n, y_n) + \mathcal{O}((e_n^2)$$

Using this again in the expression for the local error $e_{n+1} = y(x_{n+1}) - y_{n+1}$ gives

$$\begin{aligned} e_{n+1} &= e_n + h(e_n f_y(x_n, y_n)) + O(h^2) \\ &= (1 + hf_y(x_n, y_n))e_n + \mathcal{O}(h^2) \end{aligned}$$

3 Runge-Kutta methods

A Runge-Kutta method of order s looks as follows

$$y_{n+1} = y_n + h(b_1 k_1 + \ldots + b_s k_s), \tag{3}$$

where for k_i, $i = 1, ..., s$ we have

$$\begin{aligned} &k_1 = f(x_0, y_0) \\ &k_2 = f(x_0 + c_2 h, y_0 + ha_{21}k_1) \\ &k_3 = f(x_0 + c_3 h, y_0 + h(a_{31}k_1 + a_{32}k_2)) \\ &... \\ &k_s = f(x_0 + c_s h, y_0 + h(a_{s1}k_1 + ... + a_{s-1}k_{s-1})). \end{aligned}$$

A one-step method is called consistent if for every initial value problem we have that $\lim_{h\to 0} \frac{e(x+h)}{h} = 0$ for $x_0 <= x < x_n$, in words this means that at any point the local error goes to zero as the step size h goes to zero.

The Runge-Kutta method is consistent if and only if we have that $\sum_{i=1}^{s} b_i = 1$. For higher order Runge-Kutta methods we also need the condition that $\sum_{j=1}^{i-1} a_{ij} = c_i$.

The Runge-Kutta method is usually written out by using a table called the Butcher tableau.

0				
c_2	a_{21}			
c_3	a_{31}	a_{32}		
.	.	.	.	
c_s	a_{s1}	a_{s2}	$a_{s,s-1}$	
	b_1	b_2	b_{s-1}	b_s

Table 1: General Butcher tableau for a Runge-Kutta method of order s.

Euler's method (10) is a first order Runge-Kutta method. Namely,

$$k_1 = f(x_0, y_0) \tag{4}$$
$$y_n = y_{n-1} + hk_1. \tag{5}$$

The corresponding Butcher tableau is then given by

0	
	1

Table 2: Butcher tableau for Euler's method.

Another example is the Heun method, also called the improved Euler method. This method is a second order method and looks as follows

$$\begin{aligned} k_1 &= f(x_0, y_0) \\ k_2 &= f(t_0 + h, y_0 + hk_1) \\ y_n &= y_{n-1} + h(\frac{1}{2}k_1 + \frac{1}{2}k_2), \end{aligned}$$

or in form of the Butcher tableau,

0		
1	1	
	$1/2$	$1/2$

Table 3: Butcher tableau for Heun's method.

For the error estimation of the Runge-Kutta method, we have that the local error for Runge-Kutta method of order p is given by $e_h \leq Ch^{p+1}$.

4 Richardson Extrapolation

By means of Richardson Extrapolation we obtain two things, first an error estimation for the approximation $y_{2\times h}$ and second an approximation for $y(x_n + 2h)$.

We use the error expressions of two different approximations using a fixed Runge-Kutta method of order p. One approximation using two steps of size h, and one of one larger step of size $2h$.

Recall that for a Runge-Kutta method of order p we have that the error $e(h) = y(h) - y_h$ satisfies $e(h) \leq Ch^{p+1}$.

First, the error of one big step of size $2h$ is given by

$$y(x_0 + 2h) - y_{2h} = C(x_0)(2h)^{p+1} + \mathcal{O}(h^{p+2}). \tag{6}$$

Second, the error of two smaller steps of size h is given by

$$\begin{aligned} y(x_0 + 2h) - y_{2\times h} &= y(x_0 + 2h) - y_h + y_h - y_{2\times h} \\ &= C(x_0 + h)(h)^{p+1} + \mathcal{O}(h^{p+2}) + y_h - y_{2\times h}. \end{aligned}$$

Generally, a one-step method is given by $y_{n+1} = y_n + h\phi(x_n, y_n)$. The function $\phi(x, y)$ is called a 'procedural function', so some general slope in the one-step method. Using such a slope $\phi(x, y)$ for the approximations y_h and $y_{2\times h}$ we get

$$\begin{aligned} y(x_0 + 2h) - y_{2\times h} &= C(x_0 + h)(h)^{p+1} + \mathcal{O}(h^{p+2}) \\ &\quad + y(x_0 + h) + h\phi(x_0 + h, y(x_0 + h)) - (y_h + h\phi(x_0 + h, y_h)). \end{aligned}$$

Since we have that

$$y(x_0 + h) - y_h = C(x_0)(h)^{p+1},$$

and also

$$C(x_0 + h) = C(x_0) + \mathcal{O}(h).$$

We obtain that

$$y(x_0 + 2h) - y_{2\times h} = 2C(x_0)(h)^{p+1} + O(h^{p+2}). \tag{7}$$

$(h\phi(x_0 + h, y(x_0 + h)) - h\phi(x_0 + h, y_h))$

Subtract 6 from 7 gives

$$\begin{aligned} y_2 - y_{2h} &= C(x_0)(2h)^{p+1} + \mathcal{O}(h^{p+2}) - (2C(x_0)(h)^{p+1} + \mathcal{O}(h^{p+2}) \\ &= 2C(x_0)(2^p h^{p+1} - h^{p+1}) + \mathcal{O}(h^{p+2}). \end{aligned}$$

From this we get that

$$2C(x_0) = \frac{y_{2\times h} - y_{2h}}{2^p - 1}(h)^{-(p+1)} + \mathcal{O}(h^{p+2}). \tag{8}$$

Finally, we use the expression (8) in the error $y(x_0 + 2h) - y_{2\times h}$ (7) to obtain another error estimation

$$y(x_n + 2h) - y_{2\times h} = \frac{y_{2\times h} - y_{2h}}{2^p - 1} + \mathcal{O}(h^{p+2}).$$

From this, we also obtain an approximation for $y(x_n + 2h)$ denoted here by w_h

$$w_h = y_{2\times h} + \frac{y_{2\times h} - y_h}{2^p - 1}.$$

5 Reconstruction method

In this section we will use a reconstruction method to find a rigorous bound for the error of the numerical solution for a different initial value problem as before.

5.1 Using Explicit Euler method

Consider the initial value problem

$$y'(x) + cy(x) = f(x),\ y(x_0) = y_0, \tag{9}$$

where c is a scalar. For this problem, the explicit Euler scheme looks as follows

$$\frac{y_n - y_{n-1}}{h} + cy_{n-1} = f(x_{n-1}), \tag{10}$$

where $h = x_n - x_{n-1}$. As discussed in section 2, the explicit Euler scheme is a first order method.

Now, we define a linear interpolant $\tilde{U}$ between the points y_{n-1} and y_n as

$$\tilde{U}(x) = y_{n-1} + (x - x_{n-1})\frac{y_n - y_{n-1}}{h}. \tag{11}$$

Since we have that

$$\tilde{U}' = \frac{y_n - y_{n-1}}{h},$$

the expression for the Euler scheme (10) is equivalent to

$$\tilde{U}'(x) + cy_{n-1} = f(x_{n-1}).$$

Which, by adding $c\tilde{U}(x)$ on both sides, can be written as

$$\tilde{U}'(x) + c\tilde{U}(x) = f(x_{n-1}) + c(\tilde{U}(x) - y_{n-1}). \tag{12}$$

This expression is in the same form as the original problem. We subtract expression (12) from the original initial value problem 9 to get the error equation

$$\tilde{e}'(x) + c\tilde{e}(x) = R_1(x), \tag{13}$$

where $\tilde{e}(x) = y(x) - \tilde{U}(x)$ and $R_1(x) = f(x) - (f(x_{n-1}) + c(\tilde{U}(x) - y_{n-1})$.

Next, we extract an error bound from this error equation using the energy method.
First we multiply by $\tilde{e}$ to get

$$\tilde{e}'\tilde{e} + c\tilde{e}^2 = R_1\tilde{e}.$$

We then integrate the error from x_0 to x_n, which gives

$$\int_{x_0}^{x_n} \tilde{e}'\tilde{e}\,dx + c\int_{x_0}^{x_n} \tilde{e}^2\,dx = \int_{x_0}^{x_n} R_1\tilde{e}\,dx.$$

($x_0 = 0$).

Now, by product rule we have $(ee)' = 2e'e$ and therefore $e'e = \frac{1}{2}(e^2)'$. Using this and $e(x_0) = 0$ gives

$$\frac{1}{2}\tilde{e}^2(x_n) + c\int_0^{x_n} \tilde{e}^2\,dx = \int_0^{x_n} R_1\tilde{e}\,dx.$$

Using $ab \leq \frac{a^2}{2c} + \frac{cb^2}{2}$ where $a = R$ and $b = \tilde{e}$ gives

$$\int_0^{x_n} R_1\tilde{e}dx \leq \int_0^{x_n} \frac{R_1^2}{2c} + \frac{c\tilde{e}^2}{2}dx.$$

From this we obtain

$$\frac{1}{2}\tilde{e}^2(x_n) + c\int_0^{x_n} \tilde{e}^2dx \leq \int_0^{x_n} \frac{R_1^2}{2c} + \frac{c\tilde{e}^2}{2}dx.$$

And finally,

$$\tilde{e}^2(x_n) + c\int_0^{x_n} \tilde{e}^2dx \leq \frac{1}{c}\int_0^{x_n} R_1^2dx. \tag{14}$$

Notice that we have an error bound that depends on the residual $R_1(x)$ that can be evaluated. Therefore an error bound can be computed.

Next we can again show the Euler method to be a first order method. For this we first simplify the error bound to

$$\tilde{e}^2(x_n) \leq \int_0^{x_n} R_1^2(x)\,dx,$$

which we then write as

$$\tilde{e}^2(x_n) \leq \sum_{k=1}^{n}\int_{x_{k-1}}^{x_k} R_1^2(x)\,dx. \tag{15}$$

We consider the residual given by $R_1 = f(x) - f(x_{n-1}) - c(\tilde{U}(x) - y_{n-1})$ in two parts.

First consider the term $f(x) - f(x_{n-1})$. The Taylor expansion of $f(x)$ around x_{n-1} is given by

$$f(x) = f(x_{n-1}) + f'(x_{n-1})(x - x_{n-1}) + \mathcal{O}((x - x_{n-1})^2).$$

Using this we get

$$f(x) - f(x_{n-1}) = f'(x_{n-1})(x - x_{n-1}) + \mathcal{O}((x - x_{n-1})^2). \qquad (16)$$

Second, for the term $c(U(x) - y_{n-1/2})$ we have that

$$\begin{aligned} c(U(x) - y_{n-1}) &= c\left(y_{n-1} + \frac{y_n - y_{n-1}}{h}(x - x_{n-1}) - y_{n-1}\right) \\ &= (x - x_{n-1})\left(c\,\frac{y_n - y_{n-1}}{h}\right). \end{aligned}$$

Then, using Euler's method (10) we can write

$$c(U(x) - y_{n-1}) = (x - x_{n-1})\left(c\left(f(x_{n-1}) - cy_{n-1}\right)\right). \qquad (17)$$

Finally we combine expressions (16) and (17) and the residual term R_1 becomes

$$R_1 = (x - x_{n-1})\left(f'(x_{n-1}) - \left(c\left(f(x_{n-1}) - cy_{n-1}\right)\right)\right).$$

We denote $a_k = \left(f'(x_{k-1}) - \left(c\left(f(x_{k-1}) - cy_{k-1}\right)\right)\right)$ and consider the integral in expression (15). We get

$$\begin{aligned} \int_{x_{k-1}}^{x_k} R_1^2(x)\,dx &= \int_{x_{k-1}}^{x_k} (x - x_{k-1})^2 (a_k)^2\,dx \\ &= (a_k)^2 \int_0^{h_k} \tilde{x}^2\,d\tilde{x} \\ &= \frac{(a_k)^2}{3} h_k^3. \end{aligned}$$

Now using this in the expression (15) again gives the error bound

$$\tilde{e}^2(x_n) \leq \sum_{k=1}^{n} \frac{a_k^2}{3}\,h_k^3.$$

Let $h_k = h$ for all k to obtain

$$\tilde{e}^2(x_n) \leq \sum_{k=1}^{n} \frac{a_k^2}{3}\,h^3 = h^3 \sum_{k=1}^{n} \frac{a_k^2}{3} \leq h^3 n \max_k \frac{a_k^2}{3} = h^2 x_n \max_k \frac{a_k^2}{3}.$$

Finally, we obtain the error bound

$$\tilde{e}(x_n) \leq h\sqrt{x_n} \max_k \frac{a_k}{\sqrt{3}}.$$

5.2 Using the Crank-Nicolson method

Now we use the same method as in the section above, only instead of the explicit Euler method we use the Crank-Nicolson method.
The Crank-Nicolson method is a combination of the implicit and the explicit Euler method. For the initial value problem (1) it would look as follows

$$y_n = y_{n-1} + \frac{1}{2}h(f(x_{n-1}, y_{n-1}) + f(x_n, y_n)).$$

The Taylor expansion of $y(x_{n+1})$ is given by

$$y(x_{n+1}) = y(x_n) + hy'(x_n) + \frac{1}{2}h^2 y''(x_n) + \mathcal{O}(h^3). \tag{18}$$

The expansion of $y'(x_n + h)$ gives

$$y'(x_{n+1}) = y'(x_n) + hy''(x_n) + \mathcal{O}(h^2),$$

therefore we have that

$$hy''(x_n) = y'(x_n + h) - y'(x_n) + \mathcal{O}(h^2). \tag{19}$$

Using expression (19) in the expansion for y_{n+1} (18), we get

$$\begin{aligned}
y(x_{n+1}) &= y(x_n) + hy'(x_n) + \frac{1}{2}h(y'(x_n + h) - y'(x_n) + \mathcal{O}(h^2)) + \mathcal{O}(h^3) \\
&= y(x_n) + \frac{1}{2}h(y'(x_n) + y'(x_n + h)) + \mathcal{O}(h^3) \\
&= y(x_n) + \frac{1}{2}h(f(x_n, y(x_n)) + f(x_n + h, y(x_n + h))) + \mathcal{O}(h^3).
\end{aligned}$$

For the local error $e_{n+1} = y(x_{n+1}) - y_{n+1}$ we then have,

$$\begin{aligned}
e_{n+1} &= y(x_{n+1}) - y_{n+1} \\
&= y(x_n) + \frac{1}{2}h(f(x_n, y(x_n)) + f(x_n + h, y(x_n + h))) + \mathcal{O}(h^3) \\
&- (y_n + \frac{1}{2}h(f(x_n, y_n) + f(x_{n+1}, y_{n+1})) \\
&= e_n + \frac{1}{2}h(f(x_n, y(x_n)) - f(x_n, y_n) + f(x_{n+1}, y(x_{n+1})) \\
&- f(x_{n+1}, y_{n+1})) + \mathcal{O}(h^3).
\end{aligned}$$

By Taylor expansion of $f(x, y)$ around (x_n, y_n), we get

$$f(x_n, y(x_n)) - f(x_n, y_n) = e_n f_y(x_n, y_n) + \mathcal{O}(e_n^2).$$

Finally, this gives

$$e_{n+1} = \frac{1 + \frac{h}{2} f_y(x_n, y_n)}{1 - \frac{h}{2} f_y(x_{n+1}, y_{n+1})} e_n + \mathcal{O}(h^3).$$

Now for the problem of the form $y' + cy = f(x)\,, y(x_0) = x_0$, the Crank-Nicolson method can be written as

$$\frac{y_n - y_{n-1}}{h} + cy_{n-1/2} = \frac{f(x_n) + f(x_{n-1})}{2}, \tag{20}$$

where $y_{n-1/2} = \frac{y_n + y_{n-1}}{2}$.

We define a linear interpolant $\phi(x)$ for the function $f(x)$ at points x_{n-1} and x_n as follows

$$\phi(x) = f(x_{n-1}) + (x - x_{n-1}) \frac{f(x_n) - f(x_{n-1})}{h}. \tag{21}$$

Observe that $\phi(x_{n-1}) = f(x_{n-1})$ and $\phi(x_n) = f(x_n)$. Also, $\phi(x_{n-1/2}) = \frac{f(x_n)+f(x_{n-1})}{2}$.
Therefore the Crank-Nicolson method (20) is equivalent to

$$\frac{y_n - y_{n-1}}{h} + cy_{n-1/2} = \phi(x_{n-1/2}). \tag{22}$$

Now we define a linear interpolant $U(x)$ between points y_n and y_{n-1} as follows

$$U(x) = y_{n-1/2} + (x - x_{n-1/2})\frac{y_n - y_{n-1}}{h}.$$

See that $U(x_{n-1/2}) = y_{n-1/2}$ and

$$\begin{aligned} U(x_n) &= y_{n-1/2} + \left(\frac{h}{2}\right)\frac{y_n - y_{n-1}}{h} \\ &= \frac{y_n + y_{n-1}}{2} + \frac{y_n - y_{n-1}}{2} = y_n \end{aligned}$$

Similarly, $U(x_{n-1}) = y_{n-1}$.

Since we have that

$$U'(x) = \frac{y_n - y_{n-1}}{h},$$

we have that the expression for the Crank-Nicolson method (22) can be written as

$$U'(x) + cy_{n-1/2} = \phi(x_{n-1/2}).$$

And by adding $cU(x)$ on both sides we can write this as

$$U'(x) + cU(x) = \phi(x_{n-1/2}) - c(y_{n-1/2} - U(x)). \tag{23}$$

This is in the same form as the original equation. So we subtract the equation (23) from the original initial value problem (9) to get the error equation

$$e(x)' + ce(x) = R_2(x), \tag{24}$$

where $e(x) = y(x) - U(x)$ and $R_2(x) = f(x) - \phi(x_{n-1/2}) - c(y_{n-1/2} - U(x))$.
As before in section (), we can obtain from this error equation the simplified error bound

$$e^2(x_n) \leq \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} R_2^2(x)\, dx. \tag{25}$$

Notice that $R_2(x)$ can be evaluated, so an error bound can be computed.
Now for a closer look at the residual R_2 to obtain the order of the method.
We first consider the term $f(x) - \phi(x_{n-1/2})$. Using the Taylor expansion for $f(x)$ around $x_{n-1/2}$, we get

$$\begin{aligned} f(x) - f(x_{n-1/2}) &= f(x_{n-1/2}) + f'(x_{n-1/2})(x - x_{n-1/2}) + ... - f(x_{n-1/2}) \\ &= f'(x_{n-1/2})(x - x_{n-1/2}) + ... \end{aligned}$$

$$f(x) - f(x_{n-1/2}) = f'(x_{n-1/2})(x - x_{n-1/2}) + ... \tag{26}$$

Second, for the term $c(U(x) - y_{n-1/2})$ we have that

$$\begin{aligned} c(U(x) - y_{n-1/2}) &= c\left(y_{n-1/2} + \frac{y_n - y_{n-1}}{h}(x - x_{n-1/2}) - y_{n-1/2}\right) \\ &= (x - x_{n-1/2})\left(c\,\frac{y_n - y_{n-1}}{h}\right). \end{aligned}$$

Then, using the Crank-Nicolson scheme we can write

$$c(U(x) - y_{n-1/2}) = (x - x_{n-1/2})\left(c\left(\phi(x_{n-1/2}) - cy_{n-1/2}\right)\right). \tag{27}$$

Combining expressions (26) and (27) the residual term R_2 becomes

$$R_2 = (x - x_{n-1/2})\left(f'(x_{n-1/2}) - c(f(x_{n-1/2}) - cy_{n-1/2})\right).$$

Denote $a_k = f'(x_{n-1/2}) - c(f(x_{n-1/2}) - cy_{n-1/2}$ and consider the integral in the error bound (25). We obtain that

$$\begin{aligned} \int_{x_{k-1}}^{x_k} R_2^2(x)\,dx &= \int_{x_{k-1}}^{x_k} (x - x_{k-1/2})^2 (a_k)^2\,dx \\ &= (a_k)^2 \int_{-h_k/2}^{h_k/2} \tilde{x}^2\,d\tilde{x} \\ &= \frac{a_k^2}{3}((\frac{h_k}{2})^3 + (\frac{h_k}{2})^3) \\ &= \frac{a_k^2}{12}h_k^3. \end{aligned}$$

Now we use this again in expression (25) and assume $h_k = h$ for all k, and we obtain the error bound

$$\begin{aligned} e^2(x_n) &\leq \sum_{k=1}^{n} \frac{a_k^2}{12}h_k^3 \\ &\leq h^2 x_n \max_k \frac{a_k^2}{12}. \end{aligned}$$

And finally,

$$e(x_n) \leq h\sqrt{x_n}\max_k \frac{a_k}{\sqrt{12}}. \tag{28}$$

We see that the error bound is of first order. However the Crank-Nicolson method is of second order. Therefore, in the next section, we will again use the same methodology, but this time using a quadratic reconstruction instead of a linear one.

5.3 Quadratic reconstruction

Start with the observation that the original initial value problem 9 is equivalent to the problem

$$y(x) = y_0 + \int_{x_0}^{x} f(s) - cy(s)\,ds.$$

Now by replacing $f(s)$ and $y(s)$ by their linear interpolants $\phi(s)$ (21) and $U(s)$ (23) respectively and starting from y_{n-1}, we define the reconstruction $\hat{U}$ as

$$\hat{U}(x) = y_{n-1} + \int_{x_{n-1}}^{x} \phi(s) - cU(s)\,ds.$$

We see that $\hat{U}(x_{n-1}) = y_{n-1}$ and for $\hat{U}(x_n)$, since $U(x)$ and $\psi(x)$ are both linear, we have by the trapezoidal rule that

$$\begin{aligned}
\hat{U}(x_n) &= y_{n-1} + \int_{x_{n-1}}^{x_n} \phi(s) - cU(s)\,ds \\
&= y_{n-1} + \frac{1}{2}(x_n - x_{n-1})(\phi(x_n) - cU(x_n) + \phi(x_{n-1}) - cU(x_{n-1}) \\
&= y_{n-1} + \frac{1}{2}(h)(f(x_n) - cy_n + f(x_{n-1}) - cy_{n-1}) \\
&= y_{n-1} + h(\phi(x_{n-1/2}) - cy_{n-1/2}) \\
&= y_{n-1} + h(\frac{y_n - y_{n-1}}{h}) = y_n
\end{aligned}$$

Since

$$\hat{U}'(x) = \phi(x) - cU(x),$$

we have that

$$\hat{U}'(x) + c\hat{U}(x) = \phi(x) + c(\hat{U}(x) - U(x)). \tag{29}$$

Now we see that this equation in the same form as the original inital value problem. Therefore, we subtract equation (29) from the original problem (9) to get the error equation

$$\hat{e}(x)' + c\hat{e}(x) = R_3(x), \tag{30}$$

where $\hat{e}(x) = y(x) - \hat{U}(x)$ and $R_3(x) = f(x) - \phi(x) - c(\hat{U}(x) - U(x))$.

As done before in both section () and (), we can obtain from this error equation the simplified error bound

$$e^2(x_n) \leq \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} R_3^2(x)\,dx. \tag{31}$$

Like before, we have that since R_3 can be evaluated, we can compute an explicit error bound.

Next we can also find the order of the method. For this, we consider the residual R_3. First consider the term $f(x) - \phi(x)$. Using the expansion for $f(x)$ around

$(x - x_{n-1})$ and expression for $\phi(x)$ (21) we get

$$\begin{aligned} f(x) - \phi(x) &= f(x_{n-1}) + f'(x_{n-1})(x - x_{n-1}) + \mathcal{O}(x - x_{n-1})^2 \\ &- (f(x_{n-1}) + (x - x_{n-1})\frac{f(x_n) - f(x_{n-1}}{h}) \\ &= (x - x_{n-1})(f'(x_{n-1}) - \frac{f(x_n) - f(x_{n-1})}{h}) + \mathcal{O}(x - x_{n-1})^2 \\ &= (x - x_{n-1})(f'(x_{n-1}) - \frac{f(x_n) - f(x_{n-1})}{h}) + (x - x_{n-1})^2 \frac{1}{2} f''(s), \end{aligned}$$

where s is between x and x_{n-1}. Use the Taylor expansion of $f(x)$ around $f(x_{n-1})$ to write

$$f(x_n) = f(x_{n-1}) + hf'(x_{n-1}) + \frac{1}{2}h^2 f''(x_{n-1}) + \mathcal{O}(h^3).$$

We then get that

$$\frac{f(x_n) - f(x_{n-1})}{h} = f'(x_{n-1}) + \frac{1}{2}hf''(x_{n-1}) + \mathcal{O}(h^2).$$

And finally,

$$f'(x_{n-1}) - \frac{f(x_n) - f(x_{n-1})}{h} = -(\frac{1}{2}hf''(x_{n-1}) + \mathcal{O}(h)^2).$$

So for the term $f(x) - \phi(x)$ we have

$$f(x) - \phi(x) = (x - x_{n-1})^2 \Big(\frac{1}{2}f''(s)\Big) + (x - x_{n-1})\Big(-\frac{1}{2}hf''(x_{n-1}) + \mathcal{O}(h)^2\Big). \quad (32)$$

Now for the term $c(\hat{U} - U)$. First, since $\phi(x)$ and $U(x)$ are linear, by the trapezoidal rule we write $\hat{U}(x)$ as

$$\hat{U}(x) = y_{n-1} + \frac{1}{2}(x - x_{n-1})(\phi(x) - cU(x) + f(x_{n-1}) - cy_{n-1}).$$

Using then the expressions for $\phi(x)$ and $U(x)$ we have

$$\begin{aligned} \hat{U}(x) = y_{n-1} + \frac{1}{2}(x - x_{n-1})\Bigg(& f(x_{n-1}) + (x - x_{n-1})\frac{f(x_n) - f(x_{n-1})}{h} \\ & - c(y_{n-1} + (x - x_{n-1})\frac{y_n - y_{n-1}}{h}) + f(x_{n-1}) - cy_{n-1}\Bigg) \end{aligned}$$

By rearranging terms by powers of $(x - x_{n-1})$ we get

$$\begin{aligned} \hat{U}(x) &= (x - x_{n-1})^2 \Big(\frac{1}{2h}(f(x_n) - f(x_{n-1}) - c(y_n - y_{n-1}))\Big) \\ &+ (x - x_{n-1})\Big(f(x_{n-1}) - cy_{n-1}\Big) + y_{n-1} \end{aligned}$$

We use this expression for $\hat{U}(x)$ to write

$$c(\hat{U}-U) = c((x-x_{n-1})^2\Big(\frac{1}{2h}(f(x_n)-f(x_{n-1})-c(y_n-y_{n-1}))\Big)$$
$$+(x-x_{n-1})\Big(f(x_{n-1})-cy_{n-1}\Big)+y_{n-1}$$
$$-(y_{n-1}+(x-x_{n-1})\frac{y_n-y_{n-1}}{h})).$$

By rearranging terms again we obtain

$$c(\hat{U}-U) = (x-x_{n-1})^2\Big(\frac{1}{2h}(f(x_n)-f(x_{n-1})-c(y_n-y_{n-1}))\Big)$$
$$+(x-x_{n-1})\Big(cf(x_{n-1})-c^2y_{n-1}-c\frac{y_n-y_{n-1}}{h}\Big).$$

For residual R_3 we then have, after again rearranging by powers of $(x-x_{n-1})$,

$$R_3 = (x-x_{n-1})^2\left(\frac{1}{2}f''(s)-\frac{1}{2h}(f(x_n)-f(x_{n-1})-c(y_n-y_{n-1}))\right)$$
$$+(x-x_{n-1})\left(f'(x_{n-1})-\frac{f(x_n)-f(x_{n-1})}{h}-cf(x_{n-1})+c^2y_{n-1}+c\frac{y_n-y_{n-1}}{h}\right).$$

We denote

$$a_k = \frac{1}{2}f''(s)-\frac{1}{2h}(f(x_n)-f(x_{n-1}))+\frac{1}{2h}(c(y_n-y_{n-1}))$$

and

$$b_k = f'(x_{n-1})-\frac{f(x_n)-f(x_{n-1})}{h}-cf(x_{n-1})+c^2y_{n-1}+c\frac{y_n-y_{n-1}}{h}.$$

First consider the expression for a_k. By Taylor expansion of $f(x)$ around (x_{n-1}) we have that

$$f(x_n)-f(x_{n-1}) = hf'(\hat{s}),$$

where $\hat{s}$ is between x_{n-1} and x_n. Now by the Crank-Nicolson method (22) we have

$$a_k = \frac{1}{2}f''(s)-\frac{1}{2}f'(\hat{s})-\frac{c}{2}(\phi(x_{n-1/2})-cy_{n-1/2}). \tag{33}$$

Second we take a closer look at the expression for b_k. We see first that for $f'(x_{n-1})-\frac{f(x_n)-f(x_{n-1})}{h}$ we have by Taylor expansion that

$$f'(x_{n-1})-\frac{f(x_n)-f(x_{n-1})}{h} = -\frac{1}{2}hf''(x_{n-1})+\mathcal{O}(h^2)).$$

Second, for $-cf(x_{n-1})+c^2y_{n-1}+c\frac{y_n-y_{n-1}}{h}$ we have by the Crank-Nicolson method (22) that

$$-cf(x_{n-1})+c^2y_{n-1}+c\frac{y_n-y_{n-1}}{h} = -cf(x_{n-1})+c^2y_{n-1}+c(\phi(x_{n-1/2})-cy_{n-1/2})$$
$$= c(\phi(x_{n-1/2})-f(x_{n-1}))+c^2(y_{n-1}-y_{n-1/2}).$$

For the first term we have by definition (21) that

$$\begin{aligned}\phi(x_{n-1/2}) - f(x_{n-1}) &= \frac{1}{2}(f(x_{n-1}) + f(x_n)) - f(x_{n-1}) \\ &= \frac{1}{2}(f(x_n) - f(x_{n-1})),\end{aligned}$$

and by Taylor expansion of $f(x)$ around x_{n-1} we have

$$f(x_n) - f(x_{n-1}) = \mathcal{O}(h).$$

Therefore we can write

$$\phi(x_{n-1/2}) - f(x_{n-1}) = \frac{1}{2}(\mathcal{O}(h)) = \mathcal{O}(h).$$

For the second term we have by the Crank-Nicolson method (22)

$$\begin{aligned}y_{n-1} - y_{n-1/2} &= y_{n-1} - \frac{1}{2}(y_n + y_{n-1}) \\ &= \frac{1}{2}(y_{n-1} - y_n) \\ &= \frac{1}{2}(h(\phi(x_{n-1/2}) - cy_{n-1/2})).\end{aligned}$$

Finally, this gives

$$b_k = -\frac{1}{2}hf''(x_{n-1}) + \mathcal{O}(h) + \frac{1}{2}(h(\phi(x_{n-1/2}) - cy_{n-1/2})). \tag{34}$$

Now we consider the integral in the error bound (31), we get that

$$\begin{aligned}\int_{x_{k-1}}^{x_k} R_3^2(x)\,dx &= \int_{x_{k-1}}^{x_k} ((x - x_{n-1})^2 a_k + (x - x_{n-1})b_k)^2\,dx \\ &\leq \int_{x_{k-1}}^{x_k} (x - x_{n-1})^4 a_k^2\,dx + \int_{x_{k-1}}^{x_k} (x - x_{n-1})^2 b_k^2\,dx \\ &\leq \int_0^{h_k} (\tilde{x})^4 a_k^2\,d\tilde{x} + \int_0^{h_k} (\tilde{x})^2 b_k^2\,d\tilde{x} \\ &= a_k^2 \frac{1}{5} h_k^5 + b_k^2 \frac{1}{3} h_k^3.\end{aligned}$$

Putting this expression back into the error bound (31) and $h_k = h$ for all k gives

$$\begin{aligned}e^2(x_n) &\leq \sum_{k=1}^{n} a_k^2 \frac{1}{5} h_k^5 + b_k^2 \frac{1}{3} h_k^3 \\ &\leq nh^5 \max_k \frac{a_k^2}{5} + nh^3 \max_k \frac{b_k^2}{3} \\ &= h^4 x_n \max_k \frac{a_k^2}{5} + h^2 x_n \max_k \frac{b_k^2}{3}\end{aligned}$$

And finally,

$$e(x_n) \leq h^2 x_n \max_k \frac{a_k}{5} + h x_n \max_k \frac{b_k}{3}. \tag{35}$$

Observe that to retrieve the second order of the Crank-Nicolson method, we need that a_k and b_k have the correct h powers. Recall expressions (33) and (34) for a_k and b_k respectively and observe that that is indeed the case.
We conclude that the error bound is of second order, like the Crank-Nicolson method is.

5.4 Numerical example

The goal of this section is to find an expression for the error bound (15) that is the result of using the Euler method for the reconstruction method, as well as check it.
In this example, we pick the values $c = 1$, $f(x) = 0$ and $y_0 = 1$ in the original initial value problem (9). For these values we know that the exact solution of the initial value problem is given by $y(x) = e^{-x}$.
Since in the picked example the solution is known, the error can be computed exactly by calculating the difference between the known solution $y(x_n)$ and the corresponding approximation y_n using Euler's method. In the figure below, this real error corresponds to the blue line.
The error bound that is calculated using expression (15) is the orange line in the figure below.

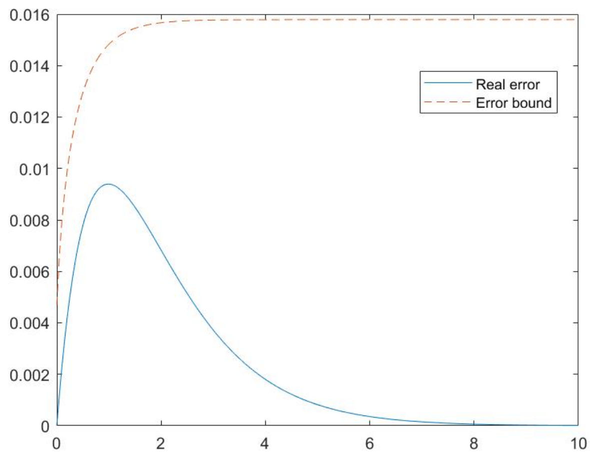

Figure 1: 1. The Euler method is used with starting point $x_0 = 0$, end point $x_{end} = 10$ and step size $h = 0.05$. The test problem is $c = 1$, $f(x) = 0$ and $y0 = 1$.

As expected, we see that the error bound is always above the real error. At the start the error bound gets quite high like the real error is as well. Later the real error gets smaller, and with that, the error bound also does not increase as much anymore.
In this example the simplified error bound (15) was used. Error bound (14), which the bound (15) is derived from, is sharper. Another way to retrieve an error bound that is arguably better, since it is exact is by solving the error

equation (13).

6 Conclusion

First we have seen some heuristic error estimations for the Euler method and Runge-Kutta methods in general. We have also seen an alternative error estimation in the form of Richardson extrapolation.
Second we have, by use of the reconstruction method, found a rigorous error bound for the Euler method as well as the Crank-Nicolson method.
Unlike the heuristic error estimations, which are not exact, the found rigorous error bound guarantees an upper bound for the error.

7 Discussion

A rigorous error bound as found could be used at end of simulation to check a certain tolerance to check if step size h was appropriately chosen. However, while in the sections above the step size h has been kept fixed, the step size may also be adapted through out a simulation based on an error estimation.
In this report the heuristic estimations and the rigorous bounds have been treated separately. That raises the question of how the two compare.
In the article by G. Akrivis, et al. [1] a method similar to the one described in this report was developed in order to find an error bound for a non-linear parabolic equation.

References

[1] G. Akrivis, C. Makridakis, and R. Nochetto. A posteriori error estimates for the Crank–Nicolson method for parabolic equations. *Mathematics of Computation*, 75(254):511–531, 2005. ISSN 0025-5718. doi: 10.1090/s0025-5718-05-01800-4.

[2] D. J. H. David F. Griffiths. *Numerical Methods for Ordinary Differential Equations*. 2010. ISBN 978-0-85729-147-9. doi: 10.1007/978-0-85729-148-6.

[3] E. Hairer, S. P. S. P. Nørsett 1944-, and G. Wanner. *Solving ordinary differential equations. I, Nonstiff problems LK - https://ut.on.worldcat.org/oclc/775677091*. Springer, Berlin ; SE - XV, 528 p. : ill. ; 24 cm, 2nd rev. ed., corr. 3rd pr. edition, 2008. ISBN 9783540566700 3540566708 9783642051630 3642051634 9783540788621 354078862X.

[4] G. Kanschat. *Numerical Analysis of Ordinary Differential Equations*. 2018. URL `https://www.mathsim.eu/~gkanscha/notes/ode.pdf`.

[5] K. Strehmel, R. Weiner, and H. Podhaisky. *Numerik gewöhnlicher Differentialgleichungen*. 2012. ISBN 9783834822635. doi: 10.1007/978-3-8348-2263-5.