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Using the θ -method to solve ODEs

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1 Introduction

- In this report we use the θ -method to solve ODE's. We begin by introducing the
- method and deriving it's truncation error. We use this to derive an expression for the
- local error. We then show an example to confirm that the correct rates of convergence are achieve.

In what follows we consider initial value problems of the form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = f(t, u) \tag{1}$$

- for t > 0 with an initial condition $u(0) = u_0$. Here, we assume that f(t,u) satisfies a
- Eipschitz condition in its second argument and that f(u,t) is bounded.
- It is also possible to use the θ -method to solve problems with spacial dependence. For example we could consider the heat equation of the form
- $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$
- for $(x,t) \in (-1,1)x(0,T]$ with boundary and initial conditions

$$u(x,0) = u_0(x) \quad for \quad -1 < x < 1,$$

$$u(-1,t) = g_1(t) \quad for \quad t > 0,$$

$$u(1,t) = g_2(t) \quad for \quad t > 0.$$

- However, we don't consider such problems here. Instead, we refer the interested
- reader to Ref. [1].

\bullet 2 The θ -method

For a general introduction to the θ method see Ref. [2]. We summarise the key points here.

In the θ -method we approximate the solution to Equation (1) at a set of discrete time points $t_n = n\Delta t$ for n = 0, ..., N where $N \geq 2$ and $N\Delta t = T$, where T is the final time. We let U_n be the numerical approximation to $u(t_n)$.

 θ -method for Equation 1 is

$$\frac{U_{n+1} - U_n}{\Delta t} = \theta f(t_{n+1}, U_n + 1) + (1 - \theta) f(t_n, U_n)$$

- Where θ is between 0 and 1. We require this equation to hold for n = 0, ..., N 1 and we apply the initial condition via $U_0 = u_0$. 3 values of θ lead to methods with a specific name:
- $\theta = 0$ is the explicit Euler scheme(also known as "forward Euler")
 - $\theta = 1$ is the implicit Euler scheme (also known as "backward Euler")
- $\theta = \frac{1}{2}$ is the Crank Nicolson scheme.

2.0.1 Truncation Error

The truncation error for the θ -method is defined as

$$T_n = \frac{u_{n+1} - u_n}{\Delta t} - \theta f(t_{n+1}, u_{n+1}) - (1 - \theta) f(t_n, u_n) , \qquad (2)$$

where $u_n = u(t_n)$ is the exact solution at the point t_n . The truncation error can be computed using Taylor series expansions about an appropriately chosen time point.

For $\theta = 0$ (i.e. explicit Euler), the expansions are usually performed about $t = t_n$, while for $\theta = 1$ (i.e. implicit Euler), the expansions are usually performed about $t = t_{n+1}$. For general values of θ it is standard to expand about $t_{n+1/2} = (t_n + t_{n+1})/2 = t_n + 1/2\Delta t$.

Note that since $u'(t_n) = f(t_n, u(t_n))$, we may re-write the expression for the truncation error

$$T_{n} = \frac{u_{n+1} - u_{n}}{\Delta t} - \theta f(t_{n+1}, u_{n+1}) - (1 - \theta) f(t_{n}, u_{n})$$

$$= \frac{u_{n+1} - u_{n}}{\Delta t} - \theta u'(t_{n+1}) - (1 - \theta) u'(t_{n}). \tag{3}$$

We have

$$u(t_n) = u(t_{n+1/2} - \Delta t/2)$$

$$= u(t_{n+1/2}) - \frac{\Delta t}{2} u'(t_{n+1/2}) + \frac{1}{2} \left(\frac{\Delta t}{2}\right)^2 u''(t_{n+1/2}) + \mathcal{O}(\Delta t^3)$$

Similarly,

$$u(t_{n+1}) = u(t_{n+1/2}) + \frac{\Delta t}{2}u'(t_{n+1/2}) + \frac{1}{2}\left(\frac{\Delta t}{2}\right)^2 u''(t_{n+1/2}) + \mathcal{O}(\Delta t^3)$$

We can also expand the first derivatives in Equation (3):

$$u'(t_n) = u'(t_{n+1/2}) - \frac{\Delta t}{2} u''(t_{n+1/2}) + \mathcal{O}(\Delta t^2) ,$$

$$u'(t_{n+1}) = u'(t_{n+1/2}) + \frac{\Delta t}{2} u''(t_{n+1/2}) + \mathcal{O}(\Delta t^2) .$$

Substituting these four expansions into (3) gives

$$T_{n} = \frac{1}{\Delta t} ((u(t_{n+1/2}) + \frac{\Delta t}{2}u'(t_{n+1/2}) + \frac{1}{2}(\frac{\Delta t}{2})^{2}u''(t_{n+1/2})) - (u(t_{n+1/2}) - \frac{\Delta t}{2}u'(t_{n+1/2}) + \frac{1}{2}(\frac{\Delta t}{2})^{2}u''(t_{n+1/2})))$$

$$-\theta(u'(t_{n+1/2}) + \frac{\Delta t}{2}u''(t_{n+1/2})) - (1 - \theta)(u'(t_{n+1/2}) - \frac{\Delta t}{2}u''(t_{n+1/2})) + O(\Delta t^{2})$$

Many of the terms in (4) cancel so the truncation error simplifies to

$$T_n = \frac{\Delta t}{2} (1 - 2\theta) u''(t_{n+1/2}) + \mathcal{O}(\Delta t^2) .$$

It can be shown by writing out the the $\mathcal{O}(\Delta t^2)$ terms in full, that they do not cancel for any value of θ .

Thus we have shown that for constant θ

$$T_n = \begin{cases} \mathcal{O}(\Delta t) & \text{for } \theta \neq 1/2 \\ \mathcal{O}(\Delta t^2) & \text{for } \theta = 1/2 \end{cases}$$

so that the truncation error of the Crank Nicolson scheme converges twice as fast as that of all other *theta*-methods.

2.1 Pointwise Errors

Recall the definition of the θ -method (??) and the corresponding truncation error (2):

$$\frac{U_{n+1} - U_n}{\Delta t} = \theta f(t_{n+1}, U_{n+1}) + (1 - \theta) f(t_n, U_n) ,$$

$$T_n = \frac{u_{n+1} - u_n}{\Delta t} - \theta f(t_{n+1}, u_{n+1}) - (1 - \theta) f(t_n, u_n) .$$

We re-arrange both of these to get

$$U_{n+1} = U_n + \Delta t \left(\theta f(t_{n+1}, U_{n+1}) + (1 - \theta) f(t_n, U_n) \right)$$
 (5)

$$u_{n+1} = u_n + \Delta t \left(\theta f(t_{n+1}, u_{n+1}) + (1 - \theta) f(t_n, u_n) \right) + \Delta t T_n \tag{6}$$

$$\implies |u_{n+1} - U_{n+1}| \le |u_n - U_n| + \theta \Delta t |f(t_{n+1}, u_{n+1}) - f(t_{n+1}, U_{n+1})| + (1 - \theta) \Delta t |f(t_n, u_n) - f(t_n, U_n)| + \Delta t |T_n|.$$
(7)

- Next suppose that the right-hand-side function f(t, u) satisfies a Lipschitz condition in its second argument, with Lipschitz constant L, so that:
- $|f(t,u)-f(t,v)| \leq L|u-v|, \quad \forall (t,u), \ (t,v) \in \Omega.$

We can use this in (7) to get

$$|u_{n+1} - U_{n+1}| \le |u_n - U_n| + \theta \Delta t L |u_{n+1} - U_{n+1}| + (1-\theta) \Delta t L |u_n - U_n| + \Delta t |T_n|$$

We can re-arrange this to get (for $\Delta t \ll 1$)

$$(1 - L\theta \Delta t)|u_{n+1} - U_{n+1}| \leq (1 + L(1 - \theta)\Delta t)|u_n - U_n| + \Delta t|T_n|$$

$$\leq (1 + L(1 - \theta)\Delta t)|u_n - U_n| + \Delta tT_{\text{max}},$$
 (8)

where

$$T_{\max} = \max_{0 \le n \le N} |T_n|$$

is an upper bound on the absolute value of the truncation error.

Now let $e_n = u_n - U_n$ denote the error at time t_n . Then (8) can be written as

$$|e_{n+1}| \leq \frac{1 + L(1-\theta)\Delta t}{1 - L\theta\Delta t}|e_n| + \frac{\Delta t T_{\text{max}}}{1 - L\theta\Delta t}. \tag{9}$$

We can show by induction that

$$|e_n| \leq \left(\frac{1 + L(1 - \theta)\Delta t}{1 - L\theta\Delta t}\right)^n |e_0| + \frac{\Delta t T_{\max}}{1 - L\theta\Delta t} \sum_{r=1}^n \left(\frac{1 + L(1 - \theta)\Delta t}{1 - L\theta\Delta t}\right)^{r-1}$$

$$\leq \left(\frac{1 + L(1 - \theta)\Delta t}{1 - L\theta\Delta t}\right)^n |e_0| + \frac{T_{\max}}{L} \left[\left(\frac{1 + L(1 - \theta)\Delta t}{1 - L\theta\Delta t}\right)^n - 1\right],$$

where the final line comes from evaluating the sum and simplifying. This holds for n = 0, 1, ..., N.

In practice, we usually set $U_0 = u_0$ which means that $e_0 = 0$. We also have

$$\frac{1 + L(1 - \theta)\Delta t}{1 - L\theta\Delta t} = 1 + \frac{L\Delta t}{1 - L\theta\Delta t}$$

$$\leq \exp\left(\frac{L\Delta t}{1 - L\theta\Delta t}\right).$$

In turn this means

$$\left(\frac{1 + L(1 - \theta)\Delta t}{1 - L\theta\Delta t}\right)^{n} \leq \left(\exp\left(\frac{L\Delta t}{1 - L\theta\Delta t}\right)\right)^{n}$$

$$\leq \exp\left(\frac{nL\Delta t}{1 - L\theta\Delta t}\right)$$

$$\leq \exp\left(\frac{LT}{1 - L\theta\Delta t}\right).$$

Thus we have

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$$|e_n| \le \frac{T_{\text{max}}}{L} \left[\exp\left(\frac{LT}{1 - L\theta\Delta t}\right) - 1 \right] ,$$
 (10)

for n = 0, 1, ..., N. This shows that the pointwise error has the same order as the truncation error.

3 Implementation

Recall that the θ -method is

$$\frac{U_{n+1} - U_n}{dt} = \theta f(t_{n+1}, U_n + 1) + (1 - \theta) f(t_n, U_n)$$

If $\theta \neq 0$ then we have an implict equation to solve for $U_n + 1$ at each timestep. We can write this equation as

$$g(U_{n+1}) := U_{n+1} - U_n - dt\theta f(t_{n+1}, U_n + 1) - dt(1 - \theta) f(t_n, U_n) = 0.$$

We can solve this using the Newton Rhapson method which is summarized in the code below.

4 Numerical Example

Consider the specific problem

$$\frac{\mathrm{d}u}{\mathrm{d}t} = loglog(4+u^2)$$

for $0 < t \le 1$ and with u(0) = 1. The numerical results are shown in Figure (1) below.

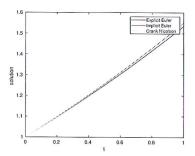


Figure 1: Numerical solution to the example problem.

(59) 4.1 Convergence results

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Since the exact solution to this problem is not known, we use a very accurate solution generated using the Crank Nicolson scheme with N=10000 to simulate the exact solution. We then consider the error at time t=1. The results are shown in the figure. We can see that the errors for implicit and explicit Euler are almost the same and converge like $\mathcal{O}(\Delta t)$, whereas the implicit Euler scheme is $\mathcal{O}(\Delta t^2)$.

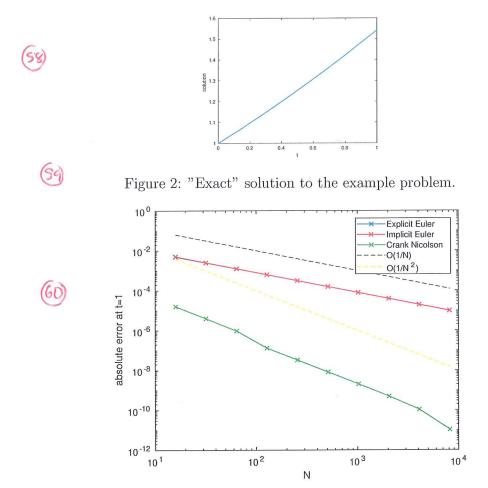


Figure 3: Convergence to the exact solution of the example problem at time t=1. The errors for implicit and explicit Euler are almost the same and have size $\mathcal{O}(\Delta t)$, whereas the Crank Nicolson error is $\mathcal{O}(\Delta t^2)$.

5 Conclusion

We have looked at the θ-method for solving initial value ordinary differential equation problems. The parameter θ is chosen to lie in the interval [0, 1]. If θ = 0 then the numerical method is explicit, otherwise it is implicit and a nonlinear equation must be solved at each timestep. If θ = ½ the method is second order accurate, otherwise the method is first oder accurate. These convergence rates were demonstrated numerically.

References



- [1] K.W. Morton and D.F. Mayers. Numerical Solution of Partial Differential Equations. Cambridge University Press, 1994.
- $[2]\,$ Süli, E. & Mayers, D. F. An Introduction to numerical analysis.