Using the θ-method to solve ODEs

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1 Introduction

1 2 In this report we use the θ-method to solve ODE’s. We begin by introducing the
3 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
4 are achieve.

In what follows we consider initial value problems of the form

5
$$\frac{\mathrm{du}}{dt} = f(t,u) \tag{1}$$

6 for $t > 0$ with an initial condition $u(0) = u_0$. Here, we assume that f(t,u) satisfies a
7 Lipschitz condition in its second argument and that f(u,t) is bounded.

8 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

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

9 for $(x,t) \in (-1,1)x(0,T]$ with boundary and initial conditions

10
$$\begin{aligned} u(x,0) &= u_0(x) \quad for -1 < x < 1, \\ u(-1,t) &= g_1(t) \quad for\ t > 0, \\ u(1,t) &= g_2(t) \quad for\ t > 0. \end{aligned}$$

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

?

12 ## 2 The θ-method

13 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 $n = 0, \ldots, N$ where $N \geq 2$ and $N\Delta t = T$, where T is the final time. We let U_n be the numerical approximation to $u(t_n)$.

14 The θ-method for Equation 1 is

15
$$\frac{U_{n+1} - U_n}{\Delta t} \quad = \quad \theta f(t_{n+1}, U_n + 1) + (1 - \theta) f(t_n, U_n)$$

16 17 Where θ is between 0 and 1. We require this equation to hold for $n = 0, \ldots, N-1$

18 and we apply the initial condition via $U_0 = u_0$. 3 values of θ lead to methods with a specific name:

19 20
- $\theta = 0$ is the explicit Euler scheme (also known as "forward Euler") ;

21
- $\theta = 1$ is the implicit Euler scheme (also known as "backward Euler") ;
- $\theta = \frac{1}{2}$ is the Crank-Nicolson scheme. ?

22 ### 2.0.1 Truncation Error

The truncation error for the θ-method is defined as

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

23 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 $t_{n+1/2} = (t_n +$

24 $t_{n+1})/2 = t_n + 1/2\Delta t$.

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

$$\begin{aligned} T_n \quad &= \quad \frac{u_{n+1} - u_n}{\Delta t} - \theta f(t_{n+1}, u_{n+1}) - (1 - \theta) f(t_n, u_n) \\ &= \quad \frac{u_{n+1} - u_n}{\Delta t} - \theta u'(t_{n+1}) - (1 - \theta) u'(t_n) \ . \end{aligned} \tag{3}$$

We have

25

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

Similarly,

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

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

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

27 Substituting these four expansions into Equation (3) gives

28, 29

$$\begin{aligned} T_n = \; & \frac{1}{\Delta t}((u(t_{n+1/2}) + \frac{\Delta t}{2} u'(t_{n+1/2}) + \frac{1}{2}(\frac{\Delta t}{2})^2 u''(t_{n+1/2})) \\ & -(u(t_{n+1/2}) - \frac{\Delta t}{2} u'(t_{n+1/2}) + \frac{1}{2}(\frac{\Delta t}{2})^2 u''(t_{n+1/2}))) \\ & -\theta(u'(t_{n+1/2}) + \frac{\Delta t}{2} u''(t_{n+1/2})) - (1-\theta)(u'(t_{n+1/2}) - \frac{\Delta t}{2} u''(t_{n+1/2})) + O(\Delta t^2) \quad (4) \end{aligned}$$

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

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

30 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

31

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

so that the truncation error of the Crank Nicolson scheme converges twice as fast as

32 that of all other *theta*-methods.

2.1 Pointwise Errors

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

$$\begin{aligned}\frac{U_{n+1}-U_n}{\Delta t} &= \theta f(t_{n+1},U_{n+1}) + (1-\theta) f(t_n,U_n)\ ,\\ T_n &= \frac{u_{n+1}-u_n}{\Delta t} - \theta f(t_{n+1},u_{n+1}) - (1-\theta) f(t_n,u_n)\ .\end{aligned}$$

We re-arrange both of these to get

34

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

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

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

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:

35

$$|f(t,u)-f(t,v)| \ \le\ L|u-v|\ , \quad \forall (t,u),\ (t,v) \in \Omega\ .$$

We can use this in (7) to get

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

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

$$\begin{aligned}(1-L\theta\Delta t)|u_{n+1}-U_{n+1}| &\le (1+L(1-\theta)\Delta t)|u_n-U_n| + \Delta t|T_n|\\ &\le (1+L(1-\theta)\Delta t)|u_n-U_n| + \Delta t T_{\max}\ ,\end{aligned} \tag{8}$$

where

37

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

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

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

We can show by induction that

$$
\begin{aligned}
|e_n| &\le \left(\frac{1+L(1-\theta)\Delta t}{1-L\theta\Delta t}\right)^n |e_0| + \frac{\Delta t T_{\max}}{1-L\theta\Delta t}\sum_{r=1}^{n}\left(\frac{1+L(1-\theta)\Delta t}{1-L\theta\Delta t}\right)^{r-1} \\
&\le \left(\frac{1+L(1-\theta)\Delta t}{1-L\theta\Delta t}\right)^n |e_0| + \frac{T_{\max}}{L}\left[\left(\frac{1+L(1-\theta)\Delta t}{1-L\theta\Delta t}\right)^n - 1\right],
\end{aligned}
$$

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

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

$$
\begin{aligned}
\frac{1+L(1-\theta)\Delta t}{1-L\theta\Delta t} &= 1 + \frac{L\Delta t}{1-L\theta\Delta t} \\
&\le \exp\left(\frac{L\Delta t}{1-L\theta\Delta t}\right).
\end{aligned}
$$

In turn this means

$$
\begin{aligned}
\left(\frac{1+L(1-\theta)\Delta t}{1-L\theta\Delta t}\right)^n &\le \left(\exp\left(\frac{L\Delta t}{1-L\theta\Delta t}\right)\right)^n \\
&\le \exp\left(\frac{nL\Delta t}{1-L\theta\Delta t}\right) \\
&\le \exp\left(\frac{LT}{1-L\theta\Delta t}\right).
\end{aligned}
$$

Thus we have

38

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

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

3 Implementation

Recall that the θ-method is

39 $$
\frac{U_{n+1}-U_n}{dt} = \theta f(t_{n+1}, U_n + 1) + (1-\theta) f(t_n, U_n)
$$

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

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

41 42 We can solve this using the Newton Rhapson method which is summarized in the code below.

43 44

```
% file mynewt.m
% this function finds a root of f(x) using Newton's method and a starting
function x=mynewt(f,fprime,xguess,tol)

x=xguess;

while abs(f(x)) > tol
    x=x-f(x)/fprime(x)
end
end
```

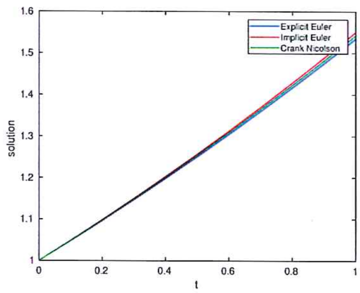
4 Numerical Example

Consider the specific problem

45
$$\frac{du}{dt} = loglog(4+u^2)$$

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

47



48 Figure 1: Numerical solution to the example problem.

4.1 Convergence results

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
49 figure. We can see that the errors for implicit and explicit Euler are almost the same
50 and converge like $\mathcal{O}(\Delta t)$, whereas the implicit Euler scheme is $\mathcal{O}(\Delta t^2)$.

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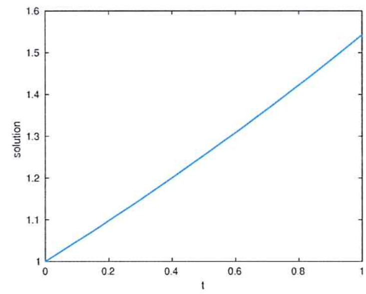

52 Figure 2: "Exact" solution to the example problem.

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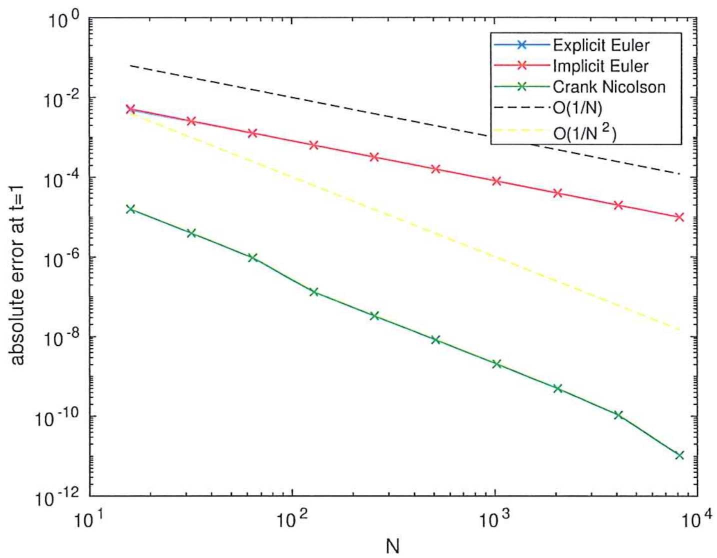

Figure 3: Convergence to the exact solution of the example problem at time $t = 1$. The errors for implicit and explicit Euler are almost the same and have size $\mathcal{O}(\Delta t)$, whereas the Crank Nicolson error is $\mathcal{O}(\Delta t^2)$.

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 $\theta = 0$ then the numerical method is explicit, otherwise it is implicit and a nonlinear equation must
54 be solved at each timestep. If $\theta = \frac{1}{2}$ the method is second order accurate, other-
55 wise 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.

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[2] Süli, E. & Mayers, D. F. An Introduction to numerical analysis.