

Study guide: Generalizations of exponential decay models

Hans Petter Langtangen^{1,2}

Center for Biomedical Computing, Simula Research Laboratory¹

Department of Informatics, University of Oslo²

Aug 4, 2015

1 Model extensions

2 Methods for general first-order ODEs

Extension to a variable coefficient; Forward and Backward Euler

$$u'(t) = -a(t)u(t), \quad t \in (0, T], \quad u(0) = I \quad (1)$$

The Forward Euler scheme:

$$\frac{u^{n+1} - u^n}{\Delta t} = -a(t_n)u^n \quad (2)$$

The Backward Euler scheme:

$$\frac{u^n - u^{n-1}}{\Delta t} = -a(t_n)u^n \quad (3)$$

Evaluating $a(t_{n+\frac{1}{2}})$ and using an average for u :

$$\frac{u^{n+1} - u^n}{\Delta t} = -a(t_{n+\frac{1}{2}}) \frac{1}{2}(u^n + u^{n+1}) \quad (4)$$

Using an average for a and u :

$$\frac{u^{n+1} - u^n}{\Delta t} = -\frac{1}{2}(a(t_n)u^n + a(t_{n+1})u^{n+1}) \quad (5)$$

The θ -rule unifies the three mentioned schemes,

$$\frac{u^{n+1} - u^n}{\Delta t} = -a((1 - \theta)t_n + \theta t_{n+1})((1 - \theta)u^n + \theta u^{n+1}) \quad (6)$$

or,

$$\frac{u^{n+1} - u^n}{\Delta t} = -(1 - \theta)a(t_n)u^n - \theta a(t_{n+1})u^{n+1} \quad (7)$$

$$[D_t^+ u = -au]^n,$$

$$[D_t^- u = -au]^n,$$

$$[D_t u = -a\bar{u}^t]^{n+\frac{1}{2}},$$

$$[D_t u = -\overline{a}u^t]^{n+\frac{1}{2}}$$

$$u'(t) = -a(t)u(t) + b(t), \quad t \in (0, T], \quad u(0) = l \quad (8)$$

$$[D_t^+ u = -au + b]^n,$$

$$[D_t^- u = -au + b]^n,$$

$$[D_t u = -a\bar{u}^t + b]^{n+\frac{1}{2}},$$

$$[D_t u = \overline{-au + b}^t]^{n+\frac{1}{2}}$$

Implementation of the generalized model problem

$$u^{n+1} = ((1-\Delta t(1-\theta)a^n)u^n + \Delta t(\theta b^{n+1} + (1-\theta)b^n))(1 + \Delta t\theta a^{n+1})^{-1} \quad (9)$$

Implementation where $a(t)$ and $b(t)$ are given as Python functions (see file `decay_vc.py`):

```
def solver(I, a, b, T, dt, theta):  
    """  
    Solve  $u' = -a(t)u + b(t)$ ,  $u(0) = I$ ,  
    for  $t$  in  $(0, T]$  with steps of  $dt$ .  
     $a$  and  $b$  are Python functions of  $t$ .  
    """  
    dt = float(dt)                # avoid integer division  
    Nt = int(round(T/dt))           # no of time intervals  
    T = Nt*dt                     # adjust T to fit time step dt  
    u = zeros(Nt+1)               # array of  $u[n]$  values  
    t = linspace(0, T, Nt+1)      # time mesh  
  
    u[0] = I                      # assign initial condition  
    for n in range(0, Nt):        #  $n=0, 1, \dots, Nt-1$   
        u[n+1] = ((1 - dt*(1-theta)*a(t[n]))*u[n] + \br/>                  dt*(theta*b(t[n+1]) + (1-theta)*b(t[n]))) / \br/>                  (1 + dt*theta*a(t[n+1]))  
    return u, t
```


Implementations of variable coefficients; functions

Plain functions:

```
def a(t):  
    return a_0 if t < tp else k*a_0  
  
def b(t):  
    return 1
```

Implementations of variable coefficients; classes

Better implementation: class with the parameters a_0 , tp , and k as attributes and a *special method* `__call__` for evaluating $a(t)$:

```
class A:
    def __init__(self, a0=1, k=2):
        self.a0, self.k = a0, k

    def __call__(self, t):
        return self.a0 if t < self.tp else self.k*self.a0

a = A(a0=2, k=1)  # a behaves as a function a(t)
```

Implementations of variable coefficients; lambda function

Quick writing: a one-liner *lambda function*

```
a = lambda t: a_0 if t < tp else k*a_0
```

In general,

```
f = lambda arg1, arg2, ...: expressin
```

is equivalent to

```
def f(arg1, arg2, ...):  
    return expression
```

One can use lambda functions directly in calls:

```
u, t = solver(1, lambda t: 1, lambda t: 1, T, dt, theta)
```

for a problem $u' = -u + 1$, $u(0) = 1$.

A lambda function can appear anywhere where a variable can appear.

Verification via trivial solutions

- Start debugging of a new code with trying a problem where $u = \text{const} \neq 0$.
- Choose $u = C$ (a constant). Choose any $a(t)$ and set $b = a(t)C$ and $I = C$.
- "All" numerical methods will reproduce $u =_{\text{const}}$ exactly (machine precision).
- Often $u = C$ eases debugging.
- In this example: *any error* in the formula for u^{n+1} make $u \neq C$!

Verification via trivial solutions; test function

```
def test_constant_solution():  
    """  
    Test problem where  $u=u_{\text{const}}$  is the exact solution, to be  
    reproduced (to machine precision) by any relevant method.  
    """  
    def exact_solution(t):  
        return u_const  
  
    def a(t):  
        return 2.5*(1+t**3)    # can be arbitrary  
  
    def b(t):  
        return a(t)*u_const  
  
    u_const = 2.15  
    theta = 0.4; I = u_const; dt = 4  
    Nt = 4    # enough with a few steps  
    u, t = solver(I=I, a=a, b=b, T=Nt*dt, dt=dt, theta=theta)  
    print u  
    u_e = exact_solution(t)  
    difference = abs(u_e - u).max()    # max deviation  
    tol = 1E-14  
    assert difference < tol
```

Verification via manufactured solutions

- Choose *any* formula for $u(t)$.
- Fit I , $a(t)$, and $b(t)$ in $u' = -au + b$, $u(0) = I$, to make the chosen formula a solution of the ODE problem.
- Then we can always have an analytical solution (!).
- Ideal for verification: testing convergence rates.
- Called the *method of manufactured solutions* (MMS)
- Special case: u linear in t , because all sound numerical methods will reproduce a linear u exactly (machine precision).
- $u(t) = ct + d$. $u(0) = 0$ means $d = I$.
- ODE implies $c = -a(t)u + b(t)$.
- Choose $a(t)$ and c , and set $b(t) = c + a(t)(ct + I)$.
- Any error in the formula for u^{n+1} makes $u \neq ct + I$!

Linear manufactured solution

$u^n = ct_n + l$ fulfills the discrete equations!

First,

$$[D_t^+ t]^n = \frac{t_{n+1} - t_n}{\Delta t} = 1, \quad (10)$$

$$[D_t^- t]^n = \frac{t_n - t_{n-1}}{\Delta t} = 1, \quad (11)$$

$$[D_t t]^n = \frac{t_{n+\frac{1}{2}} - t_{n-\frac{1}{2}}}{\Delta t} = \frac{(n + \frac{1}{2})\Delta t - (n - \frac{1}{2})\Delta t}{\Delta t} = 1 \quad (12)$$

Forward Euler:

$$[D^+ u = -au + b]^n$$

$a^n = a(t_n)$, $b^n = c + a(t_n)(ct_n + l)$, and $u^n = ct_n + l$ results in

$$c = -a(t_n)(ct_n + l) + c + a(t_n)(ct_n + l) = c$$

Test function for linear manufactured solution

```
def test_linear_solution():  
    """  
    Test problem where  $u=c*t+I$  is the exact solution, to be  
    reproduced (to machine precision) by any relevant method.  
    """  
    def exact_solution(t):  
        return c*t + I  
  
    def a(t):  
        return t**0.5 # can be arbitrary  
  
    def b(t):  
        return c + a(t)*exact_solution(t)  
  
    theta = 0.4; I = 0.1; dt = 0.1; c = -0.5  
    T = 4  
    Nt = int(T/dt) # no of steps  
    u, t = solver(I=I, a=a, b=b, T=Nt*dt, dt=dt, theta=theta)  
    u_e = exact_solution(t)  
    difference = abs(u_e - u).max() # max deviation  
    print difference  
    tol = 1E-14 # depends on c!  
    assert difference < tol
```


Sample system:

$$u' = au + bv \quad (13)$$

$$v' = cu + dv \quad (14)$$

The Forward Euler method:

$$u^{n+1} = u^n + \Delta t(au^n + bv^n) \quad (15)$$

$$v^{n+1} = v^n + \Delta t(cu^n + dv^n) \quad (16)$$

The Backward Euler method gives a system of algebraic equations

The Backward Euler scheme:

$$u^{n+1} = u^n + \Delta t(au^{n+1} + bv^{n+1}) \quad (17)$$

$$v^{n+1} = v^n + \Delta t(cu^{n+1} + dv^{n+1}) \quad (18)$$

which is a 2×2 linear system:

$$(1 - \Delta ta)u^{n+1} + bv^{n+1} = u^n \quad (19)$$

$$cu^{n+1} + (1 - \Delta td)v^{n+1} = v^n \quad (20)$$

Crank-Nicolson also gives a 2×2 linear system.

1 Model extensions

2 Methods for general first-order ODEs

Generic form

The standard form for ODEs:

$$u' = f(u, t), \quad u(0) = l \quad (21)$$

u and f : scalar or vector.

Vectors in case of ODE systems:

$$u(t) = (u^{(0)}(t), u^{(1)}(t), \dots, u^{(m-1)}(t))$$

$$\begin{aligned} f(u, t) = & (f^{(0)}(u^{(0)}, \dots, u^{(m-1)}) \\ & f^{(1)}(u^{(0)}, \dots, u^{(m-1)}), \\ & \vdots \\ & f^{(m-1)}(u^{(0)}(t), \dots, u^{(m-1)}(t))) \end{aligned}$$

The θ -rule

$$\frac{u^{n+1} - u^n}{\Delta t} = \theta f(u^{n+1}, t_{n+1}) + (1 - \theta)f(u^n, t_n) \quad (22)$$

Bringing the unknown u^{n+1} to the left-hand side and the known terms on the right-hand side gives

$$u^{n+1} - \Delta t \theta f(u^{n+1}, t_{n+1}) = u^n + \Delta t (1 - \theta) f(u^n, t_n) \quad (23)$$

This is a *nonlinear* equation in u^{n+1} (unless f is linear in u)!

Implicit 2-step backward scheme

$$u'(t_{n+1}) \approx \frac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t}$$

Scheme:

$$u^{n+1} = \frac{4}{3}u^n - \frac{1}{3}u^{n-1} + \frac{2}{3}\Delta t f(u^{n+1}, t_{n+1})$$

Nonlinear equation for u^{n+1} .

The Leapfrog scheme

Idea:

$$u'(t_n) \approx \frac{u^{n+1} - u^{n-1}}{2\Delta t} = [D_{2t}u]^n \quad (24)$$

Scheme:

$$[D_{2t}u = f(u, t)]^n$$

or written out,

$$u^{n+1} = u^{n-1} + \Delta t f(u^n, t_n) \quad (25)$$

- Some other scheme must be used as starter (u^1).
- Explicit scheme - a nonlinear f (in u) is trivial to handle.
- Downside: Leapfrog is always unstable after some time.

The filtered Leapfrog scheme

After computing u^{n+1} , stabilize Leapfrog by

$$u^n \leftarrow u^n + \gamma(u^{n-1} - 2u^n + u^{n+1}) \quad (26)$$

Forward-Euler + approximate Crank-Nicolson:

$$u^* = u^n + \Delta t f(u^n, t_n), \quad (27)$$

$$u^{n+1} = u^n + \Delta t \frac{1}{2} (f(u^n, t_n) + f(u^*, t_{n+1})) \quad (28)$$

4th-order Runge-Kutta scheme

- The most famous and widely used ODE method
- 4 evaluations of f per time step
- Its [derivation](#) is a very good illustration of numerical thinking!

2nd-order Adams-Bashforth scheme

$$u^{n+1} = u^n + \frac{1}{2}\Delta t (3f(u^n, t_n) - f(u^{n-1}, t_{n-1})) \quad (29)$$

3rd-order Adams-Bashforth scheme

$$u^{n+1} = u^n + \frac{1}{12} (23f(u^n, t_n) - 16f(u^{n-1}, t_{n-1}) + 5f(u^{n-2}, t_{n-2})) \quad (30)$$

The Odespy software

Odespy features simple Python implementations of the most fundamental schemes as well as Python interfaces to several famous packages for solving ODEs: [ODEPACK](#), [Vode](#), [rk4.f](#), [rkf45.f](#), [Radau5](#), as well as the ODE solvers in [SciPy](#), [SymPy](#), and [odelab](#).

Typical usage:

```
# Define right-hand side of ODE
def f(u, t):
    return -a*u

import odespy
import numpy as np

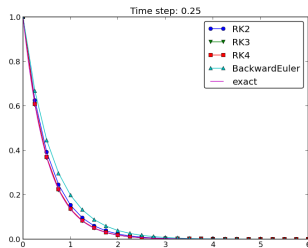
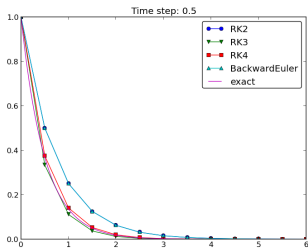
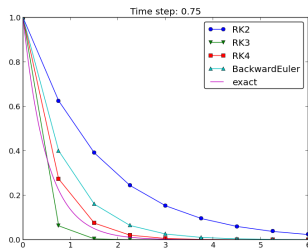
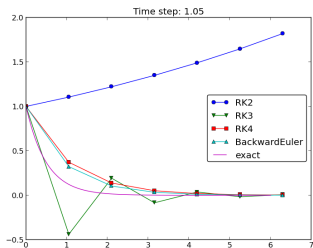
# Set parameters and time mesh
I = 1; a = 2; T = 6; dt = 1.0
Nt = int(round(T/dt))
t_mesh = np.linspace(0, T, Nt+1)

# Use a 4th-order Runge-Kutta method
solver = odespy.RK4(f)
solver.set_initial_condition(I)
u, t = solver.solve(t_mesh)
```

Example: Runge-Kutta methods

```
solvers = [odespy.RK2(f),  
            odespy.RK3(f),  
            odespy.RK4(f),  
            odespy.BackwardEuler(f, nonlinear_solver='Newton')]  
  
for solver in solvers:  
    solver.set_initial_condition(I)  
    u, t = solver.solve(t)  
  
# + lots of plot code...
```

Plots from the experiments



The 4-th order Runge-Kutta method (RK4) is the method of choice!

Example: Adaptive Runge-Kutta methods

- Adaptive methods find "optimal" locations of the mesh points to ensure that the error is less than a given tolerance.
- Downside: approximate error estimation, not always optimal location of points.
- "Industry standard ODE solver": Dormand-Prince 4/5-th order Runge-Kutta (MATLAB's famous ode45).

