

# Study guide: Generalizations of exponential decay models

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Oct 10, 2015

1 Model extensions

2 Computing convergence rates

3 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  $u$ :

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

## Extension to a variable coefficient; $\theta$ -rule

The  $\theta$ -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,

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

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

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

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

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

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

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

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

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

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

# 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] + \  
                  dt*(theta*b(t[n+1]) + (1-theta)*b(t[n]))) / \  
                  (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 u_exact(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 = u_exact(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  $d = 0$
- 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

$u^n = ct_n + I$  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:

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

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

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

# 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 u_exact(t):  
        return c*t + I  
  
    def a(t):  
        return t**0.5 # can be arbitrary  
  
    def b(t):  
        return c + a(t)*u_exact(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 = u_exact(t)  
    difference = abs(u_e - u).max() # max deviation  
    print difference  
    tol = 1E-14 # depends on c!  
    assert difference < tol
```



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Frequent assumption on the relation between the numerical error  $E$  and some discretization parameter  $\Delta t$ :

$$E = C\Delta t^r, \tag{13}$$

- Unknown:  $C$  and  $r$ .
- Goal: estimate  $r$  (and  $C$ ) from numerical experiments

## Estimating the convergence rate $r$

Perform numerical experiments:  $(\Delta t_i, E_i)$ ,  $i = 0, \dots, m - 1$ . Two methods for finding  $r$  (and  $C$ ):

- 1 Take the logarithm of (13),  $\ln E = r \ln \Delta t + \ln C$ , and fit a straight line to the data points  $(\Delta t_i, E_i)$ ,  $i = 0, \dots, m - 1$ .
- 2 Consider two consecutive experiments,  $(\Delta t_i, E_i)$  and  $(\Delta t_{i-1}, E_{i-1})$ . Dividing the equation  $E_{i-1} = C \Delta t_{i-1}^r$  by  $E_i = C \Delta t_i^r$  and solving for  $r$  yields

$$r_{i-1} = \frac{\ln(E_{i-1}/E_i)}{\ln(\Delta t_{i-1}/\Delta t_i)} \quad (14)$$

for  $i = 1, \dots, m - 1$ .

Method 2 is best.

Compute  $r_0, r_1, \dots, r_{m-2}$  from  $E_i$  and  $\Delta t_i$ :

```
def compute_rates(dt_values, E_values):  
    m = len(dt_values)  
    r = [log(E_values[i-1]/E_values[i])/  
          log(dt_values[i-1]/dt_values[i])  
          for i in range(1, m, 1)]  
    # Round to two decimals  
    r = [round(r_, 2) for r_ in r]  
    return r
```

## We embed the code in a real test function

```
def test_convergence_rates():
    # Create a manufactured solution
    # define u_exact(t), a(t), b(t)

    dt_values = [0.1*2**(-i) for i in range(7)]
    I = u_exact(0)

    for theta in (0, 1, 0.5):
        E_values = []
        for dt in dt_values:
            u, t = solver(I=I, a=a, b=b, T=6, dt=dt, theta=theta)
            u_e = u_exact(t)
            e = u_e - u
            E = sqrt(dt*sum(e**2))
            E_values.append(E)
        r = compute_rates(dt_values, E_values)
        print 'theta=%g, r: %s' % (theta, r)
        expected_rate = 2 if theta == 0.5 else 1
        tol = 0.1
        diff = abs(expected_rate - r[-1])
        assert diff < tol
```

# The manufactured solution can be computed by sympy

We choose  $u_e(t) = \sin(t)e^{-2t}$ ,  $a(t) = t^2$ , fit  $b(t) = u'(t) - a(t)$ :

```
# Create a manufactured solution with sympy
import sympy as sym
t = sym.symbols('t')
u_exact = sym.sin(t)*sym.exp(-2*t)
a = t**2
b = sym.diff(u_exact, t) + a*u_exact

# Turn sympy expressions into Python function
u_exact = sym.lambdify([t], u_exact, modules='numpy')
a = sym.lambdify([t], a, modules='numpy')
b = sym.lambdify([t], b, modules='numpy')
```

Complete code: [decay\\_vc.py](#).

# Execution

```
Terminal> python decay_vc.py
```

```
...
```

```
theta=0, r: [1.06, 1.03, 1.01, 1.01, 1.0, 1.0]
```

```
theta=1, r: [0.94, 0.97, 0.99, 0.99, 1.0, 1.0]
```

```
theta=0.5, r: [2.0, 2.0, 2.0, 2.0, 2.0, 2.0]
```

# Debugging via convergence rates

Potential bug: missing  $a$  in the denominator,

$$u[n+1] = (1 - (1-\theta)a*dt)/(1 + \theta*dt)*u[n]$$

Running `decay_convrate.py` gives same rates.

Why? The value of  $a...$  ( $a = 1$ )

0 and 1 are *bad values* in tests!

Better:

```
Terminal> python decay_convrate.py --a 2.1 --I 0.1 \
          --dt 0.5 0.25 0.1 0.05 0.025 0.01
```

```
...
```

```
Pairwise convergence rates for theta=0:
```

```
1.49 1.18 1.07 1.04 1.02
```

```
Pairwise convergence rates for theta=0.5:
```

```
-1.42 -0.22 -0.07 -0.03 -0.01
```

```
Pairwise convergence rates for theta=1:
```

```
0.21 0.12 0.06 0.03 0.01
```

Forward Euler works...because  $\theta = 0$  hides the bug.



Sample system:

$$u' = au + bv \quad (15)$$

$$v' = cu + dv \quad (16)$$

The Forward Euler method:

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

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

# The Backward Euler method gives a system of algebraic equations

The Backward Euler scheme:

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

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

which is a  $2 \times 2$  linear system:

$$(1 - \Delta ta)u^{n+1} + bv^{n+1} = u^n \quad (21)$$

$$cu^{n+1} + (1 - \Delta td)v^{n+1} = v^n \quad (22)$$

Crank-Nicolson also gives a  $2 \times 2$  linear system.

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# Generic form

The standard form for ODEs:

$$u' = f(u, t), \quad u(0) = I \quad (23)$$

$u$  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 $\theta$ -rule

$$\frac{u^{n+1} - u^n}{\Delta t} = \theta f(u^{n+1}, t_{n+1}) + (1 - \theta)f(u^n, t_n) \quad (24)$$

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

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

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:

$$u'(t_n) \approx \frac{u^{n+1} - u^{n-1}}{2\Delta t} = [D_{2t}u]^n \quad (26)$$

Scheme:

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

or written out,

$$u^{n+1} = u^{n-1} + \Delta t f(u^n, t_n) \quad (27)$$

- 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

$$u^n \leftarrow u^n + \gamma(u^{n-1} - 2u^n + u^{n+1}) \quad (28)$$



Forward-Euler + approximate Crank-Nicolson:

$$u^* = u^n + \Delta t f(u^n, t_n), \quad (29)$$

$$u^{n+1} = u^n + \Delta t \frac{1}{2} (f(u^n, t_n) + f(u^*, t_{n+1})) \quad (30)$$

# 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!

$$u^{n+1} = u^n + \frac{1}{2}\Delta t (3f(u^n, t_n) - f(u^{n-1}, t_{n-1})) \quad (31)$$

## 3rd-order Adams-Bashforth scheme

$$u^{n+1} = u^n + \frac{1}{12} (23f(u^n, t_n) - 16f(u^{n-1}, t_{n-1}) + 5f(u^{n-2}, t_{n-2})) \quad (32)$$

# 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

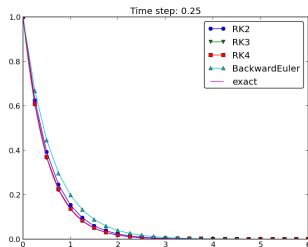
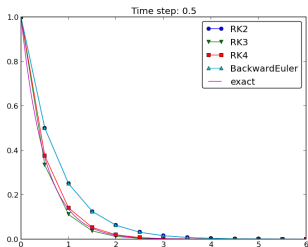
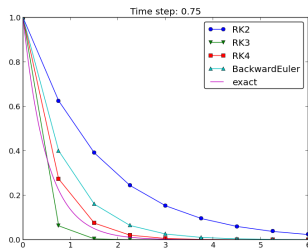
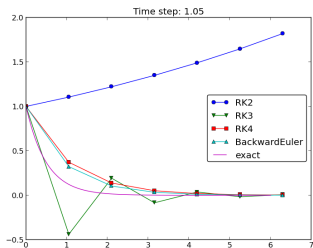
# Set parameters and time mesh
I = 1; a = 2; T = 6; dt = 1.0
Nt = int(round(T/dt))
t_mesh = np.linspace(0, T, Nt+1)

# 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).

