Study guide: Generalizations of exponential decay models

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Extension to a variable coefficient; Forward and Backward Euler

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

The Forward Euler scheme:

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

The Backward Euler scheme:

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

Extension to a variable coefficient; Crank-Nicolson

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

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

Using an average for a and u:

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

Extension to a variable coefficient; θ-rule

The θ-rule unifies the three mentioned schemes,

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

or,

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

Extension to a variable coefficient; operator notation

$$\begin{aligned}
[D_t^+ u &= -au]^n,\\
[D_t^- u &= -au]^n,\\
[D_t u &= -a\overline{u}^t]^{n+\frac{1}{2}},\\
[D_t u &= -\overline{au}^t]^{n+\frac{1}{2}}
\end{aligned}$$

Extension to a source term

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

$$\begin{aligned}
[D_t^+ u &= -au + b]^n,\\
[D_t^- u &= -au + b]^n,\\
[D_t u &= -a\overline{u}^t + b]^{n+\frac{1}{2}},\\
[D_t u &= \overline{-au + b}^t]^{n+\frac{1}{2}}
\end{aligned}$$

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,...,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 `a0`, `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_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 $d = I$
- 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

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

First,

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

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

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

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

```python
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
```

Computing convergence rates

Frequent assumption on the relation between the numerical error E and some discretization parameter Δt:

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

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

Estimating the convergence rate r

Perform numerical experiments: $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$. 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 $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$.
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

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

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

Method 2 is best.

Brief implementation

Compute $r_0, r_1, \ldots, r_{m-2}$ from E_i and Δt_i:

```python
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.

Extension to systems of ODEs

Sample system:

$$u' = au + bv \tag{15}$$
$$v' = cu + dv \tag{16}$$

The Forward Euler method:

$$u^{n+1} = u^n + \Delta t(au^n + bv^n) \tag{17}$$
$$v^{n+1} = u^n + \Delta t(cu^n + dv^n) \tag{18}$$

The Backward Euler method gives a system of algebraic equations

The Backward Euler scheme:

$$u^{n+1} = u^n + \Delta t(au^{n+1} + bv^{n+1}) \tag{19}$$
$$v^{n+1} = v^n + \Delta t(cu^{n+1} + dv^{n+1}) \tag{20}$$

which is a 2×2 linear system:

$$(1 - \Delta ta)u^{n+1} + bv^{n+1} = u^n \tag{21}$$
$$cu^{n+1} + (1 - \Delta td)v^{n+1} = v^n \tag{22}$$

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

Generic form

The standard form for ODEs:

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

u and f: scalar or vector.

Vectors in case of ODE systems:

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

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

The θ-rule

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

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

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

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:

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

Scheme:

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

or written out,

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

- 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

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

2nd-order Runge-Kutta scheme

Forward-Euler + approximate Crank-Nicolson:

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

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

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!

2nd-order Adams-Bashforth scheme

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

3rd-order Adams-Bashforth scheme

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

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, rkc.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)
```

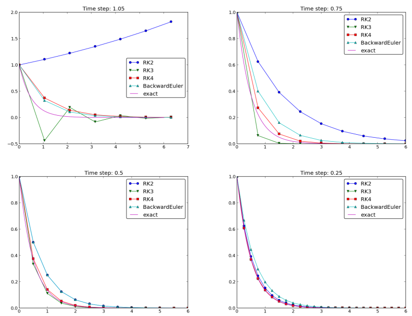
Example: Runge-Kutta methods

```
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`).