Experiments with Schemes for Exponential Decay

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Abstract

This report investigates the accuracy of three finite difference schemes for the ordinary differential equation u' = -au with the aid of numerical experiments. Numerical artifacts are in particular demonstrated.

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1 Mathematical problem

We address the initial-value problem

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

$$u(0) = I, (2)$$

where a, I, and T are prescribed parameters, and u(t) is the unknown function to be estimated. This mathematical model is relevant for physical phenomena featuring exponential decay in time, e.g., vertical pressure variation in the atmosphere, cooling of an object, and radioactive decay.

2 Numerical solution method

We introduce a mesh in time with points $0 = t_0 < t_1 \cdots < t_{N_t} = T$. For simplicity, we assume constant spacing Δt between the mesh points: $\Delta t = t_n - t_{n-1}$, $n = 1, \ldots, N_t$. Let u^n be the numerical approximation to the exact solution at t_n .

The θ -rule [1] is used to solve (1) numerically:

$$u^{n+1} = \frac{1 - (1 - \theta)a\Delta t}{1 + \theta a\Delta t}u^n,$$

for $n = 0, 1, \dots, N_t - 1$. This scheme corresponds to

- The Forward Euler¹ scheme when $\theta = 0$
- The Backward Euler² scheme when $\theta = 1$
- The Crank-Nicolson³ scheme when $\theta = 1/2$

3 Implementation

The numerical method is implemented in a Python function [2] solver (found in the model⁴ module):

```
def solver(I, a, T, dt, theta):

"""Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    dt = float(dt)
                                  # avoid integer division
    Nt = int(round(T/dt))
                                 # no of time intervals
                                  # adjust T to fit time step dt # array of u[n] values
    T = Nt*dt
    u = zeros(Nt+1)
    t = linspace(0, T, Nt+1) # time mesh
                                  # assign initial condition
    for n in range(0, Nt):
                                # n=0,1,...,Nt-1
         u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return u, t
def exact_solution(t, I, a):
    return I*exp(-a*t)
def explore(I, a, T, dt, theta=0.5):
    Run a case with the solver, compute error measure,
    and plot the numerical and exact solutions (if makeplot=True).
    u, t = solver(I, a, T, dt, theta)
                                               # Numerical solution
    u_e = exact_solution(t, I, a)
    e = u_e - u
    E = \overline{sqrt(dt*sum(e**2))}
    figure()
                                           # create new plot
    t_e = linspace(0, T, 1001)
u_e = exact_solution(t_e, I, a)
                                          # very fine mesh for u_e
    plot(t, u, 'r--o')
plot(t_e, u_e, 'b-')
legend(['numerical', 'exact'])
                                          # dashed red line with circles
                                          # blue line for u_e
    xlabel('t')
    ylabel('u')
```

¹http://en.wikipedia.org/wiki/Forward_Euler_method

²http://en.wikipedia.org/wiki/Backward_Euler_method

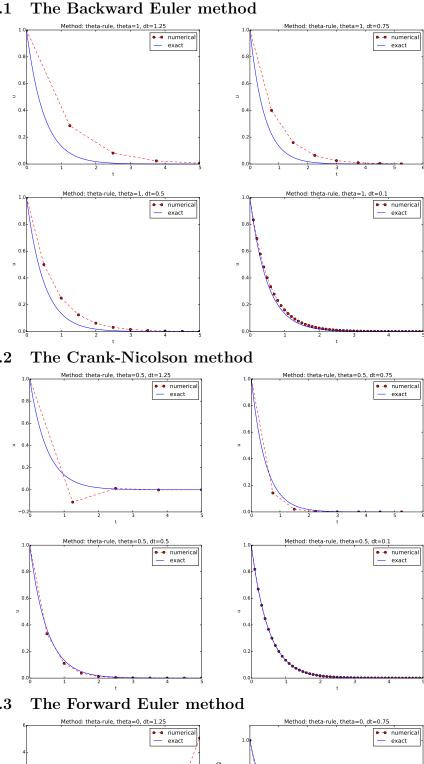
http://en.wikipedia.org/wiki/Crank-Nicolson

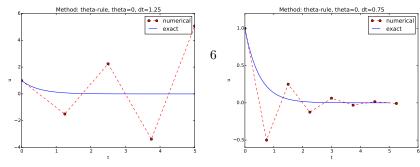
⁴https://github.com/hplgit/INF5620/blob/gh-pages/src/decay/experiments/dc_mod.py

```
title('Method: theta-rule, theta=%g, dt=%g' % (theta, dt))
theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
savefig('%s_%g.png' % (theta2name[theta], dt), dpi=150)
savefig('%s_%g.pdf' % (theta2name[theta], dt))
#show() # run in batch
return F
     return E
def define_command_line_options():
     import argparse
     parser = argparse.ArgumentParser()
     parser.add_argument('--I', '--initial_condition', type=float,
                              default=1.0, help='initial condition, u(0)',
                              metavar='I')
     parser.add_argument('--a', type=float,
                               default=1.0, help='coefficient in ODE',
                              metavar='a')
     parser.add_argument('--T', '--stop_time', type=float,
                              default=1.0, help='end time of simulation',
                              metavar='T')
     parser.add_argument('--dt', '--time_step_values', type=float,
                              default=[1.0], help='time step values',
metavar='dt', nargs='+', dest='dt_values')
     return parser
def read_command_line():
     parser = define_command_line_options()
     args = parser.parse_args()
     return args.I, args.a, args.T, args.dt_values
def main():
     """Conduct experiments with theta and dt values."""
     I, a, T, dt_values = read_command_line()
     for theta in 0, 0.5, 1:
          for dt in dt_values:
               E = explore(I, a, T, dt, theta)
print '%3.1f %6.2f: %12.3E' % (theta, dt, E)
if __name__ == '__main__':
     main()
```

4 Numerical experiments

We define a set of numerical experiments where I, a, and T are fixed, while Δt and θ are varied. In particular, I = 1, a = 2, $\Delta t = 1.25, 0.75, 0.5, 0.1$.





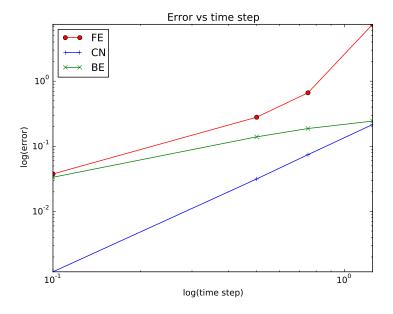


Figure 1: Variation of the error with the time step.



Observe:

The data points for the three largest Δt values in the Forward Euler method are not relevant as the solution behaves non-physically.

The numbers corresponding to the figure above are given in the table below.

Δt	$\theta = 0$	$\theta = 0.5$	$\theta = 1$
1.25	7.4630	0.2161	0.2440
0.75	0.6632	0.0744	0.1875
0.50	0.2797	0.0315	0.1397
0.10	0.0377	0.0012	0.0335



Summary

- 1. $\theta = 1$: $E \sim \Delta t$ (first-order convergence).
- 2. $\theta = 0.5$: $E \sim \Delta t^2$ (second-order convergence).
- 3. $\theta = 1$ is always stable and gives qualitatively corrects results.

- 4. $\theta=0.5$ never blows up, but may give oscillating solutions if Δt is not sufficiently small.
- 5. $\theta = 0$ suffers from fast-growing solution if Δt is not small enough, but even below this limit one can have oscillating solutions (unless Δt is sufficiently small).

References

- [1] A. Iserles. A First Course in the Numerical Analysis of Differential Equations. Cambridge University Press, second edition, 2009.
- [2] H. P. Langtangen. A Primer on Scientific Programming With Python. Springer, fourth edition, 2014.