Study guide: Analysis of exponential decay models

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• Analysis of finite difference equations

Analysis of finite difference equations

Model:

$$u'(t) = -au(t), \quad u(0) = I$$
 (1)

Method:

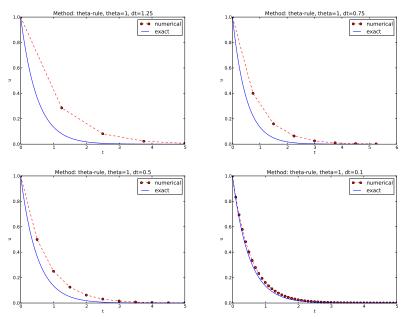
$$u^{n+1} = \frac{1 - (1 - \theta)a\Delta t}{1 + \theta a\Delta t} u^n \tag{2}$$

Problem setting

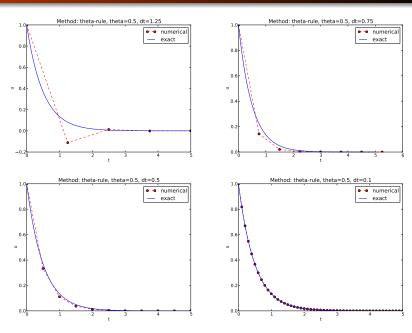
How good is this method? Is it safe to use it?

Encouraging numerical solutions

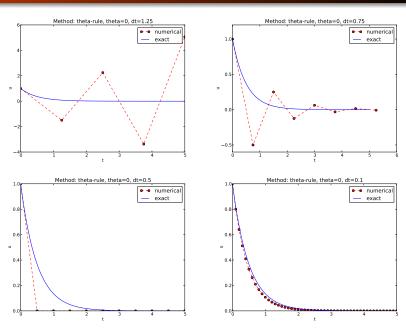
I = 1, a = 2, $\theta = 1, 0.5, 0$, $\Delta t = 1.25, 0.75, 0.5, 0.1$.



Discouraging numerical solutions; Crank-Nicolson



Discouraging numerical solutions; Forward Euler



Summary of observations

The characteristics of the displayed curves can be summarized as follows:

- The Backward Euler scheme always gives a monotone solution, lying above the exact curve.
- ullet The Crank-Nicolson scheme gives the most accurate results, but for $\Delta t=1.25$ the solution oscillates.
- The Forward Euler scheme gives a growing, oscillating solution for $\Delta t=1.25$; a decaying, oscillating solution for $\Delta t=0.75$; a strange solution $u^n=0$ for $n\geq 1$ when $\Delta t=0.5$; and a solution seemingly as accurate as the one by the Backward Euler scheme for $\Delta t=0.1$, but the curve lies below the exact solution.

Problem setting

Goal

We ask the question

• Under what circumstances, i.e., values of the input data I, a, and Δt will the Forward Euler and Crank-Nicolson schemes result in undesired oscillatory solutions?

Techniques of investigation:

- Numerical experiments
- Mathematical analysis

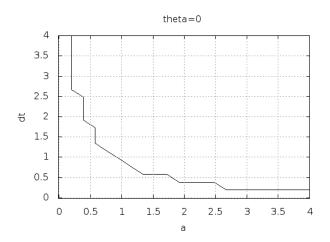
Another question to be raised is

• How does Δt impact the error in the numerical solution?

Experimental investigation of oscillatory solutions

The solution is oscillatory if

$$u^n > u^{n-1}$$



Exact numerical solution

Starting with $u^0 = I$, the simple recursion (2) can be applied repeatedly n times, with the result that

$$u^{n} = IA^{n}, \quad A = \frac{1 - (1 - \theta)a\Delta t}{1 + \theta a\Delta t}$$
 (3)

Such an exact discrete solution is unusual, but very handy for analysis.

Stability

Since $u^n \sim A^n$,

- A < 0 gives a factor $(-1)^n$ and oscillatory solutions
- |A| > 1 gives growing solutions
- Recall: the exact solution is monotone and decaying
- If these qualitative properties are not met, we say that the numerical solution is unstable

Computation of stability in this problem

A < 0 if

$$\frac{1-(1-\theta)a\Delta t}{1+\theta a\Delta t}<0$$

To avoid oscillatory solutions we must have A > 0 and

$$\Delta t < \frac{1}{(1-\theta)a} \tag{4}$$

- Always fulfilled for Backward Euler
- \bullet $\Delta t \leq 1/a$ for Forward Euler
- $\Delta t \le 2/a$ for Crank-Nicolson

Computation of stability in this problem

 $|A| \leq 1$ means $-1 \leq A \leq 1$

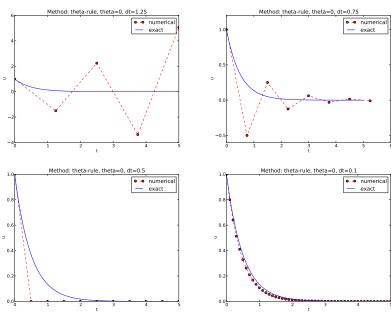
$$-1 \le \frac{1 - (1 - \theta)a\Delta t}{1 + \theta a\Delta t} \le 1 \tag{5}$$

-1 is the critical limit:

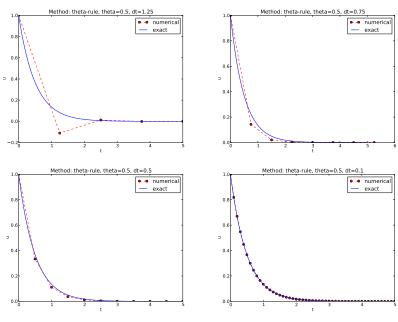
$$\Delta t \leq \frac{2}{(1-2\theta)a}, \quad \theta < \frac{1}{2}$$
 $\Delta t \geq \frac{2}{(1-2\theta)a}, \quad \theta > \frac{1}{2}$

- Always fulfilled for Backward Euler and Crank-Nicolson
- $\Delta t \leq 2/a$ for Forward Euler

Explanation of problems with Forward Euler



Explanation of problems with Crank-Nicolson



Summary of stability

- Forward Euler is conditionally stable
 - $\Delta t < 2/a$ for avoiding growth
 - $\Delta t \leq 1/a$ for avoiding oscillations
- The Crank-Nicolson is unconditionally stable wrt growth and conditionally stable wrt oscillations
 - $\Delta t < 2/a$ for avoiding oscillations
- Backward Euler is unconditionally stable

Comparing amplification factors

 u^{n+1} is an amplification A of u^n :

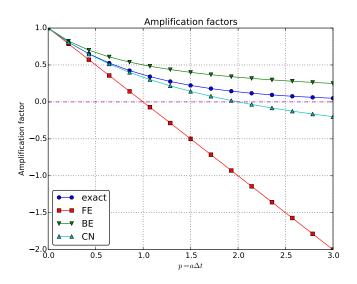
$$u^{n+1} = Au^n$$
, $A = \frac{1 - (1 - \theta)a\Delta t}{1 + \theta a\Delta t}$

The exact solution is also an amplification:

$$u(t_{n+1}) = A_e u(t_n), \quad A_e = e^{-a\Delta t}$$

A possible measure of accuracy: $A_{\rm e}-A$

Plot of amplification factors



$p=a\Delta t$ is the important parameter for numerical performance

- ullet $p=a\Delta t$ is a dimensionless parameter
- all expressions for stability and accuracy involve p
- Note that Δt alone is not so important, it is the combination with a through $p=a\Delta t$ that matters

Another "proof" why $p = a\Delta t$ is key

If we scale the model by $\overline{t}=at,\ \overline{u}=u/I,$ we get $d\,\overline{u}/d\overline{t}=-\overline{u},$ $\overline{u}(0)=1$ (no physical parameters!). The analysis show that $\Delta\,\overline{t}$ is key, corresponding to $a\Delta\,t$ in the unscaled model.

Series expansion of amplification factors

To investigate $A_{\rm e}-A$ mathematically, we can Taylor expand the expression, using $p=a\Delta t$ as variable.

```
>>> from sympy import *
>>> # Create p as a mathematical symbol with name 'p'
>>> p = Symbol('p')
>>> # Create a mathematical expression with p
>>> A_e = exp(-p)
>>>
>>> # Find the first 6 terms of the Taylor series of A_e
>>> A_e.series(p, 0, 6)
1 + (1/2)*p**2 - p - 1/6*p**3 - 1/120*p**5 + (1/24)*p**4 + 0(p**6)
>>> theta = Symbol('theta')
>>> A = (1-(1-theta)*p)/(1+theta*p)
\Rightarrow FE = A_e.series(p, 0, 4) - A.subs(theta, 0).series(p, 0, 4)
>>> BE = A_e.series(\bar{p}, 0, 4) - A.subs(theta, 1).series(\bar{p}, 0, 4)
\Rightarrow half = Rational(1,2) # exact fraction 1/2
>>> CN = A_e.series(p, 0, 4) - A.subs(theta, half).series(p, 0, 4)
>>> FF.
(1/2)*p**2 - 1/6*p**3 + 0(p**4)
>>> BE
-1/2*p**2 + (5/6)*p**3 + 0(p**4)
>>> CN
(1/12)*p**3 + 0(p**4)
```

Error in amplification factors

Focus: the error measure $A-A_{\rm e}$ as function of Δt (recall that $p=a\Delta t$):

$$A - A_{\rm e} = \left\{ egin{array}{ll} \mathcal{O}(\Delta t^2), & {\sf Forward and Backward Euler}, \\ \mathcal{O}(\Delta t^3), & {\sf Crank-Nicolson} \end{array} \right.$$
 (6)

The fraction of numerical and exact amplification factors

Focus: the error measure $1 - A/A_{\rm e}$ as function of $p = a\Delta t$:

```
>>> FE = 1 - (A.subs(theta, 0)/A_e).series(p, 0, 4)
>>> BE = 1 - (A.subs(theta, 1)/A_e).series(p, 0, 4)
>>> CN = 1 - (A.subs(theta, half)/A_e).series(p, 0, 4)
>>> FE
(1/2)*p**2 + (1/3)*p**3 + 0(p**4)
>>> BE
-1/2*p**2 + (1/3)*p**3 + 0(p**4)
>>> CN
(1/12)*p**3 + 0(p**4)
```

Same leading-order terms as for the error measure $A-A_{
m e}$.

The true/global error at a point

- The error in A reflects the *local error* when going from one time step to the next
- What is the global (true) error at t_n ? $e^n = u_e(t_n) - u^n = Ie^{-at_n} - IA^n$
- Taylor series expansions of eⁿ simplify the expression

Computing the global error at a point

```
>>> n = Symbol('n')
>>> u_e = exp(-p*n)  # I=1
>>> u_n = A**n  # I=1
>>> FE = u_e.series(p, 0, 4) - u_n.subs(theta, 0).series(p, 0, 4)
>>> BE = u_e.series(p, 0, 4) - u_n.subs(theta, 1).series(p, 0, 4)
>>> CN = u_e.series(p, 0, 4) - u_n.subs(theta, half).series(p, 0, 4)
>>> FE
(1/2)*n*p**2 - 1/2*n**2*p**3 + (1/3)*n*p**3 + 0(p**4)
>>> BE
(1/2)*n**2*p**3 - 1/2*n*p**2 + (1/3)*n*p**3 + 0(p**4)
>>> CN
(1/12)*n*p**3 + 0(p**4)
```

Substitute *n* by $t/\Delta t$:

- ullet Forward and Backward Euler: leading order term ${1\over2}ta^2\Delta t$
- Crank-Nicolson: leading order term $\frac{1}{12}ta^3\Delta t^2$

Convergence

The numerical scheme is convergent if the global error $e^n \to 0$ as $\Delta t \to 0$. If the error has a leading order term Δt^r , the convergence rate is of order r.

Integrated errors

Focus: norm of the numerical error

$$||e^n||_{\ell^2} = \sqrt{\Delta t \sum_{n=0}^{N_t} (u_e(t_n) - u^n)^2}$$

Forward and Backward Euler:

$$||e^n||_{\ell^2} = \frac{1}{4} \sqrt{\frac{T^3}{3}} a^2 \Delta t$$

Crank-Nicolson:

$$||e^n||_{\ell^2} = \frac{1}{12} \sqrt{\frac{T^3}{3}} a^3 \Delta t^2$$

Summary of errors

Analysis of both the pointwise and the time-integrated true errors:

Truncation error

- How good is the discrete equation?
- \bullet Possible answer: see how well u_e fits the discrete equation

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

i.e.,

$$\frac{u^{n+1}-u^n}{\Delta t}=-au^n$$

Insert u_e (which does not in general fulfill this equation):

$$\frac{u_{\rm e}(t_{n+1}) - u_{\rm e}(t_n)}{\Delta t} + au_{\rm e}(t_n) = R^n \neq 0 \tag{7}$$

Computation of the truncation error

- The residual R^n is the truncation error.
- How does R^n vary with Δt ?

Tool: Taylor expand u_e around the point where the ODE is sampled (here t_n)

$$u_{e}(t_{n+1}) = u_{e}(t_{n}) + u'_{e}(t_{n})\Delta t + \frac{1}{2}u''_{e}(t_{n})\Delta t^{2} + \cdots$$

Inserting this Taylor series in (7) gives

$$R^n = u_{\mathsf{e}}'(t_n) + rac{1}{2}u_{\mathsf{e}}''(t_n)\Delta t + \ldots + \mathsf{a}u_{\mathsf{e}}(t_n)$$

Now, $u_{\rm e}$ solves the ODE $u_{\rm e}'=-au_{\rm e}$, and then

$$R^n pprox rac{1}{2} u_{
m e}''(t_n) \Delta t$$

This is a mathematical expression for the truncation error.

The truncation error for other schemes

Backward Euler:

$$R^n pprox -rac{1}{2}u''_{\mathsf{e}}(t_n)\Delta t$$

Crank-Nicolson:

$$R^{n+\frac{1}{2}} pprox \frac{1}{24} u_{\rm e}^{\prime\prime\prime}(t_{n+\frac{1}{2}}) \Delta t^2$$

Consistency, stability, and convergence

- Truncation error measures the residual in the difference equations. The scheme is *consistent* if the truncation error goes to 0 as $\Delta t \rightarrow 0$. Importance: the difference equations approaches the differential equation as $\Delta t \rightarrow 0$.
- Stability means that the numerical solution exhibits the same qualitative properties as the exact solution. Here: monotone, decaying function.
- Convergence implies that the true (global) error $e^n = u_{\rm e}(t_n) u^n \to 0$ as $\Delta t \to 0$. This is really what we want!

The Lax equivalence theorem for *linear* differential equations: consistency + stability is equivalent with convergence.

(Consistency and stability is in most problems much easier to establish than convergence.)