Analysis of exponential decay models

MATMEK-4270

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Recap - Finite differencing of exponential decay

The ordinary differential equation

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

where $a > 0$ is a constant.

Solve the ODE by finite difference methods:

- Discretize in time:

$$
0 = t_0 < t_1 < t_2 < \cdots < t_{N_t - 1} < t_{N_t} = T
$$

- Satisfy the ODE at N_t discrete time steps:

$$
\begin{aligned}
u'(t_n) &= -au(t_n), && n \in [1, \ldots, N_t], \text{ or} \\
u'(t_{n+\frac{1}{2}}) &= -au(t_{n+\frac{1}{2}}), && n \in [0, \ldots, N_t - 1]
\end{aligned}
$$

Finite difference algorithms

- Discretization by a generic θ-rule

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

$$\begin{cases} \theta = 0 & \text{Forward Euler} \\ \theta = 1 & \text{Backward Euler} \\ \theta = 1/2 & \text{Crank-Nicolson} \end{cases}$$

Note $u^n = u(t_n)$

- Solve recursively: Set $u^0 = I$ and then

$$u^{n+1} = \frac{1 - (1-\theta)a\triangle t}{1 + \theta a \triangle t} u^n \quad \text{for } n = 0, 1, \ldots$$

Analysis of finite difference equations

Model:

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

Method:

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

Problem setting

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

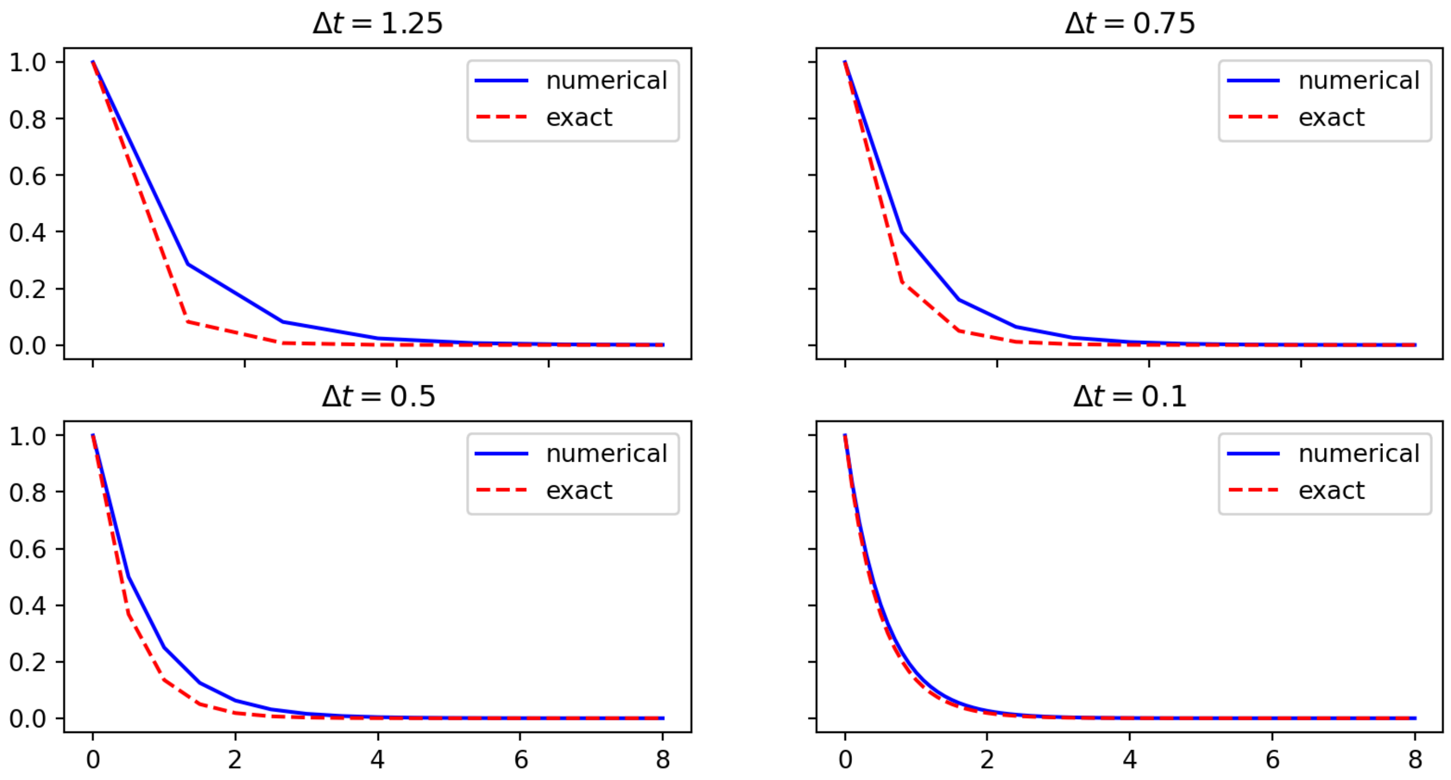
Solver

We already have a solver that we can use to experiment with. Lets run it for a range of different timesteps.

```
import numpy as np
def solver(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0, T] with steps of dt."""
    Nt = int(T/dt)                    # no of time intervals
    T = Nt*dt                         # adjust T to fit time step dt
    u = np.zeros(Nt+1)                   # array of u[n] values
    t = np.linspace(0, T, Nt+1)  # time mesh
    u[0] = I                          # assign initial condition
    u[1:] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    u[:] = np.cumprod(u)
    return u, t
```

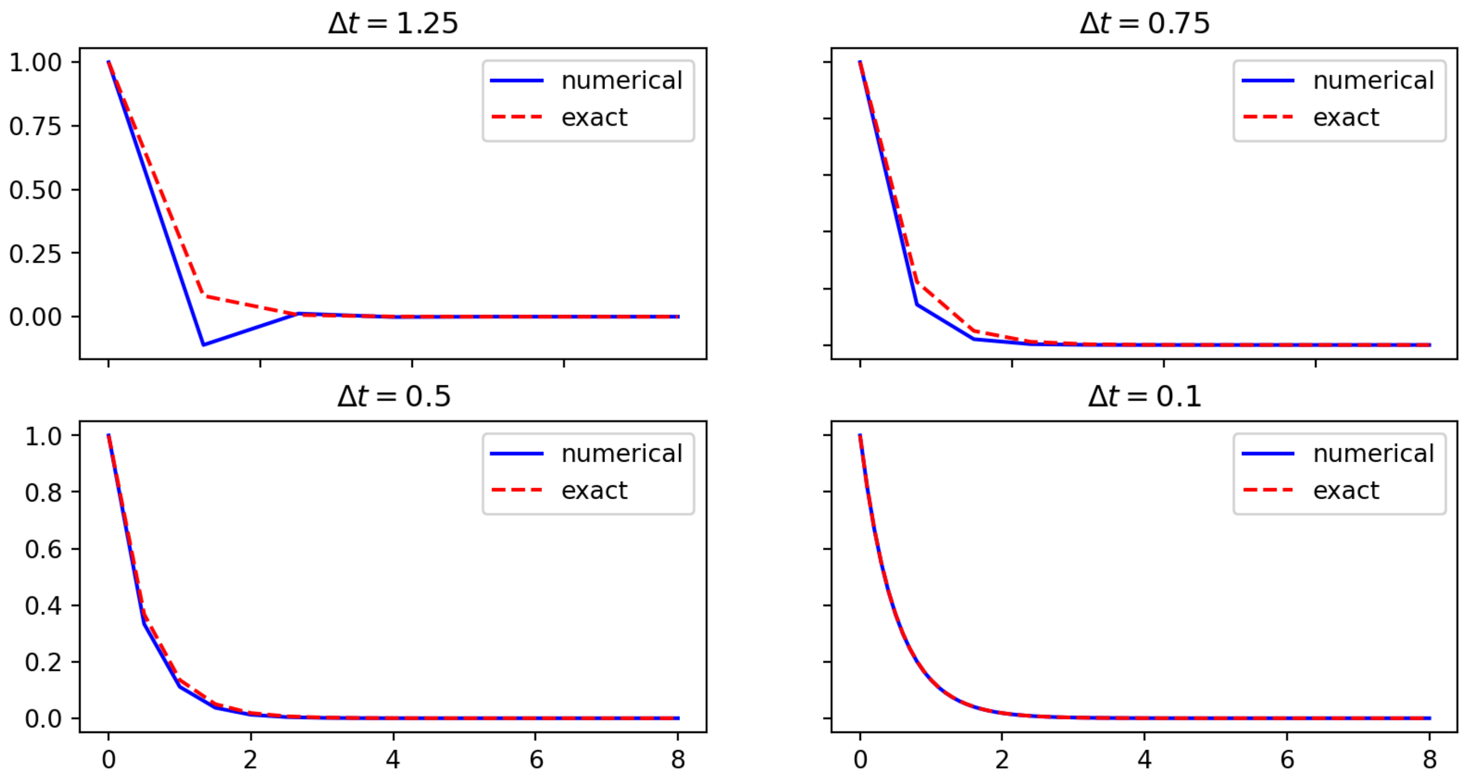
Encouraging numerical solutions - Backwards Euler

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



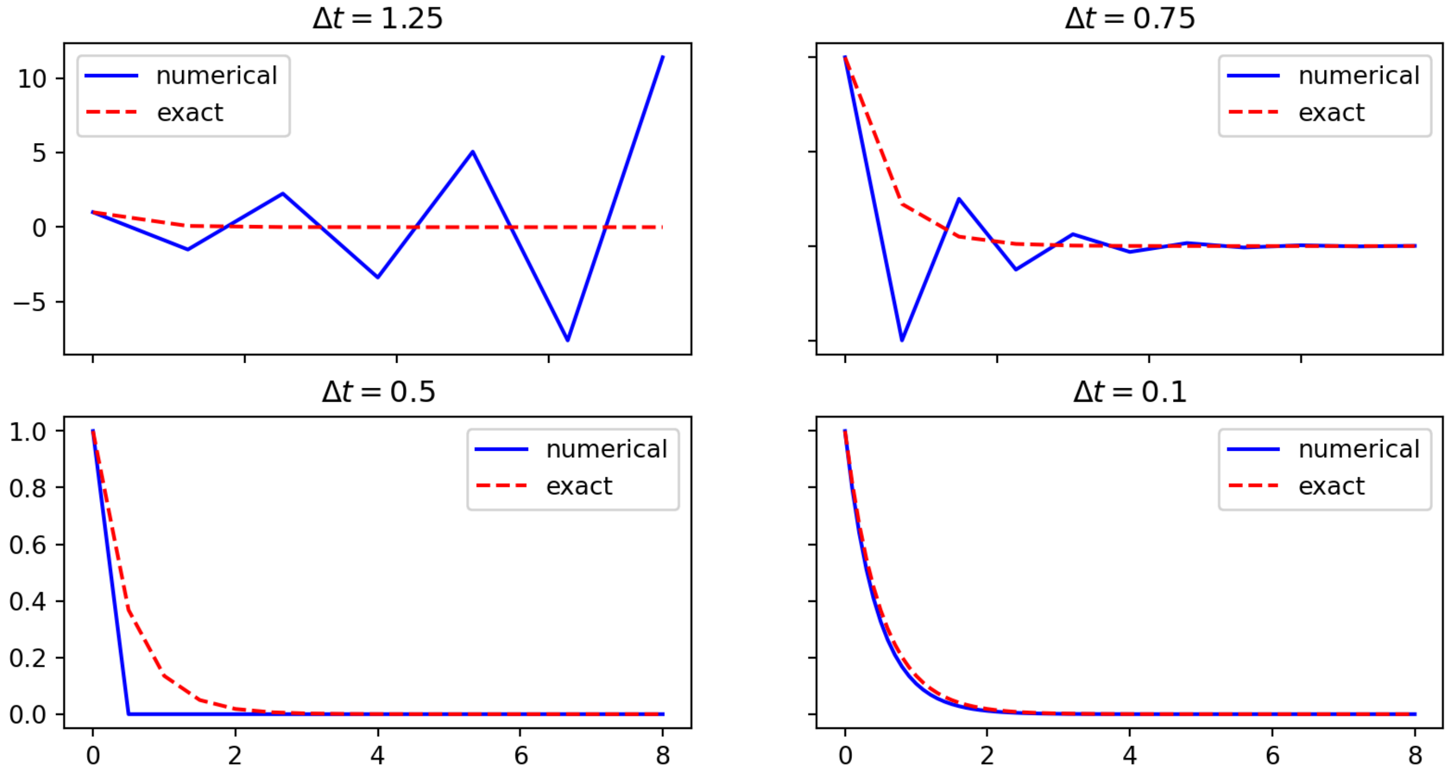
Discouraging numerical solutions - Crank-Nicolson

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



Discouraging numerical solutions - Forward Euler

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



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 solution.
- 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.
- Small enough Δt gives stable and accurate solution for all methods!

Problem setting

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?

Exact numerical solution

For the simple exponential decay problem we are lucky enough to have an exact numerical solution

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

Such a formula for the exact discrete solution is unusual to obtain in practice, but very handy for our analysis here.

Note

An exact dicrete solution fulfills a discrete equation (without round-off errors), whereas an exact solution fulfills the original mathematical equation.

Stability

Since $u^n = IA^n$,

- $A < 0$ 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*

For stability we need

$$A > 0 \quad \text{and} \quad |A| \leq 1$$

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 $A > 0$, which happens for

$$\Delta t < \frac{1}{(1-\theta)a}, \quad \text{for}\, \theta < 1$$

- Always fulfilled for Backward Euler ($\theta = 1 \rightarrow A = 1/(1+a\Delta t) > 0$)
- $\Delta t \leq 1/a$ for Forward Euler ($\theta = 0$)
- $\Delta t \leq 2/a$ for Crank-Nicolson ($\theta = 0.5$)

We get oscillatory solutions for FE when $\Delta t \leq 1/a$ and for CN when $\Delta t \leq 2/a$

Computation of stability in this problem

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

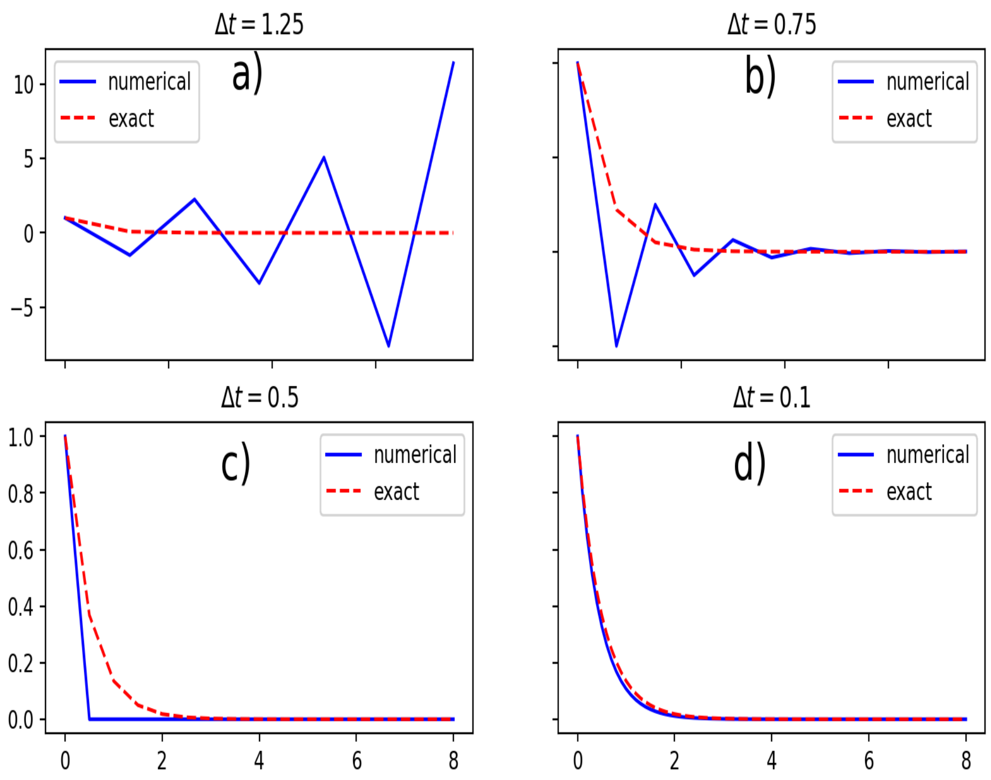
$$-1 \leq \frac{1-(1-\theta)a\Delta t}{1+\theta a\Delta t} \leq 1$$

- -1 is the critical limit (because $A \leq 1$ is always satisfied).
- $-1 < A$ is always fulfilled for Backward Euler ($\theta = 1$) and Crank-Nicolson ($\theta = 0.5$).
- For forward Euler or simply $\theta < 0.5$ we have

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

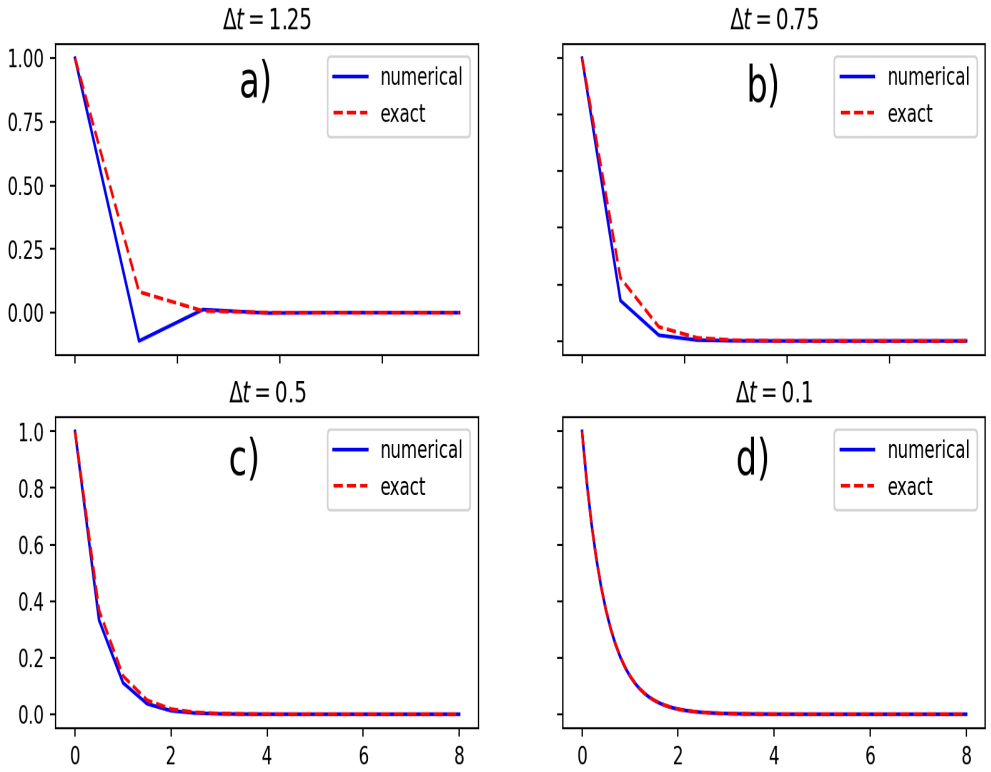
and thus $\Delta t \leq 2/a$ for stability of the forward Euler ($\theta = 0$) method

Explanation of problems with forward Euler



a. $a\Delta t = 2 \cdot 1.25 = 2.5$ and $A = -1.5$: oscillations and growth
b. $a\Delta t = 2 \cdot 0.75 = 1.5$ and $A = -0.5$: oscillations and decay
c. $\Delta t = 0.5$ and $A = 0$: $u^n = 0$ for $n > 0$
d. Smaller Δt: qualitatively correct solution

Explanation of problems with Crank-Nicolson



a. $\Delta t = 1.25$ and $A = -0.25$: oscillatory solution

Never any growing solution

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:

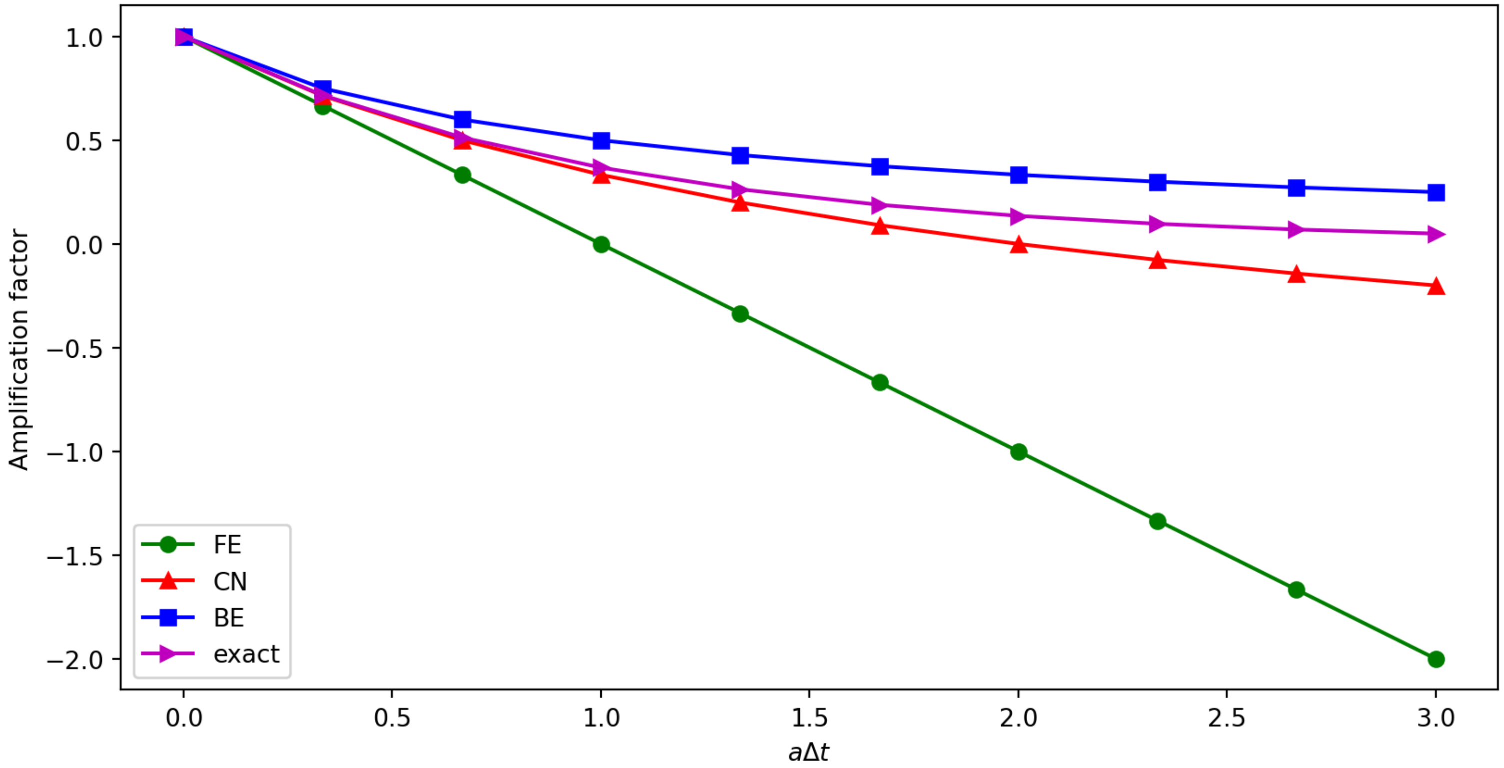
$$u^{n+1} = Au^n, \quad A = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a\Delta t}$$

The exact solution is also an amplification:

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

A possible measure of accuracy: $A_e - A$

Plotting amplification factors



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

- $p = a\Delta t$ 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 evidence why $p = a\Delta t$ is key

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

Series expansion of amplification factors

To investigate $A_e - A$ mathematically, we can Taylor expand the expression, using $p = a\Delta t$ as variable.

```python
from sympy import *
# Create p as a mathematical symbol with name 'p'
p = Symbol('p', positive=True)
# 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)
```

$$1 - p + \frac{p^2}{2} - \frac{p^3}{6} + \frac{p^4}{24} - \frac{p^5}{120} + O\left(p^6\right)$$

This is the Taylor expansion of the exact amplification factor. How does it compare with the numerical amplification factors?

Numerical amplification factors

Compute the Taylor expansions of $A_e - A$

```
from IPython.display import display
theta = Symbol('theta', positive=True)
A = (1-(1-theta)*p)/(1+theta*p)
FE = A_e.series(p, 0, 4) - A.subs(theta, 0).series(p, 0, 4)
BE = A_e.series(p, 0, 4) - A.subs(theta, 1).series(p, 0, 4)
half = Rational(1, 2)  # exact fraction 1/2
CN = A_e.series(p, 0, 4) - A.subs(theta, half).series(p, 0, 4)
display(FE)
display(BE)
display(CN)
```

$$\frac{p^2}{2} - \frac{p^3}{6} + O\left(p^4\right)$$

$$-\frac{p^2}{2} + \frac{5p^3}{6} + O\left(p^4\right)$$

$$\frac{p^3}{12} + O\left(p^4\right)$$

- Forward/backward Euler have leading error p^2, or more commonly Δt^2
- Crank-Nicolson has leading error p^3, or Δt^3

The true/global error at a point

- The error in A reflects the **local (amplification) 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 e^n simplify the expression

Computing the global error at a point

```
n = Symbol('n', integer=True, positive=True)
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)
display(simplify(FE))
display(simplify(BE))
display(simplify(CN))
```

$$\frac{np^2}{2} + \frac{np^3}{3} - \frac{n^2p^3}{2} + O\left(p^4\right)$$

$$-\frac{np^2}{2} + \frac{np^3}{3} + \frac{n^2p^3}{2} + O\left(p^4\right)$$

$$\frac{np^3}{12} + O\left(p^4\right)$$

Substitute n by $t/\Delta t$ and p by $a\Delta t$:

- Forward and Backward Euler: leading order term $\frac{1}{2}ta^2\Delta t$
- 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 $(\Delta t)^r$, the convergence rate is of order r.

Integrated errors

The ℓ^2 norm of the numerical error is computed as

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

We can compute this using Sympy. Forward/Backward Euler has $e^n \sim np^2/2$

```python
h, N, a, T = symbols('h,N,a,T') # h represents Delta t
simplify(sqrt(h * summation((n*p**2/2)**2, (n, 0, N))).subs(p, a*h).subs(N, T/h))
```

$$\frac{\sqrt{6} a^2 h^2 \sqrt{T \left(\frac{2T^2}{h^2} + \frac{3T}{h} + 1 \right)}}{12}$$

If we keep only the leading term in the parenthesis, we get the first order

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

Crank-Nicolson

For Crank-Nicolson the pointwise error is $e^n \sim np^3/12$. We get

```
simplify(sqrt(h * summation((n*p**3/12)**2, (n, 0, N))).subs(p, a*h).subs(N, T/h))
```

$$\frac{\sqrt{6}a^3h^3\sqrt{T\left(\frac{2T^2}{h^2}+\frac{3T}{h}+1\right)}}{72}$$

which is simplified to the second order accurate

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

Summary of errors

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

- 1st order for Forward and Backward Euler
- 2nd order for Crank-Nicolson

Truncation error

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

Consider the forward difference equation

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

Insert u_e to obtain a truncation error R^n

$$\frac{u_e(t_{n+1}) - u_e(t_n)}{\Delta t} + au_e(t_n) = R^n \neq 0$$

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 for u_e in the forward difference equation

$$R^n = \frac{u_e(t_{n+1}) - u_e(t_n)}{\Delta t} + au_e(t_n)$$

to get

$$R^n = u_e'(t_n) + \frac{1}{2}u_e''(t_n)\Delta t + \ldots + au_e(t_n)$$

The truncation error forward Euler

We have

$$R^n = u_e'(t_n) + \frac{1}{2}u_e''(t_n)\Delta t + \ldots + au_e(t_n)$$

Since u_e solves the ODE $u_e'(t_n) = -au_e(t_n)$, we get that $u_e'(t_n)$ and $au_e(t_n)$ cancel out. We are left with leading term

$$R^n \approx \frac{1}{2}u_e''(t_n)\Delta t$$

This is a mathematical expression for the truncation error.

The truncation error for other schemes

Backward Euler:

$$R^n \approx -\frac{1}{2}u_e''(t_n)\Delta t$$

Crank-Nicolson:

$$R^{n+\frac{1}{2}} \approx \frac{1}{24}u_e'''(t_{n+\frac{1}{2}})\Delta t^2$$

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 $e^n = u_e(t_n) - u^n \rightarrow 0$ as $\Delta t \rightarrow 0$. 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.)

Numerical computation of convergence rate

We assume that the ℓ^2 error norm on the mesh with level i can be written as

$$E_i = C(\Delta t_i)^r$$

where C is a constant. This way, if we have the error on two levels, then we can compute

$$\frac{E_{i-1}}{E_i} = \frac{(\Delta t_{i-1})^r}{(\Delta t_i)^r} = \left(\frac{\Delta t_{i-1}}{\Delta t_i}\right)^r$$

and isolate r by computing

$$r = \frac{\log \frac{E_{i-1}}{E_i}}{\log \frac{\Delta t_{i-1}}{\Delta t_i}}$$

Function for convergence rate

```python
u_exact = lambda t, I, a: I*np.exp(-a*t)

def l2_error(I, a, theta, dt):
    u, t = solver(I, a, T, dt, theta)
    en = u_exact(t, I, a) - u
    return np.sqrt(dt*np.sum(en**2))

def convergence_rates(m, I=1, a=2, T=8, theta=1, dt=1.):
    dt_values, E_values = [], []
    for i in range(m):
        E = l2_error(I, a, theta, dt)
        dt_values.append(dt)
        E_values.append(E)
        dt = dt/2
    # Compute m-1 orders that should all be the same
    r = [np.log(E_values[i-1]/E_values[i])/
         np.log(dt_values[i-1]/dt_values[i])
         for i in range(1, m, 1)]
    return r
```

Test convergence rates

Backward Euler:

```python
I, a, T, dt, theta = 1., 2., 8., 0.1, 1.
convergence_rates(4, I, a, T, theta, dt)
```

```
[np.float64(0.9619265651066382),
 np.float64(0.98003334385805),
 np.float64(0.9897576131285538)]
```

Forward Euler:

```python
I, a, T, dt, theta = 1., 2., 8., 0.1, 0.
convergence_rates(4, I, a, T, theta, dt)
```

```
[np.float64(1.0472640894307232),
 np.float64(1.0222599097461846),
 np.float64(1.0108154242259877)]
```

Crank-Nicolson:

```python
I, a, T, dt, theta = 1., 2., 8., 0.1, 0.5
convergence_rates(4, I, a, T, theta, dt)
```

```
[np.float64(2.0037335266421343),
 np.float64(2.0009433957768175),
 np.float64(2.000236481071457)]
```

All in good agreement with theory:-)