Study guide: Algorithms and implementations for exponential decay models

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Slides selected and modified by Mikael Mortensen

MAT-MEK4270 in a nutshell

- Numerical methods for partial differential equations (PDEs)
- How do we solve a PDE in practice and produce numbers?
- How do we trust the answer?
- Approach: simplify, understand, generalize
- IN5670 -> IN5270 -> MAT-MEK4270 Lots of old material

After the course. You see a PDE and can't wait to program a method and visualize a solution! Somebody asks if the solution is right and you can give a convincing answer.

The new official six-point course description

After having completed MAT-MEK4270 you

• can derive methods and implement them to solve frequently arising partial differential equations (PDEs) from physics and mechanics.

- have a good understanding of finite difference and finite element methods and how they are applied in linear and nonlinear PDE problems.
- can identify numerical artifacts and perform mathematical analysis to understand and cure non-physical effects.
- can apply sophisticated programming techniques in Python, combined with Cython, C, C++, and Fortran code, to create modern, flexible simulation programs.
- can construct verification tests and automate them.
- have experience with project hosting sites (GitHub), version control systems (Git), report writing (IATEX), and Python scripting for performing reproducible computational science.

More specific contents: finite difference methods

- Simple ODEs
- Exponential decay $u_t = -au(t)$ in time
- the wave equation $u_{tt} = \nabla^2 u$ in 1D, 2D, 3D
- write your own software from scratch
- understand how the methods work and why they fail

More specific contents: Variational methods (Galerkin)

- stationary diffusion equations $u_{xx} = f$ in 1D
- time-dependent diffusion and wave equations in 1D
- PDEs in 2D and 3D by use of the FEniCS and Shenfun softwares
- perform hand-calculations, write your own software (1D)
- understand how the methods work and why they fail

Philosophy: simplify, understand, generalize

- Start with simplified ODE/PDE problems
- Learn to reason about the discretization
- Learn to implement, verify, and experiment
- Understand the method, program, and results
- Generalize the problem, method, and program

This is the power of applied mathematics!

Required software

- Our software platform: Python (sometimes combined with Cython, Fortran, C, C++)
- Important Python packages: numpy, scipy, matplotlib, sympy, fenics, shenfun, ...
- Anaconda Python

Assumed/ideal background

- IN1900: Python programming, solution of ODEs
- Some experience with finite difference methods
- Some analytical and numerical knowledge of PDEs
- Much experience with calculus and linear algebra
- Much experience with programming of mathematical problems
- Experience with mathematical modeling with PDEs (from physics, mechanics, geophysics, or ...)

Start-up example for the course

What if you don't have this ideal background?

- Students come to this course with very different backgrounds
- First task: summarize assumed background knowledge by going through a simple example
- Also in this example:

- Some fundamental material on software implementation and software testing
- Material on analyzing numerical methods to understand why they can fail
- Applications to real-world problems

Start-up example

ODE problem.

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

where a > 0 is a constant.

Everything we do is motivated by what we need as building blocks for solving Partial Differential Equations (PDEs)!

What to learn in the start-up example; standard topics

- How to think when constructing finite difference methods, with special focus on the Forward Euler, Backward Euler, and Crank-Nicolson (midpoint) schemes
- How to formulate a computational algorithm and translate it into Python code
- How to make curve plots of the solutions
- How to compute numerical errors
- How to compute convergence rates

What to learn in the start-up example; programming topics

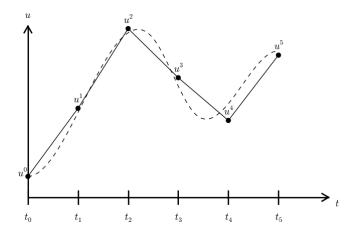
- How to verify an implementation and automate verification through nose tests in Python
- How to structure code in terms of functions, classes, and modules
- How to work with Python concepts such as arrays, lists, dictionaries, lambda functions, functions in functions (closures), doctests, unit tests, command-line interfaces, graphical user interfaces
- How to perform array computing and understand the difference from scalar computing
- How to conduct and automate large-scale numerical experiments
- How to generate scientific reports

What to learn in the start-up example; mathematical analysis

- How to uncover numerical artifacts in the computed solution
- How to analyze the numerical schemes mathematically to understand why artifacts occur
- How to derive mathematical expressions for various measures of the error in numerical methods, frequently by using the sympy software for symbolic computation
- Introduce concepts such as finite difference operators, mesh (grid), mesh functions, stability, truncation error, consistency, and convergence

Finite difference methods

- The finite difference method is the simplest method for solving differential equations
- Fast to learn, derive, and implement
- A very useful tool to know, even if you aim at using the finite element or the finite volume method



Topics in the first intro to the finite difference method Contents.

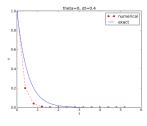
- How to think about finite difference discretization
- Key concepts:
 - mesh
 - mesh function
 - finite difference approximations
- The Forward Euler, Backward Euler, and Crank-Nicolson methods
- Finite difference operator notation
- How to derive an algorithm and implement it in Python
- How to test the implementation

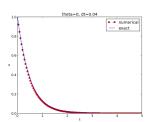
A basic model for exponential decay

The world's simplest (?) ODE:

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

Observation. We can learn a lot about numerical methods, computer implementation, program testing, and real applications of these tools by using this very simple ODE as example. The teaching principle is to keep the math as simple as possible while learning computer tools.





The ODE model has a range of applications in many fields

- Growth and decay of populations (cells, animals, human)
- Growth and decay of a fortune
- Radioactive decay
- Cooling/heating of an object

- Pressure variation in the atmosphere
- Vertical motion of a body in water/air
- Time-discretization of diffusion PDEs by Fourier techniques

See the text for details.

The ODE problem has a continuous and discrete version Continuous problem.

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

(varies with a continuous t)

Discrete problem. Numerical methods applied to the continuous problem turns it into a discrete problem

$$u^{n+1} = \text{const} \cdot u^n, \quad n = 0, 1, \dots N_t - 1, \quad u^n = I$$
 (2)

(varies with discrete mesh points t_n)

The steps in the finite difference method

Solving a differential equation by a finite difference method consists of four steps:

- 1. discretizing the domain,
- 2. fulfilling the equation at discrete time points,
- 3. replacing derivatives by finite differences,
- 4. solve the discretized problem. (Often with a recursive algorithm in 1D)

Step 1: Discretizing the domain

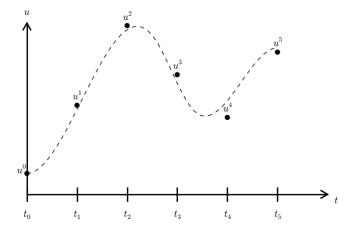
The time domain [0,T] is represented by a mesh: a finite number of N_t+1 points

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

- We seek the solution u at the mesh points: $u(t_n)$, $n = 1, 2, \ldots, N_t$.
- Note: u^0 is known as I.
- Notational short-form for the numerical approximation to $u(t_n)$: u^n
- ullet In the differential equation: u is the exact solution
- In the numerical method and implementation: u^n is the numerical approximation, $u_e(t)$ is the exact solution

Step 1: Discretizing the domain

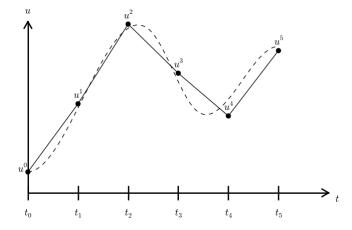
 u^n is a mesh function, defined at the mesh points $t_n,\, n=0,\dots,N_t$ only.



What about a mesh function between the mesh points?

Can extend the mesh function to yield values between mesh points by $\it linear interpolation$:

$$u(t) \approx u^n + \frac{u^{n+1} - u^n}{t_{n+1} - t_n} (t - t_n)$$
 (3)



Step 2: Fulfilling the equation at discrete time points

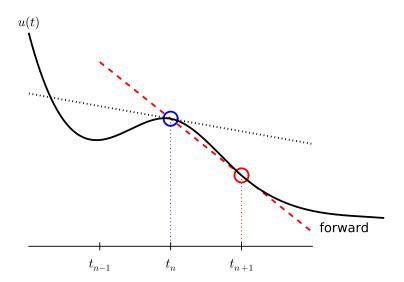
- The ODE holds for all $t \in (0, T]$ (infinite no of points)
- Idea: let the ODE be valid at the mesh points only (finite no of points)

$$u'(t_n) = -au(t_n), \quad n = 1, \dots, N_t$$
(4)

Step 3: Replacing derivatives by finite differences

Now it is time for the *finite difference* approximations of derivatives:

$$u'(t_n) \approx \frac{u^{n+1} - u^n}{t_{n+1} - t_n}$$
 (5)



Step 3: Replacing derivatives by finite differences

Inserting the finite difference approximation in

$$u'(t_n) = -au(t_n)$$

gives

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -au^n, \quad n = 0, 1, \dots, N_t - 1$$
(6)

(Known as discrete equation, or discrete problem, or finite difference method/scheme)

Step 4: Formulating a recursive algorithm

How can we actually compute the u^n values?

- given $u^0 = I$
- compute u^1 from u^0
- compute u^2 from u^1
- compute u^3 from u^2 (and so forth)

In general: we have u^n and seek u^{n+1}

The Forward Euler scheme. Solve wrt u^{n+1} to get the computational formula:

$$u^{n+1} = u^n - a(t_{n+1} - t_n)u^n (7)$$

Let us apply the scheme by hand

Assume constant time spacing: $\Delta t = t_{n+1} - t_n = \text{const}$

$$u_0 = I,$$

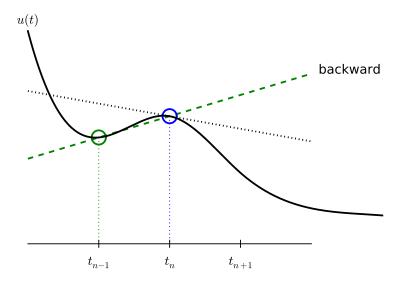
 $u_1 = u^0 - a\Delta t u^0 = I(1 - a\Delta t),$
 $u_2 = I(1 - a\Delta t)^2,$
 $u^3 = I(1 - a\Delta t)^3,$
 \vdots
 $u^{N_t} = I(1 - a\Delta t)^{N_t}$

Ooops - we can find the numerical solution by hand (in this simple example)! No need for a computer (yet)...

A backward difference

Here is another finite difference approximation to the derivative (backward difference):

$$u'(t_n) \approx \frac{u^n - u^{n-1}}{t_n - t_{n-1}}$$
 (8)



The Backward Euler scheme

Inserting the finite difference approximation in $u'(t_n) = -au(t_n)$ yields the Backward Euler (BE) scheme:

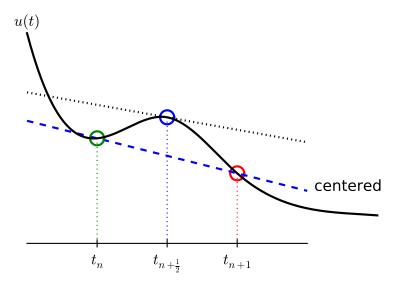
$$\frac{u^n - u^{n-1}}{t_n - t_{n-1}} = -au^n \tag{9}$$

Solve with respect to the unknown u^{n+1} :

$$u^{n+1} = \frac{1}{1 + a(t_{n+1} - t_n)} u^n \tag{10}$$

A centered difference

Centered differences are better approximations than forward or backward differences.



The Crank-Nicolson scheme; ideas

Idea 1: let the ODE hold at $t_{n+\frac{1}{2}}$

$$u'(t_{n+\frac{1}{2}}) = -au(t_{n+\frac{1}{2}})$$

Idea 2: approximate $u'(t_{n+\frac{1}{2}})$ by a centered difference

$$u'(t_{n+\frac{1}{2}}) \approx \frac{u^{n+1} - u^n}{t_{n+1} - t_n} \tag{11}$$

Problem: $u(t_{n+\frac{1}{2}})$ is not defined, only $u^n=u(t_n)$ and $u^{n+1}=u(t_{n+1})$ Solution:

$$u(t_{n+\frac{1}{2}}) \approx \frac{1}{2}(u^n + u^{n+1})$$

The Crank-Nicolson scheme; result

Result:

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -a\frac{1}{2}(u^n + u^{n+1})$$
(12)

Solve wrt to u^{n+1} :

$$u^{n+1} = \frac{1 - \frac{1}{2}a(t_{n+1} - t_n)}{1 + \frac{1}{2}a(t_{n+1} - t_n)}u^n$$
(13)

This is a Crank-Nicolson (CN) scheme or a midpoint or centered scheme.

The unifying θ -rule

The Forward Euler, Backward Euler, and Crank-Nicolson schemes can be formulated as one scheme with a varying parameter θ :

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -a(\theta u^{n+1} + (1 - \theta)u^n)$$
(14)

- $\theta = 0$: Forward Euler
- $\theta = 1$: Backward Euler
- $\theta = 1/2$: Crank-Nicolson
- We may alternatively choose any $\theta \in [0, 1]$.

 u^n is known, solve for u^{n+1} :

$$u^{n+1} = \frac{1 - (1 - \theta)a(t_{n+1} - t_n)}{1 + \theta a(t_{n+1} - t_n)} u^n$$
(15)

Constant time step

Very common assumption (not important, but exclusively used for simplicity hereafter): constant time step $t_{n+1} - t_n \equiv \Delta t$

Summary of schemes for constant time step.

$$u^{n+1} = (1 - a\Delta t)u^n$$
 Forward Euler (16)

$$u^{n+1} = \frac{1}{1 + a\Delta t}u^n$$
 Backward Euler (17)

$$u^{n+1} = \frac{1 - \frac{1}{2}a\Delta t}{1 + \frac{1}{2}a\Delta t}u^n \qquad \text{Crank-Nicolson}$$
 (18)

$$u^{n+1} = \frac{1 - (1 - \theta)a\Delta t}{1 + \theta a\Delta t}u^n \quad \text{The } \theta - \text{rule}$$
 (19)

Test the understanding!

Derive Forward Euler, Backward Euler, and Crank-Nicolson schemes for Newton's law of cooling:

$$T' = -k(T - T_s), \quad T(0) = T_0, \ t \in (0, t_{end}]$$

Physical quantities:

- T(t): temperature of an object at time t
- \bullet k: parameter expressing heat loss to the surroundings
- T_s : temperature of the surroundings
- T_0 : initial temperature

Compact operator notation for finite differences

- Finite difference formulas can be tedious to write and read/understand
- Handy tool: finite difference operator notation
- Advantage: communicates the nature of the difference in a compact way

$$[D_t^- u = -au]^n \tag{20}$$

Specific notation for difference operators

Forward difference:

$$[D_t^+ u]^n = \frac{u^{n+1} - u^n}{\Delta t} \approx \frac{d}{dt} u(t_n)$$
(21)

Centered difference (around t_n):

$$[D_t u]^n = \frac{u^{n+\frac{1}{2}} - u^{n-\frac{1}{2}}}{\Delta t} \approx \frac{d}{dt} u(t_n),$$
 (22)

Backward difference:

$$[D_t^- u]^n = \frac{u^n - u^{n-1}}{\Delta t} \approx \frac{d}{dt} u(t_n)$$
 (23)

The Backward Euler scheme with operator notation

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

Common to put the whole equation inside square brackets:

$$[D_t^- u = -au]^n \tag{24}$$

The Forward Euler scheme with operator notation

$$[D_t^+ u = -au]^n \tag{25}$$

The Crank-Nicolson scheme with operator notation

Introduce an averaging operator:

$$[\overline{u}^t]^n = \frac{1}{2}(u^{n-\frac{1}{2}} + u^{n+\frac{1}{2}}) \approx u(t_n)$$
 (26)

The Crank-Nicolson scheme can then be written as

$$[D_t u = -a\overline{u}^t]^{n+\frac{1}{2}} \tag{27}$$

Test: use the definitions and write out the above formula to see that it really is the Crank-Nicolson scheme!

Implementation

Model:

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

Numerical method:

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

for $\theta \in [0, 1]$. Note

- $\theta = 0$ gives Forward Euler
- $\theta = 1$ gives Backward Euler
- $\theta = 1/2$ gives Crank-Nicolson

Requirements of a program

- Compute the numerical solution u^n , $n = 1, 2, ..., N_t$
- Display the numerical and exact solution $u_e(t) = e^{-at}$
- Bring evidence to a correct implementation (verification)
- Compare the numerical and the exact solution in a plot
- Compute the error $u_{\mathbf{e}}(t_n) u^n$

Tools to learn

- Basic Python programming
- Array computing with numpy
- Plotting with matplotlib.pyplot
- File writing and reading

Why implement in Python?

- Python has a very clean, readable syntax (often known as "executable pseudo-code").
- Python code is very similar to MATLAB code (and MATLAB has a particularly widespread use for scientific computing).
- Python is a full-fledged, very powerful programming language.
- Python is similar to, but much simpler to work with and results in more reliable code than C++.

Why implement in Python?

- Python has a rich set of modules for scientific computing, and its popularity in scientific computing is rapidly growing.
- Python was made for being combined with compiled languages (C, C++, Fortran) to reuse existing numerical software and to reach high computational performance of new implementations.
- Python has extensive support for administrative task needed when doing large-scale computational investigations.
- Python has extensive support for graphics (visualization, user interfaces, web applications).
- FEniCS, a very powerful tool for solving PDEs by the finite element method, is most human-efficient to operate from Python.

Algorithm

- Store u^n , $n = 0, 1, \ldots, N_t$ in an array **u**.
- Algorithm:
 - 1. initialize u^0
 - 2. for $t = t_n, n = 1, 2, ..., N_t$: compute u_n using the θ -rule formula

Translation to Python function

Note about the for loop: range(0, Nt, s) generates all integers from 0 to Nt in steps of s (default 1), but not including Nt (!). Sample call:

```
u, t = solver(I=1, a=2, T=8, dt=0.8, theta=1)
```

Integer division

Python applies integer division: 1/2 is 0, while 1./2 or 1.0/2 or 1/2. or 1/2.0 or 1.0/2.0 all give 0.5.

A safer solver function (dt = float(dt) - guarantee float):

```
from numpy import *
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
   T = Nt*dt
                            # adjust T to fit time step dt
                      # array of u[n] values
   u = zeros(Nt+1)
   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 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
   return u, t
```

Doc strings

- First string after the function heading
- Used for documenting the function
- Automatic documentation tools can make fancy manuals for you
- Can be used for automatic testing

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

    u'(t) = -a*u(t),

with initial condition u(0)=I, for t in the time interval
    (0,T]. The time interval is divided into time steps of
length dt.
```

```
theta=1 corresponds to the Backward Euler scheme, theta=0 to the Forward Euler scheme, and theta=0.5 to the Crank-Nicolson method.
```

Formatting of numbers

Can control formatting of reals and integers through the *printf* format:

```
print('t=%6.3f u=%g' % (t[i], u[i]))
```

Or the alternative format string syntax:

```
print('t={t:6.3f} u={u:g}'.format(t=t[i], u=u[i]))
```

Or even better through the alternative f-string syntax:

```
print(f't={t[i]:6.3f} u={u[i]:g}')
```

Running the program

How to run the program decay_v1.py.

```
Terminal> python decay_v1.py
```

Can also run it as "normal" Unix programs: ./decay_v1.py if the first line is

```
"#!/usr/bin/env python"
```

Then

```
Terminal> chmod a+rx decay_v1.py
Terminal> ./decay_v1.py
```

Plotting the solution

Basic syntax:

```
from matplotlib.pyplot import *
plot(t, u)
show()
```

Can (and should!) add labels on axes, title, legends.

Comparing with the exact solution

Python function for the exact solution $u_e(t) = Ie^{-at}$:

```
def u_exact(t, I, a):
    return I*exp(-a*t)
```

Quick plotting:

```
u_e = u_exact(t, I, a)
plot(t, u, t, u_e)
```

Problem: $u_{e}(t)$ applies the same mesh as u^{n} and looks as a piecewise linear function.

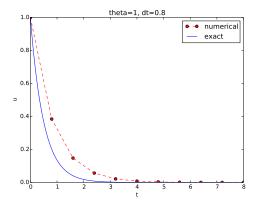
Remedy: Introduce a very fine mesh for u_e .

```
t_e = linspace(0, T, 1001)  # fine mesh
u_e = u_exact(t_e, I, a)

plot(t_e, u_e, 'b-',  # blue line for u_e
    t, u, 'r--o')  # red dashes w/circles
```

Add legends, axes labels, title, and wrap in a function

```
def plot_numerical_and_exact(theta, I, a, T, dt):
    """Compare the numerical and exact solution in a plot."""
    u, t = solver(I=I, a=a, T=T, dt=dt, theta=theta)
    t_e = linspace(0, T, 1001)  # fine mesh for u_e
    u_e = u_exact(t_e, I, a)
    plot(t, u, 'r--o', t_e, u_e, 'b-')
    legend(['numerical', 'exact'])
    xlabel('t'); ylabel('u')
    title('theta=%g, dt=%g' % (theta, dt))
    savefig('plot_%s_%g.png' % (theta, dt))
```



Verifying the implementation

- Verification = bring evidence that the program works
- Find suitable test problems
- Make function for each test problem
- Later: put the verification tests in a professional testing framework

Simplest method: run a few algorithmic steps by hand

Use a calculator $(I = 0.1, \theta = 0.8, \Delta t = 0.8)$:

$$A \equiv \frac{1 - (1 - \theta)a\Delta t}{1 + \theta a\Delta t} = 0.298245614035$$

$$u^{1} = AI = 0.0298245614035,$$

 $u^{2} = Au^{1} = 0.00889504462912,$
 $u^{3} = Au^{2} = 0.00265290804728$

See the function test_solver_three_steps in decay_v3.py.

Comparison with an exact discrete solution

Best verification. Compare computed numerical solution with a closed-form *exact discrete solution* (if possible).

Define

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

Repeated use of the θ -rule:

$$u^{0} = I,$$

$$u^{1} = Au^{0} = AI$$

$$u^{n} = A^{n}u^{n-1} = A^{n}I$$

Making a test based on an exact discrete solution

The exact discrete solution is

$$u^n = IA^n \tag{28}$$

Question. Understand what n in u^n and in A^n means! Test if

$$\max_{n} |u^n - u_e(t_n)| < \epsilon \sim 10^{-15}$$

Implementation in decay_verf2.py.

Computing the numerical error as a mesh function

Task: compute the numerical error $e^n = u_e(t_n) - u^n$ Exact solution: $u_e(t) = Ie^{-at}$, implemented as

```
def u_exact(t, I, a):
    return I*exp(-a*t)
```

Compute e^n by

```
u, t = solver(I, a, T, dt, theta) # Numerical solution
u_e = u_exact(t, I, a)
e = u_e - u
```

Array arithmetics - we compute on entire arrays!

- u_exact(t, I, a) works with t as array
- Must have exp from numpy (not math)
- e = u_e u: array subtraction
- Array arithmetics gives shorter and much faster code

Computing the norm of the error

- e^n is a mesh function
- Usually we want one number for the error
- Use a norm of e^n

Norms of a function f(t):

$$||f||_{L^2} = \left(\int_0^T f(t)^2 dt\right)^{1/2}$$
 (29)

$$||f||_{L^1} = \int_0^T |f(t)|dt \tag{30}$$

$$||f||_{L^{\infty}} = \max_{t \in [0,T]} |f(t)| \tag{31}$$

Norms of mesh functions

- Problem: $f^n = f(t_n)$ is a mesh function and hence not defined for all t. How to integrate f^n ?
- Idea: Apply a numerical integration rule, using only the mesh points of the mesh function.

The Trapezoidal rule:

$$||f^n|| = \left(\Delta t \left(\frac{1}{2}(f^0)^2 + \frac{1}{2}(f^{N_t})^2 + \sum_{n=1}^{N_t-1}(f^n)^2\right)\right)^{1/2}$$

Common simplification yields the L^2 norm of a mesh function:

$$||f^n||_{\ell^2} = \left(\Delta t \sum_{n=0}^{N_t} (f^n)^2\right)^{1/2}$$

Norms - notice!

Notice.

- The continuous norms use capital L^2, L^1, L^{∞}
- The discrete norm uses lowercase ℓ^2

Implementation of the norm of the error

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

Python w/array arithmetics:

```
e = u_exact(t) - u
E = sqrt(dt*sum(e**2))
```

Comment on array vs scalar computation

Scalar computing of E = sqrt(dt*sum(e**2)):

```
m = len(u)  # length of u array (alt: u.size)
u_e = zeros(m)
t = 0
for i in range(m):
    u_e[i] = u_exact(t, a, I)
    t = t + dt
e = zeros(m)
for i in range(m):
    e[i] = u_e[i] - u[i]
s = 0  # summation variable
for i in range(m):
    s = s + e[i]**2
error = sqrt(dt*s)
```

Scalar computing. takes more code, is less readable and runs much slower

Rule. Compute on entire arrays (when possible)! Vectorization!