App.E: Programming of differential equations

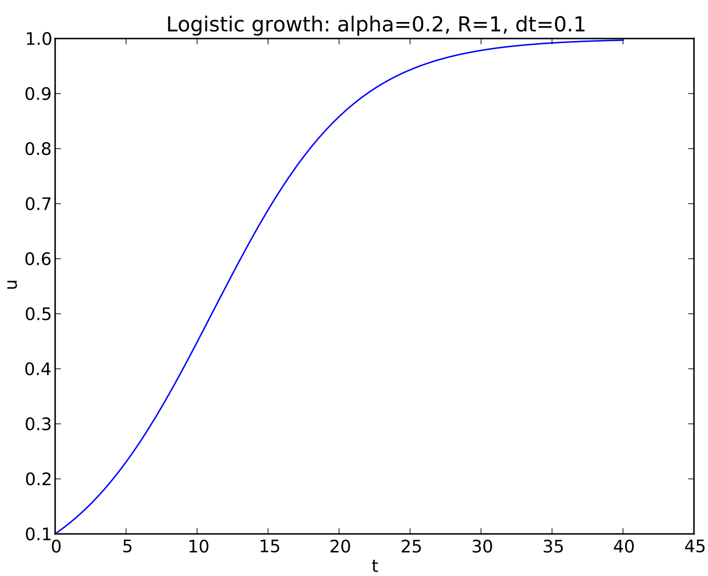
Hans Petter Langtangen[1,2]

[1]Simula Research Laboratory
[2]University of Oslo, Dept. of Informatics

Aug 15, 2015

How to solve any ordinary scalar differential equation

$$
\begin{aligned}
u'(t) &= \alpha u(t)(1 - R^{-1}u(t)) \\
u(0) &= U_0
\end{aligned}
$$



Examples on scalar differential equations (ODEs)

Terminology:

- *Scalar ODE*: a single ODE, one unknown function
- *Vector ODE* or *systems of ODEs*: several ODEs, several unknown functions

Examples:

$$
\begin{aligned}
u' &= \alpha u \quad \text{exponential growth}\\
u' &= \alpha u\left(1-\frac{u}{R}\right) \quad \text{logistic growth}\\
u' + b|u|u = g &\quad \text{falling body in fluid}
\end{aligned}
$$

We shall write an ODE in a generic form: $u' = f(u,t)$

- Our methods and software should be applicable to *any* ODE
- Therefore we need an abstract notation for an arbitrary ODE

$$u'(t) = f(u(t), t)$$

The three ODEs on the last slide correspond to

$$
\begin{aligned}
f(u,t) &= \alpha u, \quad \text{exponential growth}\\
f(u,t) &= \alpha u\left(1-\frac{u}{R}\right), \quad \text{logistic growth}\\
f(u,t) &= -b|u|u + g, \quad \text{body in fluid}
\end{aligned}
$$

Our task: write functions and classes that take f as input and produce u as output

What is the $f(u,t)$?

Problem: Given an ODE,

$$\sqrt{u}u' - \alpha(t)u^{3/2}(1 - \frac{u}{R(t)}) = 0,$$

what is the $f(u,t)$?

Solution: The target form is $u' = f(u,t)$, so we need to isolate u' on the left-hand side:

$$u' = \underbrace{\alpha(t)u(1 - \frac{u}{R(t)})}_{f(u,t)}$$

Such abstract f functions are widely used in mathematics

We can make generic software for:

- Numerical differentiation: $f'(x)$
- Numerical integration: $\int_a^b f(x)dx$
- Numerical solution of algebraic equations: $f(x) = 0$

Applications:

1. $\frac{d}{dx}x^a \sin(wx)$: $f(x) = x^a \sin(wx)$
2. $\int_{-1}^{1}(x^2 \tanh^{-1} x - (1+x^2)^{-1})dx$: $f(x) = x^2 \tanh^{-1} x - (1+x^2)^{-1}$, $a = -1$, $b = 1$
3. Solve $x^4 \sin x = \tan x$: $f(x) = x^4 \sin x - \tan x$

We use finite difference approximations to derivatives to turn an ODE into a difference equation

$u' = f(u,t)$**.** Assume we have computed u at discrete time points $t_0, t_1, \ldots, t_k$. At t_k we have the ODE

$$u'(t_k) = f(u(t_k), t_k)$$

Approximate $u'(t_k)$ by a forward finite difference,

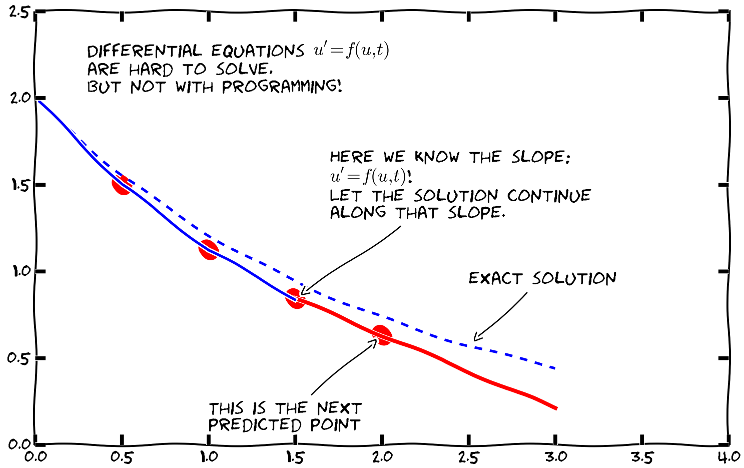
$$u'(t_k) \approx \frac{u(t_{k+1}) - u(t_k)}{\Delta t}$$

Insert in the ODE at $t = t_k$:

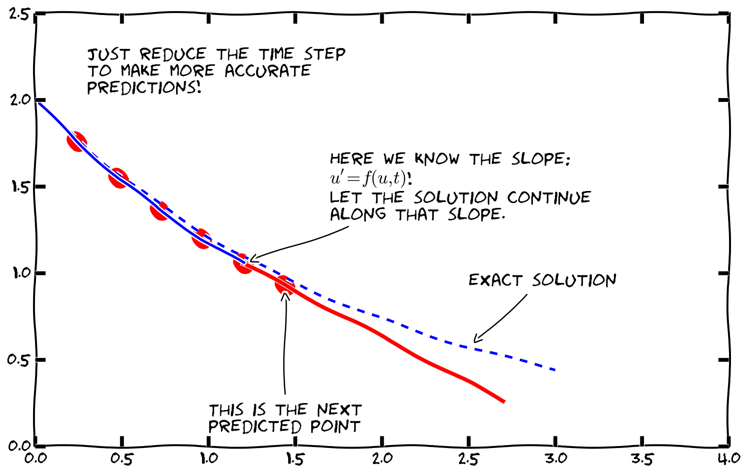
$$\frac{u(t_{k+1}) - u(t_k)}{\Delta t} = f(u(t_k), t_k)$$

Terms with $u(t_k)$ are known, and this is an algebraic (difference) equation for $u(t_{k+1})$

The Forward Euler (or Euler's) method; idea



The Forward Euler (or Euler's) method; idea



The Forward Euler (or Euler's) method; mathematics

Solving with respect to $u(t_{k+1})$

$$u(t_{k+1}) = u(t_k) + \Delta t f(u(t_k), t_k)$$

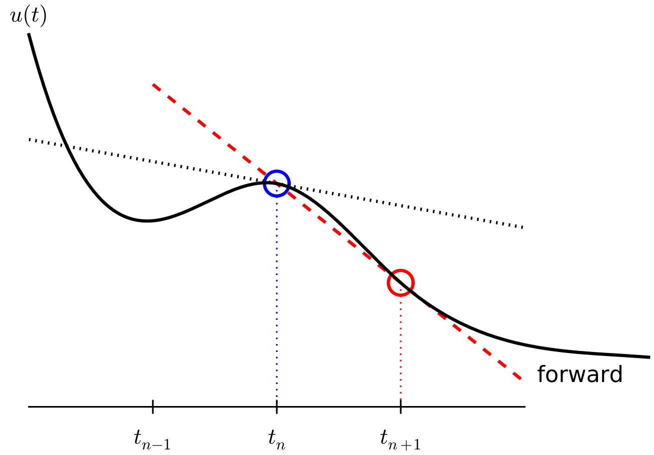
This is a very simple formula that we can use repeatedly for $u(t_1)$, $u(t_2)$, $u(t_3)$ and so forth.

Difference equation notation: Let u_k denote the numerical approximation to the exact solution $u(t)$ at $t = t_k$.

$$u_{k+1} = u_k + \Delta t f(u_k, t_k)$$

This is an ordinary difference equation we can solve!

Illustration of the forward finite difference



Let's apply the method!

Problem: The world's simplest ODE.

$$u' = u, \quad t \in (0, T]$$

Solve for u at $t = t_k = k\Delta t$, $k = 0, 1, 2, \ldots, t_n$, $t_0 = 0$, $t_n = T$

Forward Euler method:

$$u_{k+1} = u_k + \Delta t\, f(u_k, t_k)$$

Solution by hand: What is f? $f(u,t) = u$

$$u_{k+1} = u_k + \Delta t f(u_k, t_k) = u_k + \Delta t u_k = (1 + \Delta t) u_k$$

First step:

$$u_1 = (1 + \Delta t) u_0$$

but what is u_0?

An ODE needs an initial condition: $u(0) = U_0$

Numerics: Any ODE $u' = f(u,t)$ *must* have an initial condition $u(0) = U_0$, with known U_0, otherwise we cannot start the method!

Mathematics: In mathematics: $u(0) = U_0$ must be specified to get a unique solution.

Example:

$$u' = u$$

Solution: $u = Ce^t$ for any constant C. Say $u(0) = U_0$: $u = U_0 e^t$.

We continue solution by hand

Say $U_0 = 2$:

$$
\begin{aligned}
u_1 &= (1+\Delta t)u_0 = (1+\Delta t)U_0 = (1+\Delta t)2 \\
u_2 &= (1+\Delta t)u_1 = (1+\Delta t)(1+\Delta t)2 = 2(1+\Delta t)^2 \\
u_3 &= (1+\Delta t)u_2 = (1+\Delta t)2(1+\Delta t)^2 = 2(1+\Delta t)^3 \\
u_4 &= (1+\Delta t)u_3 = (1+\Delta t)2(1+\Delta t)^3 = 2(1+\Delta t)^4 \\
u_5 &= (1+\Delta t)u_4 = (1+\Delta t)2(1+\Delta t)^4 = 2(1+\Delta t)^5 \\
\vdots &= \vdots \\
u_k &= 2(1+\Delta t)^k
\end{aligned}
$$

Actually, we found a formula for u_k! No need to program...

How accurate is our numerical method?

- Exact solution: $u(t) = 2e^t$, $u(t_k) = 2e^{k\Delta t} = 2(e^{\Delta t})^k$
- Numerical solution: $u_k = 2(1+\Delta t)^k$

When going from t_k to t_{k+1}, the solution is amplified by a factor:

- Exact: $u(t_{k+1}) = e^{\Delta t}u(t_k)$
- Numerical: $u_{k+1} = (1+\Delta t)u_k$

Using Taylor series for e^x we see that

$$
e^{\Delta t} - (1+\Delta t) = 1 + \Delta t + \frac{\Delta t^2}{2} + frac\Delta t^3 6 + \cdots - (1+\Delta t) = frac\Delta t^3 6 + \mathcal{O}(\Delta t^4)
$$

This error approaches 0 as $\Delta t \to 0$.

What about the general case $u' = f(u,t)$?

Given any U_0:

$$
\begin{aligned}
u_1 &= u_0 + \Delta t f(u_0, t_0) \\
u_2 &= u_1 + \Delta t f(u_1, t_1) \\
u_3 &= u_2 + \Delta t f(u_2, t_2) \\
u_4 &= u_3 + \Delta t f(u_3, t_3) \\
&\vdots
\end{aligned}
$$

No general formula in this case...

Rule of thumb: When hand calculations get boring, let's program!

We start with a specialized program for $u' = u$, $u(0) = U_0$

Algorithm: Given Δt (`dt`) and n

- Create arrays `t` and `u` of length $n + 1$
- Set initial condition: `u[0]` $= U_0$, `t[0]=0`
- For $k = 0, 1, 2, \ldots, n - 1$:
  - `t[k+1] = t[k] + dt`
  - `u[k+1] = (1 + dt)*u[k]`

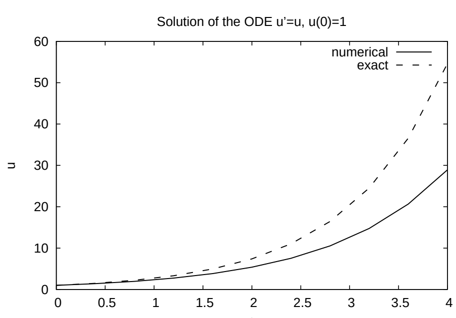
We start with a specialized program for $u' = u$, $u(0) = U_0$

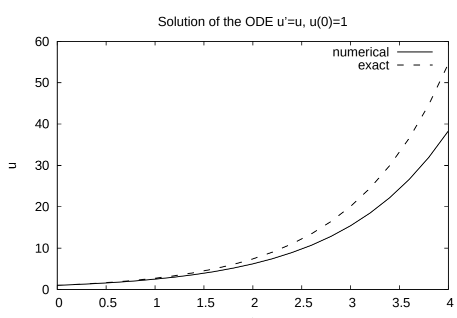
Program:

```
import numpy as np
import sys

dt = float(sys.argv[1])
U0 = 1
T = 4
n = int(T/dt)

t = np.zeros(n+1)
u = np.zeros(n+1)

t[0] = 0
u[0] = U0
for k in range(n):
    t[k+1] = t[k] + dt
    u[k+1] = (1 + dt)*u[k]

# plot u against t
```

The solution if we plot u against t

$\Delta t = 0.4$ and $\Delta t = 0.2$:





The algorithm for the general ODE $u' = f(u, t)$

Algorithm: Given Δt (`dt`) and n

- Create arrays `t` and `u` of length $n + 1$
- Create array `u` to hold u_k and
- Set initial condition: `u[0]` $= U_0$, `t[0]=0`
- For $k = 0, 1, 2, \ldots, n - 1$:
  - `u[k+1] = u[k] + dt*f(u[k], t[k])` (the only change!)
  - `t[k+1] = t[k] + dt`

Implementation of the general algorithm for $u' = f(u, t)$

General function:

```
def ForwardEuler(f, U0, T, n):
    """Solve u'=f(u,t), u(0)=U0, with n steps until t=T."""
    import numpy as np
    t = np.zeros(n+1)
    u = np.zeros(n+1)  # u[k] is the solution at time t[k]

    u[0] = U0
    t[0] = 0
    dt = T/float(n)

    for k in range(n):
        t[k+1] = t[k] + dt
        u[k+1] = u[k] + dt*f(u[k], t[k])

    return u, t
```

Magic: This simple function can solve any ODE (!)

Example on using the function

Mathematical problem: Solve $u' = u$, $u(0) = 1$, for $t \in [0, 4]$, with $\Delta t = 0.4$
Exact solution: $u(t) = e^t$.

Basic code:

```
def f(u, t):
    return u

U0 = 1
T = 3
n = 30
u, t = ForwardEuler(f, U0, T, n)
```

Compare exact and numerical solution:

```
from scitools.std import plot, exp
u_exact = exp(t)
plot(t, u, 'r-', t, u_exact, 'b-',
     xlabel='t', ylabel='u', legend=('numerical', 'exact'),
     title="Solution of the ODE u'=u, u(0)=1")
```

Now you can solve any ODE!

Recipe:

- Identify $f(u, t)$ in your ODE
- Make sure you have an initial condition U_0
- Implement the $f(u, t)$ formula in a Python function `f(u, t)`
- Choose Δt or no of steps n
- Call `u, t = ForwardEuler(f, U0, T, n)`
- `plot(t, u)`

Warning: The Forward Euler method may give very inaccurate solutions if Δt is not sufficiently small. For some problems (like $u'' + u = 0$) other methods should be used.

Let us make a class instead of a function for solving ODEs

Usage of the class:

```
method = ForwardEuler(f, dt)
method.set_initial_condition(U0, t0)
u, t = method.solve(T)
plot(t, u)
```

How?

- Store f, Δt, and the sequences u_k, t_k as attributes
- Split the steps in the `ForwardEuler` function into four methods:
  - the constructor (`__init__`)
  - `set_initial_condition` for $u(0) = U_0$
  - `solve` for running the numerical time stepping
  - `advance` for isolating the numerical updating formula
    (new numerical methods just need a different `advance` method, the rest is the same)

The code for a class for solving ODEs (part 1)

```
import numpy as np

class ForwardEuler_v1:
    def __init__(self, f, dt):
        self.f, self.dt = f, dt

    def set_initial_condition(self, U0):
        self.U0 = float(U0)
```

The code for a class for solving ODEs (part 2)

```
class ForwardEuler_v1:
    ...
    def solve(self, T):
        """Compute solution for 0 <= t <= T."""
        n = int(round(T/self.dt))  # no of intervals
        self.u = np.zeros(n+1)
        self.t = np.zeros(n+1)
        self.u[0] = float(self.U0)
        self.t[0] = float(0)

        for k in range(self.n):
            self.k = k
            self.t[k+1] = self.t[k] + self.dt
            self.u[k+1] = self.advance()
        return self.u, self.t

    def advance(self):
        """Advance the solution one time step."""
        # Create local variables to get rid of "self." in
        # the numerical formula
        u, dt, f, k, t = self.u, self.dt, self.f, self.k, self.t

        unew = u[k] + dt*f(u[k], t[k])
        return unew
```

Alternative class code for solving ODEs (part 1)

```
# Idea: drop dt in the constructor.
# Let the user provide all time points (in solve).

class ForwardEuler:
    def __init__(self, f):

        # test that f is a function
        if not callable(f):
            raise TypeError('f is %s, not a function' % type(f))
        self.f = f

    def set_initial_condition(self, U0):
        self.U0 = float(U0)
```

```
    def solve(self, time_points):
        ...
```

Alternative class code for solving ODEs (part 2)

```
class ForwardEuler:
    ...
    def solve(self, time_points):
        """Compute u for t values in time_points list."""
        self.t = np.asarray(time_points)
        self.u = np.zeros(len(time_points))

        self.u[0] = self.U0

        for k in range(len(self.t)-1):
            self.k = k
            self.u[k+1] = self.advance()
        return self.u, self.t

    def advance(self):
        """Advance the solution one time step."""
        u, f, k, t = self.u, self.f, self.k, self.t

        dt = t[k+1] - t[k]
        unew = u[k] + dt*f(u[k], t[k])
        return unew
```

Verifying the class implementation; mathematics

Mathematical problem: Important result: the numerical method (and most others) will exactly reproduce u if it is linear in t (!):

$$\begin{aligned} u(t) &= at + b = 0.2t + 3 \\ h(t) &= u(t) \\ u'(t) &= 0.2 + (u - h(t))^4, \quad u(0) = 3, \quad t \in [0, 3] \end{aligned}$$

This u should be reproduced to machine precision for any Δt.

Verifying the class implementation; implementation

Code:

```
def test_ForwardEuler_against_linear_solution():
    def f(u, t):
        return 0.2 + (u - h(t))**4

    def h(t):
        return 0.2*t + 3

    solver = ForwardEuler(f)
    solver.set_initial_condition(U0=3)
```

```
dt = 0.4; T = 3; n = int(round(float(T)/dt))
time_points = np.linspace(0, T, n+1)
u, t = solver.solve(time_points)
u_exact = h(t)
diff = np.abs(u_exact - u).max()
tol = 1E-14
success = diff < tol
assert success
```

Using a class to hold the right-hand side $f(u, t)$

Mathematical problem:

$$u'(t) = \alpha u(t)\left(1 - \frac{u(t)}{R}\right), \quad u(0) = U_0, \quad t \in [0, 40]$$

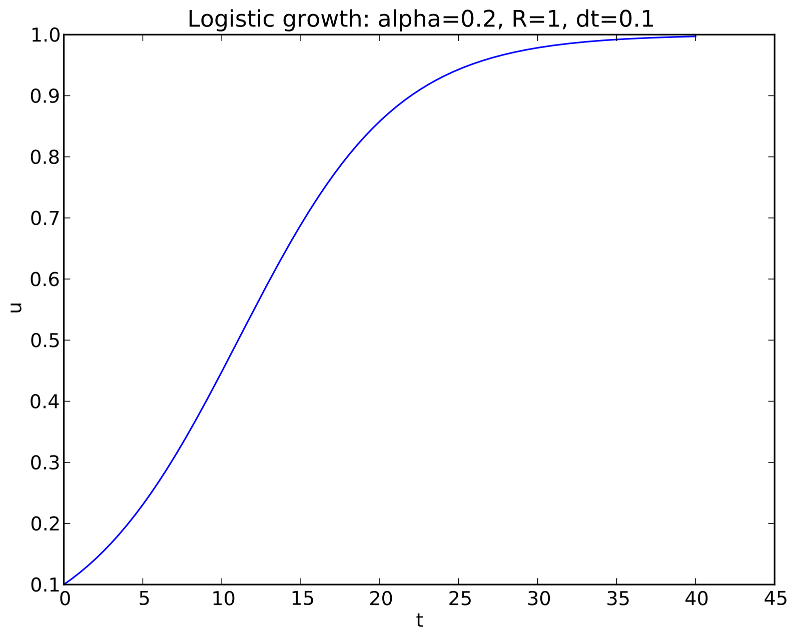
Class for right-hand side $f(u, t)$:

```
class Logistic:
    def __init__(self, alpha, R, U0):
        self.alpha, self.R, self.U0 = alpha, float(R), U0

    def __call__(self, u, t):   # f(u,t)
        return self.alpha*u*(1 - u/self.R)
```

Main program:

```
problem = Logistic(0.2, 1, 0.1)
time_points = np.linspace(0, 40, 401)
method = ForwardEuler(problem)
method.set_initial_condition(problem.U0)
u, t = method.solve(time_points)
```

Figure of the solution



Numerical methods for ordinary differential equations

Forward Euler method:

$$u_{k+1} = u_k + \Delta t\, f(u_k, t_k)$$

4th-order Runge-Kutta method:

$$u_{k+1} = u_k + \frac{1}{6}\,(K_1 + 2K_2 + 2K_3 + K_4)$$

$$\begin{aligned}
K_1 &= \Delta t\, f(u_k, t_k)\\
K_2 &= \Delta t\, f(u_k + \frac{1}{2}K_1, t_k + \frac{1}{2}\Delta t)\\
K_3 &= \Delta t\, f(u_k + \frac{1}{2}K_2, t_k + \frac{1}{2}\Delta t)\\
K_4 &= \Delta t\, f(u_k + K3, t_k + \Delta t)
\end{aligned}$$

And lots of other methods! How to program a wide collection of methods? Use object-oriented programming!

A superclass for ODE methods

Common tasks for ODE solvers:

- Store the solution u_k and the corresponding time levels t_k, $k = 0, 1, 2, \ldots, n$
- Store the right-hand side function $f(u, t)$
- Set and store the initial condition
- Run the loop over all time steps

Principles:

- Common data and functionality are placed in superclass `ODESolver`
- Isolate the numerical updating formula in a method `advance`
- Subclasses, e.g., `ForwardEuler`, just implement the specific numerical formula in `advance`

The superclass code

```
class ODESolver:
    def __init__(self, f):
        self.f = f

    def advance(self):
        """Advance solution one time step."""
        raise NotImplementedError  # implement in subclass

    def set_initial_condition(self, U0):
        self.U0 = float(U0)

    def solve(self, time_points):
        self.t = np.asarray(time_points)
        self.u = np.zeros(len(self.t))
        # Assume that self.t[0] corresponds to self.U0
        self.u[0] = self.U0

        # Time loop
        for k in range(n-1):
            self.k = k
            self.u[k+1] = self.advance()
        return self.u, self.t

    def advance(self):
        raise NotImplemtedError # to be impl. in subclasses
```

Implementation of the Forward Euler method

Subclass code:

```
class ForwardEuler(ODESolver):
    def advance(self):
        u, f, k, t = self.u, self.f, self.k, self.t

        dt = t[k+1] - t[k]
        unew = u[k] + dt*f(u[k], t)
        return unew
```

Application code for $u' - u = 0$, $u(0) = 1$, $t \in [0, 3]$, $\Delta t = 0.1$:

```
from ODESolver import ForwardEuler
def test1(u, t):
    return u

method = ForwardEuler(test1)
method.set_initial_condition(U0=1)
u, t = method.solve(time_points=np.linspace(0, 3, 31))
plot(t, u)
```

The implementation of a Runge-Kutta method

Subclass code:

```
class RungeKutta4(ODESolver):
    def advance(self):
        u, f, k, t = self.u, self.f, self.k, self.t

        dt = t[k+1] - t[k]
        dt2 = dt/2.0
        K1 = dt*f(u[k], t)
        K2 = dt*f(u[k] + 0.5*K1, t + dt2)
        K3 = dt*f(u[k] + 0.5*K2, t + dt2)
        K4 = dt*f(u[k] + K3, t + dt)
        unew = u[k] + (1/6.0)*(K1 + 2*K2 + 2*K3 + K4)
        return unew
```

Application code (same as for ForwardEuler):

```
from ODESolver import RungeKutta4
def test1(u, t):
    return u

method = RungeKutta4(test1)
method.set_initial_condition(U0=1)
u, t = method.solve(time_points=np.linspace(0, 3, 31))
plot(t, u)
```

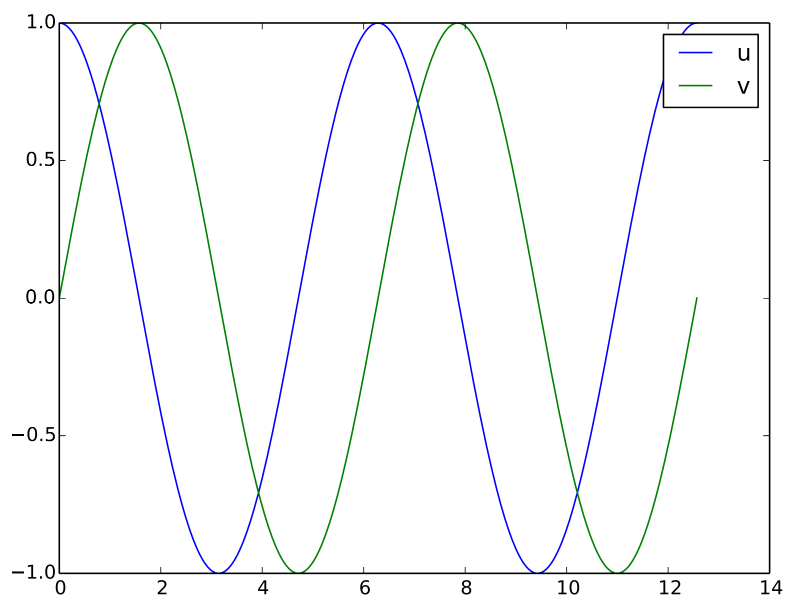
The user should be able to check intermediate solutions and terminate the time stepping

- Sometimes a property of the solution determines when to stop the solution process: e.g., when $u < 10^{-7} \approx 0$.
- Extension: `solve(time_points, terminate)`
- `terminate(u, t, step_no)` is called at every time step, is user-defined, and returns `True` when the time stepping should be terminated
- Last computed solution is `u[step_no]` at time `t[step_no]`

```
def terminate(u, t, step_no):
    eps = 1.0E-6                        # small number
    return abs(u[step_no,0]) < eps     # close enough to zero?
```

Systems of differential equations (vector ODE)

$$
\begin{aligned}
u' &= v \\
v' &= -u \\
u(0) &= 1 \\
v(0) &= 0
\end{aligned}
$$



Example on a system of ODEs (vector ODE)

Two ODEs with two unknowns $u(t)$ and $v(t)$:

$$
\begin{aligned}
u'(t) &= v(t)\\
v'(t) &= -u(t)
\end{aligned}
$$

Each unknown must have an initial condition, say

$$u(0) = 0, \quad v(0) = 1$$

In this case, one can derive the exact solution to be

$$u(t) = \sin(t), \quad v(t) = \cos(t)$$

Systems of ODEs appear frequently in physics, biology, finance, ...

The ODE system that is the final project in the course

Model for spreading of a disease in a population:

$$
\begin{aligned}
S' &= -\beta SI\\
I' &= \beta SI - \nu R\\
R' &= \nu I
\end{aligned}
$$

Initial conditions:

$$
\begin{aligned}
S(0) &= S_0\\
I(0) &= I_0\\
R(0) &= 0
\end{aligned}
$$

Another example on a system of ODEs (vector ODE)

Second-order ordinary differential equation, for a spring-mass system (from Newton's second law):

$$mu'' + \beta u' + ku = 0, \quad u(0) = U_0,\ u'(0) = 0$$

We can rewrite this as a system of two *first-order* equations, by introducing two new unknowns

$$u^{(0)}(t) \equiv u(t), \quad u^{(1)}(t) \equiv u'(t)$$

The first-order system is then

$$
\begin{aligned}
\frac{d}{dt}u^{(0)}(t) &= u^{(1)}(t)\\
\frac{d}{dt}u^{(1)}(t) &= -m^{-1}\beta u^{(1)} - m^{-1}ku^{(0)}
\end{aligned}
$$

Initial conditions: $u^{(0)}(0) = U_0$, $u^{(1)}(0) = 0$

Making a flexible toolbox for solving ODEs

- For scalar ODEs we could make one general class hierarchy to solve "all" problems with a range of methods
- Can we easily extend class hierarchy to systems of ODEs?
- Yes!
- The example here can easily be extended to professional code (Odespy)

Vector notation for systems of ODEs: unknowns and equations

General software for any vector/scalar ODE demands a general mathematical notation. We introduce n unknowns

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

in a system of n ODEs:

$$
\begin{aligned}
\frac{d}{dt}u^{(0)} &= f^{(0)}(u^{(0)}, u^{(1)}, \ldots, u^{(n-1)}, t)\\
\frac{d}{dt}u^{(1)} &= f^{(1)}(u^{(0)}, u^{(1)}, \ldots, u^{(n-1)}, t)\\
\vdots &= \qquad \vdots\\
\frac{d}{dt}u^{(n-1)} &= f^{(n-1)}(u^{(0)}, u^{(1)}, \ldots, u^{(n-1)}, t)
\end{aligned}
$$

Vector notation for systems of ODEs: vectors

We can collect the $u^{(i)}(t)$ functions and right-hand side functions $f^{(i)}$ in vectors:

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

$$f = (f^{(0)}, f^{(1)}, \ldots, f^{(n-1)})$$

The first-order system can then be written

$$u' = f(u,t), \quad u(0) = U_0$$

where u and f are vectors and U_0 is a vector of initial conditions

The magic of this notation: Observe that the notation makes a scalar ODE and a system look the same, and we can easily make Python code that can handle both cases within the same lines of code (!)

How to make class ODESolver work for systems of ODEs

- Recall: ODESolver was written for a scalar ODE
- Now we want it to work for a system $u' = f$, $u(0) = U_0$, where u, f and U_0 are vectors (arrays)
- What are the problems?

Forward Euler applied to a system:

$$\underbrace{u_{k+1}}_{\text{vector}} = \underbrace{u_k}_{\text{vector}} + \Delta t\, \underbrace{f(u_k, t_k)}_{\text{vector}}$$

In Python code:

```
unew = u[k] + dt*f(u[k], t)
```

where

- `u` is a two-dim. array (`u[k]` is a row)
- `f` is a function returning an array (all the right-hand sides $f^{(0)}, \ldots, f^{(n-1)}$)

The adjusted superclass code (part 1)

To make ODESolver work for systems:

- Ensure that `f(u,t)` returns an array.
  This can be done be a general adjustment in the superclass!
- Inspect U_0 to see if it is a number or list/tuple and make corresponding `u` 1-dim or 2-dim array

```python
class ODESolver:
    def __init__(self, f):
        # Wrap user's f in a new function that always
        # converts list/tuple to array (or let array be array)
        self.f = lambda u, t: np.asarray(f(u, t), float)

    def set_initial_condition(self, U0):
        if isinstance(U0, (float,int)):  # scalar ODE
            self.neq = 1                 # no of equations
            U0 = float(U0)
        else:                            # system of ODEs
            U0 = np.asarray(U0)
            self.neq = U0.size           # no of equations
        self.U0 = U0
```

The superclass code (part 2)

```python
class ODESolver:
    ...
    def solve(self, time_points, terminate=None):
        if terminate is None:
            terminate = lambda u, t, step_no: False

        self.t = np.asarray(time_points)
        n = self.t.size
        if self.neq == 1:  # scalar ODEs
            self.u = np.zeros(n)
        else:              # systems of ODEs
            self.u = np.zeros((n,self.neq))

        # Assume that self.t[0] corresponds to self.U0
        self.u[0] = self.U0

        # Time loop
        for k in range(n-1):
            self.k = k
            self.u[k+1] = self.advance()
            if terminate(self.u, self.t, self.k+1):
                break  # terminate loop over k
        return self.u[:k+2], self.t[:k+2]
```

All subclasses from the scalar ODE works for systems as well

Example on how to use the general class hierarchy

Spring-mass system formulated as a system of ODEs:

$$mu'' + \beta u' + ku = 0, \quad u(0),\ u'(0) \text{ known}$$

$$
\begin{aligned}
u^{(0)} &= u, \quad u^{(1)} = u' \\
u(t) &= (u^{(0)}(t), u^{(1)}(t)) \\
f(u,t) &= (u^{(1)}(t), -m^{-1}\beta u^{(1)} - m^{-1}ku^{(0)}) \\
u'(t) &= f(u,t)
\end{aligned}
$$

Code defining the right-hand side:

```
def myf(u, t):
    # u is array with two components u[0] and u[1]:
    return [u[1],
            -beta*u[1]/m - k*u[0]/m]
```

Alternative implementation of the f function via a class

Better (no global variables):

```
class MyF:
    def __init__(self, m, k, beta):
        self.m, self.k, self.beta = m, k, beta

    def __call__(self, u, t):
        m, k, beta = self.m, self.k, self.beta
        return [u[1], -beta*u[1]/m - k*u[0]/m]
```

Main program:

```
from ODESolver import ForwardEuler
# initial condition:
U0 = [1.0, 0]
f = MyF(1.0, 1.0, 0.0)    # u'' + u = 0 => u(t)=cos(t)
solver = ForwardEuler(f)
solver.set_initial_condition(U0)

T = 4*pi; dt = pi/20; n = int(round(T/dt))
time_points = np.linspace(0, T, n+1)
u, t = solver.solve(time_points)

# u is an array of [u0,u1] arrays, plot all u0 values:
u0_values = u[:,0]
u0_exact = cos(t)
plot(t, u0_values, 'r-',  t, u0_exact, 'b-')
```

Throwing a ball; ODE model

Newton's 2nd law for a ball's trajectory through air leads to

$$\frac{dx}{dt} = v_x$$
$$\frac{dv_x}{dt} = 0$$
$$\frac{dy}{dt} = v_y$$
$$\frac{dv_y}{dt} = -g$$

Air resistance is neglected but can easily be added!

- 4 ODEs with 4 unknowns:
  - the ball's position $x(t)$, $y(t)$
  - the velocity $v_x(t)$, $v_y(t)$

Throwing a ball; code

Define the right-hand side:

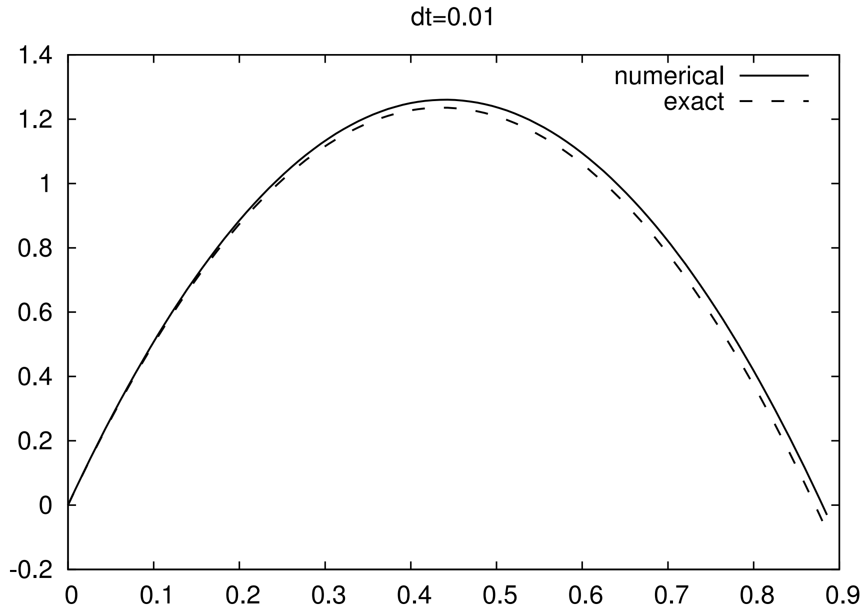
```
def f(u, t):
    x, vx, y, vy = u
    g = 9.81
    return [vx, 0, vy, -g]
```

Main program:

```
from ODESolver import ForwardEuler
# t=0: prescribe x, y, vx, vy
x = y = 0                       # start at the origin
v0 = 5;  theta = 80*pi/180      # velocity magnitude and angle
vx = v0*cos(theta)
vy = v0*sin(theta)
# Initial condition:
U0 = [x, vx, y, vy]

solver= ForwardEuler(f)
solver.set_initial_condition(u0)
time_points = np.linspace(0, 1.2, 101)
u, t = solver.solve(time_points)

# u is an array of [x,vx,y,vy] arrays, plot y vs x:
x = u[:,0];  y = u[:,2]
plot(x, y)
```

Throwing a ball; results

Comparison of exact and Forward Euler solutions



Logistic growth model; ODE and code overview

Model:

$$u' = \alpha u(1 - u/R(t)), \quad u(0) = U_0$$

R is the maximum population size, which can vary with changes in the environment over time

Implementation features:

- Class Problem holds "all physics": α, $R(t)$, U_0, T (end time), $f(u,t)$ in ODE
- Class Solver holds "all numerics": Δt, solution method; solves the problem and plots the solution
- Solve for $t \in [0,T]$ but terminate when $|u - R| < \text{tol}$

Logistic growth model; class Problem (f)

```
class Problem:
    def __init__(self, alpha, R, U0, T):
        self.alpha, self.R, self.U0, self.T = alpha, R, U0, T

    def __call__(self, u, t):
```

```
        """Return f(u, t)."""
        return self.alpha*u*(1 - u/self.R(t))

    def terminate(self, u, t, step_no):
        """Terminate when u is close to R."""
        tol = self.R*0.01
        return abs(u[step_no] - self.R) < tol

problem = Problem(alpha=0.1, R=500, U0=2, T=130)
```

Logistic growth model; class Solver

```
class Solver:
    def __init__(self, problem, dt,
                 method=ODESolver.ForwardEuler):
        self.problem, self.dt = problem, dt
        self.method = method

    def solve(self):
        solver = self.method(self.problem)
        solver.set_initial_condition(self.problem.U0)
        n = int(round(self.problem.T/self.dt))
        t_points = np.linspace(0, self.problem.T, n+1)
        self.u, self.t = solver.solve(t_points,
                                      self.problem.terminate)

    def plot(self):
        plot(self.t, self.u)

problem = Problem(alpha=0.1, U0=2, T=130,
                  R=lambda t: 500 if t < 60 else 100)
solver = Solver(problem, dt=1.)
solver.solve()
solver.plot()
print 'max u:', solver.u.max()
```

Logistic growth model; results