App.E: Programming of differential equations

Hans Petter Langtangen 1,2

Simula Research Laboratory ¹

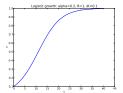
University of Oslo, Dept. of Informatics ²

Oct 20, 2014

How to solve any ordinary scalar differential equation

$$u'(t) = \alpha u(t)(1 - R^{-1}u(t))$$

 $u(0) = U_0$



Examples on scalar differential equations (ODEs)

Terminolog

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

Examples:

$$u' = \alpha u$$
 exponential growth

$$u' = \alpha u \left(1 - \frac{u}{R}\right)$$
 logistic growth

$$u' = -b|u|u + g$$
 body in fluid

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

- Numerical solution methods do not depend on how the ODE looks like
- Method and software aim at 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

$$f(u, t) = \alpha u$$
, exponential growth

$$f(u,t) = \alpha u \left(1 - \frac{u}{R}\right)$$
, logistic growth

$$f(u,t) = -b|u|u+g$$
, body in fluid

Our task: write functions and classes that take \boldsymbol{f} and produces the solution \boldsymbol{u}

What is the f(u, t)?

Proble

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:

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

How to solve a general ODE numerically by the Forward Euler method

u'=f(u,t)

Assume we have computed u at discrete time points $t_0, t_1, \ldots, t_n.$ 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,

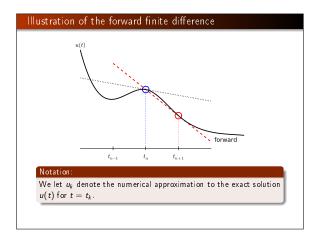
$$u'(t_k) \approx \frac{u(t_{k+1}) - u(t_k)}{\wedge t}$$

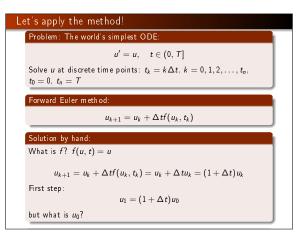
Insert in the ODE at $t=t_k$:

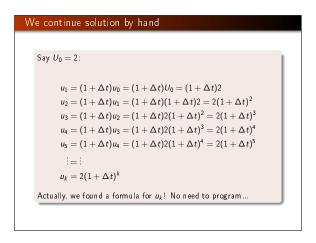
$$\frac{u(t_{k+1})-u(t_k)}{\Delta t}=f(u(t_k),t_k)$$

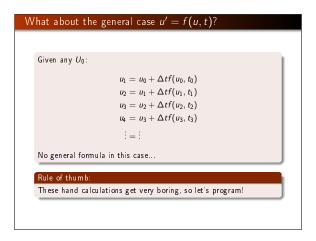
Everything with $u(t_k)$ is known, $u(t_{k+1})$ is unknown

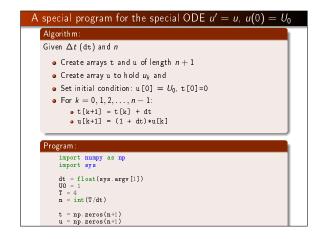
$$u(t_{k+1}) = u(t_k) + \Delta t f(u(t_k), t_k)$$

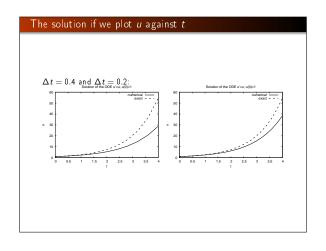












The algorithm for the general ODE u'=f(u,t)Algorithm: Given Δt (dt) and n• Create arrays t and u of length n+1• Create array u to hold u_k and • Set initial condition: $u[0] = U_0$, t[0] = 0• For $k = 0, 1, 2, \ldots, n-1$: • u[k+1] = u[k] + dt*f(u[k], t[k])textcolorred(the only change!) • t[k+1] = t[k] + dt

```
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 \Delta t or no of steps n
• Call u,t= ForwardEuler (f,U_0,T,n)
• plot (t,u)

Warning:

The Forward Euler method may give very inaccurate solutions if \Delta t is not sufficiently small. For some problems (like u''+u=0) other methods should be used.
```

```
A class for solving ODEs

Instead of a function for solving any ODE we now want to make a class and use it like this:

method = ForwardEuler(f, dt)
method.set_initial_condition(UO, tO)
u, t = method.solve(T)
plot(t, u)

How?

• Store f, Δt, and the sequences uk, tk as attributes
• Split the steps in the ForwardEuler function into three methods:

• the constructor (__init__)
• set_initial_condition for u(0) = U_0
• solve for running the Forward Euler algorithm
• advance for isolating the numerical updating formula (new numerical methods just need a different advance method, the rest is the same)
```

```
import numpy as np
class ForwardEuler_vi:
    def __init__(solf, 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)) self. u = pn.zeros(n+1) self. t = np.zeros(n+1) self. t[0] = float(self.U0) self. k[0] = float(self.U0) for k in range(self.n): self. k = k self. t[k] = self. dt self. dvance() return self.u, self. t def advance(self): """dvance the solution one time step.""" u, dt, f, k, t = self.u, self.dt, self.f, self.k, self.t unew = u[k] + dt*f(u[k], t[k])

```
Alternative class code solving ODEs (part 1)

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

class ForwardBuler:
    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_init__condition(self, UO):
        self.UO = float(UO)

def solve(self, time_points):
```

class ForwardEuler: def solve(self, time_points): """Compute u for t values in time_points list.""" self it = pn_asarray(time_points) self u = pn_zeros(len(time_points)) self u[0] = self .U0 for k in range(len(self it)-i): self it k = k self.u(k+i] = self.advance() return self u, self.t def advance(self): """downce the solution one time step.""" u, f, k, t = self.u, self.f, self.k, self.t dt = t[k+i] - t[k] unew = u[k] + dt*f(u[k], t[k]) return unew

```
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

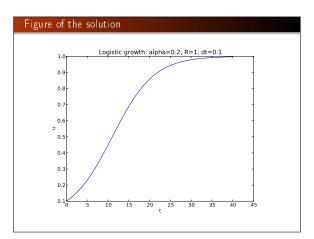
        solver = ForwardEuler(f)
        solver.set initial_condition(UO=3)
        dt = 0.4; T = 3; n = int(round(float(T)/dt))
        time_points = np. linepace(0, T, n*1)
        u_t = solver_solve(time_points)
        u_exact = h(t)
        diff = np.abs(u_exact - u).max()
        tol = 1E-14
        success = diff < tol
        assert success</pre>
```

```
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):
\text{class Logistic:} \quad \text{def \_init\_(self, alpha, R, U0):} \quad \text{self.alpha, self. R, self. U0 = alpha, float(R), U0}
\text{def \_call\_(self, u, t):} \quad \text{$f(u,t)$} \quad \text{return self.alpha*u*}(1 - u/\text{self.R})

Main program:
\text{problem = Logistic}(0,2,1,0.1) \quad \text{time\_points = np linepace}(0,40,401) \quad \text{method. set. initial condition(problem. U0)} \quad \text{u, t = method. solve}(\text{time\_points})
```



Numerical methods for ordinary differential equations $u_{k+1} = u_k + \Delta t \, f(u_k, t_k)$ 4 th-order Runge-Kutta method: $u_{k+1} = u_k + \frac{1}{6} \left(K_1 + 2 K_2 + 2 K_3 + K_4 \right)$ where $K_1 = \Delta t \, f(u_k, t_k)$ $K_2 = \Delta t \, f(u_k + \frac{1}{2} K_1, t_k + \frac{1}{2} \Delta t)$ $K_3 = \Delta t \, f(u_k + \frac{1}{2} K_2, t_k + \frac{1}{2} \Delta t)$ $K_4 = \Delta t \, f(u_k + K_3, t_k + \Delta t)$ And lots of other methods! How to program a collection of methods?

A superclass 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

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

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

    def set _initial_condition(self, UO):
        self.UO = float (UO)

    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.UO
        self.u[O] = self.UO

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

    def advance(self):
        raise NotImplemetdError # 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 ∈ [0, 3], Δt = 0.1:

from ODESolver import ForwardEuler
def testi(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

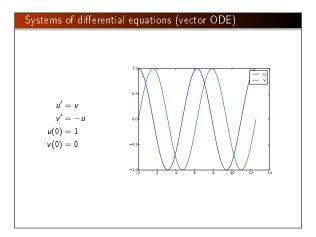
    K1 = dt*f(u[k] + 0.5*K1, t + dt2)
    K3 = dt*f(u[k] + 0.5*K1, t + dt2)
    K4 = dt*f(u[k] + 3.5 * 4.2)
    K4 = dt*f(u[k] + 3.5 * 4.2)
    unev = u[k] + (1/6.0)*(K1 + 2*K2 + 2*K3 + K4)
    return unev

Application code (same as for ForwardEuler):
    from ODESolver import RungeKutta4
    def testf(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]



Example on a system of ODEs (vector ODE)

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

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

$$v'(t) = -u(t)$$

Each unknown must have an initial condition, say

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

In this case, one can derive the exact solution

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

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:

$$S' = -\beta SI$$

$$I' = \beta SI - \nu R$$

$$R' = \nu I$$

$$S(0) = S_0$$

$$I(0) = I_0$$

$$R(0) = 0$$

Another example on a system of ODEs (vector ODE)

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

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

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

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

Initial conditions:

 $u^{(0)}(0) = U_0 \quad u^{(1)}(0) = 0$

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:

$$\frac{d}{dt}u^{(0)} = f^{(0)}(u^{(0)}, u^{(1)}, \dots, u^{(n-1)}, t)
\frac{d}{dt}u^{(1)} = f^{(1)}(u^{(0)}, u^{(1)}, \dots, u^{(n-1)}, t)
\vdots =$$

$$\frac{d}{dt}u^{(n-1)}=f^{(n-1)}(u^{(0)},u^{(1)},\ldots,u^{(n-1)},t)$$

Vector notation for systems of ODEs: vectors

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

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

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

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)
- ullet f is a function returning an array (all the right-hand sides $f^{(0)},\ldots,f^{(n-1)})$
- Result: ODESolver will work for systems!

The adjusted superclass code (part 1)

```
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
        Self.neq = U0.size  # no of equations
        self.U0 = U0
```

The superclass code (part 2)

Example on how to use the general class hierarchy

Spring-mass system formulated as a system of ODEs:

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

$$u^{(0)} = u, \quad u^{(1)} = u'$$

$$u(t) = (u^{(0)}(t), u^{(1)}(t))$$

$$f(u, t) = (u^{(1)}(t), -m^{-1}\beta u^{(1)} - m^{-1}ku^{(0)})$$

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

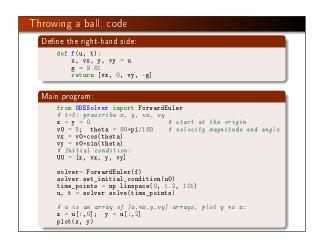
Code defining the right-hand side:

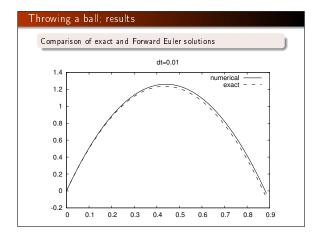
```
def myf(u, t):

$ u is array with two components u[0] and u[1]:
return [u[1],
-beta*u[i]/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[i], -beta*u[i]/m - k*u[0]/m] Main program: from DBSsolver import ForwardEuler # initial condition: Uo = [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(UO) T = 4*pi; dt = pi/20; n = int(round(T/dt)) time_points = np_linspace(0, T, n*t) u, t = solver.selve(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 dx V_{χ} dt $\frac{dv_x}{dx} = 0$ Ω dt $\frac{dy}{dt} =$ V_y $\frac{dv_y}{dv_y} = 0$ -gdt Air resistance is neglected but can easily be added! • 4 ODEs with 4 unknowns: • the ball's position x(t), y(t)• the velocity $v_x(t)$, $v_y(t)$





```
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.alphau*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)
```

