### App.E: Programming of differential equations

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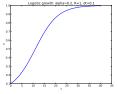
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### How to solve any ordinary scalar differential equation

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



### 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  $u'=\alpha u\left(1-rac{u}{R}
ight)$  logistic growth  $u'+b|u|u=g$  falling body in fluid

### 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

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

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

### 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:

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

### 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:

- $\int_{-1}^{1} (x^2 \tanh^{-1} x (1+x^2)^{-1}) dx:$   $f(x) = x^2 \tanh^{-1} x (1+x^2)^{-1}, \ a = -1, \ b = 1$
- 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

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

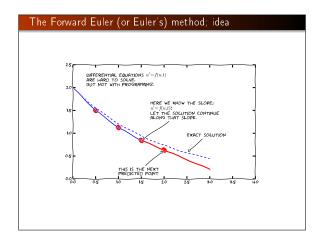
Approximate  $u'(t_k)$  by a forward finite difference,

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

Insert in the ODE at  $t = t_k$ :

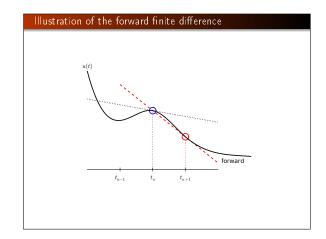
$$\frac{u(t_{k+1})-u(t_k)}{\Delta t}=f(u(t_k),t_k)$$

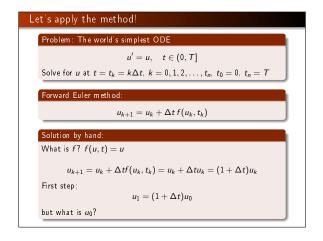
Terms with  $u(t_k)$  are known, and this is an algebraic (difference) equation for  $u(t_{k+1})$ 



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### 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  $u(0) = U_0$ :  $u = U_0e^t$ .

### We continue solution by hand

Say 
$$U_0=2$$
: 
$$u_1=(1+\Delta t)u_0=(1+\Delta t)U_0=(1+\Delta t)2$$
 
$$u_2=(1+\Delta t)u_1=(1+\Delta t)(1+\Delta t)2=2(1+\Delta t)^2$$
 
$$u_3=(1+\Delta t)u_2=(1+\Delta t)2(1+\Delta t)^2=2(1+\Delta t)^3$$
 
$$u_4=(1+\Delta t)u_3=(1+\Delta t)2(1+\Delta t)^3=2(1+\Delta t)^4$$
 
$$u_5=(1+\Delta t)u_4=(1+\Delta t)2(1+\Delta t)^4=2(1+\Delta t)^5$$
 
$$\vdots=\vdots$$
 
$$u_k=2(1+\Delta t)^k$$
 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

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

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

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

### Given any $U_0$ :

$$u_1 = u_0 + \Delta t f(u_0, t_0)$$
  
 $u_2 = u_1 + \Delta t f(u_1, t_1)$ 

$$u_3 = u_2 + \Delta t f(u_2, t_2)$$

$$u_4 = u_3 + \Delta t f(u_3, t_3)$$

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No general formula in this case...

### Rule of thumb:

When hand calculations get boring, let's program!

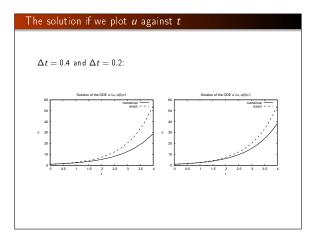
### We start with a specialized program for u'=u, $u(0)=U_0$

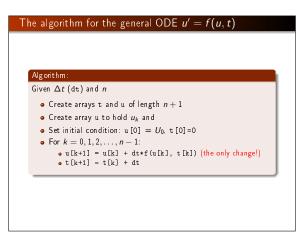
### Algorithm:

Given  $\Delta t$  (dt) and n

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

### Program: import numpy as np import sys dt = float(sys.argv[i]) 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+i] = t [k] + dt u [k+i] = (i + dt)\*u[k] # plot u against t





## | Implementation of the general algorithm for u' = f(u, t) | General function: | def ForwardEuler(f, U0, T, n): | """Solve $u^2 = f(u, t)$ , u(0) = U0, with n steps until t = T.""" | import numpy as np | t = np.zeros(n+1) | u = np.zeros(n+1) | u = np.zeros(n+1) | su[k] is the solution at time t[k] | | u[0] = U0 | t[0] = 0 | dt = T/float(n) | | for k in range(n): | t[x+1] = t[k] + dt | u[k] + dt\*f(u[k], t[k]) | | return u, t | | Magic: | This simple function 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 \Delta t 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 \Delta t is not sufficiently small. For some problems (like u''+u=0) other methods should be used.
```

## 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_vi:

...

def solve(self, T):

"""Compute solution for 0 <= t <= T."""

n = int(round(T)self.dt))  # no of intervals

self.u = np.zeros(n*i)

self.t = np.zeros(n*i)

self.u(0] = float(self.U0)

self.t[0] = float(0)

for k in range(self.n):
 self.k = k

self.t[k*i] = self.t[k] + self.dt

self.u[k*i] = self.advance()

return self.u, self.t

def advance(self):

"""dwance 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
```

```
# 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):
```

```
class ForwardEuler:

def solve(self, time_points):
    """Compute u for t values in time_points list."""
    self. t = np.saarray(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!] = self.advance()
    return self.u, self.t

def advance(self):
    """Idvance 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
```

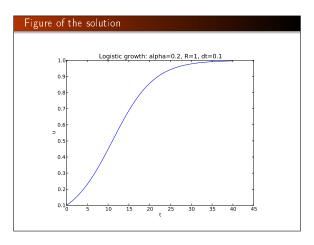
```
Code:

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</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): $\text{class Logistic:} \quad \text{def \__init\_}(\text{self, alpha, R, U0):} \quad \text{self.alpha, self.R, self.U0 = alpha, float(R), U0}$ $\text{def \_\_call\_\_(\text{self, u, t}): \quad \text{if } f(u,t) \quad \text{return self.alpha+u+(1 - u/\text{self.R})}$ Main program: $\text{problem = Logistic(0.2, 1, 0.1)} \quad \text{time_points = np linepace(0, 40, 401)} \quad \text{method = ForwardBuler(problem)} \quad \text{method -set initial.condition(problem.U0)} \quad \text{u, t = method.solve(time_points)}$



```
Numerical methods for ordinary differential equations u_{k+1} = u_k + \Delta t \, f(u_k, t_k) 4 \text{th-order Runge-Kutta method:} u_{k+1} = u_k + \frac{1}{6} \left( K_1 + 2K_2 + 2K_3 + K_4 \right) 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 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

• Sub classes, e.g., ForwardEuler, just implement the specific numerical formula in advance
```

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

def advance(self):
    """ddvance 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. saarray(time.points)
        self.u = np. zeros(len(self.t))
        # Assume that self.t[0] corresponds to self.U0

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

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

```
Subclass code:

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

    dt = t[k+i] - t[k]
    unew = u[k] + d + f(u[k], t)
    return unew

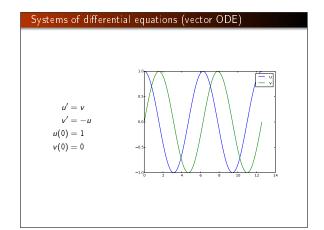
Application code for u' − u = 0, u(0) = 1, t ∈ [0,3]. Δt = 0.1:

from ODESolver import ForwardEuler
def testl(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(DDESolver): def advance(self): u, f, k, t = self.u, self.f, self.k, self.t dt = t[k+1] - t[k] dt 2 = 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] + 0.5\*X + dt2) K4 = dt \*f(u[k] + 0.5\*X + t+ dt2) unew = u[k] + (1/6.0)\*(K1 + 2\*K2 + 2\*K3 + K4) 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<sup>-7</sup> ≈ 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 return abs(u[step\_no,0]) < eps # small number return abs(u[step\_no,0]) < eps # close enough to zero?



### 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 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:

$$S' = -\beta SI$$

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

$$R' = \nu I$$

Initial conditions:

$$S(0) = S_0$$
  
 $I(0) = I_0$   
 $R(0) = 0$ 

### 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

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

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?
- The example here can easily be extended to professional code (Odespy)

### Vector notation for systems of ODEs: unknowns and

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)
- 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

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

### The superclass code (part 2) class ODESolver:

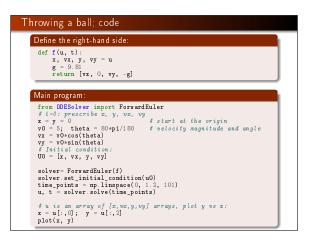
```
def solve(self, time_points, terminate=None):
    if terminate is None:
        terminate = lambda u, t, step_no: False
          self.t = np.asarray(time_points)
         self.t.size
if self.neq == 1: # scalar ODEs
self.u = np.zeros(n)
else: # systems of ODEs
self.u = np.zeros((n, self.neq))
         # Assume that self.t[0] corresponds to self.U0 self.u[0] = self.U0
          # Time loop
         for k in range(n-1):
        sof 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]
```

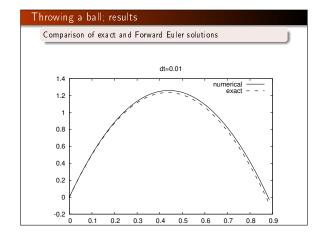
All subclasses from the scalar ODE works for systems as well

### Example on how to use the general class hierarchy $\begin{aligned} &\text{Spring-mass system formulated as a system of ODEs:} \\ &mu'' + \beta u' + ku = 0, \quad u(0), \quad u'(0) \text{ kn own} \end{aligned}$ $u^{(0)} = u, \quad u^{(1)} = u' \\ u(t) = (u^{(0)}(t), u^{(1)}(t)) \\ f(u,t) = (u^{(1)}(t), -m^{-1}\beta u^{(1)} - m^{-1}ku^{(0)}) \\ u'(t) = f(u,t) \end{aligned}$ $\begin{aligned} &\text{Code defining the right-hand side:} \\ &\text{def myf}(u, t): \\ & f \text{ u is array with two components u[0] and u[1]:} \\ &\text{return [u[1], -beta*u[1]/m - k*u[0]/m]} \end{aligned}$

## 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[i1], -beta\*u[i]/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\*pl; dt = pl/20; n = int(round(T/dt)) time\_points = mp\_linspace(0, T, n+i) 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 $v_x(t)$ , $v_y(t)$



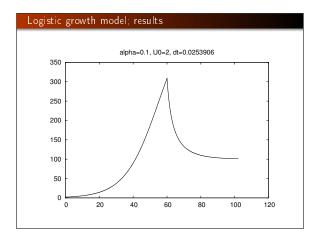


```
class Problem:
    def __init__(self, alpha, R, U0, T):
        self.alpha, self R, self.U0, self.T = alpha, R, U0, T

    def __call__(self, u, t):
        """Return f(u, t)."""
        return self.alphaeve(i - 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)
```



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