

## 4. Ordinary Differential Equations

## initial value problem (IVP)

### Definition [system of ordinary differential equations]

- ▶ explicit, first order form of ODE

$$\frac{du(t)}{dt} = f(t, u(t))$$

- ▶ function  $f(t, u)$

$$f : [0, T] \times \mathbb{R}^n \rightarrow \mathbb{R}^n$$

- ▶ models how change of  $u(t)$  depends on  $u(t)$
  - ▶ initial value:  $u(0) = u_0$
  - ▶ **IVP:** *find  $u(t)$  with  $u(0) = u_0$  and which satisfies ODE*

## example: growth and decay

- ▶ models change in amount of some quantity  $u(t)$  over time
- ▶ ode

$$\frac{du}{dt} = \alpha - \beta u$$

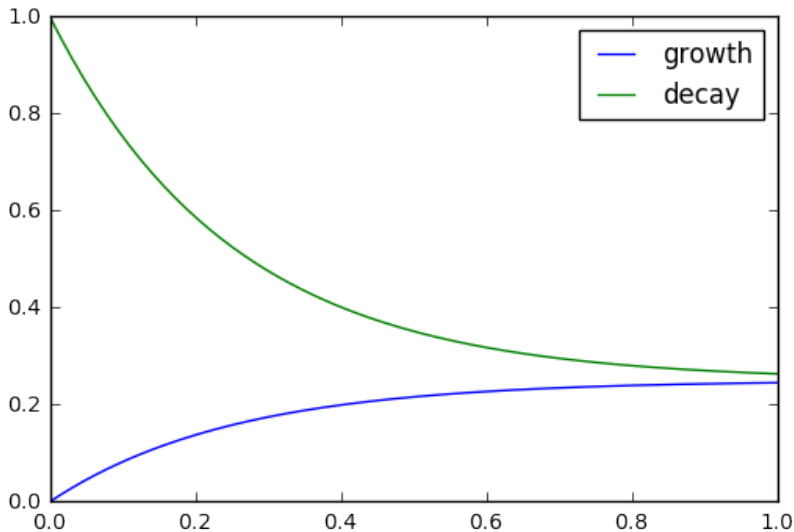
- ▶  $\alpha$ : growth,  $\beta$ : decay
- ▶ stationary solution  $u(t) = \alpha/\beta$
- ▶ general solution

$$u(t) = e^{-\beta t} u_0 + (1 - e^{-\beta t}) \frac{\alpha}{\beta}$$

## plot of exact solution

```
T = 1.0
t = np.linspace(0,T,129)
u = lambda t, u0, T=T, alpha=1.0, beta = 4.0 : \
    np.exp(-beta*t)*u0 + (1-np.exp(-beta*t))*alpha/beta
```

```
plt.plot(t,u(t,u0=0),label='growth')  
plt.plot(t,u(t,u0=1),label='decay');  
plt.legend();
```

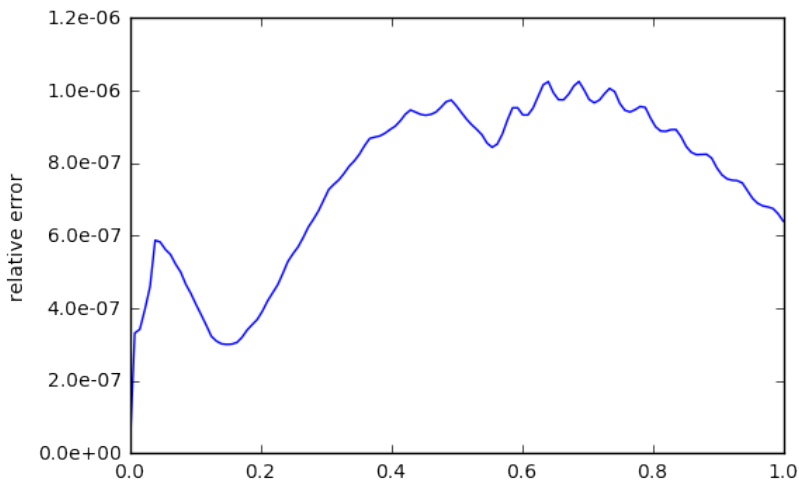


## solving with scipy

```
f = lambda t, u, alpha=1.0, beta=4.0 : alpha - beta*u
solver = scint.ode(f)
u0 = 1.0
solver.set_initial_value(u0,0.0)
unum = [u0,]
for tk in t[1:]:
    #print(tk)
    unum.append(solver.integrate(tk)[0])

#help(scint.ode)
```

```
#plt.plot(t,np.array(unum));  
plt.plot(t,(np.array(unum)-u(t,u0))/u(t,u0)); plt.ylabel('relative error')  
plt.gca().yaxis.set_major_formatter(mtick.FormatStrFormatter('%1.2e'))
```



## example: mechanics

- ▶ Damped spring oscillator, Newton's 2nd law

$$mx'' = -m\beta x' - \gamma x$$

- ▶ first order system  $u_1 = x$  and  $u_2 = x'$

$$\frac{du}{dt} = f(u)$$

where

$$f = \begin{bmatrix} u_2 \\ -(\beta u_2 + \gamma u_1/m) \end{bmatrix}$$

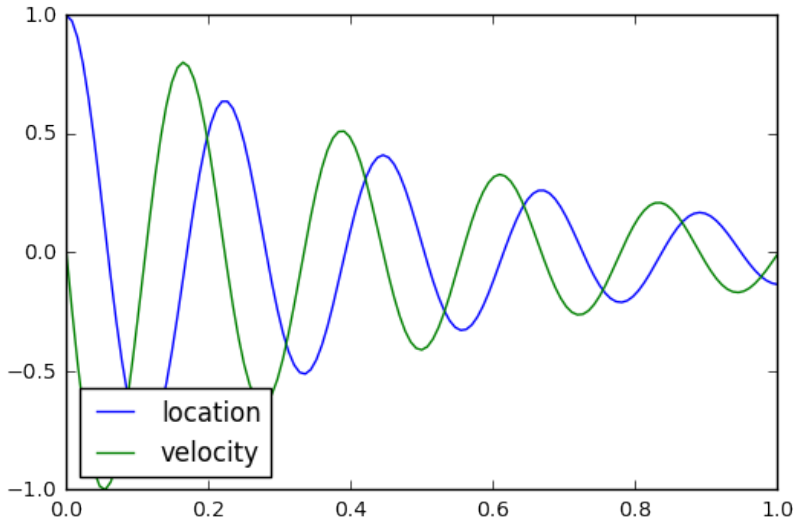


## solving with scipy

```
f = lambda t, u, m=0.5, beta = 4, gamma = 400.0 :\
    np.array((u[1], -(beta*u[1]+gamma*u[0]/m)))

solver = scint.ode(f)
u0 = np.array([1.0,0.0])
solver.set_initial_value(u0,0.0)
unum = [u0,]
for tk in t[1:]:
    unum.append(solver.integrate(tk))
```

```
max_disp = np.max(abs(np.array(unum)[: ,0]))  
max_vel = np.max(abs(np.array(unum)[: ,1]))  
plt.plot(t, np.array(unum)[: ,0]/max_disp, label='location')  
plt.plot(t, (np.array(unum)[: ,1])/max_vel, label='velocity')
```



## example: chemical reaction

- ▶ burning hydrogen  $2H + O \rightarrow H_2O$
- ▶  $u_1, u_2, u_3$  are concentrations of  $H, O$  and  $H_2O$ , respectively
- ▶ system of ODEs from law of mass action

$$\frac{du}{dt} = f(u)$$

with

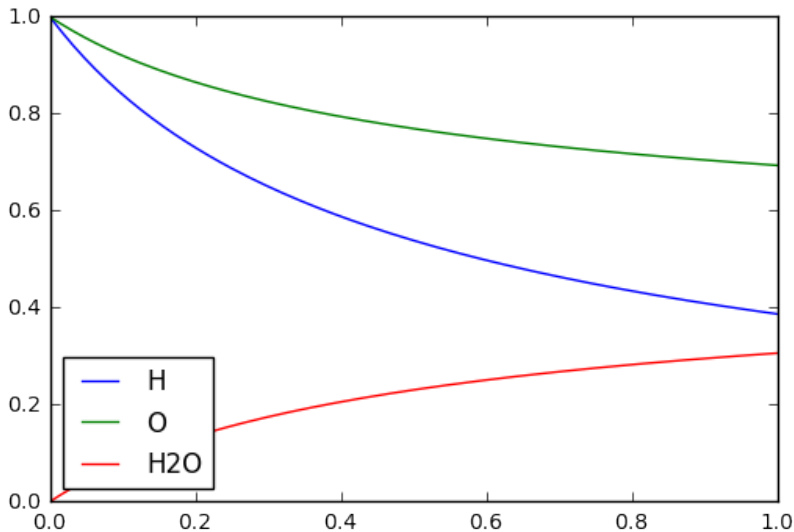
$$f(u) = \kappa u_1^2 u_2 \begin{bmatrix} -2 \\ -1 \\ 1 \end{bmatrix}$$

- ▶ note that  $u_1 + 2u_3$  and  $u_2 + u_3$  are constant (total amount of  $H$  and  $O$  atoms)

## solving with scipy

```
f = lambda t, u, kappa=1.0 : \  
    kappa*u[0]**2*u[1]*np.array((-2.0,-1.0,1.0))  
solver = scint.ode(f)  
u0 = np.array([1.0,1.0,0.0])  
solver.set_initial_value(u0,0.0)  
unum = [u0,]  
for tk in t[1:]:  
    unum.append(solver.integrate(tk))
```

```
plt.plot(t, np.array(unum)[: ,0],label='H')  
plt.plot(t, np.array(unum)[: ,1],label='O')  
plt.plot(t, (np.array(unum)[: ,2])), label='H2O');plt.legend
```



## example: epidemiology

- ▶ SIR model (susceptibles, infectives, removed)
- ▶  $u_1, u_2, u_3$  are number of susceptibles, infectives and recovered
- ▶ system of ODES

$$\frac{du}{dt} = f(u)$$

with

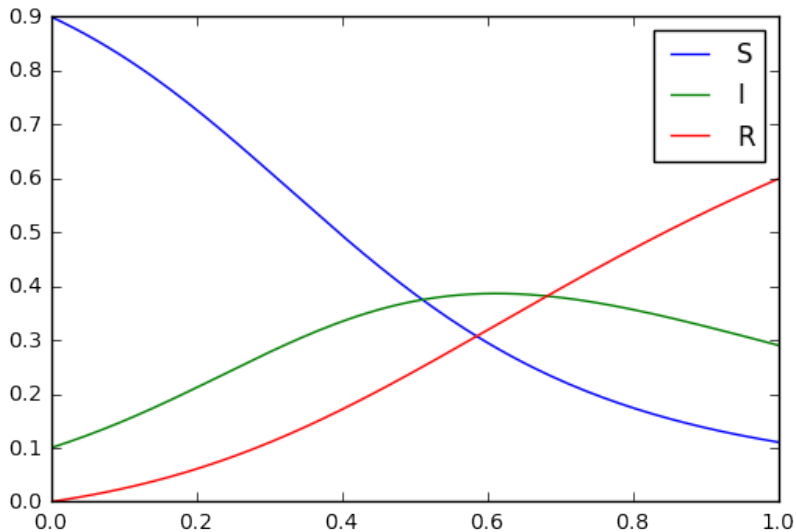
$$f(u) = \begin{bmatrix} -\beta u_1 u_2 \\ \beta u_1 u_2 - \gamma u_2 \\ \gamma u_2 \end{bmatrix}$$

- ▶  $\beta$  fixed number of contacts per day
- ▶  $\gamma$  fixed number of recovered people per day
- ▶ total population size  $u_1 + u_2 + u_3$  constant

## solving with scipy

```
f = lambda t, u, beta=7.0,gamma=2.0 : \  
    beta*u[0]*u[1]*np.array((-1.0,1.0,0.0))\  
    +gamma*u[1]*np.array((0.0,-1.0,1.0))  
solver = scint.ode(f)  
u0 = np.array([0.9,0.1,0.0])  
solver.set_initial_value(u0,0.0)  
unum = [u0,]  
for tk in t[1:]:  
    unum.append(solver.integrate(tk))
```

```
plt.plot(t, np.array(unum)[: ,0],label='S')  
plt.plot(t, np.array(unum)[: ,1],label='I')  
plt.plot(t, (np.array(unum)[: ,2]), label='R');plt.legend(10
```





## example: heat

- ▶ diffusion, discretised in space
- ▶  $\lambda > 0$ : diffusion coefficient, heat conductivity
- ▶  $u_k(t)$  is temperature at location  $x_k = kh$  in 1D medium
- ▶ system of ODEs

$$\frac{du}{dt} = -Au$$

where

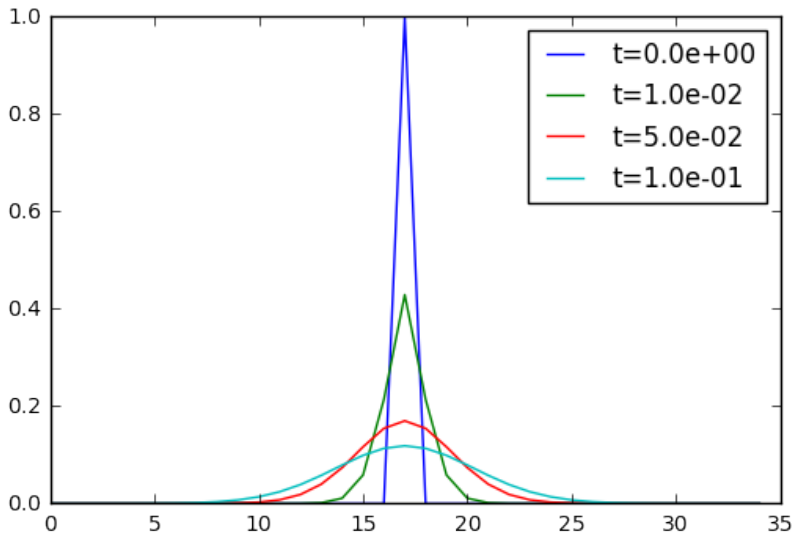
$$A = \frac{\lambda}{h^2} \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}$$

## solving with scipy

```
def f(t,u,lam=0.05):  
    n = u.shape[0]  
    df = -2*lam*u  
    df[:-1] += lam*u[1:]  
    df[1:] += lam*u[:-1]  
    return df*(n-1)**2  
  
def heat():  
    n = 35  
    solver = scint.ode(f)  
    u0 = np.zeros(n);  
    u0[n//2] = 1.0  
    print(n//2)  
    solver.set_initial_value(u0,0.0)  
    plt.plot(u0,label='t={:2.1e}'.format(0.0))  
    for tk in (0.01,0.05,0.1):  
        unum = solver.integrate(tk)  
        plt.plot(unum,label='t={:2.1e}'.format(tk))
```

heat()

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## autonomous form

$$\frac{du}{dt} = f(u)$$

- ▶ function  $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$
- ▶ by adding  $u_0(t) = t$  with ODE  $u'_0 = 1$  and  $u_0(0) = 0$   
reformulate more general ODE as autonomous

## implicit higher order form

(1)

$$F(u(t), u'(t), \dots, u^{(s)}(t), t) = 0$$

- ▶ function  $F(u_1, \dots, u_{s+1}, t)$

$$F : \mathbb{R}^n \times \dots \times \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R}^n$$

- ▶ transform higher order implicit form to first order explicit form:
  - ▶ reduce to first order system by replacing  $u(t)$  by vector  $(u_1(t), u_2(t), \dots, u_s(t))$  where  $u_k(t) = u^{(k-1)}(t)$
  - ▶ add the equations  $u'_k(t) - u_{k+1}(t) = 0$  to  $F$
  - ▶ resulting first order implicit form with extended  $F$  and  $u(t)$ :

$$F(u(t), u'(t), t) = 0$$

- ▶ solve for  $u'(t)$  to get explicit form

## remarks

- ▶ for most ordinary differential equations the solution is not known
- ▶ solution of ordinary differential equations is not unique
  - ▶ initial value problem:  $u(0) = u_0$
  - ▶ boundary value problem:  $B(u(0), u(T)) = 0$
  - ▶ solution of boundary value problem with “shooting method”:
    - ▶ solve initial value problem for general initial value  $u_0$  to get  $u_T = g(u_0)$  for some function  $g$
    - ▶ then solve the boundary equations for  $u_0$

$$B(u_0, g(u_0)) = 0$$

- ▶ here we only consider the initial value problem

# linear systems of ODEs

- ▶ important class of ODEs with known solution: linear ODEs where  $f(t, u) = Au$

$$\frac{du}{dt} = Au$$

- \* solution of the initial value problem

$$u(t) = \exp(At)u_0$$

## reformulate IVP as integral equation

- ▶ integrate the explicit form to get

(2)

$$u(t) = u_0 + \int_0^t f(s, u(s)) ds, \quad t \in [0, T]$$

- ▶ this is a **Volterra integral equation of the 2nd kind**
- ▶ why reformulate?
  - ▶ allows application of functional analysis to show existence and uniqueness of solution
  - ▶ starting point for development and theory of numerical techniques using quadrature methods



## theory

- ▶ existence, uniqueness, stability and bounds on solutions, properties like positivity, symmetry and conserved quantities
- ▶ these theoretical aspects are important for numerical solution
- ▶ theory uses computational concepts

### **Reference** (advanced)

Gerald Teschl, *Ordinary Differential Equations and Dynamical Systems*, Amer. Math. Soc 2011

see your own lecture notes from ODE course

# existence and uniqueness theorem

## **Theorem** Picard-Lindelof theorem

If

- ▶  $f(t, u)$  is continuous in a neighborhood of  $(t_0, u_0)$
- ▶  $f(t, \cdot)$  is Lipschitz continuous with Lipschitz constant  $L$  which is independent of  $t$ , then there exists a unique continuous  $u(t)$  which satisfies the initial value problem for  $t \in [t_0, t_0 + 1/L]$

## mathematical algorithm: Picard iteration

- ▶ aim: compute solution of ODE in  $[t, t + h]$  where  $h \leq 1/L$  (Lipschitz constant)
- ▶ integral operator:

$$F_h(u)(t) = u_0 + \int_{t_0}^t f(s, u(s)) ds, \quad t \in [t_0, t_0 + h]$$

- ▶ initialise:  $u^0 = u_0$
- ▶ iterate:  $u^{k+1} = F_h(u^k)$  for  $k = 0, 1, 2, \dots$  until convergence

## comments

- ▶ proof of theorem by Picard iteration and fixed point theorem
- ▶ in practical algorithms,  $F_h(u)$  is approximated
- ▶ theorem shows the way how to design numerical algorithms: compute  $u(t)$  for  $t \in [t, t + h]$  from

$$u(t) = u_0 + \int_{t_0}^t f(s, u(s)) ds, \quad t \in [t_0, t_0 + h]$$

- ▶ obtain approximation by approximating the integral using quadrature methods