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 $f(t, u)$

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

- 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*

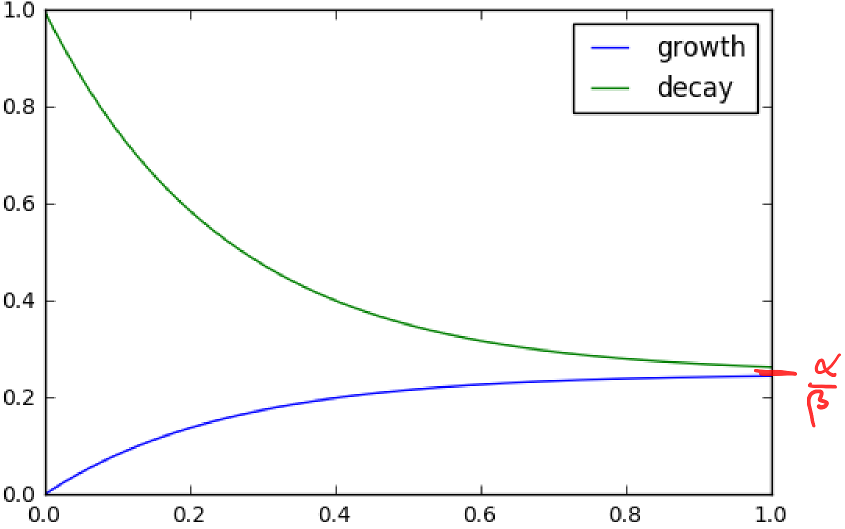
example: growth and decay

- models change in amount of some quantity $u(t)$ over time
- ode
$$\frac{du}{dt} = \alpha - \beta u$$
  - α: growth, β: 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
```

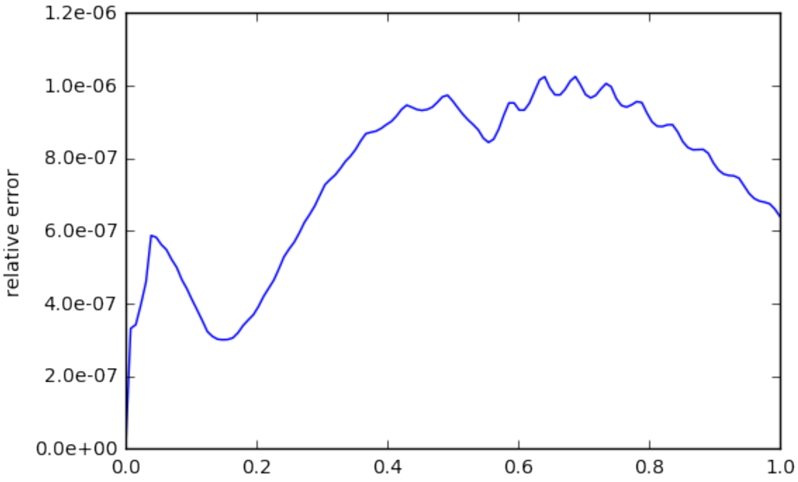
```
plt.plot(t,u(t,u0=0),label='growth')
plt.plot(t,u(t,u0=1),label='decay'); plt.legend();
```



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:]:
    unum.append(solver.integrate(tk)[0])
```

```
plt.plot(t,(np.array(unum)-u(t,u0))/u(t,u0)); plt.ylabel('r
plt.gca().yaxis.set_major_formatter(mtick.FormatStrFormatte
```



example: mechanics

Corr

- particle affected by friction and gravity, Newton's 3rd law

$$m x'' = -\beta x'^2 - \gamma/x^2$$

- first order system $u_1 = x$ and $u_2 = \cancel{x}'$ mx' momentum

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

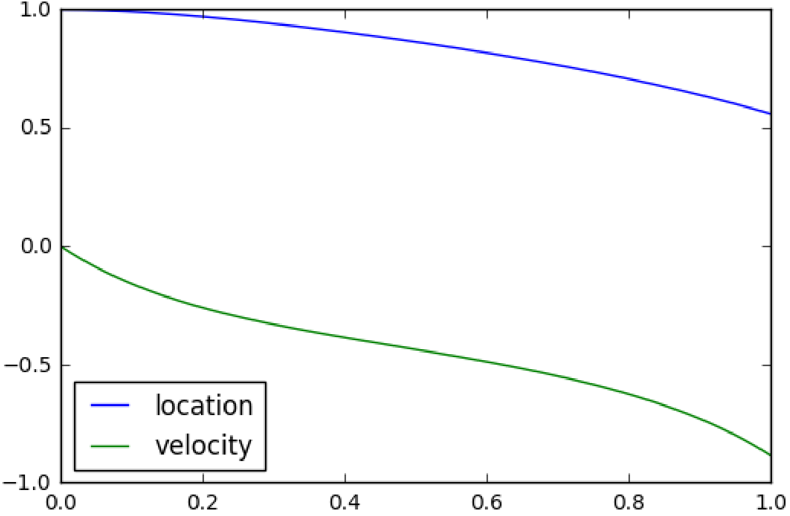
where

$$f = \cancel{\frac{1}{m}} \begin{bmatrix} u_2/m \\ -\beta u_2^2 - \gamma/u_1^2 \end{bmatrix}$$

solving with scipy

```
f = lambda t, u, m=1.0, beta = 5, gamma = 2 :\
    np.array((u[1],-beta*u[1]-gamma/u[0]**2))
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))
```

```
plt.plot(t, np.array(unum)[:,0],label='location')
plt.plot(t, (np.array(unum)[:,1]), label='velocity');plt.le
```



example: "chemical" reaction

- burning hydrogen $2H + O \to H_2O$
- 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

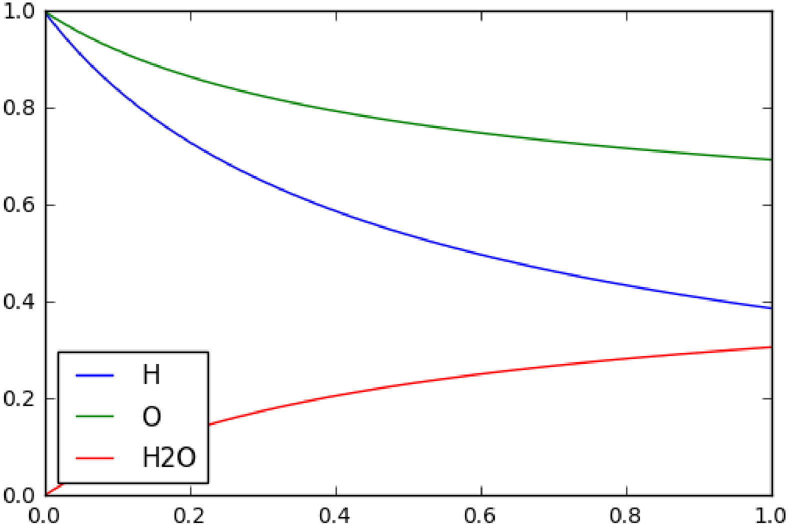
$$f(u) = \kappa u_1^2 u_2 \begin{bmatrix} -2 \\ -1 \\ 1 \end{bmatrix}$$

- note that $u_1 + 2u_3$ and $u_1 + u_3$ 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 removed
- system of ODES

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

  with

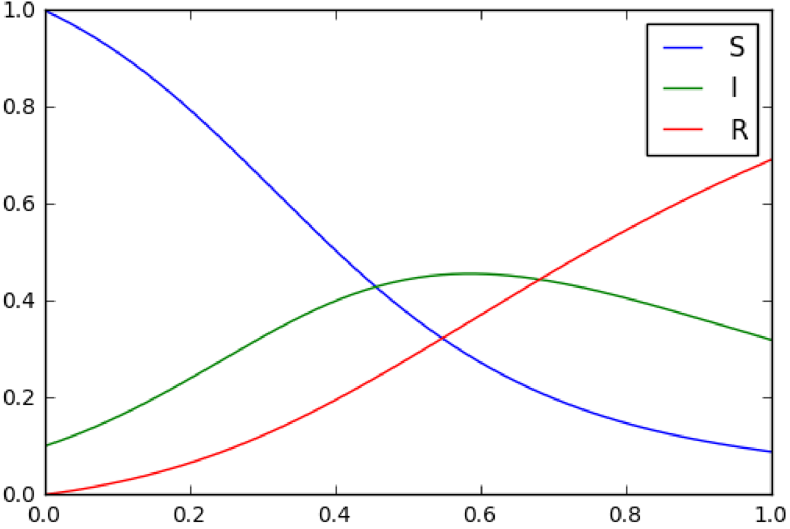
  $$f(u) = \begin{bmatrix} \underline{-\beta u_1 u_2} \\ \underline{\beta u_1 u_2} - \gamma u_2 \\ \gamma u_2 \end{bmatrix}$$

- 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([1.0,0.1,0.0])
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(lo
```



example: heat

- diffusion, discretised in space
- $u_k(t)$ is temperature at location $x_k = kh$ in 1D medium
- system of ODEs

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

where

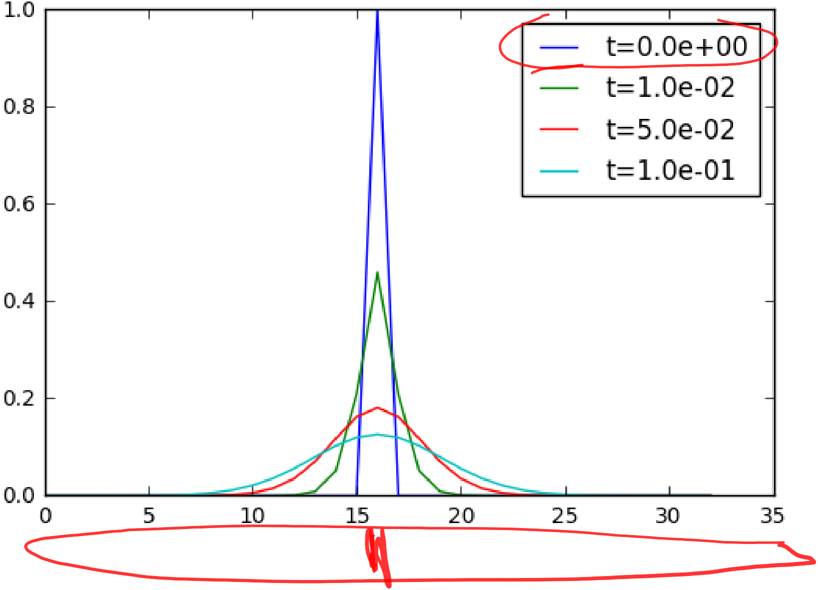
$$A = \frac{\lambda}{h^2} \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}$$

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 = 33
    solver = scint.ode(f)
    u0 = np.zeros(n); u0[n//2] = 1.0
    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))
    plt.legend();
```

heat()



1.0
0.8
0.6
0.4
0.2
0.0
0
5
10
15
20
25
30
35
t=0.0e+00
t=1.0e-02
t=5.0e-02
t=1.0e-01

autonomous form

$$\int \frac{du}{dt}\frac{dt}{f(u)} = \int_{u_0}^{u} \frac{du}{f(u)} = t$$

$$\boxed{\frac{du}{dt} = f(u)} \qquad \cancel{t}$$

- function $f : \mathbb{R}^n \to \mathbb{R}^n$
- 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 $F(u_1, \dots, u_{s+1}, t)$

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

- 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 intial 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

x_0, Ax_0, A^2x_0

$f: M_{n\times n} \to M_{n\times n}$

$$\frac{dB}{dt} = AB$$

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

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

$\begin{cases} u' = 4u \\ u(0) = 1 \end{cases} \to \underline{\underline{e^{4t} = u(t)}}$

$e^x = 1 + x + \frac{x^2}{2} + \cdots$

* solution of the initial value problem

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

$$e^{At} = I + At + \frac{A^2t^2}{2} + \cdots$$

$$= Q \begin{bmatrix} e^{\lambda_1 t} & & \\ & \ddots & \\ & & e^{\lambda_n t} \end{bmatrix} Q^T$$

$$A = Q \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} Q^T$$

reformulate IVP as integral equation

$$\int_0^t u'(s)\,ds = u(t) - u(0) \qquad \frac{du}{dt} = f(u), \quad u(0) = u_0$$

- integrate the explicit form to get

2.

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

- 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

$u' = f(u,t)$

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 $t \in [t_0, t_0 + 1/L]$

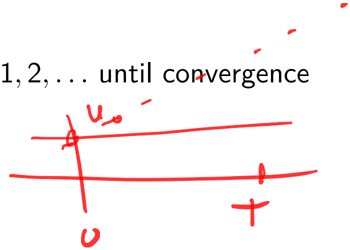
mathematical algorithm: Picard iteration

- aim: compute solution of ODE in $[t, t+h]$ where $h \leq L$ (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: $u^0(t) = u_0$
- iterate: $u^{k+1} = F_h(u^k)$ for $k = 0, 1, 2, \ldots$ until convergence

u^0



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

Euler