L06-ODEsI

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Supporting textbook chapters for week 6: Chapters 8.1, 8.2, 8.5.1 to 8.5.3

Lecture 6, topics: * Euler method * Runge-Kutta methods * Leapfrog and Verlet Methods — energy conservation

1 Intro

Consider ODE(s) with some initial condition(s): * 1D: $\dfrac{dx}{dt} = f(x,t) \quad \text{with} \quad x(t=0) = x_0$. * nD: $\dfrac{dx_i}{dt} = f_i(x_1, \ldots, x_n, t) \quad \text{with} \quad x_i(t=0) = x_{i0}$. * higher order, e.g.:

$$\frac{d^3x}{dt^3} = f(x,t) \quad \Leftrightarrow \quad \frac{dx}{dt} = v, \; \frac{dv}{dt} = a, \; \frac{da}{dt} = f.$$

These equations can be impossible to solve anaytically, but easy to solve on a computer.

1.1 `odeint`

- Python has a built in ODE solver called `odeint` located in the `scipy.integrate` module. (Aside: This module also contains a bunch of integration functions that can do Gaussian quadrature, Simpson's rule etc.).
- See http://docs.scipy.org/doc/scipy/reference/tutorial/integrate.html
- Functions as a black box and you don't know how accurate your solution is (you don't know what method was used).
- If that doesn't matter to your specific application, then just use `odeint`. However, if it does matter, then you can write your own ODE solver with the method that you want.

2 Euler method

Let's solve for

$$\frac{dx}{dt} = -x^3(t) + \sin(t)$$

```
In [ ]: # %load euler-odeint.py
        # From Newman's euler-odeint
        # Paul J. Kushner added comparison with odeint
```

```
# I (NG) made it more PEP8 compliant, and added figure options

#do euler.py solution for odeint
from math import sin
from numpy import arange
from pylab import plot, xlabel, ylabel, show, legend, figure, grid, autoscale
from scipy.integrate import odeint

def f(x, t):
    return -x**3 + sin(t)

a = 0.0  # Start of the interval
b = 10.0  # End of the interval
N = 100  # Number of steps
h = (b-a)/N  # Size of a single step
x = 0.0  # Initial condition

tpoints = arange(a, b, h)
xpoints = []
for t in tpoints:
    xpoints.append(x)
    x += h*f(x, t)

# also solve by odeint (PJK)
x_new = odeint(func=f, y0=0, t=tpoints)
```

```
In [ ]: figure()  # NG
        plot(tpoints, xpoints, label='Euler')
        xlabel("t")
        ylabel("x(t)")
        plot(tpoints, x_new+0.2, '--', label='odeint+0.2')  # PJK
        autoscale(enable=True, axis='x', tight=True)  # NG
        grid()  # NG
        legend()
```

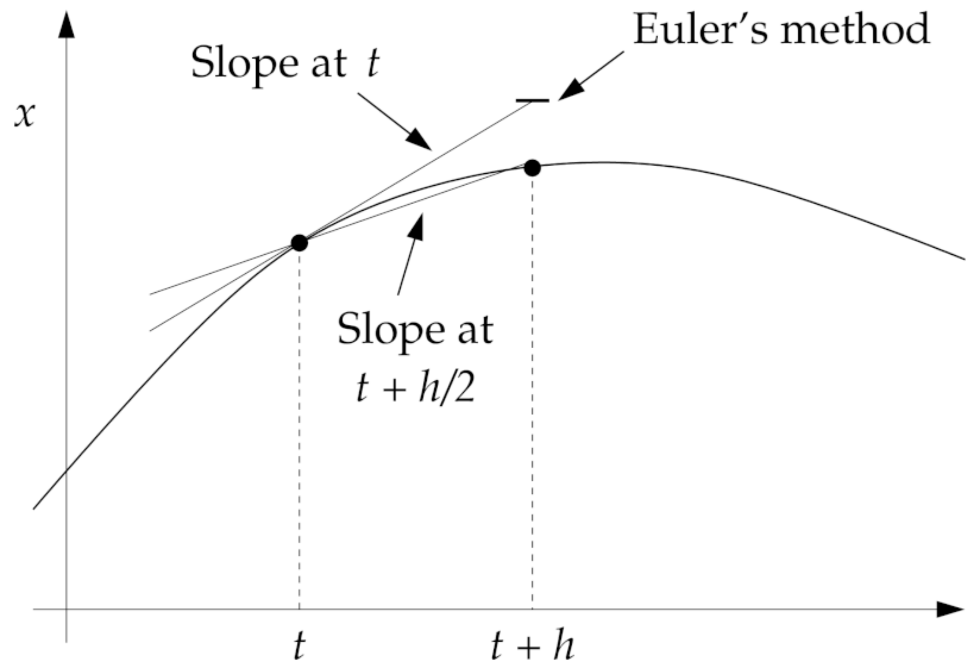
- The Euler method is has error $O(h^2)$ at each step (error $= O(h^2)$),
- integrating across the whole interval: global error is $O(h)$.
- We can do better!

3 Runge-Kutta methods

3.1 2nd-order Runge-Kutta (RK2) method

- Use the middle point, $t + h/2$,
- Evaluate

$$x\left(t + \frac{h}{2}\right) \approx x(t) + \frac{h}{2} f(x(t), t) \qquad \text{(Euler's method)}$$



Newman's Fig. 8.2

- Slope at $t + \frac{h}{2} \approx f\left(x(t) + \frac{h}{2} f(x(t), t), t + \frac{h}{2}\right)$

$$\Rightarrow \boxed{x(t+h) = x(t) + hf\left(x(t) + \frac{h}{2} f(x(t), t), t + \frac{h}{2}\right)}$$

RK2 usually coded by defining intermediate quantities: * $k_1 = hf(x, t)$ as preliminary step before $x(t + h/2)$, * $k_2 = hf\left(x + \frac{k_1}{2}, t + \frac{h}{2}\right)$, * $x(t+h) = x(t) + k_2$.

RK2: $O(h^3)$ step-by-step error, usually $O(h^2)$ global error.

Coding Euler:

```
In [ ]: for t in tpoints:
            x += h*f(x, t)
```

Coding RK2:

```
In [ ]: for t in tpoints:
            k1 = h*f(x, t)
            k2 = h*f(x + 0.5*k1, t+0.5*h)
            x += k2
```

3.2 4th-order Runge-Kutta method (RK4)

- Perform various Taylor expansions at various points in the interval $\Rightarrow$ higher-order RK's.
- RK4 is usually a very good compromise to code oneself. Higher-order methods come in canned routines.

- If Newman says the algebra is tedious, it has got to be.
- End result:
  - $k_1 = hf(x,t)$,
  - $k_2 = hf\left(x + \frac{k_1}{2}, t + \frac{h}{2}\right)$,
  - $k_3 = hf\left(x + \frac{k_2}{2}, t + \frac{h}{2}\right)$,
  - $k_4 = hf\left(x + k_3, t + h\right)$,
  - $x(t+h) = x(t) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$.

Coding Euler:

```
In [ ]: for t in tpoints:
            x += h*f(x, t)
```

Coding RK2:

```
In [ ]: for t in tpoints:
            k1 = h*f(x, t)
            k2 = h*f(x + 0.5*k1, t+0.5*h)
            x += k2
```

Coding RK4:

```
In [ ]: for t in tpoints:
            k1 = h*f(x, t)
            k2 = h*f(x+0.5*k1, t+0.5*h)
            k3 = h*f(x+0.5*k2, t+0.5*h)
            k4 = h*f(x+k3, t+h)
            x += (k1 + 2*k2 + 2*k3 + k4)/6
```

- RK4 carries $O(h^4)$ error globally,
- Many small things to keep track of: easy to introduce a coding error!

4 Leapfrog methods

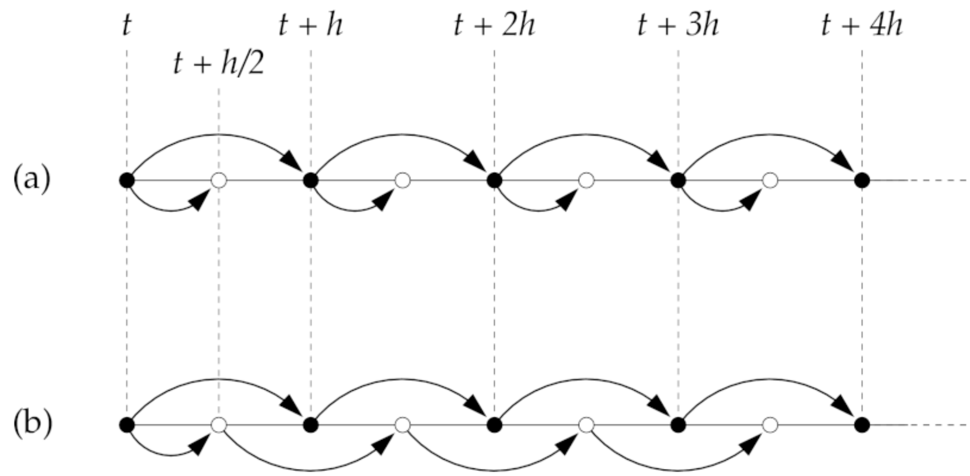
- RK2: Use mid-point location as clutch to jump to $t+h$, and restart.

$$x(t+h) = x(t) + hf\left(x + \frac{h}{2}f(x,t), t + \frac{h}{2}\right)$$

- Leapfrog: use each point as a mid-point.

$$x(t+h) = x(t) + hf\left(x + \frac{h}{2}f(x,t), t + \frac{h}{2}\right),$$

$$x\left(t + \frac{3}{2}h\right) = x\left(t + \frac{h}{2}\right) + hf(x(t+h), t+h).$$

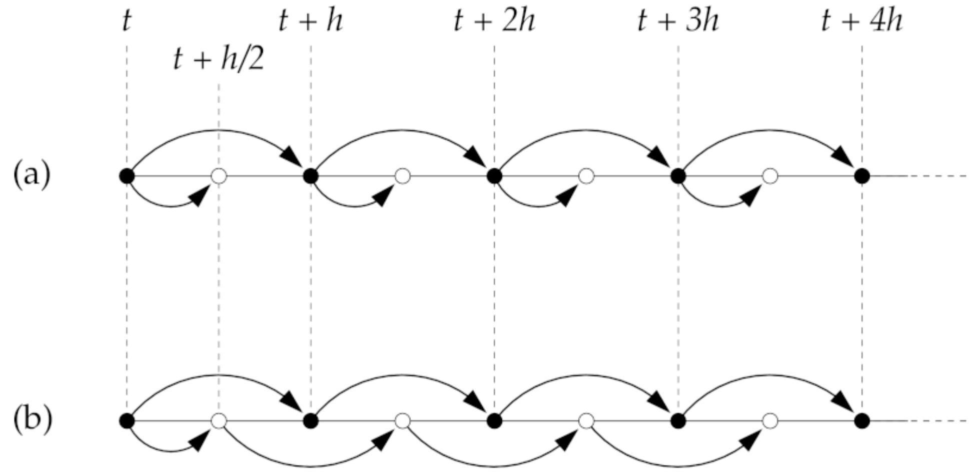


Newman's fig. 8.9

- Also $O(h^2)$ global error,
- Not RK4-able. Not trivially at least (cf. Yoshida algorithms).
- So, is it just cute?

- No: it is **time-reversible**!
- Emmy Noether (from Wikipedia): > If a system has a continuous symmetry property, then there are corresponding quantities whose values are conserved in time.
- Invariance in time of the laws of Physics $\Rightarrow$ conservation of energy.
- **Leapfrog timestepping is reversible!**

Leapfrog timestepping is reversible!
Forward leapfrog:
$x(t+h) = x(t) + hf\left(x\left(t+\frac{h}{2}\right), t+\frac{h}{2}\right)$,
$x\left(t+\frac{3}{2}h\right) = x\left(t+\frac{h}{2}\right) + hf(x(t+h), t+h)$.
Backward Leapfrog: $h \to -h$
$x(t-h) = x(t) - hf\left(x\left(t-\frac{h}{2}\right), t-\frac{h}{2}\right)$,
$x\left(t-\frac{3}{2}h\right) = x\left(t-\frac{h}{2}\right) - hf(x(t-h), t-h)$.
Shift things in time (just to reveal the similarity): $t \to t + 3h/2$
$x\left(t+\frac{h}{2}\right) = x\left(t+\frac{3}{2}h\right) - hf\left(x\left(t+h\right), t+h\right)$,
$x\left(t\right) = x\left(t+h\right) - hf\left(x\left(t+\frac{h}{2}\right), t+\frac{h}{2}\right)$.
With RK2:
$x\left(t+\frac{h}{2}\right) = x(t) + \frac{h}{2}f(x(t), t)$
$x(t+h) = x(t) + hf\left(x\left(t+\frac{h}{2}\right), t+\frac{h}{2}\right)$
Backward RK2: $h \to -h$
$x\left(t-\frac{h}{2}\right) = x(t) - \frac{h}{2}f(x(t), t)$
$x(t-h) = x(t) - hf\left(x\left(t-\frac{h}{2}\right), t-\frac{h}{2}\right)$
Shift things in time (just to reveal the similarity): $t \to t + h$



Newman's fig. 8.9

$x\left(t+\frac{h}{2}\right) = \underbrace{x\left(t+h\right)}_{\neq\ reset} - \frac{h}{2} f\left(x\left(t+h\right), t+h\right)$

$x\left(t\right) = x\left(t+h\right) - hf\left(x\left(t+\frac{h}{2}\right), t+\frac{h}{2}\right)$

- Because everything gets "reset" at $t+h$, the info a the mid-point is lost and the RK2 reverse path is not a "retracing of the steps".
- Graphically, reverse RK2 is not like drawing the arrows in reverse on the top panel of Newman's figure:

Energy of a nonlinear pendulum:

5 Leapfrog to Verlet

- Leapfrog:

$$x(t+h) = x(t) + hf\left(x\left(t+\frac{h}{2}\right), t+\frac{h}{2}\right),$$

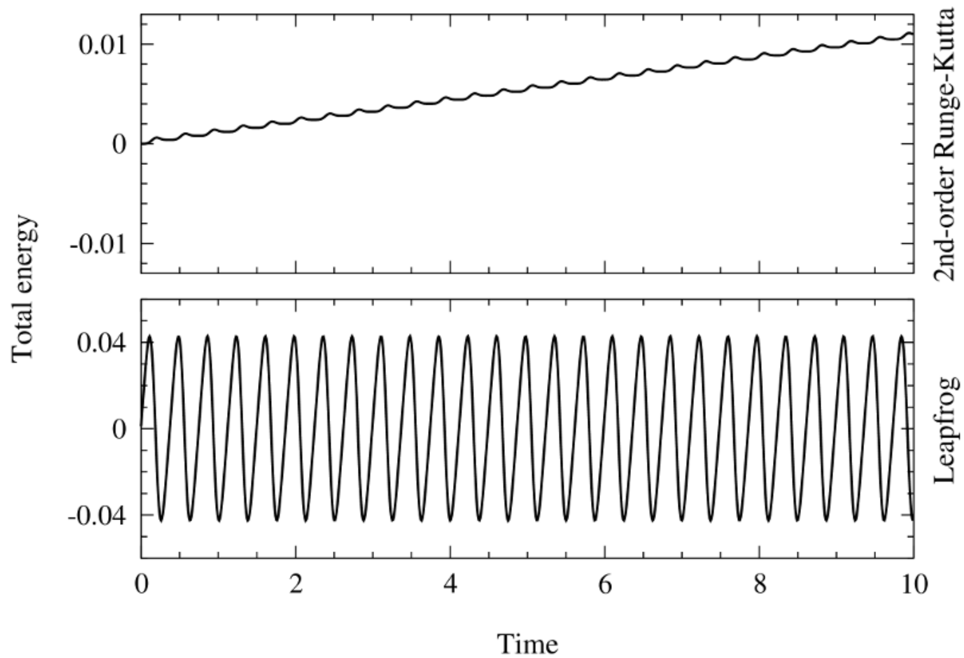
$$x\left(t+\frac{3}{2}h\right) = x\left(t+\frac{h}{2}\right) + hf(x(t+h), t+h).$$

- Extension to two (or n) coupled ODEs: cf. §§ 8.2, 8.3.

- For the special case of two coupled ODEs, with LHS and RHS having separated variables. Like for Newton's 2nd law:

$$\frac{d^2x}{dt^2} = \frac{F(x,t)}{m} \quad \Rightarrow \quad \frac{dx}{dt} = v \quad \text{and} \quad \frac{dv}{dt} = \frac{F(x,t)}{m}.$$

  1st ODE: x on LHS, v on RHS; 2nd ODE: v on LHS, x on RHS.



Newman's Fig. 8.10

- Verlet method:

$$x(t+h) = x(t) + hv\left(t + \frac{h}{2}\right),$$

$$v\left(t + \frac{3}{2}h\right) = v\left(t + \frac{h}{2}\right) + h\frac{F(x(t+h), t+h)}{m}.$$

- Verlet is a 2-variable leapfrog method at 1/2 the cost.
- It conserves energy too.
- If diagnostics (like energy) are needed at specific time steps, we need to recompute the half-step quantities.

RK2: * $\oplus$ Easily extended to RK4 * $\oplus$ Possible to use adaptive time step (see next week) * $\ominus$ not time-reversible * $\ominus$ not accurate

RK4: * $\oplus$ accuracy * $\oplus$ Possible to use adaptive time step (see next week) * $\ominus$ not time-reversible

Leapfrog: * $\oplus$ time-reversible * $\oplus$ basis for higher-order methods (Bulirsch-Stoer, see next week) * $\ominus$ not accurate * $\ominus$ time step has to be constant.