Computational Physics Lab

Ordinary Differential Equations & Initial Value Problems

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Ordinary Differential Equations

READ Discussions in

Chapter 8 Sections 1-4

Recall from Exercise 7

Radioactive Decays

$$\frac{dN(t)}{dt} = \frac{-N(t)}{\tau}$$

we used the forward difference and found a solution:

$$N(t+h) \simeq N(t) - h\frac{N(t)}{\tau} = N(t) + h f(N,t)$$

$$x(t+h) = x(t) + h f(x,t) + O(h^2)$$

Euler's Method for solving differential equations

Initial Value Problem

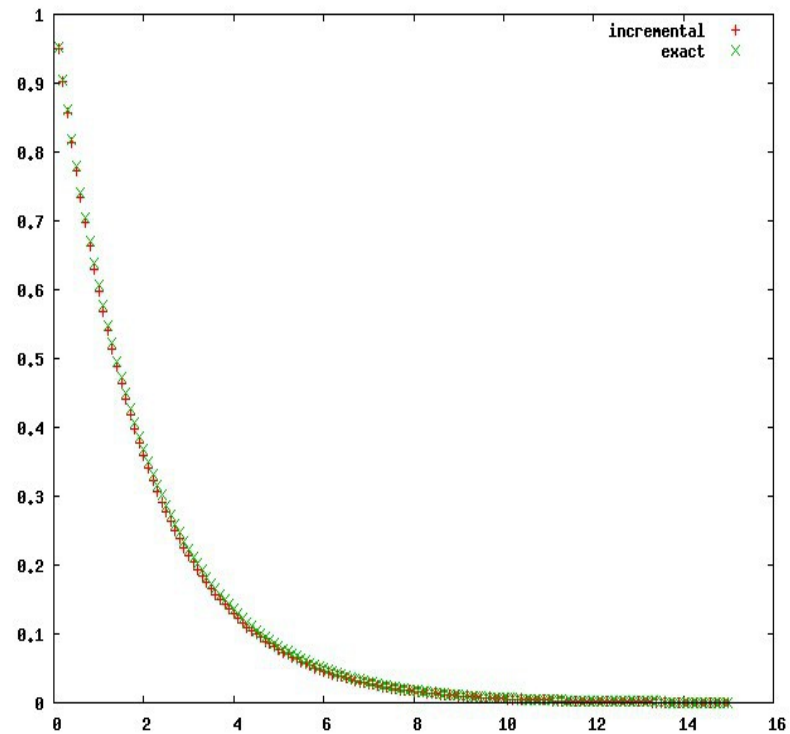
To determine a solution we need its initial or boundary conditions

```
def f(N, t):
    tau = 2.0
    return  -N/tau

h, tMin, tMax = 0.1,  0, 15

# Set initial conditions:  at t=0, N(t) = 100%
time = [tMin]
N = [1]

for i, t in enumerate( np.arange(tMin, tMax, h) ):
    time += [ t ]
    N += [ N[i] + h * f(N[i], t) ]

plt.plot( time, N, "*" )
plt.show()
```

$$N(t)=N(t_0)e^{\left(\frac{-\Delta t}{\tau}\right)}$$

exact

t_i	N_i	$N(t)$
0.1	0.95	0.951229
0.2	0.9025	0.904837
0.3	0.857375	0.860708
0.4	0.814506	0.818731
0.5	0.773781	0.778801
0.6	0.735092	0.740818
...		



Simultaneous Differential Equations

Two 1st-Order Differential Equations

$$\frac{dx}{dt} = f_x(x, y, t) \qquad \frac{dy}{dt} = f_y(x, y, t)$$

Using **vectorized notation**

$$\frac{d\mathbf{r}}{dt} = \boldsymbol{f}(\mathbf{r}, t)$$

$$where\ \mathbf{r} = \begin{bmatrix} x \\ y \end{bmatrix}$$

$$and\ \boldsymbol{f}(\mathbf{r}, t) = \begin{bmatrix} f_x(\mathbf{r}, t) \\ f_y(\mathbf{r}, t) \end{bmatrix}$$

Solution using Euler's method

$$\mathbf{r}(t+h) = \mathbf{r}(t) + h\,\boldsymbol{f}(\mathbf{r}, t)$$

$$\boxed{\begin{aligned} x(t+h) &= x(t) + h\,f_x(x, y, t) \\ y(t+h) &= y(t) + h\,f_y(x, y, t) \end{aligned}}$$

Nth-order Differential Equations

Problems Involving Nth-order Ordinary Differential Equations Can Always be Reduced to the Study of a set of 1st-Order Differential Equations

Nth-order ODE Transformed to N 1st-order ODEs

Example:

$$\frac{d^2y}{dt^2} + f(t)\frac{dy}{dt} = g(t)$$

$$\frac{dy}{dt} = v(t)$$

$$\frac{dv}{dt} = g(t) - f(t)v(t)$$

Differential Equations

$$y(t+h) = y(t) + h\,v(t) \qquad v(t+h) = v(t) + h\big(g(t) - f(t)\,v(t)\big)$$

```
for i, t in enumerate(np.arange(h, tMax, h)):
    tPoints += [t]
    yPoints += [yPoints[i] + h * fy(yPoints[i],vPoints[i], t)]
    vPoints += [vPoints[i] + h * fv(yPoints[i],xPoints[t], t)]
```

Be aware that order matters

```
for i, t in enumerate(np.arange(h, tMax, h)):
    tPoints += [t]
    vPoints += [vPoints[i] + h * fv(yPoints[i],xPoints[t], t)]
    yPoints += [yPoints[i] + h * fy(yPoints[i],vPoints[i], t)]
```

ODE & Diff. Eq. Errors

Uses info at 1 point "t"

O(h²)

Forward difference

truncation error

$$x(t+h) = x(t) + h\,x'(t) + \frac{h^2}{2}x''(t) + \ldots$$

Central difference

$$x(t+h) = x(t) + h\ x'(x(t+h/2), t+h/2) + O(h^3)$$

Uses info at 2 points to improve accuracy

ODE & Diff. Eq. Errors

Uses info at 1 point "t"

O(h²)

Forward difference

truncation error

$$x(t+h) = x(t) + h\,x'(t) + \frac{h^2}{2}x''(t) + \ldots$$

Central difference

$$x(t+h) = x(t) + h\; x'(x(t+h/2), t+h/2) + O(h^3)$$

Uses info at 2 points to improve accuracy

General Runge-Kutta Method

$$x(t+h) = x(t) + h\left(\sum_i^N c_i\, x'(x_i, t_i)\right) + O(h^{N+1})$$

Use info at many points to further increase accuracy

Fourth-Order Runge-Kutta

$$\frac{dx}{dt} = f(x,t)$$

$$x(t+h) = x(t) + \frac{1}{6}(k_1 + 2\mathrm{k}_2 + 2\mathrm{k}_3 + k_4)$$

$$k_1 = h f(x,t)$$

$$k_2 = h f(x + \frac{1}{2}k_{1,} t + \frac{1}{2}h)$$

$$k_3 = h f(x + \frac{1}{2}k_{2,} t + \frac{1}{2}h)$$

$$k_4 = h f(x + k_{3,} t + h)$$

The Most Commonly Used Method!

$O(h^5)$

truncation error

Fourth-Order Runge-Kutta using <u>vectorized notation</u>

$$\frac{d\boldsymbol{r}}{dt} = \boldsymbol{f}(\boldsymbol{r}, t)$$

$$\boldsymbol{r}(t+h) = \boldsymbol{r}(t) + \frac{1}{6}(\boldsymbol{k}_1 + 2\boldsymbol{k}_2 + 2\boldsymbol{k}_3 + \boldsymbol{k}_4)$$

$$\boldsymbol{k}_1 = h f(\boldsymbol{r}, t)$$

$$\boldsymbol{k}_2 = h f(\boldsymbol{r} + \frac{1}{2}\boldsymbol{k}_{1,}\, t + \frac{1}{2}h)$$

$$\boldsymbol{k}_3 = h f(\boldsymbol{r} + \frac{1}{2}\boldsymbol{k}_{2,}\, t + \frac{1}{2}h)$$

$$\boldsymbol{k}_4 = h f(\boldsymbol{r} + k_{3,}\, t + h)$$

Implementing Runge Kutta

Because of Python's Dynamic Typing and Vectorization,
one function works for any dimension!

```
def rung_kutta4(f, r, t, h):
    """ 4th order Runge-Kutta method
        …
    """
    k1 = h*f(r,t)
    k2 = h*f(r+0.5*k1,t+0.5*h)
    k3 = h*f(r+0.5*k2,t+0.5*h)
    k4 = h*f(r+k3,t+h)
    return (k1 + 2*k2 + 2*k3 + k4)/6
```

```
def fN(N, t):
    """ 1 dimensional function"""
    tau = 2.0
    return - N/tau

N, NPoints = 1, []
for t in tPoints:
    NPoints += [N]
    N += runge_kutta4(fN, N, t, h)

plt.plot(tPoints, NPoints)
```

```
def f2D(r, t):
    """ 2 dimensional function"""
    g, L = 9.81, 0.1
    theta, omega = r[0], r[1]
    fTheta = omega
    fOmega = -g/L * theta
    return np.array([fTheta, fOmega],\
                    float)

r = np.array([10*np.pi/180, 0], float)
for t in tPoints:
    thetaPoints += [r[0]]
     omegaPoints += [r[1]]
    r += runge_kutta4(f2D, r, t, h)

plt.plot(tPoints, thetaPoints)
```

The van der Pol oscillator

The van der Pol oscillator appears in electronic circuits and in laser physics

$$\frac{d^2x}{dt^2} - \mu\left(1 - x^2\right)\frac{dx}{dt} + \omega^2 x = 0$$

Solve with initial conditions x = 1 and dx/dt = 0.

The van der Pol oscillator

The van der Pol oscillator appears in electronic circuits and in laser physics

$$\frac{d^2x}{dt^2} - \mu\left(1 - x^2\right)\frac{dx}{dt} + \omega^2 x = 0$$

Solve with initial conditions x = 1 and dx/dt = 0.

$$\boldsymbol{f}\left(\boldsymbol{r}, t\right) = \begin{bmatrix} \dfrac{dx}{dt} = v \\ \dfrac{dv}{dt} = -\omega^2 x + \mu\left(1 - x^2\right) v \end{bmatrix}$$

The van der Pol oscillator

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$$\frac{d^2 x}{dt^2} - \mu \left(1 - x^2\right) \frac{dx}{dt} + \omega^2 x = 0$$

Solve with initial conditions x = 1 and dx/dt = 0.

$$\boldsymbol{f}\left(\boldsymbol{r}, t\right) = \begin{bmatrix} \dfrac{dx}{dt} = v \\ \dfrac{dv}{dt} = -\omega^2 x + \mu \left(1 - x^2\right) v \end{bmatrix}$$

```
def f_vanderPol(r, t):
    """ vectorized function for the van der Pol oscillator """
    mu, omega = 3.0, 1.0         # constants
    x = r[0]
    v = r[1]
    fx = v
    fv = -omega**2 * x  +  mu * (1 - x**2) * v
    return np.array([fx, fv], float)
```

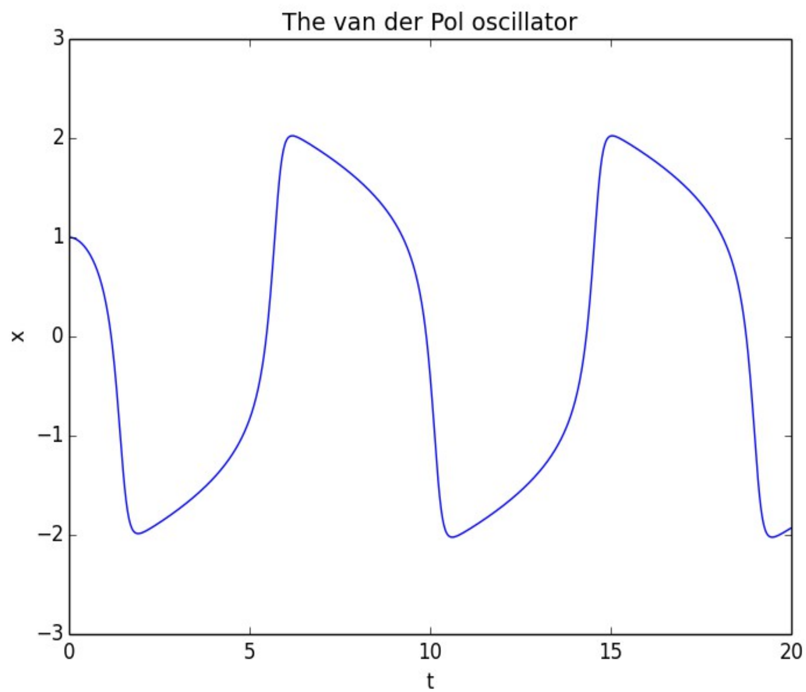
The van der Pol oscillator

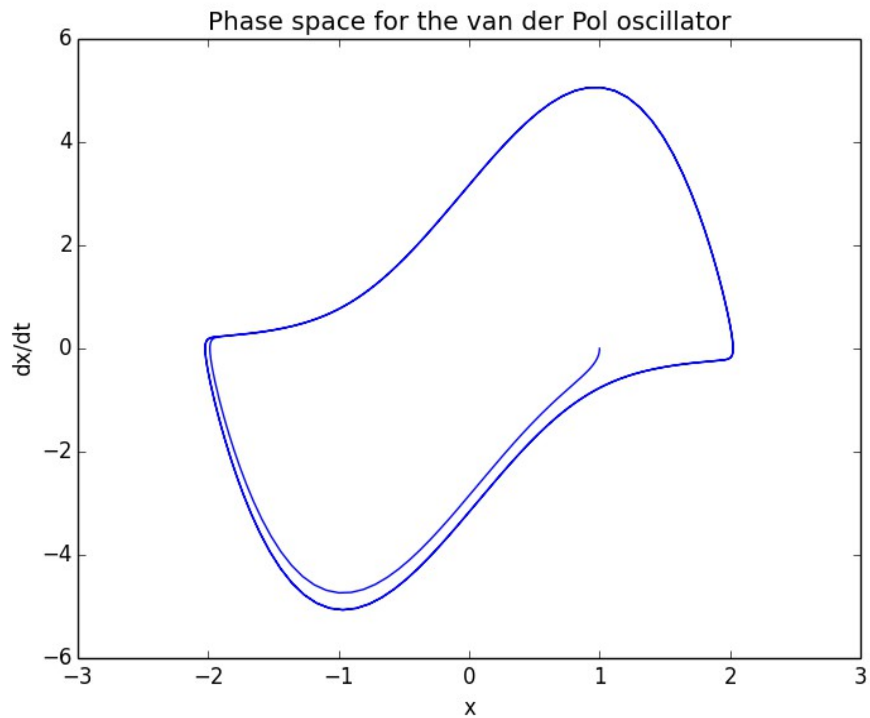
The van der Pol oscillator appears in electronic circuits and in laser physics

```
#
# main

# initialization
N = 1000                          # Number of steps
tMin, tMax = 0.0, 20.0      # time range
tStep = (tMax – tMin) / N       # time step

# define time values
time = np.arange(tMin, tMax, tStep)

# creating lists for plotting
xPoints, vPoints = [],[]

# set initial conditions
x0,v0 = 1.0,0.0
r = np.array([x0,v0], float)
```

```
# find numerical solution to Dif. Eq.
for t in time:
    xPoints += [r[0]]
    vPoints += [r[1]]
    r +=  runge_kutta4(f_vanderPol, \
            r,  t, tStep)

# Now generate plots
    ...
```

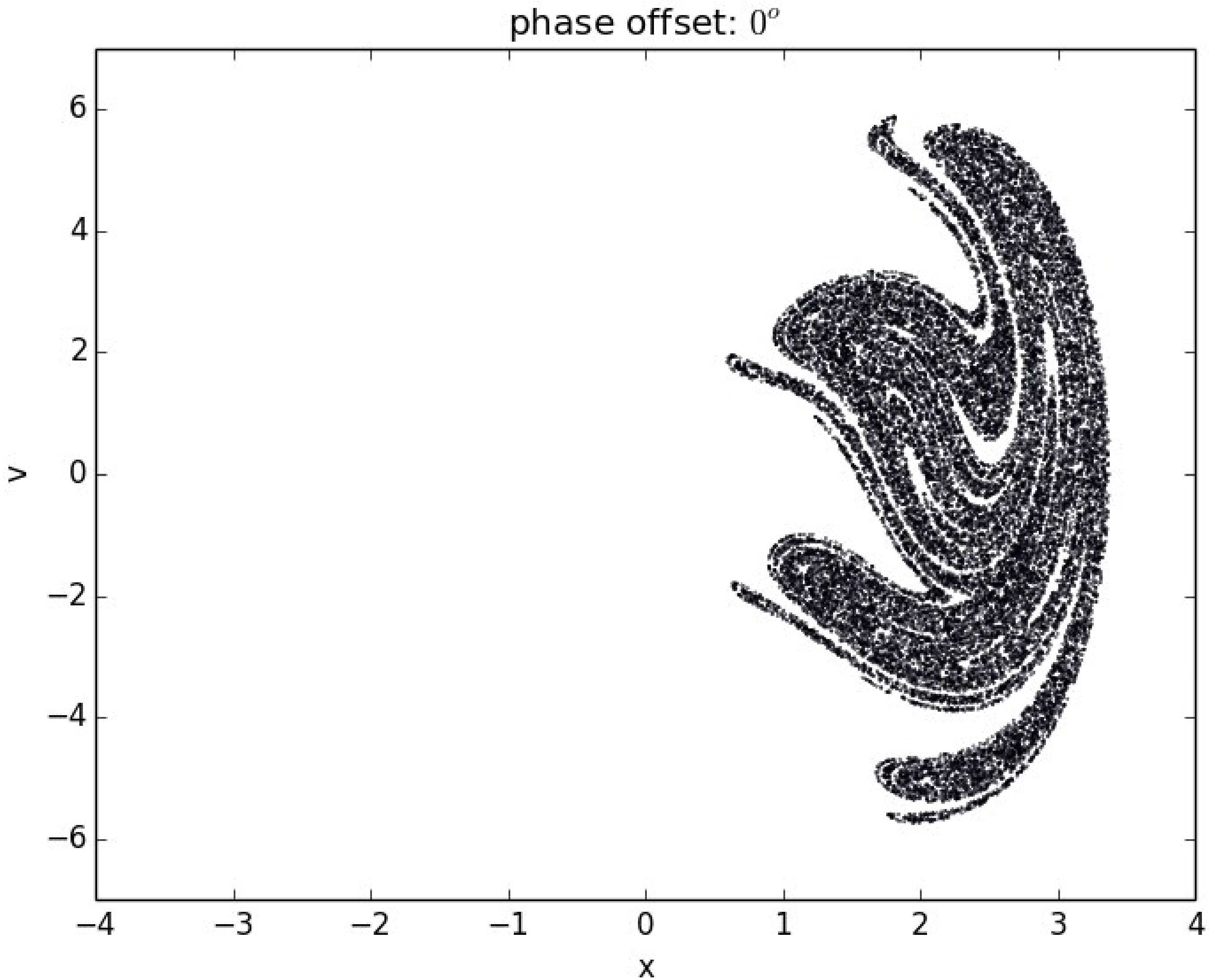
The van der Pol oscillator





See Python source code: vanderpol.py

Poincare' sections from Exercise 9



click on plot to see animated plot