L07-ODEsII

October 23, 2018

Author: Nico Grisouard, nicolas.grisouard@physics.utoronto.ca

Supporting textbook chapters for week 7: Chapters 8.4, 8.2, 8.5.5, 8.6

Lecture 7, topics: * Adaptive step size for RK schemes, * Bulirsch-Stoer method, * Boundary value problems, * Stability issues.

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

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

1 Runge-Kutta methods

1.1 2nd-order Runge-Kutta (RK2) method

RK2: * $\oplus$ Easily extended to RK4 * $\oplus$ Possible to use adaptive time step (this week) * $\ominus$ time-reversible * $\ominus$ accuracy

RK4: * $\oplus$ accuracy * $\oplus$ Possible to use adaptive time step (this week) * $\ominus$ time-reversible

Leapfrog: * $\oplus$ time-reversible * $\oplus$ basis for higher-order methods (Bulirsch-Stoer, this week) * $\ominus$ accuracy * $\ominus$ time step has to be constant (not exactly true, as we will see).

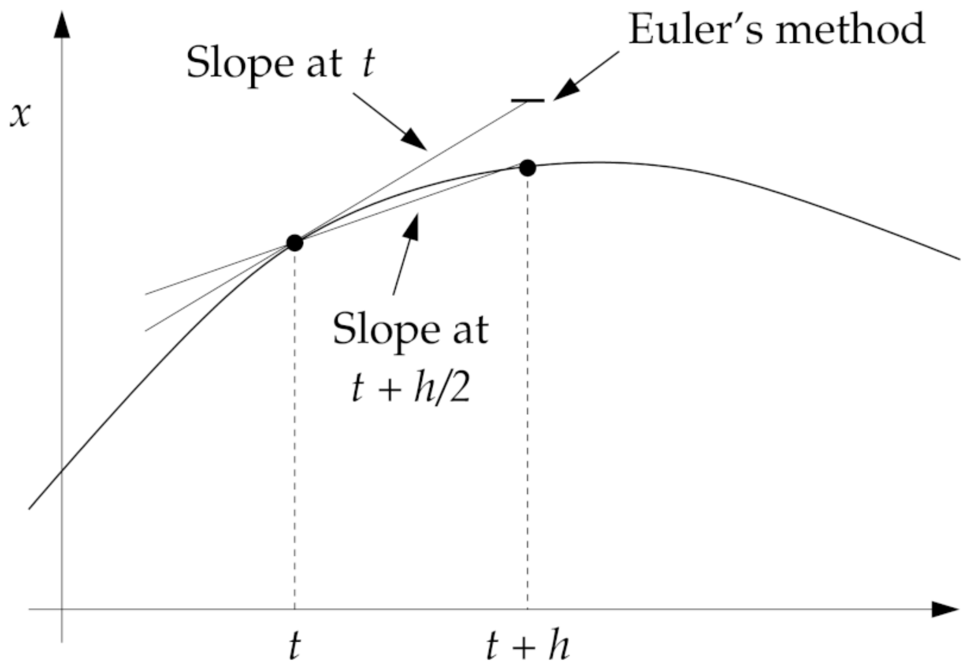
2 Adaptive 4th-order Runge-Kutta method (RK4)

2.1 Error of RK4

- End result:
  - $k_1 = hf(x,t)$,
  - $k_2 = hf\left(x + \frac{k_1}{2}, t + \frac{h}{2}\right)$,
  - $k_3 = hf\left(x + \frac{k_2}{2}, t + \frac{h}{2}\right)$,
  - $k_4 = hf\left(x + k_3, t + h\right)$,
  - $x(t+h) = x(t) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$.
- Very accurate method: error is $\epsilon = c \times h^5$ at each time step h, c constant.

- Very accurate method: error is $\epsilon = c \times h^5$ at each time step h, c constant.

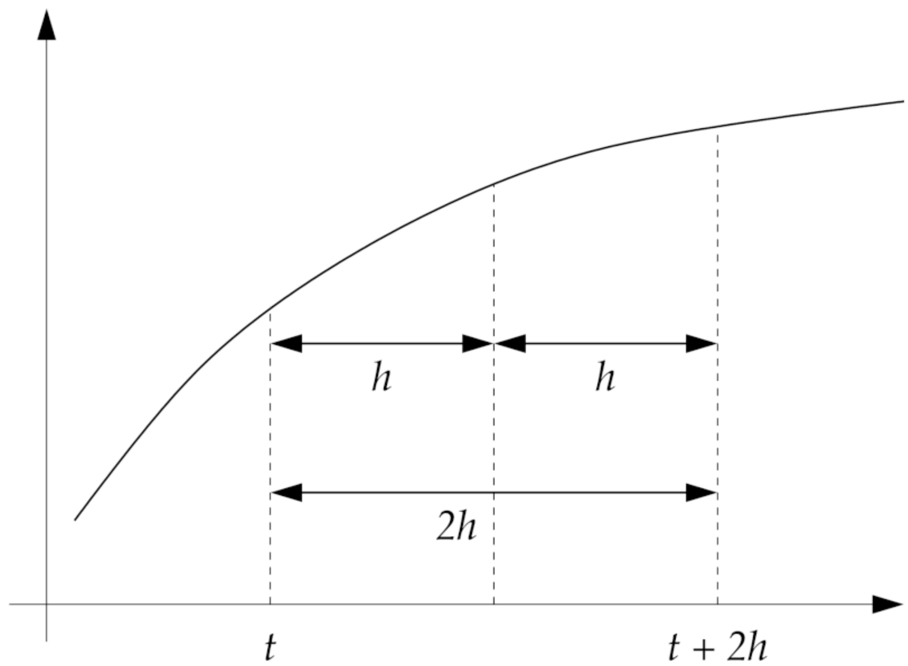
- Error after 2 time steps? $\approx 2ch^5$.



Newman's Fig. 8.2

- Error after 1 time step of $2h$? $c(2h)^5 = 32ch^5 \gg 2ch^5$
- The difference is $(32-2)ch^5 = 30ch^5$.
- To estimate error: run ODE solver once with h (to get x_1), once with $2h$ (to get x_2), divide difference by 30.

$$\epsilon = ch^5 = \frac{1}{30}(x_1 - x_2).$$



2.2 Adaptive time stepping

- Suppose target error is δ *per unit time*. If

$$\rho = \frac{h\delta}{\epsilon} = \frac{30h\delta}{|x_1 - x_2|} = \frac{30\delta}{ch^4} > 1,$$

  h is too small and can be adjusted to $h' = h\rho^{1/4}$ to get $\rho' = 1$, i.e., without missing target accuracy.

  – This saves calculation time.

- If $\rho < 1$, the time step is too large and needs to be adjusted down by the same factor.

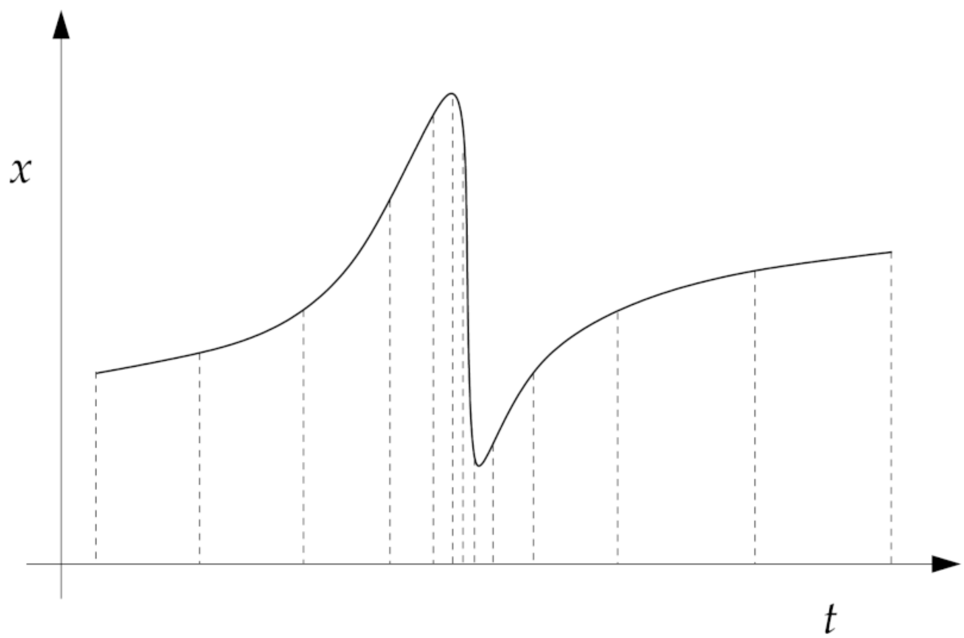
  – We also need to repeat our calculation to get the desired accuracy.
  – This will guarantee meeting error target.

- We test if we need to adjust by performing the calculation twice (we retrieve x_1 and x_2), testing if we met the target, and adjusting h.
- Overall, despite extra work (up to 3 RK4 steps per time step), program often faster because resolution focused where it's needed.

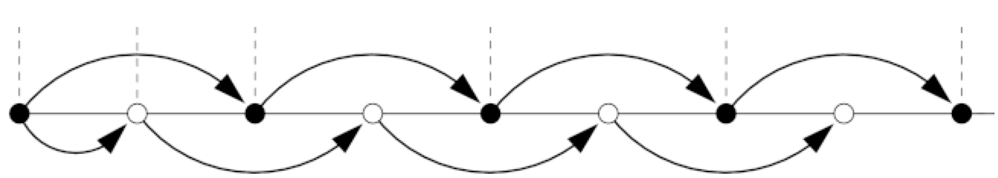
3 From Leapfrog to Bulirsch-Stoer

3.1 Leapfrog error

- Leapfrog is timestep-reversible.



Newman 8.6



Newman’s fig. 8.9, focus on leapfrog

- $\Rightarrow$ error ϵ is an **odd** function of h:
$$\epsilon(-h) = -\epsilon(h)$$
$\Rightarrow$ Taylor expansion is made of **odd** powers of h.
- $\Rightarrow$ cumulative error is **even** in h,
- Each improvement we apply $\Rightarrow$ we can get two orders of accuracy, if we play it right.

3.2 Modified mid-point (MMP) method

- Integration from t to $t + H$, with $n + 1$ time steps:

$$\begin{aligned}
x_0 &= x(t) \\
x_{1/2} &= x_0 + hf(x_0, t)/2 \quad \text{(Initial Euler 1/2-step} \Rightarrow \text{lots of even powers in } \epsilon\text{!)} \\
x_1 &= x_0 + hf(x_{1/2}, t + h/2) \\
x_{3/2} &= x_{1/2} + hf(x_1, t + h) \\
&\dots
\end{aligned}$$

- $\dots$ and keep going until you reach the end.

- Then, do **both** the whole integer **and** the backward Euler.

$$\begin{aligned}
x_{n-1/2} &= x_{n-3/2} + hf(x_{n-1}, t + H - h), \\
x_n &= x_{n-1} + hf(x_{n-1/2}, t + H - h/2) \approx x(t + H) \\
x'_n &= x_{n-1/2} + hf(x_n, t + H) \qquad \text{(But do this adjustment...)} \\
x(t + H)_{final} &= \frac{x_n + x'_n}{2} \qquad \text{(... and you have canceled the even powers (MMP)).}
\end{aligned}$$

This is not a trivial result (cf. Gragg 1965 for proof).

3.3 Bulirsch-Stoer method

- MMP method rarely used by itself, but is the basis for the powerful Bulirsch-Stoer method.
- Method:
  - Take 1 single MMP step of size $h_1 = H$ to get estimate of
  $$x(t + H) = R_{1,1}.$$
  (R stands for "Richardson extrapolation")
  - Now take 2 MMP steps of size $h_2 = H/2$ to get second estimate of
  $$x(t + H) = R_{2,1}.$$
  - Since we know the MMP has 2nd order and even total error, we can write both of these estimates as
  $$\begin{aligned}
  x(t + H) &= R_{1,1} + c_1 h_1^2 + O(h_1^4) \quad \text{and} \\
  x(t + H) &= R_{2,1} + c_1 h_2^2 + O(h_2^4).
  \end{aligned}$$

Recall

$$x(t+H) = R_{1,1} + c_1 h_1^2 + O(h_1^4) \quad \text{and}$$
$$x(t+H) = R_{2,1} + c_1 h_2^2 + O(h_2^4).$$

* Using the relationship between the step sizes: $h_1 = 2h_2$, we can equate these expressions to get

$$R_{1,1} + 4c_1 h_2^2 + O(h_2^4) = R_{2,1} + c_1 h_2^2 + O(h_2^4)$$
$$\Rightarrow \; c_1 h_2^2 = \frac{1}{3}(R_{2,1} - R_{1,1}) + O(h_2^4).$$

* If we plug this back in to the expression for $x(t+H)$ above we get a new estimate called $R_{2,2}$:

$$x(t+H) \approx R_{2,2} = R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1}) + \underbrace{O(h_2^4)}.$$

$$x(t+H) \approx R_{2,2} = R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1}) + \underbrace{O(h_2^4)}.$$

* 2 different grid spacings (H and $H/2$) $\rightarrow$ expression for the leading error term $\rightarrow$ replace it with our estimates for these grid spacings, i.e., $R_{1,1}$ and $R_{2,2}$. * We have reduced the error in our estimate by 2 orders! *(which was possible because the errors were even)*

Why stop there?

- Take another grid spacing, to estimate the **new** leading order error term and then replace for that.
- E.g., with $h_3 = H/3$,
$$x(t+H) = R_{3,1} + c_1 h_3^2 + O(h_3^4).$$
- E.g., with $h_3 = H/3$,
$$\begin{aligned} x(t+H) &= R_{3,1} + c_1 h_3^2 + O(h_3^4), \\ &= R_{2,1} + c_1 \left(\frac{3}{2} h_3\right)^2 + O(h_3^4), \\ \Rightarrow R_{3,1} + c_1 h_3^2 + O(h_3^4) &= R_{2,1} + c_1 \frac{9}{4} h_3^2 + O(h_3^4) \\ \Rightarrow c_1 h_3^2 &= \frac{4}{5}(R_{3,1} - R_{2,1}) + O(h_3^4) \end{aligned}$$
- Now plugging this into our expression for $x(t+H)$ and calling it $R_{3,2}$,
$$x(t+H) \approx R_{3,2} + c_2 h_3^4 + \underbrace{O(h_3^6)},$$
$$\text{where } R_{3,2} = R_{3,1} + \frac{4}{5}(R_{3,1} - R_{2,1}),$$
and where c_2 is a new constant that we need to find an expression for…
- Equating $R_{3,2}$ and $R_{2,2}$ allows to find c_2:
$$\begin{aligned} x(t+H) &\approx R_{2,2} + c_2 h_2^4 + \underbrace{O(h_2^6)} \\ &\approx R_{3,2} + c_2 h_3^4 + \underbrace{O(h_3^6)} \end{aligned}$$
$$h_3 = 2h_2/3 \Rightarrow c_2 h_3^4 = \frac{16}{65}(R_{3,2} - R_{2,2})$$

- Plugging this back in and calling the new result $R_{3,3}$ yields

$$x(t+H) \approx R_{3,3} + O(h_3^6),$$

$$\text{where } R_{3,3} = R_{3,2} + \frac{16}{65}(R_{3,2} - R_{2,2}),$$

- and so on.

- The power in this method is that you keep cancelling 2 powers in the error for every new grid spacing you consider.
- Typically, you continue the refinement until you reach the error tolerance you want.
- Summary of method:
  - Take $h = H$, set $n = 1$ and use MMP to find $x(t+H)$,
  - Continue to refine grid to find new estimates and error estimates.
  - When error is acceptable, stop.

- The iteration can be expressed:

$$x(t+H) = R_{n,m+1} + O(h_n^{2m+2}), \qquad \text{where}$$

$$R_{n,m+1} = R_{n,m} + \frac{R_{n,m} - R_{n-1,m}}{[n/(n-1)]^{2m} - 1} \quad \text{and} \quad h_n = \left(\frac{n-1}{n}\right) h_{n-1}.$$

Let's look at `bulirsch.py` from Newman's book.
Equations solved: nonlinear pendulum,

$$\frac{d\theta}{dt} = \omega, \qquad \frac{d\omega}{dt} = -\frac{g}{\ell}\sin\theta.$$

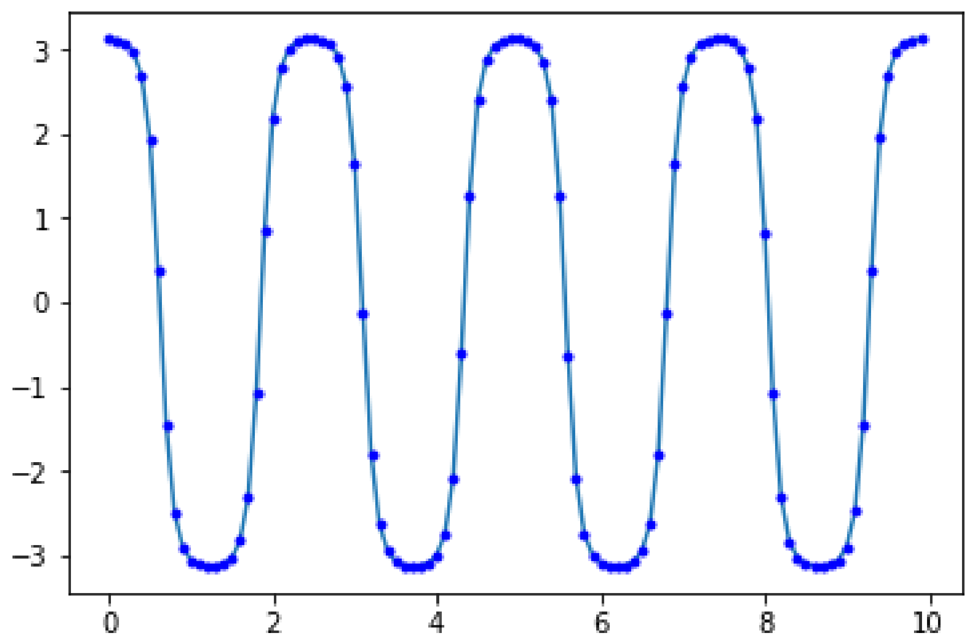
Extrapolation table:

$$\begin{array}{llll}
n = 1 : R_{1,1} & & & \\
 & \searrow & & \\
n = 2 : R_{2,1} & \to R_{2,2} & & \\
 & \searrow & \searrow & \\
n = 3 : R_{3,1} & \to R_{3,2} & \to R_{3,3} & \\
 & \searrow & \searrow & \searrow \\
n = 4 : \underbrace{R_{4,1}}_{MMP} & \to R_{4,2} & \to R_{4,3} & \to R_{4,4}
\end{array}$$

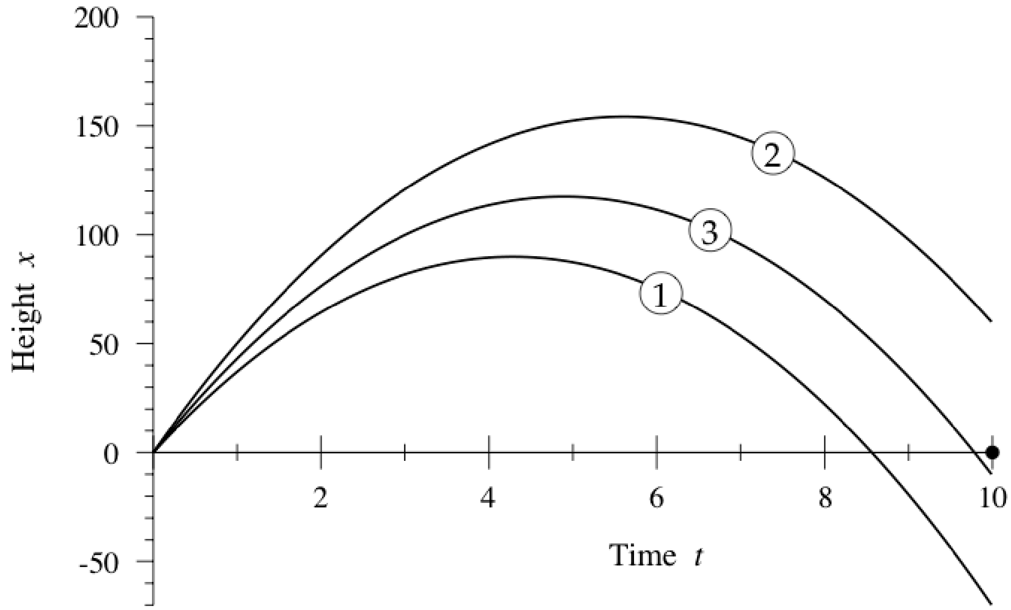
In [2]:
```
# load bulirsch.py from Newman
from math import sin, pi

from numpy import empty, array, arange
from pylab import plot, show

g = 9.81
ell = 0.1
theta0 = 179*pi/180
```

```
a = 0.0
b = 10.0
N = 100  # Number of "big steps"
H = (b-a)/N  # Size of "big steps"
delta = 1e-8  # Required position accuracy per unit time


def f(r):
    theta = r[0]
    omega = r[1]
    ftheta = omega
    fomega = -(g/ell)*sin(theta)
    return array([ftheta, fomega], float)


tpoints = arange(a, b, H)
thetapoints = []
r = array([theta0, 0.0], float)

# Do the "big steps" of size H
for t in tpoints:

    thetapoints.append(r[0])

    # Do one modified midpoint step to get things started
    n = 1
    r1 = r + 0.5*H*f(r)
    r2 = r + H*f(r1)

    # The array R1 stores the first row of the
    # extrapolation table, which contains only the single
    # modified midpoint estimate of the solution at the
    # end of the interval
    R1 = empty([1, 2], float)
    R1[0] = 0.5*(r1 + r2 + 0.5*H*f(r2))

    # Now increase n until the required accuracy is reached
    error = 2*H*delta
    while error > H*delta:

        n += 1
        h = H/n

        # Modified midpoint method
        r1 = r + 0.5*h*f(r)
        r2 = r + h*f(r1)
        for i in range(n-1):
```

```
            r1 += h*f(r2)
            r2 += h*f(r1)

        # Calculate extrapolation estimates.  Arrays R1 and R2
        # hold the two most recent lines of the table
        R2 = R1
        R1 = empty([n, 2], float)
        R1[0] = 0.5*(r1 + r2 + 0.5*h*f(r2))
        for m in range(1, n):
            epsilon = (R1[m-1]-R2[m-1])/((n/(n-1))**(2*m)-1)
            R1[m] = R1[m-1] + epsilon
        error = abs(epsilon[0])  # epsilon[0] is theta error

    # Set r equal to the most accurate estimate we have,
    # before moving on to the next big step
    r = R1[n-1]

# Plot the results
plot(tpoints, thetapoints)
plot(tpoints, thetapoints, "b.")
show()
```



- Notes: This only calculates really accurate values for $x(t+H)$, not the region in between.
- Common practice (helps with efficiency/speed):
  - If your solution doesn't reach your tolerance level in some `nmax` steps (usually `nmax` $\sim 8-10$), half your interval and redo in smaller H regions.



Newman's fig. 8.11

- Iterate until your regions are small enough that you reach the tolerance level in `nmax` steps.
- "Adaptive" B-S Method!

4 Boundary Value Problems

4.1 Shooting method

- Suppose we wanted to choose an initial velocity v_0 for a projectile to land after $t_l = 10$ s.
- x(v_0, t) is a nonlinear function of v_0, and finding $x(v_0, t = t_l)$ can be done using root finding method (binary search, secant...)
- **Shooting method:** integrate the equations and adjust v_0 until you locate root.

In [ ]:
```
# %load throw.py
from numpy import array, arange

g = 9.81  # Acceleration due to gravity
a = 0.0  # Initial time
b = 10.0  # Final time
N = 1000  # Number of Runge-Kutta steps
h = (b-a)/N  # Size of Runge-Kutta steps
target = 1e-10  # Target accuracy for binary search


def f(r):
    """Function for Runge-Kutta calculation"""
    x = r[0]
    y = r[1]
```

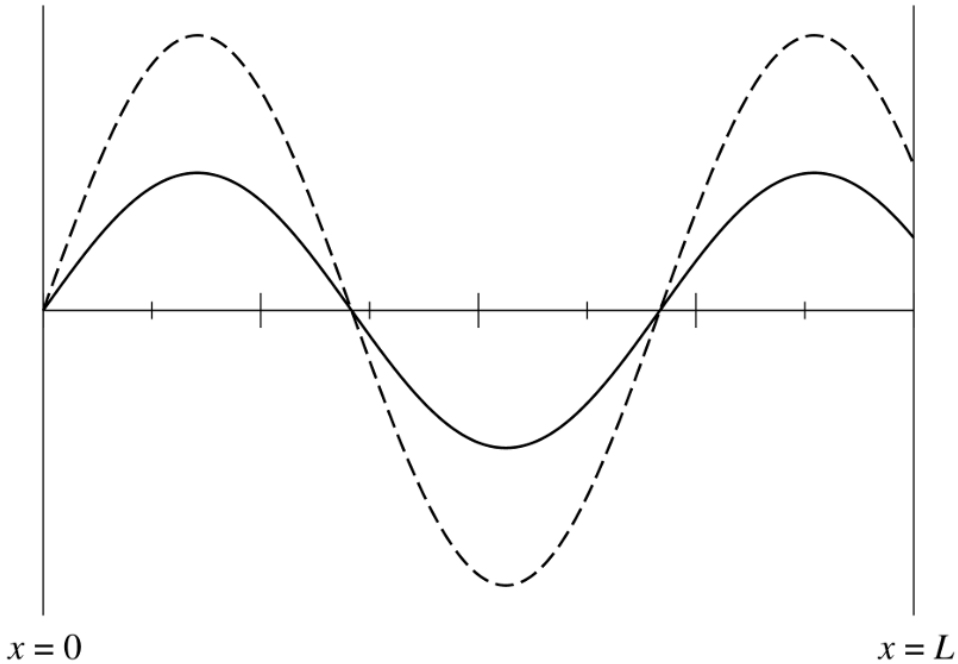
```
    fx = y
    fy = -g
    return array([fx, fy], float)


def height(v):
    """Function to solve the equation and calculate the final height"""
    r = array([0.0, v], float)
    for t in arange(a, b, h):
        k1 = h*f(r)
        k2 = h*f(r+0.5*k1)
        k3 = h*f(r+0.5*k2)
        k4 = h*f(r+k3)
        r += (k1+2*k2+2*k3+k4)/6
    return r[0]


# Main program performs a binary search
v1 = 0.01
v2 = 1000.0
h1 = height(v1)
h2 = height(v2)

while abs(h2-h1) > target:
    vp = (v1+v2)/2
    hp = height(vp)
    if h1*hp > 0:
        v1 = vp
        h1 = hp
    else:
        v2 = vp
        h2 = hp

v = (v1+v2)/2
print("The required initial velocity is", v, "m/s")
```

4.2 Eigenvalue problems

$$-\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi,$$
$$\psi(x=0) = \psi(x=L) = 0.$$

- But this approach does not work for finding wavefunctions that satisfy two boundary conditions, as in QM square well, except for valid eigenvalues E.

- So for these problems, E is the parameter that must be varied instead of the leftmost slope of wavefunction.



Newman's fig. 8.12

5 A word on stability

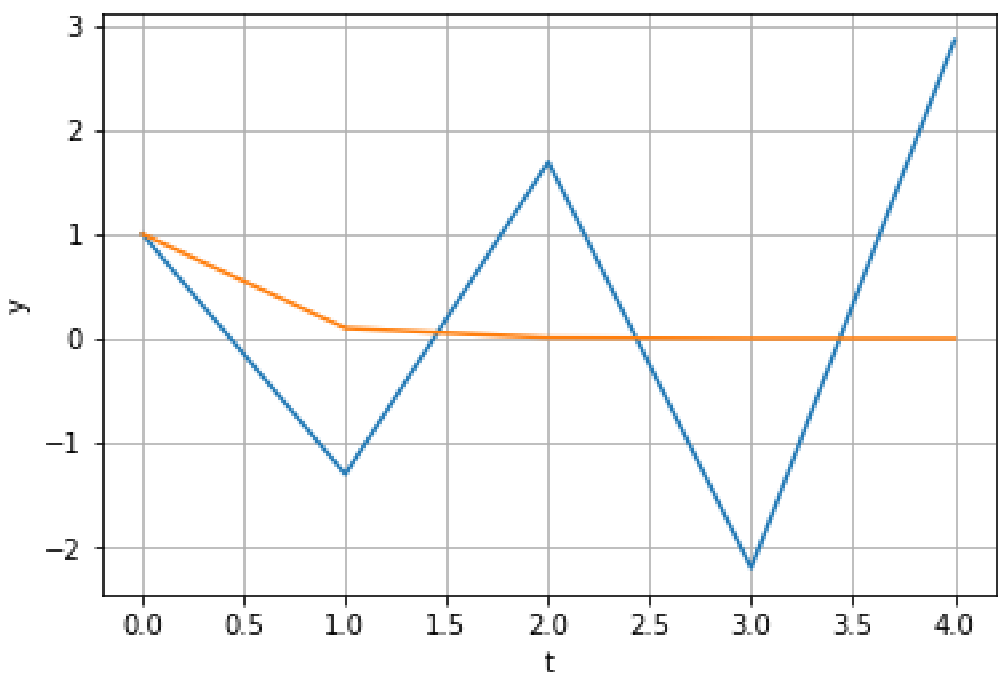
- We have focused on accuracy and speed in investigating our solutions to ODEs.
- But stability is also important. The stability of solutions tells us how fast initially close solutions diverge from each other.
- Some systems are inherently unstable and so will always be challenging to simulate.

- Stability or instability of a system can be determined from small perturbations to a solution of the ODE.
- But even for stable systems, numerical methods can be unstable and give truncation errors that grow.
- Example: $y' = -2.3y$ is a stable system (tends to a finite number). Forward Euler stable for $h = 0.7$ but unstable for $h = 1$.

In [5]:
```
import numpy as np

y0 = 1.
a = 0.
b = 5.
h = 1.
N = int((b-a)/h)

y = np.empty(N)
time = np.zeros(N)  # I will use this for plotting
y[0] = y0
for k in range(1, N):
```

```
        time[k] = k*h
        y[k] = y[k-1] + h*(-2.3*y[k-1])  # Euler time step

    y_a = np.exp(-2.3*time)  # analytical solution
```

```
In [6]: import matplotlib.pyplot as plt
        plt.figure()
        plt.plot(time, y, label='Euler, h={0:.1f}'.format(h))
        plt.plot(time, y_a, label='Analytical')
        plt.xlabel('t')
        plt.ylabel('y')
        plt.grid()
```



- Why is forward Euler unstable in some cases?
- Explicitly write the solution: for each time step,

$$y_{k+1} = y_k + h_k \lambda y_k \qquad \text{(here, } \lambda = -2.3\text{)}$$

- And for k time steps,

$$y_k = (1 + h_k \lambda)^k y_0.$$

- For the method to be stable, the magnitude of growth factor

$$|1 + h_k \lambda| \leq 1 \quad \Rightarrow \quad \lambda < 0,\ h_k \leq |2/\lambda|.$$

- We will investigate more of this in the coming labs.