Notebook

September 6, 2017

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2 Solving Ordinary Differential Equations with the Runge-Kutta Methods

2.1 List of Problems

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2.2 Objectives

In this lab, you will explore Runge-Kutta methods for solving ordinary differential equations. The goal is to gain a better understanding of some of the more popular Runge-Kutta methods and the corresponding numerical code.

Specifically you will be able to:

- describe the mid-point method
- construct a Runge-Kutta tableau from equations or equations from a tableau
- describe how a Runge-Kutta method estimates truncation error
- edit a working Octave code to use a different method or solve a different problem

2.3 Readings

There is no required reading for this lab, beyond the contents of the lab itself. However, if you would like additional background on any of the following topics, then refer to the sections indicated below.

Runge-Kutta Methods:

```
-   Newman, Chapter 8

-   Press, et al.  Section 16.1

-   Burden & Faires  Section 5.4
```

2.4 Introduction

Ordinary differential equations (ODEs) arise in many physical situations. For example, there is the first-order Newton cooling equation discussed in , and perhaps the most famous equation of all, the second-order Newton's Second Law of Mechanics $F = ma$.

In general, higher-order equations, such as Newton's force equation, can be rewritten as a system of first-order equations . So the generic problem in ODEs is a set of N coupled first-order differential equations of the form,

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

where $\mathbf{y}$ is a vector of variables.

For a complete specification of the solution, boundary conditions for the problem must be given. Typically, the problems are broken up into two classes:

- **Initial Value Problem (IVP)**: the initial values of $\mathbf{y}$ are specified.

- **Boundary Value Problem (BVP)**: **y** is specified at the initial and final times.

For this lab, we are concerned with the IVP's. BVP's tend to be much more difficult to solve and involve techniques which will not be dealt with in this set of labs.

Now as was pointed out in , in general, it will not be possible to find exact, analytic solutions to the ODE. However, it is possible to find an approximate solution with a finite difference scheme such as the forward Euler method . This is a simple first-order, one-step scheme which is easy to implement. However, this method is rarely used in practice as it is neither very stable nor accurate.

The higher-order Taylor methods discussed in are one alternative but involve higher-order derivatives that must be calculated by hand or worked out numerically in a multi-step scheme. Like the forward Euler method, stability is a concern.

The Runge-Kutta methods are higher-order, one-step schemes that makes use of information at different *stages* between the beginning and end of a step. They are more stable and accurate than the forward Euler method and are still relatively simple compared to schemes such as the multi-step predictor-corrector methods or the Bulirsch-Stoer method. Though they lack the accuracy and efficiency of these more sophisticated schemes, they are still powerful methods that almost always succeed for non-stiff IVPs.

2.5 Runge-Kutta methods

2.5.1 The Midpoint Method: A Two-Stage Runge-Kutta Method

The forward Euler method takes the solution at time t_n and advances it to time t_{n+1} using the value of the derivative $f(y_n, t_n)$ at time t_n

$$y_{n+1} = y_n + hf(y_n, t_n)$$

where $h \equiv \Delta t$.

```
In [41]: from IPython.display import Image
         Image(filename="images/euler.png")
```

```
Out[41]:
```

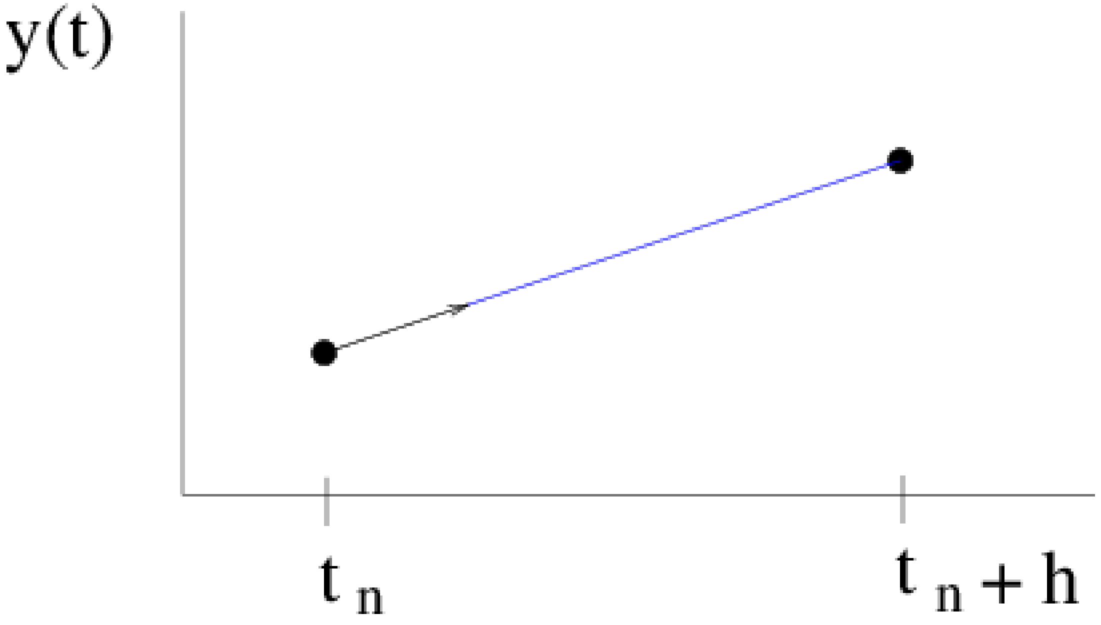


Figure euler: The forward Euler method is essentially a straight-line approximation to the solution, over the interval of one step, using the derivative at the starting point as the slope.

The idea of the Runge-Kutta schemes is to take advantage of derivative information at the times between t_n and t_{n+1} to increase the order of accuracy.

For example, in the midpoint method, the derivative at the initial time is used to approximate the derivative at the midpoint of the interval, $f(y_n + \frac{1}{2}hf(y_n, t_n), t_n + \frac{1}{2}h)$. The derivative at the midpoint is then used to advance the solution to the next step. The method can be written in two *stages* k_i,

$$\begin{aligned} k_1 &= hf(y_n, t_n) \\ k_2 &= hf(y_n + \tfrac{1}{2}k_1, t_n + \tfrac{1}{2}h) \quad \text{eq : midpoint} \\ y_{n+1} &= y_n + k_2 \end{aligned}$$

The midpoint method is known as a 2-stage Runge-Kutta formula.

```
In [42]: Image(filename='images/midpoint.png')
```

```
Out[42]:
```

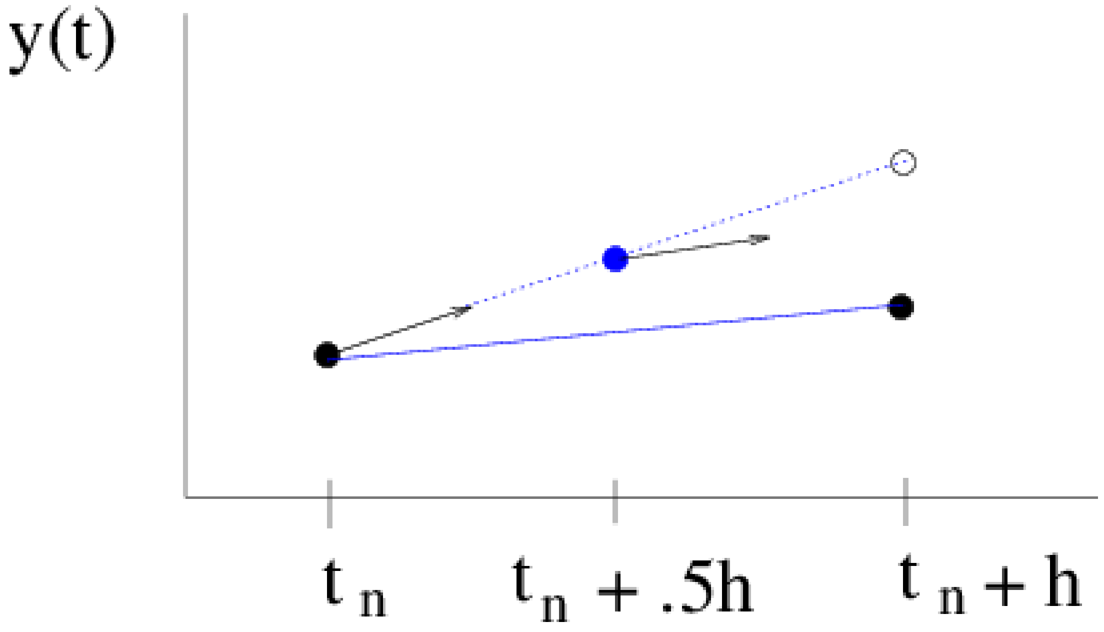


Figure midpoint: The midpoint method again uses the derivative at the starting point to approximate the solution at the midpoint. The derivative at the midpoint is then used as the slope of the straight-line approximation.

2.5.2 Second-Order Runge-Kutta Methods

As was shown in lab 2 , the error in the forward Euler method is proportional to h. In other words, the forward Euler method has an accuracy which is *first order* in h.

The advantage of the midpoint method is that the extra derivative information at the midpoint results in the first order error term cancelling out, making the method *second order* accurate. This can be shown by a Taylor expansion of equation Section **??**

Problem midpoint: Even though the midpoint method is second-order accurate, it may still be less accurate than the forward Euler method. In the demo below, compare the accuracy of the two methods on the initial value problem

$$\frac{dy}{dt} = -y + t + 1, \quad y(0) = 1 \;\; \textbf{eq: linexp}$$

which has the exact solution

$$y(t) = t + e^{-t}$$

1. Why is it possible that the midpoint method may be less accurate than the forward Euler method, even though it is a higher order method?

2. Based on the numerical solutions of (eq: linexp), which method appears more accurate?

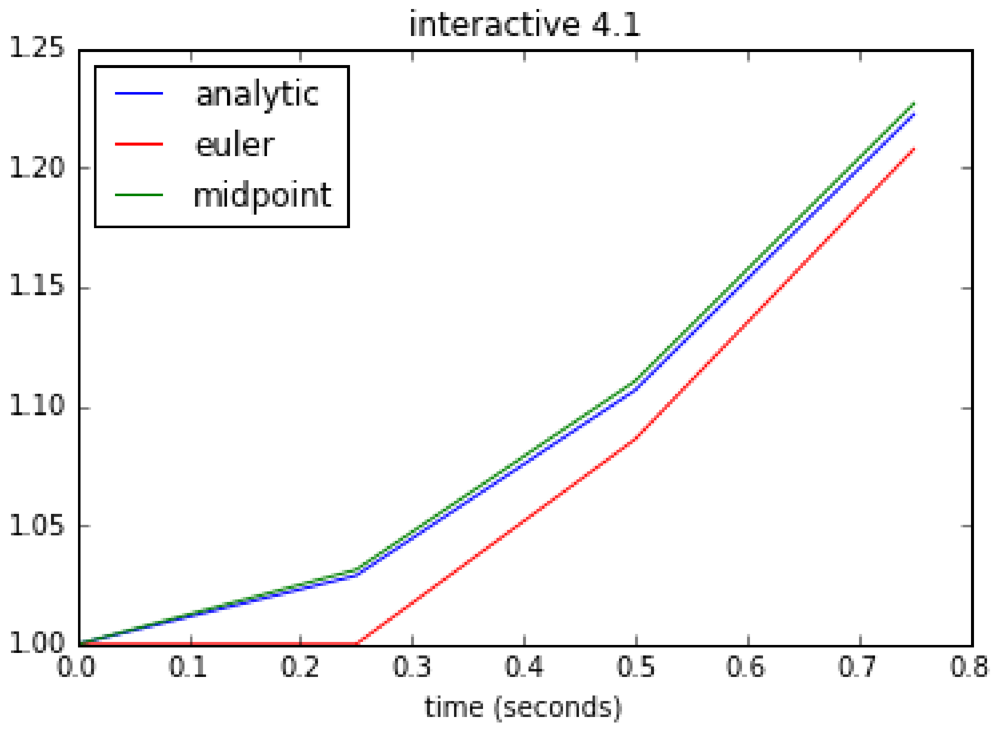
3. Cut the stepsize in half and check the error at a given time. Repeat a couple of more times. How does the error drop relative to the change in stepsize?

4. How do the numerical solutions compare to $y(t) = t + e^{-t}$ when you change the initial time? Why?

```
In [43]: %matplotlib inline
         from numlabs.lab4.lab4_functions import initinter41,eulerinter41,midpointinter41
         import numpy as np
         from matplotlib import pyplot as plt

         initialVals={'yinitial': 1,'t_beg':0.,'t_end':1.,'dt':0.25,'c1':-1.,'c2':1.,'c3':1.}
         coeff = initinter41(initialVals)
         timeVec=np.arange(coeff.t_beg,coeff.t_end,coeff.dt)
         nsteps=len(timeVec)
         ye=[]
         ym=[]
         y=coeff.yinitial
         ye.append(coeff.yinitial)
         ym.append(coeff.yinitial)
         for i in np.arange(1,nsteps):
             ynew=eulerinter41(coeff,y,timeVec[i-1])
             ye.append(ynew)
             ynew=midpointinter41(coeff,y,timeVec[i-1])
             ym.append(ynew)
             y=ynew
         analytic=timeVec + np.exp(-timeVec)
         theFig,theAx=plt.subplots(1,1)
         l1=theAx.plot(timeVec,analytic,'b-',label='analytic')
         theAx.set_xlabel('time (seconds)')
         l2=theAx.plot(timeVec,ye,'r-',label='euler')
         l3=theAx.plot(timeVec,ym,'g-',label='midpoint')
         theAx.legend(loc='best')
         theAx.set_title('interactive 4.1')

Out[43]: <matplotlib.text.Text at 0x1145690b8>
```



In general, an *explicit* 2-stage Runge-Kutta method can be written as,

$$k_1 = hf(y_n, t_n)$$
$$k_2 = hf(y_n + b_{21}k_1, t_n + a_2 h) \quad \textbf{eq: explicitrk2}$$
$$y_{n+1} = y_n + c_1 k_1 + c_2 k_2$$

The scheme is said to be *explicit* since a given stage does not depend *implicitly* on itself, as in the backward Euler method , or on a later stage.

Other explicit second-order schemes can be derived by comparing the formula Section **??** to the second-order Taylor method and matching terms to determine the coefficients a_2, b_{21}, c_1 and c_2.

See Section **??** for the derivation of the midpoint method.

2.5.3 The Runge-Kutta Tableau

A general s-stage Runge-Kutta method can be written as,

$$k_i = hf(y_n + \sum_{j=1}^{s} b_{ij}k_j, t_n + a_i h), \quad i = 1, ..., s$$
$$y_{n+1} = y_n + \sum_{j=1}^{s} c_j k_j$$

An *explicit* Runge-Kutta method has $b_{ij} = 0$ for $i \leq j$, i.e. a given stage k_i does not depend on itself or a later stage k_j.

The coefficients can be expressed in a tabular form known as the Runge-Kutta tableau.

i	a_i	b_{ij}				c_i
1	a_1	b_{11}	b_{12}	...	b_{1s}	c_1
2	a_2	b_{21}	b_{22}	...	b_{2s}	c_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
s	a_s	b_{s1}	b_{s2}	...	b_{ss}	c_s
$j =$		1 2		...	s	

An explicit scheme will be strictly lower-triangular.
For example, a general 2-stage Runge-Kutta method,

$$\begin{aligned}
k_1 &= hf(y_n + b_{11}k_1 + b_{12}k_2, t_n + a_1 h) \\
k_2 &= hf(y_n + b_{21}k_1 + b_{22}k_2, t_n + a_2 h) \\
y_{n+1} &= y_n + c_1 k_1 + c_2 k_2
\end{aligned}$$

has the coefficients,

i	a_i	b_{ij}		c_i
1	a_1	b_{11}	b_{12}	c_1
2	a_2	b_{21}	b_{22}	c_2
$j =$		1	2	

In particular, the midpoint method is given by the tableau,

i	a_i	b_{ij}		c_i
1	0	0	0	0
2	$\frac{1}{2}$	$\frac{1}{2}$	0	1
$j =$		1	2	

Problem tableau Write out the tableau for

1. Section **??**
2. the fourth-order Runge-Kutta method ([lab4:eq:rk4]) discussed in the next section.

2.5.4 Explicit Fourth-Order Runge-Kutta Method

Explicit Runge-Kutta methods are popular as each stage can be calculated with one function evaluation. In contrast, implicit Runge-Kutta methods usually involves solving a non-linear system of equations in order to evaluate the stages. As a result, explicit schemes are much less expensive to implement than implicit schemes.

However, there are cases in which implicit schemes are necessary and that is in the case of *stiff* sets of equations. See section 16.6 of Press et al. for a discussion. For these labs, we will focus on non-stiff equations and on explicit Runge-Kutta methods.

The higher-order Runge-Kutta methods can be derived by in manner similar to the midpoint formula. An s-stage method is compared to a Taylor method and the terms are matched up to the desired order.

Methods of order $M > 4$ require $M + 1$ or $M + 2$ function evaluations or stages, in the case of explicit Runge-Kutta methods. As a result, fourth-order Runge-Kutta methods have achieved great popularity over the years as they require only four function evaluations per step. In particular, there is the classic fourth-order Runge-Kutta formula:

$$\begin{aligned}
k_1 &= hf(y_n, t_n)\\
k_2 &= hf(y_n + \tfrac{k_1}{2}, t_n + \tfrac{h}{2})\\
k_3 &= hf(y_n + \tfrac{k_2}{2}, t_n + \tfrac{h}{2})\\
k_4 &= hf(y_n + k_3, t_n + h)\\
y_{n+1} &= y_n + \tfrac{k_1}{6} + \tfrac{k_2}{3} + \tfrac{k_3}{3} + \tfrac{k_4}{6}
\end{aligned}$$

Problem rk4: In the demo below, compare compare solutions to the test problem (eq: test)

$$\frac{dy}{dt} = -y + t + 1, \quad y(0) = 1 \quad \textbf{eq : test}$$

generated with the fourth-order Runge-Kutta method to solutions generated by the forward Euler and midpoint methods.

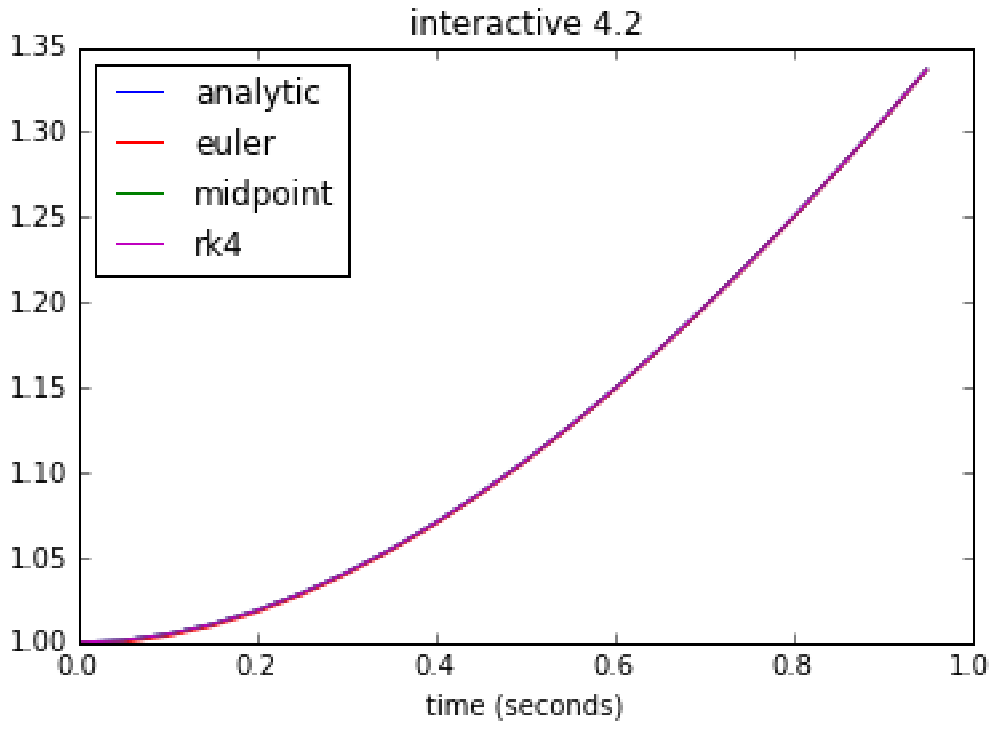
1. Based on the numerical solutions of (eq: test), which of the three methods appears more accurate?

2. Again determine how the error changes relative to the change in stepsize, as the stepsize is halved.

```
In [44]: from numlabs.lab4.lab4_functions import initinter41,eulerinter41,midpointinter41,\
                                                rk4ODEinter41
         initialVals={'yinitial': 1,'t_beg':0.,'t_end':1.,'dt':0.05,'c1':-1.,'c2':1.,'c3':1.}
         coeff = initinter41(initialVals)
         timeVec=np.arange(coeff.t_beg,coeff.t_end,coeff.dt)
         nsteps=len(timeVec)
         ye=[]
         ym=[]
         yrk=[]
         y=coeff.yinitial
         ye.append(coeff.yinitial)
         ym.append(coeff.yinitial)
         yrk.append(coeff.yinitial)
         for i in np.arange(1,nsteps):
             ynew=eulerinter41(coeff,y,timeVec[i-1])
             ye.append(ynew)
             ynew=midpointinter41(coeff,y,timeVec[i-1])
             ym.append(ynew)
             ynew=rk4ODEinter41(coeff,y,timeVec[i-1])
             yrk.append(ynew)
             y=ynew
         analytic=timeVec + np.exp(-timeVec)
         theFig=plt.figure(0)
         theFig.clf()
         theAx=theFig.add_subplot(111)
         l1=theAx.plot(timeVec,analytic,'b-',label='analytic')
         theAx.set_xlabel('time (seconds)')
```

```
l2=theAx.plot(timeVec,ye,'r-',label='euler')
l3=theAx.plot(timeVec,ym,'g-',label='midpoint')
l4=theAx.plot(timeVec,yrk,'m-',label='rk4')
theAx.legend(loc='best')
theAx.set_title('interactive 4.2')
```

```
Out[44]: <matplotlib.text.Text at 0x1146ced30>
```



2.5.5 Embedded Runge-Kutta Methods: Estimate of the Truncation Error

It is possible to find two methods of different order which share the same stages k_i and differ only in the way they are combined, i.e. the coefficients c_i. For example, the original so-called embedded Runge-Kutta scheme was discovered by Fehlberg and consisted of a fourth-order scheme and fifth-order scheme which shared the same six stages.

In general, a fourth-order scheme embedded in a fifth-order scheme will share the stages

$$\begin{aligned}
&k_1 = hf(y_n, t_n)\\
&k_2 = hf(y_n + b_{21}k_1, t_n + a_2 h)\\
&\vdots\\
&k_6 = hf(y_n + b_{51}k_1 + ... + b_{56}k_6, t_n + a_6 h)
\end{aligned}$$

The fifth-order formula takes the step:

$$y_{n+1} = y_n + c_1k_1 + c_2k_2 + c_3k_3 + c_4k_4 + c_5k_5 + c_6k_6$$

while the embedded fourth-order formula takes a different step:

$$y^*_{n+1} = y_n + c^*_1 k_1 + c^*_2 k_2 + c^*_3 k_3 + c^*_4 k_4 + c^*_5 k_5 + c^*_6 k_6$$

If we now take the difference between the two numerical estimates, we get an estimate Δ_{spec} of the truncation error for the fourth-order method,

$$\Delta_{\text{est}}(i) = y_{n+1}(i) - y^*_{n+1}(i) = \sum_{i=1}^{6}(c_i - c^*_i)k_i$$

This will prove to be very useful in the next lab where we provide the Runge-Kutta algorithms with adaptive stepsize control. The error estimate is used as a guide to an appropriate choice of stepsize.

An example of an embedded Runge-Kutta scheme was found by Cash and Karp and has the tableau:

i	a_i	b_{ij}						c_i	c^*_i
1								$\frac{37}{378}$	$\frac{2825}{27648}$
2	$\frac{1}{5}$	$\frac{1}{5}$						0	0
3	$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$					$\frac{250}{621}$	$\frac{18575}{48384}$
4	$\frac{3}{5}$	$\frac{3}{10}$	$-\frac{9}{10}$	$\frac{6}{5}$				$\frac{125}{594}$	$\frac{13525}{55296}$
5	1	$-\frac{11}{54}$	$\frac{5}{2}$	$-\frac{70}{27}$	$\frac{35}{27}$			0	$\frac{277}{14336}$
6	$\frac{7}{8}$	$\frac{1631}{55296}$	$\frac{175}{512}$	$\frac{575}{13824}$	$\frac{44275}{110592}$	$\frac{253}{4096}$		$\frac{512}{1771}$	$\frac{1}{4}$
$j =$		1	2	3	4	5	6		

Problem embedded Though the error estimate is for the embedded fourth-order Runge-Kutta method, the fifth-order method can be used in practice for calculating the solution, the assumption being the fifth-order method should be at least as accurate as the fourth-order method. In the demo below, compare solutions of the test problem (eq: test2])

$$\frac{dy}{dt} = -y + t + 1, \quad y(0) = 1 \quad \textbf{eq : test2}$$

generated by the fifth-order method with solutions generated by the standard fourth-order Runge-Kutta method. Which method is more accurate? Again, determine how the error decreases as you halve the stepsizes.

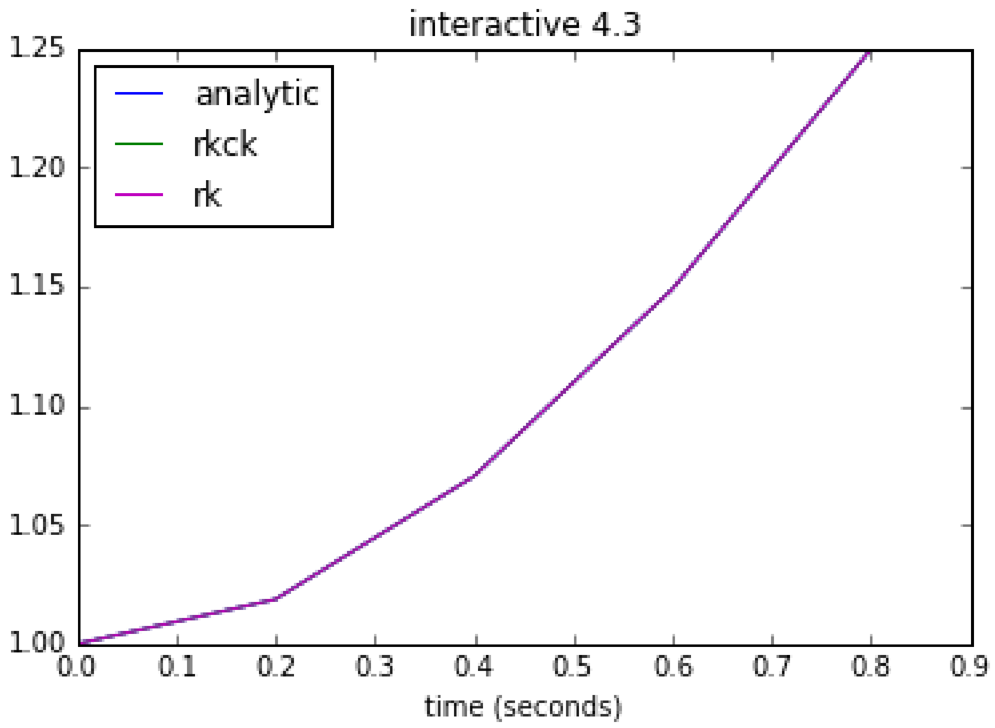
```
In [45]: import numpy as np
         from matplotlib import pyplot as plt

         from numlabs.lab4.lab4_functions import initinter41,rk4ODEinter41,rkckODEinter41
         initialVals={'yinitial': 1,'t_beg':0.,'t_end':1.,'dt':0.2,'c1':-1.,'c2':1.,'c3':1.}
         coeff = initinter41(initialVals)

         timeVec=np.arange(coeff.t_beg,coeff.t_end,coeff.dt)
         nsteps=len(timeVec)
         ye=[]
         ym=[]
         yrk=[]
         yrkck=[]
```

```
y1=coeff.yinitial
y2=coeff.yinitial
yrk.append(coeff.yinitial)
yrkck.append(coeff.yinitial)
for i in np.arange(1,nsteps):
    ynew=rk4ODEinter41(coeff,y1,timeVec[i-1])
    yrk.append(ynew)
    y1=ynew
    ynew=rkckODEinter41(coeff,y2,timeVec[i-1])
    yrkck.append(ynew)
    y2=ynew
analytic=timeVec + np.exp(-timeVec)
theFig,theAx=plt.subplots(1,1)
l1=theAx.plot(timeVec,analytic,'b-',label='analytic')
theAx.set_xlabel('time (seconds)')
l2=theAx.plot(timeVec,yrkck,'g-',label='rkck')
l3=theAx.plot(timeVec,yrk,'m-',label='rk')
theAx.legend(loc='best')
theAx.set_title('interactive 4.3')
```

```
Out[45]: <matplotlib.text.Text at 0x1148d59e8>
```



2.6 Python: moving from a notebook to a library

If we want our ODE routines to be more generally useful, we need to lift two restrictions from the code:

1. Inital conditions are currently specified in the main script as a dictionary, e.g.:

   ```
   initialVals={'yinitial': 1,'t_beg':0.,'t_end':1.,
                'dt':0.2,'c1':-1.,'c2':1.,'c3':1.}
   ```

   and then converted to a named tuple in initinter41

   We need to move this into an external configuration file that we can keep track of using version control, so we can keep the library code and the input and output files in separate folders and keep a record of our runs.

2. The derivatives are hardwired into the library, for example in eulerinter41, . We need to be able to have integrators work with any derivative function.

2.6.1 Writing a config file

Python has a variety of configuration libraries, including configparser in the standard library. This is overkill, however, for our simple programs. We just need a way to input and output a dictionary in human readable form. One example of how to do this is write_init.py:

```
"""
  write the initial condition file for the simple oscillator
  example
"""

import json

initialVals={'yinitial': [0.,1.],'t_beg':0.,'t_end':40.,'dt':0.1,'c1':0.,'c2':1.}
initialVals['comment'] = 'written Sep. 29, 2015'
initialVals['plot_title'] = 'simple damped oscillator run 1'

with open('run_1.json','w') as f:
      f.write(json.dumps(initialVals,indent=4))
```

When you run this from the command line or IPython with:

```
In [19]: run write_init
```

you get a json Javascript Object Notation file that looks like this:

```
{
    "t_beg": 0.0,
    "c1": 0.0,
```

```
        "c2": 1.0,
        "t_end": 40.0,
        "dt": 0.1,
        "plot_title": "simple damped oscillator run 1",
        "comment": "written Sep. 29, 2015",
        "yinitial": [
            0.0,
            1.0
        ]
    }
```

This format is simple enough to change with a text editor.
To load this into a program, do something like read_init.py:

```
import json
from collections import namedtuple

with open('run_1.json','r') as f:
      init_dict=json.load(f)

print('as a dictionary:\n{}\n'.format(init_dict))

#either use this as a dict or convert to a namedtuple
initvals=namedtuple('initvals','dt c1 c2 t_beg t_end yinitial comment plot_title')
theCoeff=initvals(**init_dict)

print('as a namedtuple:\n{}'.format(theCoeff))
```

which produces:

```
In [21]: run read_init
as a dictionary:
{'yinitial': [0.0, 1.0], 'c2': 1.0, 'plot_title': 'simple damped oscillator run 1', 'comment': '

as a namedtuple:
initvals(dt=0.1, c1=0.0, c2=1.0, t_beg=0.0, t_end=40.0, yinitial=[0.0, 1.0], comment='written Se
```

2.6.2 Passing a derivative function to an integrator

In python, functions are first class objects, which means you can pass them around like any other datatype, no need to get function handles as in matlab or Fortran. The integrators in test.py have been written to accept a derivative function of the form:

```
def derivs4(coeff, y):
```

i.e. as long as the derivative can be written in terms of coefficients and the previous value of y, the integrator will move the ode ahead one timestep. If we wanted coefficients that were a function of time, we would need to also include those functions the coeff namedtuple, and add keep track of the timestep through the integration.

Here's an example using foward euler to integrate the harmonic oscillator

```
In [46]: %matplotlib inline

         import json
         from numlabs.lab4.example.test import read_init,euler4
         #
         # specify the derivs function
         #
         def derivs(coeff, y):
           f=np.empty_like(y) #create a 2 element vector to hold the derivitive
           f[0]=y[1]
           f[1]= -1.*coeff.c1*y[1] - coeff.c2*y[0]
           return f
         #
         # first make sure we have an input file in this directory
         #
         initialVals={'yinitial': [0.,1.],'t_beg':0.,'t_end':40.,'dt':0.1,'c1':0.,'c2':1.}
         initialVals['comment'] = 'written Sep. 29, 2015'
         initialVals['plot_title'] = 'simple damped oscillator run 1'

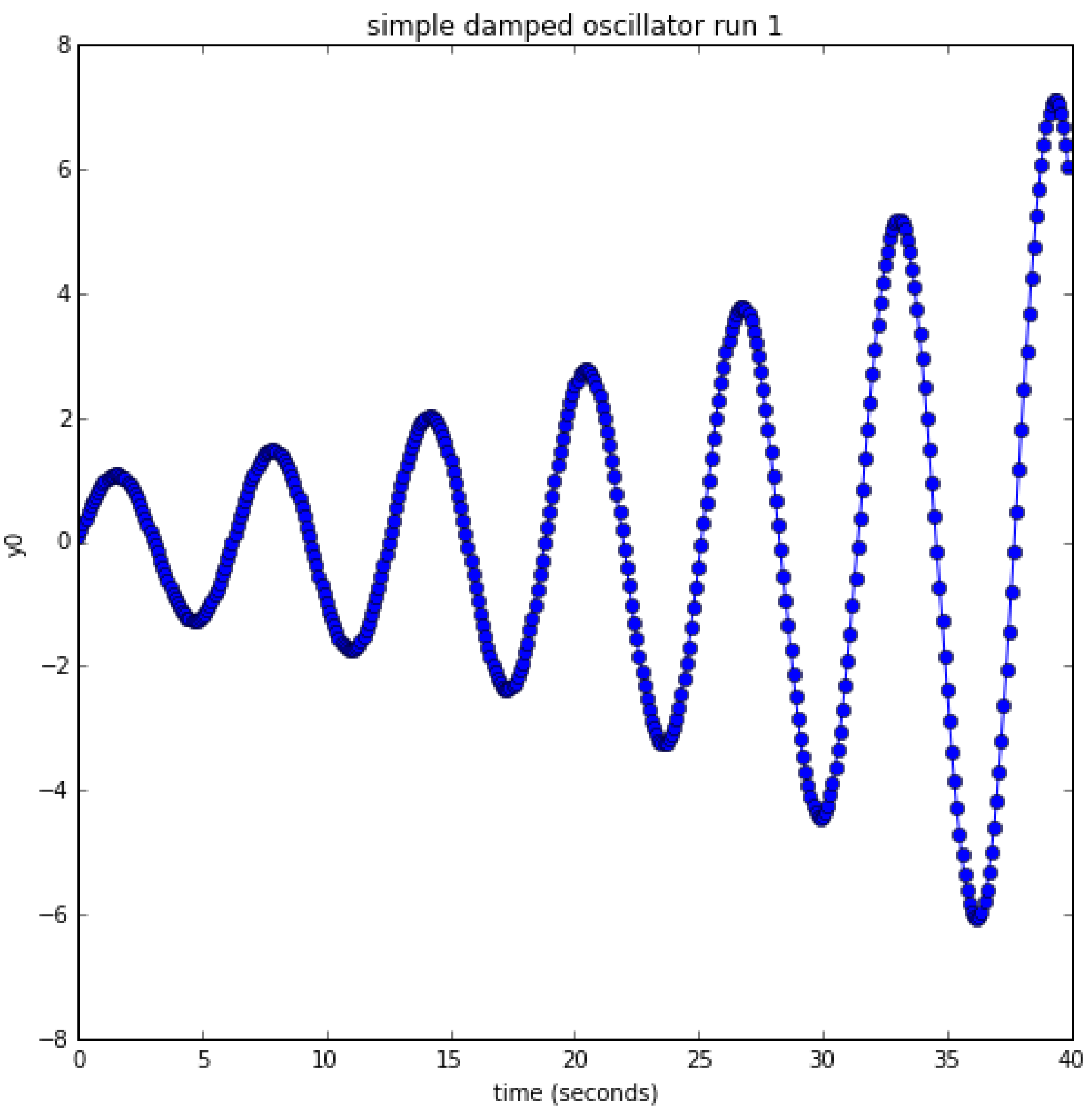
         infile='run_1.json'
         with open(infile,'w') as f:
               f.write(json.dumps(initialVals,indent=4))
         #
         #  now read the initial information into a namedtuple coeff
         #

         infile='run_1.json'
         coeff=read_init(infile)

         #
         # integrate and save the result in savedata
         #
         time=np.arange(coeff.t_beg,coeff.t_end,coeff.dt)
         y=coeff.yinitial
         nsteps=len(time)
         savedata=np.empty([nsteps],np.float64)
         for i in range(nsteps):
             y=euler4(coeff,y,derivs)
             savedata[i]=y[0]

         theFig,theAx=plt.subplots(1,1,figsize=(8,8))
         theAx.plot(time,savedata,'o-')
         theAx.set_title(coeff.plot_title)
         theAx.set_xlabel('time (seconds)')
         theAx.set_ylabel('y0')

Out[46]: <matplotlib.text.Text at 0x1149a8eb8>
```



problem coding A Try out the lab4 example:

As set up above, test.py solved the damped, harmonic oscillator with the (unstable) forward Euler method.

1. Write a new routine that solves the harmonic oscilator using Section **??** along the lines of the routines in lab4_functions.py

   Hand in a notebook with the code and a plot.

problem coding B

1. Now solve the following test equation by both the midpoint and Heun's method and compare.

$$f(y,t) = t - y + 1.0$$

Choose two sets of initial conditions and investigate the behaviour.

2. Is there any difference between the two methods when applied to either problem? Should there be? Explain by analyzing the steps that each method is taking.

problem coding C

6. Solve the Newtonian cooling equation of lab 1 by any of the above methods.

7. Hand in some sample plots along with the parameter values and initial conditions used.

2.7 Mathematical Notes

2.7.1 Note on the Derivation of the Second-Order Runge-Kutta Methods

A general s-stage Runge-Kutta method can be written as,

$$\begin{aligned} k_i &= hf(y_n + \sum_{j=1}^{s} b_{ij}k_j, t_n + a_i h), \quad i = 1, ..., s \\ y_{n+1} &= y_n + \sum_{j=1}^{s} c_j k_j \end{aligned}$$

where
$\sum_{j=1}^{s} b_{ij} = a_i$.

In particular, an *explicit* 2-stage Runge-Kutta method can be written as,

$$\begin{aligned} k_1 &= hf(y_n, t_n) \\ k_2 &= hf(y_n + ak_1, t_n + ah) \\ y_{n+1} &= y_n + c_1k_1 + c_2k_2 \end{aligned}$$

where
$b_{21} = a_2 \equiv a$.

So we want to know what values of a, c_1 and c_2 leads to a second-order method, i.e. a method with an error proportional to h^3.

To find out, we compare the method against a second-order Taylor expansion,

$$y(t_n + h) = y(t_n) + hy'(t_n) + \frac{h^2}{2}y''(t_n) + O(h^3)$$

So for the y_{n+1} to be second-order accurate, it must match the Taylor method. In other words, $c_1k_1 + c_2k_2$ must match $hy'(t_n) + \frac{h^2}{2}y''$. To do this, we need to express k_1 and k_2 in terms of derivatives of y at time t_n.

First note, $k_1 = hf(y_n, t_n) = hy'(t_n)$.

Next, we can expand k_2 about $(y_n.t_n)$,

$$k_2 = hf(y_n + ak_1, t_n + ah) = h(f + haf_t + haf_y y' + O(h^2))$$

However, we can write y'' as,

$$y'' = \frac{df}{dt} = f_t + f_y y'$$

This allows us to rewrite k_2 in terms of y'',

$$k_2 = h(y' + hay'' + O(h^2))$$

Substituting these expressions for k_i back into the Runge-Kutta formula gives us,

$$y_{n+1} = y_n + c_1 hy' + c_2 h(y' + hay'')$$

or

$$y_{n+1} = y_n + h(c_1 + c_2)y' + h^2(c_2 a)y''$$

If we compare this against the second-order Taylor method, we see that we need,

$$\begin{aligned} c_1 + c_2 &= 1 \\ ac_2 &= \tfrac{1}{2} \end{aligned}$$

for the Runge-Kutta method to be second-order.

If we choose $a = 1/2$, this implies $c_2 = 1$ and $c_1 = 0$. This gives us the midpoint method.

However, note that other choices are possible. In fact, we have a *one-parameter family* of second-order methods. For example if we choose, $a = 1$ and $c_1 = c_2 = \frac{1}{2}$, we get the *modified Euler method,*

$$\begin{aligned} k_1 &= hf(y_n, t_n) \\ k_2 &= hf(y_n + k_1, t_n + h) \\ y_{n+1} &= y_n + \tfrac{1}{2}(k_1 + k_2) \end{aligned}$$

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while the choice
```

$a = \frac{2}{3}$, $c_1 = \frac{1}{4}$ and $c_2 = \frac{3}{4}$, gives us *Heun's method,*

$$\begin{aligned} k_1 &= hf(y_n, t_n) \\ k_2 &= hf(y_n + \tfrac{2}{3}k_1, t_n + \tfrac{2}{3}h) \\ y_{n+1} &= y_n + \tfrac{1}{4}k_1 + \tfrac{3}{4}k_2 \end{aligned}$$

2.8 Glossary

- **driver** A routine that calls the other routines to solve the problem.
- **embedded Runge-Kutta methods**: Two Runge-Kutta methods that share the same stages. The difference between the solutions give an estimate of the local truncation error.
- **explicit** In an explicit numerical scheme, the calculation of the solution at a given step or stage does not depend on the value of the solution at that step or on a later step or stage.
- **fourth-order Runge-Kutta method** A popular fourth-order, four-stage, explicit Runge-Kutta method.
- **implicit**: In an implicit numerical scheme, the calculation of the solution at a given step or stage does depend on the value of the solution at that step or on a later step or stage. Such methods are usually more expensive than implicit schemes but are better for handling stiff ODEs.

- **midpoint method** : A two-stage, second-order Runge-Kutta method.
- **stages**: The approximations to the derivative made in a Runge-Kutta method between the start and end of a step.
- **tableau** The tableau for a Runge-Kutta method organizes the coefficients for the method in tabular form.

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