Adaptive-time-stepping-v3

April 1, 2025

1 Adaptive time stepping

[166]:
```
# Load important libraries
import numpy as np
import matplotlib.pyplot as plt
```

1.0.1 Basic RK4

We implement simple RK4 and its caller function.

[167]:
```
# Basic Runge Kutta 4
def rk4(fn, x, y, h):
    k1 = h*fn(x, y)
    k2 = h*fn(x+h/2, y+k1/2)
    k3 = h*fn(x+h/2, y+k2/2)
    k4 = h*fn(x+h, y+k3)
    return y + (k1+2*k2+2*k3+k4)/6

# A caller function
def caller(my_method, fn, y_ini, x0, xT, h):
    # generate x values from x0 to xT
    xs = np.arange(x0, xT, h)

    # calculate the number of steps
    N = len(xs)

    # initialize y
    y = y_ini

    # initialize storage to keep y values
    ys = np.zeros((N, len(y_ini)))

    # for each i
    for i in range(N):
        ys[i,:] = y             # store y
        x = xs[i]               # get x
        y = my_method(fn,x,y,h)  # update y
```

```
    # return all y
    return ys
```

1.0.2 Apply on a simple ODE whose solution has a rapid change and a flat profile

The ODE function is

$$\frac{dy}{dx} = f(x, y) = -y$$

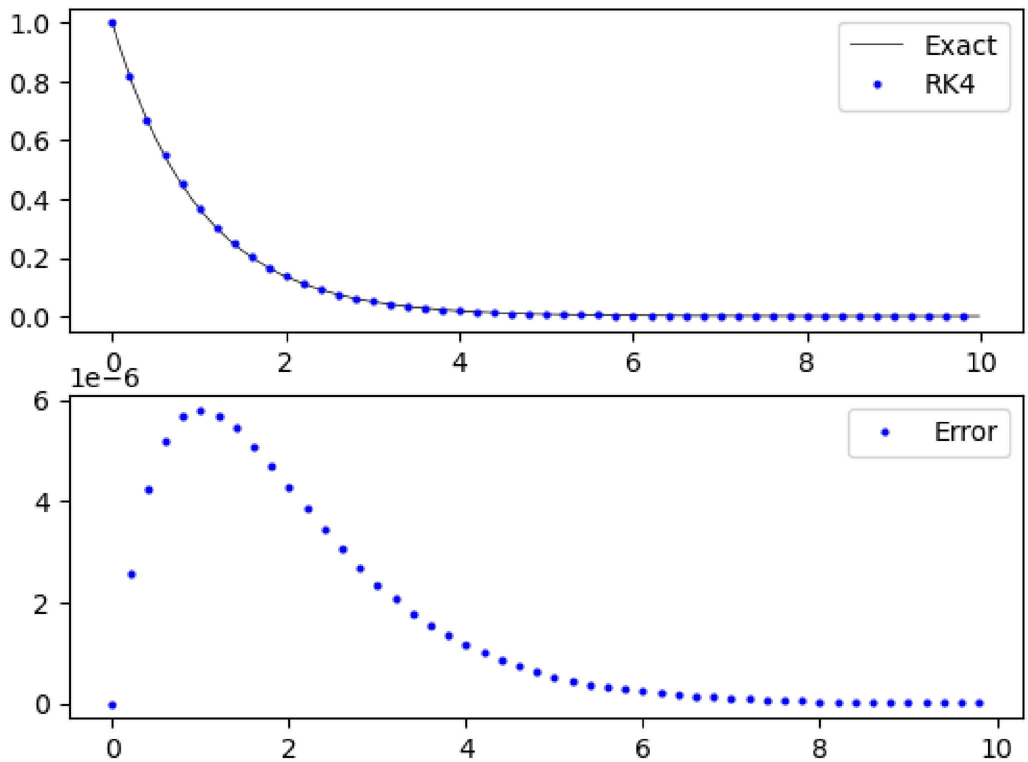
[168]:
```
# for dy/dx = f(x,y)
# define f(x,y)
def f(x, y):
    return -y

# Step size h
h = 0.2

# Time span
x0 = 0.0
xT = 10.0

# Generate x values (for plotting and comparison)
xs = np.arange(x0, xT, h)
N = len(xs)

# Initialize y
y_ini = np.asarray([1.0])

# Final call: returns y values
ysrk4 = caller(rk4, f, y_ini, x0, xT, h)
```

1.0.3 Plot the solution and also the error.

[169]:
```
# Finely sampled solution for drawing a line
xfine = np.arange(x0, xT, h/10)
yfine = np.exp(-xfine)

# Also the exact solution
yexact = np.exp(-xs)

# Plot using subplots
plt.subplot(2,1,1)
plt.plot(xfine, yfine, 'k-',linewidth=0.5,label='Exact')
plt.plot(xs, ysrk4,'bo',markersize=2,label='RK4')
plt.legend()
plt.subplot(2,1,2)
yerror = [ysrk4[i][0] - yexact[i] for i in range(len(yexact))]
plt.plot(xs, yerror,'bo',markersize=2,label='Error')
```

```python
plt.legend()
```

```
[169]: <matplotlib.legend.Legend at 0x7fa8cb7328d0>
```



1.1 Butcher tableau and RK methods

The Butcher tableau for a general $ s $-stage Runge-Kutta method is written as:

$$\begin{array}{c|c} a & B \\ \hline & c^T \end{array}$$

where: $+ a = (a\_1, a\_2, \ldots, a\_s)$ is the vector of node values (stage times). $+ B = (b\_\{ij\})$ is an $s \times s$ matrix of coefficients that define the intermediate steps, $+ c = (c\_1, c\_2, \ldots, c\_s)$ is the weight vector,

1.1.1 Summation Formulation

A general Runge-Kutta method computes the solution at $t\_\{n+1\}$ using intermediate stages:

$$y_{n+1} = y_n + h \sum_{i=1}^{s} c_i k_i$$

where the stage values k_i are computed as:

$$k_i = f\left(t_n + a_i h, y_n + h\sum_{j=1}^{s} b_{ij} k_j\right), \quad i = 1, 2, \ldots, s$$

Here: + h is the step size, + $f(t, y)$ represents the derivative function $\frac{dy}{dt}$, + k_i are the intermediate function evaluations.

[170]:
```
# Dormand-Prince in matrix form
a = [0.2, 0.3, 0.8, 8/9, 1.0, 1.0]
b = [
    [1/5, 0, 0, 0, 0, 0],
    [3/40, 9/40, 0, 0, 0, 0],
    [44/45, -56/15, 32/9, 0, 0, 0],
    [19372/6561, -25360/2187, 64448/6561, -212/729, 0, 0],
    [9017/3168, -355/33, 46732/5247, 49/176, -5103/18656, 0],
    [35/384, 0, 500/1113, 125/192, -2187/6784, 11/84]
]
c = [35/384, 0, 500/1113, 125/192, -2187/6784, 11/84, 0]

# Dormand-Prince
a2 = 1/5;  b21 = 1/5;
a3 = 3/10; b31 = 3/40;       b32 = 9/40;
a4 = 4/5;  b41 = 44/45;      b42 = -56/15;      b43 = 32/9;
a5 = 8/9;  b51 = 19372/6561; b52 = -25360/2187; b53 = 64448/6561; b54 =-212/729;
a6 = 1;    b61 = 9017/3168;  b62 = -355/33;     b63 = 46732/5247; b64 = 49/176; b65 = -5103/18656;
a7 = 1;    b71 = 35/384;     b72 = 0;           b73 = 500/1113;   b74 = 125/192; b75 = -2187/6784;  b76 = 11/84;

c1 = 35/384; c2 = 0; c3 = 500/1113; c4 = 125/192; c5=-2187/6784; c6 = 11/84; c7 = 0;
c1s = 5179/57600; c2s = 0; c3s = 7571/16695; c4s = 393/640; c5s = -92097/339200; c6s = 187/2100; c7s = 1/40;
```

1.1.2 An implementation of 4th and 5th order embedded RK methods using Butcher tableau

[171]:
```
# Embedded Runge-Kutta formulas
def erk54(f, x, y, h):
    k1 = h*f(x, y)
    k2 = h*f(x + a2*h, y + b21*k1)
    k3 = h*f(x + a3*h, y + b31*k1 + b32*k2)
    k4 = h*f(x + a4*h, y + b41*k1 + b42*k2 + b43*k3)
    k5 = h*f(x + a5*h, y + b51*k1 + b52*k2 + b53*k3 + b54*k4)
    k6 = h*f(x + a6*h, y + b61*k1 + b62*k2 + b63*k3 + b64*k4 + b65*k5)
```

```python
    y5 = y + c1*k1 + c2*k2 + c3*k3 + c4*k4 + c5*k5 + c6*k6
    k7 = h*f(x + a7*h, y5)
    y4 = y + c1s*k1 + c2s*k2 + c3s*k3 + c4s*k4 + c5s*k5 + c6s*k6 + c7s*k7
    return y5, y4

# A caller function
def caller5(my_method, fn, y_ini, x0, xT, h):
    # x values uniformly sampled
    xs = np.arange(x0, xT, h)
    # number of points
    N = len(xs)
    # Initialize
    y = np.asarray(y_ini)
    # Initialize storage
    ys = np.zeros((N, len(y_ini)))
    # Loop over all xs
    for i in range(N):
        # store and ...
        ys[i,:] = y
        x = xs[i]
        # ... update
        y, y4 = my_method(fn,x,y,h)
    return ys


def caller4(my_method, fn, y_ini, x0, xT, h):
    # x values uniformly sampled
    xs = np.arange(x0, xT, h)
    # number of points
    N = len(xs)
    # Initialize
    y = np.asarray(y_ini)
    # Initialize storage
    ys = np.zeros((N, len(y_ini)))
    # Loop over all xs
    for i in range(N):
        # store and ...
        ys[i,:] = y
        x = xs[i]
        # ... update
        y5, y = my_method(fn,x,y,h)
    return ys
```

[172]:

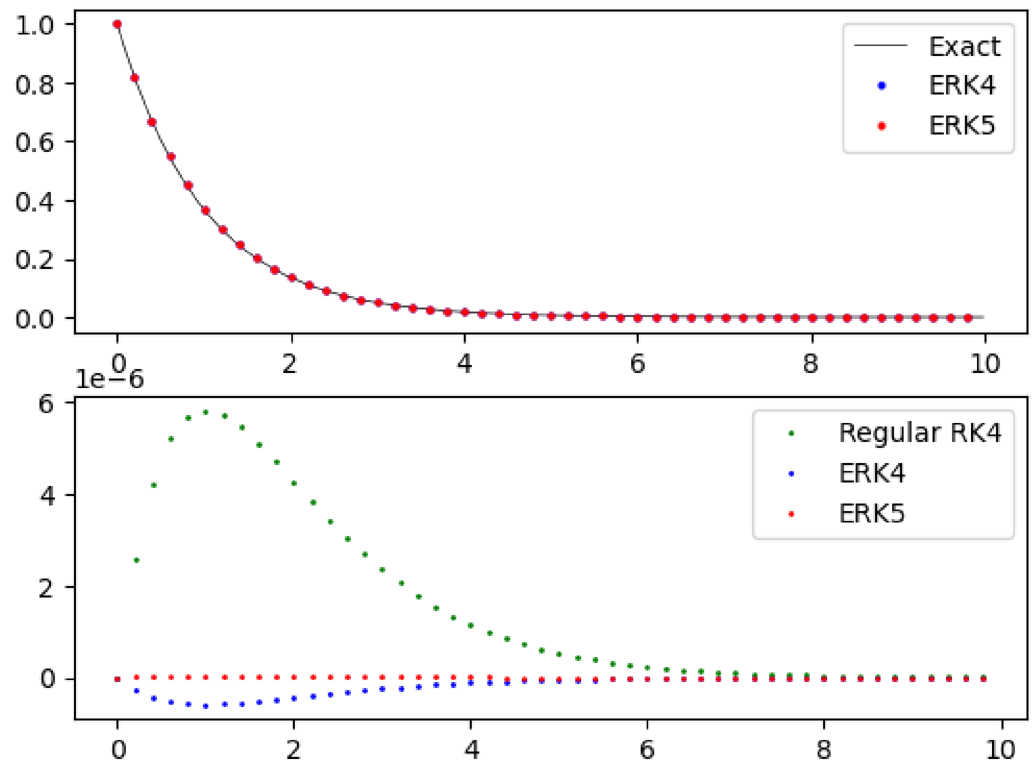
```python
# Define the function
def f(x,y):
    return -1.0*np.asarray(y)
```

```python
# Initialize the parameters
max_iter = 500
abstol = 1.0e-6
reltol = 1.0e-6
y_ini = [1.0]
x0 = 0.0
xT = 10.0
h = 0.2
xs = np.arange(x0, xT, h)

# Caller functions provide the solutions
yserk5 = caller5(erk54, f, y_ini, x0, xT, h)
yserk4 = caller4(erk54, f, y_ini, x0, xT, h)
```

1.1.3 plot solutions and errors

[173]:
```python
plt.subplot(2,1,1)
plt.plot(xfine, yfine, 'k-',linewidth=0.5,label='Exact')
plt.plot(xs, yserk4,'bo',markersize=2,label='ERK4')
plt.plot(xs, yserk5,'ro',markersize=2,label='ERK5')
plt.legend()

yerror4 = [yserk4[i][0] - yexact[i] for i in range(len(yexact))]
yerror5 = [yserk5[i][0] - yexact[i] for i in range(len(yexact))]
plt.subplot(2,1,2)
plt.plot(xs, yerror,'g.',markersize=2,label='Regular RK4')
plt.plot(xs, yerror4,'b.',markersize=2,label='ERK4')
plt.plot(xs, yerror5,'r.',markersize=2,label='ERK5')
plt.legend()
```

[173]:
```
<matplotlib.legend.Legend at 0x7fa8cb231d30>
```



2 Predictor-Corrector Method for RK45

The **Runge-Kutta-Fehlberg (RK45)** method is an **adaptive step-size** technique used for solving ordinary differential equations (ODEs). It employs a **predictor-corrector** approach using **two different Runge-Kutta formulas**—one of **4th-order** (predictor) and one of **5th-order** (corrector)—to estimate the error and adjust the step size dynamically.

2.1 Step-by-Step Description

2.1.1 1. Predictor Step (4th-Order RK)

We first compute an approximation $y_{n+1}^{(4)}$ using the **4th-order Runge-Kutta** formula:

$$y_{n+1}^{(4)} = y_n + h \sum_{i=1}^{6} b_i^{(4)} k_i$$

where the intermediate function evaluations k_i are given by:

$$k_i = f\left(t_n + c_i h, y_n + h\sum_{j=1}^{i-1} a_{ij} k_j\right)$$

for $i = 1, 2, \ldots, 6$.

2.1.2 2. Corrector Step (5th-Order RK)

Next, we compute a more accurate approximation $y_{n+1}^{(5)}$ using the **5th-order Runge-Kutta** formula:

$$y_{n+1}^{(5)} = y_n + h\sum_{i=1}^{6} b_i^{(5)} k_i$$

where the same k_i values are reused.

2.1.3 3. Error Estimation

The local error estimate is obtained as the difference between the two approximations:

$$E = y_{n+1}^{(5)} - y_{n+1}^{(4)}$$

Since the 5th-order solution is more accurate, the error gives a measure of how much the 4th-order solution deviates.

2.1.4 4. Step Size Adjustment

The step size h is adjusted based on the error E:

$$h_{\text{new}} = h_{\text{old}} \times \left(\frac{\epsilon}{|E|}\right)^{\frac{1}{5}}$$

where ϵ is the desired tolerance. If the error is too large, h is reduced; if it's small, h is increased to improve efficiency.

[174]:
```python
# Predictor-Corrector
# Embedded Runge-Kutta formulas
def erk54h(f, x, y, h, k7bh):
    # Implement FSAL (first same as last)
    # The first
    # k1 = k7bh, unless k1 is zero (initially)
    if sum(k7bh)==0:
        k1 = h*f(x, y)
    else:
        k1 = k7bh*h

    # Implement rest of the Butcher table
```

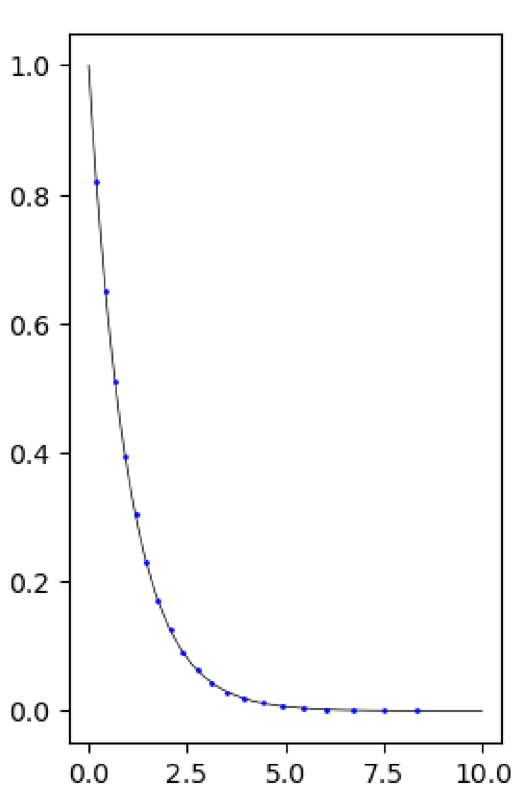
```
    k2 = h*f(x + a2*h, y + b21*k1)
    k3 = h*f(x + a3*h, y + b31*k1 + b32*k2)
    k4 = h*f(x + a4*h, y + b41*k1 + b42*k2 + b43*k3)
    k5 = h*f(x + a5*h, y + b51*k1 + b52*k2 + b53*k3 + b54*k4)
    k6 = h*f(x + a6*h, y + b61*k1 + b62*k2 + b63*k3 + b64*k4 + b65*k5)

    # get y fifth-order correct
    y5 = y + c1*k1 + c2*k2 + c3*k3 + c4*k4 + c5*k5 + c6*k6 # c7 = 0

    # FSAL -> the last
    k7bh = f(x + a7*h, y5)

    #@printf("%.6f %.6f %.6f %.6f\n",x, y[1], y5[1], k7bh[1])

    # get y fourth-order correct
    y4 = y + c1s*k1 + c2s*k2 + c3s*k3 + c4s*k4 + c5s*k5 + c6s*k6 + c7s*k7bh*h

    # return y, error, k7bh
    err = abs(y5 - y4)
    return y5, err, k7bh

def caller54(fn, y_ini, x0, xT, h0, max_iter, abstol, reltol):
    y = np.asarray(y_ini); h = h0;
    ys = np.zeros((max_iter, len(y_ini)))
    xs = np.zeros((max_iter, 1))
    xs[0] = x0; ys[0,:] = y
    x = x0; i = 0; k = 1
    k7bh = np.zeros(len(y_ini))
    while x<=xT and i<max_iter:

        # calculate the tolerance
        if i == 0:
            tol = abstol + reltol*np.linalg.norm(ys[i,:])
        else:
            tol = abstol + reltol*np.max([np.linalg.norm(ys[i,:]), np.linalg.
 ↪norm(ys[i-1,:])])

        # get the next y and the error
        y, err, k7bh = erk54h(fn,xs[i],ys[i,:],h, k7bh)

        # get max error and the scale factor
        merr = np.max(err)
        #scale_factor = (tol/merr)^0.2

        # for debugging
        #print("%2d %.4f %.6f %.6f %g"%(i,xs[i],ys[i],h,merr))
```

```
        if merr == 0.0:
            merr = tol/100

        # If the step is valid (less error than tol)
        # then we proceed
        if merr<tol:
            x += h
            i += 1
            xs[i] = x
            ys[i,:] = y
            #k7 = k7t
            #print("%2d %.4f %.6f %.6f"%(i,xs[i],ys[i],k7[1]))

        # anyway we update h every time
        h = 0.9*h*(tol/merr)**0.2

    # if the maximum number of steps exceeded
    if i>=max_iter:
        println(i," Increase max_iter.")
        return None

    # return the usable portion of the array
    return xs[1:i-1], ys[1:i-1,:]
```

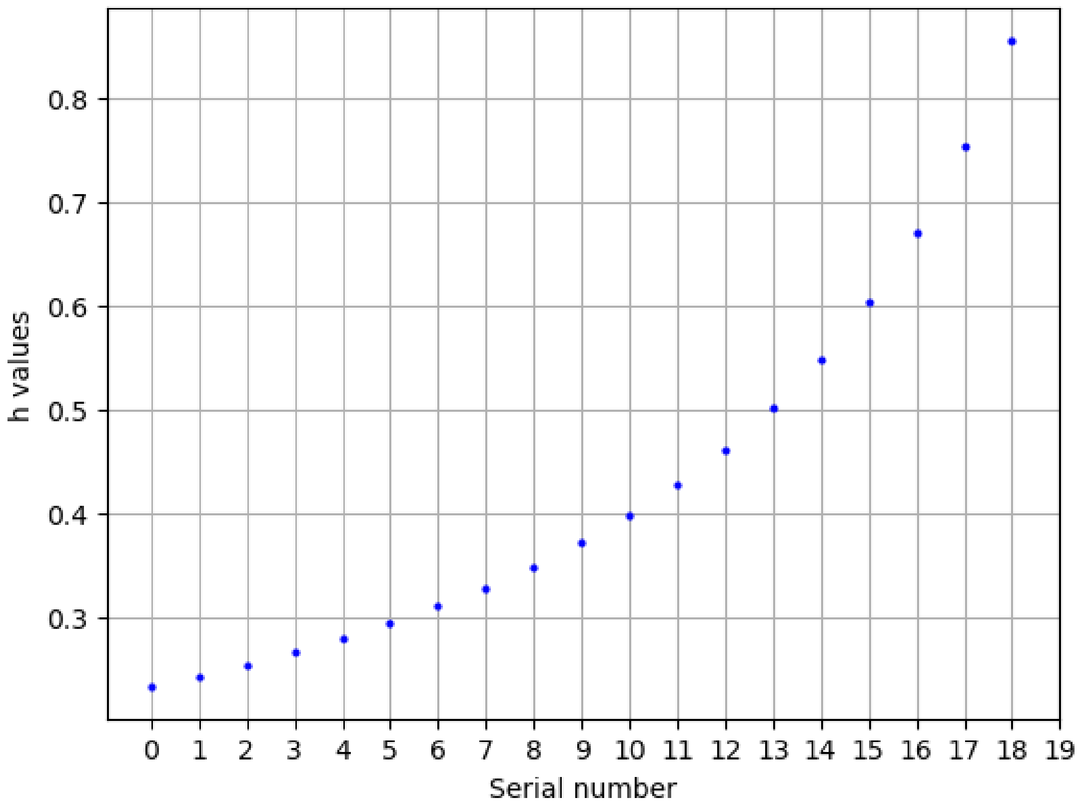
[175]:
```
# Initialize parameters
max_iter = 2000
abstol = 1.0e-6
reltol = 1.0e-8
y_ini = [1.0]
x0 = 0.0
xT = 10.0
h0 = 0.2

# Final call
xs54, yserk54 = caller54(f, y_ini, x0, xT, h0, max_iter, abstol, reltol)
```

[176]:
```
plt.subplot(1,2,1)
plt.plot(xfine, yfine, 'k-',linewidth=0.5)
plt.plot(xs54, yserk54, 'b.', markersize=2)

yexact = np.exp(-xs54)
error54 = [yserk54[i][0] - yexact[i] for i in range(len(xs54))]

plt.subplot(1,2,2)
plt.plot(xs54, error54,'g.',markersize=2)
```

[176]:
```
[<matplotlib.lines.Line2D at 0x7fa8cb2ce330>]
```



[177]:
```
xs54l = [xs54[i][0] for i in range(len(xs54))]
plt.plot(np.diff(xs54l),'bo',markersize=2)
plt.xlabel('Serial number')
plt.ylabel('h values')
plt.xticks([i for i in range(20)])
plt.grid()
```



0.8
0.7
0.6
0.5
0.4
0.3
h values
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
Serial number


```
[ ]:
```