

Ay 190 Assignment 6

Linear Systems of Equations

February 7, 2013

1 Solving Large Linear Systems of Equations

1.1 The given linear systems of equations

Five linear systems of equations (LSEs) downloaded from http://www.tapir.caltech.edu/~cott/ay190/stuff/LSEi_m.dat and http://www.tapir.caltech.edu/~cott/ay190/stuff/LSEi_bvec.dat with $i = 1..5$. The properties of the LSEs and whether or not a unique solution exists (i.e. $\det A \neq 0$) can be found in Table 1.

1.2 Solving the LSEs

A routine written by Isaac Evan (available at <https://github.com/ievans/GaussianElimination/blob/master/gaussianeelimination.py>, see also Appendix A) was used to solve the LSEs using Gauss elimination and back-substitution. As a comparison, the LSEs were also solved using NumPy's `linalg.solve` routine, which employs LU decomposition, partial pivoting, and row swapping. The performance of both routines on the 5 LSEs are shown in Table 1.

Table 1: Dimensions and solution speeds of the 5 given LSEs

i	dim A	dim b	Gauss Elimination	NumPy solver
1	10×10	10	0.000598 s	0.000256 s
2	100×100	100	0.256901 s	0.002186 s
3	200×200	200	1.979687	0.006756 s
4	1000×1000	1000	247.190892 s	0.278832 s
5	2000×2000	2000	1940.300075	1.819025

2 Stiff ODE Systems

Here we will solve the stiff ODE

$$\begin{aligned}\frac{d}{dt}Y_1 &= Y_1 - 99Y_2 \\ \frac{d}{dt}Y_2 &= -Y_1 + 99Y_2\end{aligned}$$

over $t = 0$ to $t = 4$ for the initial conditions $Y_1(0) = 1$, $Y_2(0) = 0$.

2.1 Analytic solution

Plugging in the ansatz $\mathbf{Y} = \mathbf{v} \exp \lambda t$ into the ODEs gives

$$\begin{aligned} v_1 \lambda e^{\lambda t} &= v_1 e^{\lambda t} - 99 v_2 e^{\lambda t} & v_2 \lambda e^{\lambda t} &= -v_1 e^{\lambda t} + 99 v_2 e^{\lambda t} \\ v_1 \lambda &= v_1 - 99 v_2 & v_2 \lambda &= -v_1 + 99 v_2 \\ v_2 &= \frac{1}{99} (1 - \lambda) v_1 & v_1 &= (99 - \lambda) v_2 \end{aligned}$$

$$\begin{aligned} v_1 &= (1 - \frac{\lambda}{99})(1 - \lambda) v_1 \\ 1 &= (1 - \frac{\lambda}{99} - \lambda + \frac{\lambda^2}{99}) \\ 0 &= \lambda(-100 + \lambda). \end{aligned}$$

Thus $\lambda = 0$ or 100 . $\lambda = 0$ yields a constant solution $\mathbf{Y} = \mathbf{v}$. For $\lambda = 100$, $v_1 = (99 - \lambda)v_2$ yields $v_1 = -v_2$. Solving for the initial conditions and adding a constant term yields the solution

$$\begin{aligned} Y_1(t) &= \frac{1}{100}(99 + e^{100t}) \\ Y_2(t) &= \frac{1}{100}(1 - e^{100t}). \end{aligned}$$

2.2 Numerical solutions

The ODEs were integrated using four different integrators: explicit Euler, 2nd and 4th order Runge-Kutta methods, and backwards Euler. Four step sizes $\Delta t = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}$ were used for each of the integrators to test for convergence. The results are shown below.

2.2.1 Explicit Euler and Runge-Kutta methods

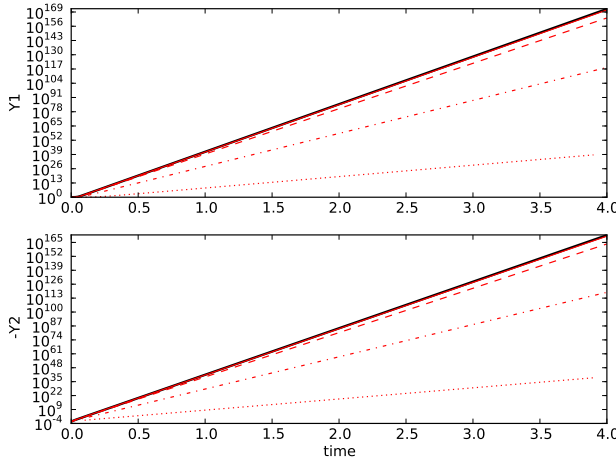


Figure 1: Solution computed using the explicit Euler method. The exact solution for both Y_1 (top) and Y_2 (bottom) is depicted in black. The solution computed with a step size of 10^{-1} is depicted with a dotted line, a step size of 10^{-2} with a dot-dashed line, a step size of 10^{-3} with a dashed line, and a step size of 10^{-4} with a solid red line. The explicit Euler method required a step size of at least 10^{-4} for convergence.

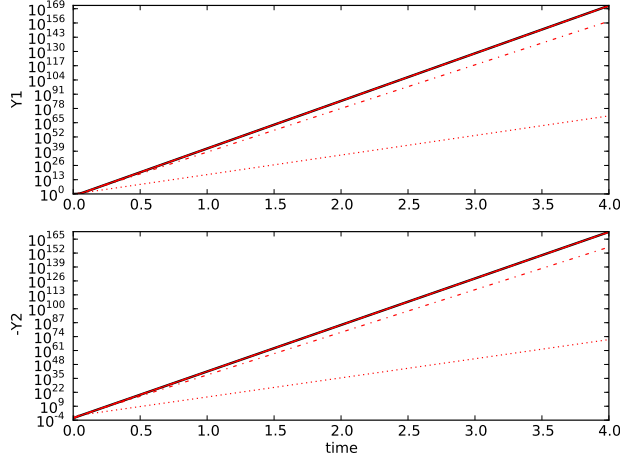


Figure 2: Similar to Figure 1, but for solutions computed using the 2nd order Runge-Kutta method. A step size of at least 10^{-3} was required for convergence.

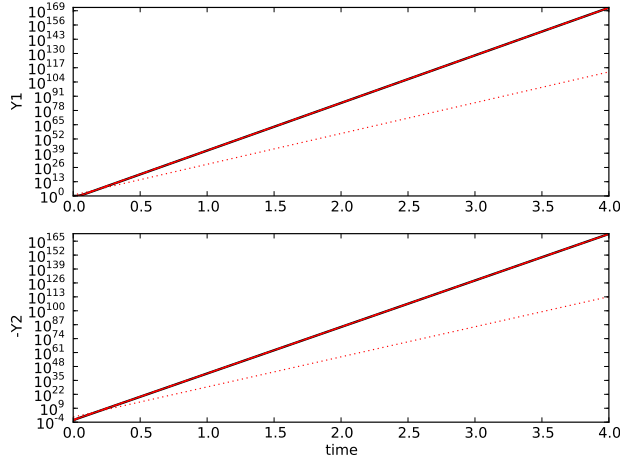


Figure 3: Similar to Figure 1, but for solutions computed using the 4th order Runge-Kutta (RK4) method. The superior convergence rate of RK4 is demonstrated here; a step size as large as 10^{-2} was sufficient for convergence.

2.2.2 Backwards Euler

For the backwards Euler method, the ODEs were written as

$$\frac{1}{\Delta t} \begin{pmatrix} Y_1^{i+1} - Y_1^i \\ Y_2^{i+1} - Y_2^i \end{pmatrix} = \begin{pmatrix} 1 & -99 \\ -1 & 99 \end{pmatrix} \begin{pmatrix} Y_1^{i+1} \\ Y_2^{i+1} \end{pmatrix}$$

Solving this system of equations for Y_1^{i+1} and Y_2^{i+1} yields

$$Y_1^{i+1} = \frac{Y_1^i(1 - 99\Delta t) - 99Y_2^i\Delta t}{1 - 100\Delta t}, \quad Y_2^{i+1} = \frac{Y_2^i(1 - \Delta t) - Y_1^i\Delta t}{1 - 100\Delta t}.$$

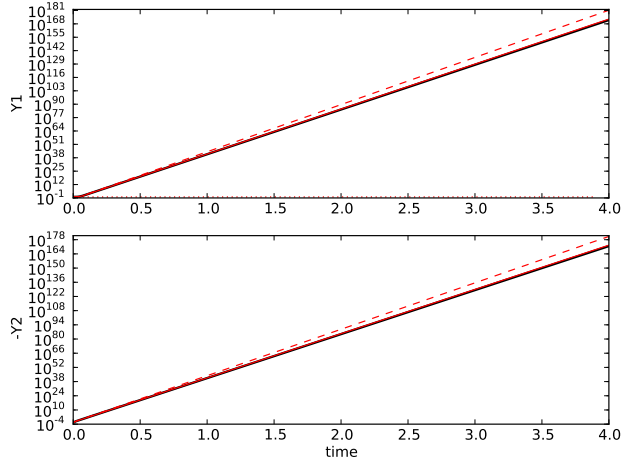


Figure 4: Similar to Figure 1, but for solutions computed using the backwards Euler method. Note that the solution is significantly erroneous (remaining constant at about 1 for Y_1 and at about 0.01 for Y_2) for a step size of 0.1. Due to a division by zero error, the solution was not calculated for a step size of 10^{-2} . At a step size of 10^{-4} , the solution was nearly (but not quite) convergent, as demonstrated in the following figure.

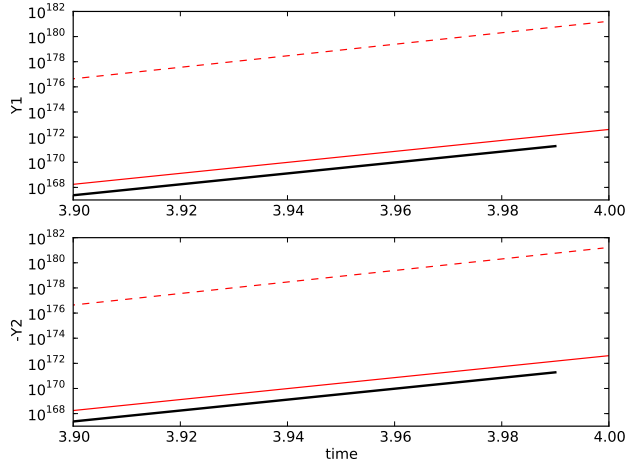


Figure 5: Close up of the tail of the solutions computed using the backwards Euler method. Even with a step size of 10^{-4} (solid red line), the solution did not converge to the exact solution.

Appendices

The Python modules and scripts used in this assignment include

- A The Gauss Elimination LSE Solver: `gaussianelimination.py` (see page 5)
- B The Runge-Kutta Routines: `rungekutta.py` (see pages 5-8)
- C Script for Set 6: `set6.py` (see pages 8-11)

A The Gauss Elimination LSE Solver: `gaussianelimination.py`

```
# Copyright (c) Isaac Evans 2011
# All rights reserved.

def myGauss(m):
    # eliminate columns
    for col in range(len(m[0])):
        for row in range(col+1, len(m)):
            r = [(rowValue * (-(m[row][col] / m[col][col])) for rowValue in m[col])
                m[row] = [sum(pair) for pair in zip(m[row], r)]
    # now backsolve by substitution
    ans = []
    m.reverse() # makes it easier to backsolve
    for sol in range(len(m)):
        if sol == 0:
            ans.append(m[sol][-1] / m[sol][-2])
        else:
            inner = 0
            # substitute in all known coefficients
            for x in range(sol):
                inner += (ans[x]*m[sol][-2-x])
            # the equation is now reduced to ax + b = c form
            # solve with (c - b) / a
            ans.append((m[sol][-1]-inner)/m[sol][-sol-2])
    ans.reverse()
    return ans
```

B The Runge-Kutta Routines: `rungekutta.py`

```
# rk4.py
# created 11/8/11 by stacy kim
#
# Computes a function given its derivative func with initial conditions x using the
# Runge-Kutta method. 2nd, 3rd, and 4th order routines and adaptive stepping are
# implemented.
#
#
# modified 11/10/11 to include adaptive step size control
# modified 1/24/12
# corrected 2-step rungekutta call (t+h/2 in second call)
```

```

#    corrected error comparison in stepper routine (element vs. list comparison)
# modified 1/31/12
#    modified error comparison in stepper (max(list) vs. element)
#    removed calculation complete status output from driver
#    added debug print stmts to stepper to check error decrease
# modified 2/6/12: removed shebang line
# modified 2/12/12
#    added t0 to the driver's parameter list
#    create min step size (abort if reached)
# modified 1/21/13
#    renamed module from rk4 to rungekutta and 4th order routine
#    implemented 2nd and 3rd order runge-kutta methods
#    modified driver and stepper routines to use the rk method of the given order
#    switched support of vector arith. from homegrown Vector module to numpy

```

```
import sys, math
```

```
MAXITER=1000
```

```
MINH=1e-8
```

```
h=1.0
```

```
# TIME-STEPPING ROUTINES -----
```

```
def driver(rk,x,t0,tf,h,f,err,fn):
```

```
    """
```

```
    Solves the differential equation 'f' using the given Runge-Kutta method
    'rk' from t0 to tf. Takes time steps of 'h' or adaptively steps to satisfy
    the given accuracy criteria 'err'. Results are printed to the file fn.
    """
```

```
    ADAPTIVE = 1 if h==0 else 0
```

```
    # Open output file and write headers
```

```
    file=open(fn,'w')
```

```
    file.write(fn)
```

```
    file.write('\nh={0},t0={5},tf={1},err={4}\n{2}{3}'.format(h,tf,'t'.rjust(19),'h'.rjust(19),err,t0))
```

```
    for i in range(len(x)): file.write('x{0}'.format(i+1).rjust(19))
```

```
    file.write('\n')
```

```
    #Iteratively calculate position and velocities using given time steps
```

```
    t=t0
```

```
    i=0
```

```
    while (t<=tf):
```

```
        # Write results to file
```

```
        file.write('{0} {1} '.format(str(t).rjust(19),str(h).rjust(19)))
```

```
        for j in range(len(x)): file.write('{0} '.format(str(x[j]).rjust(19)))
```

```
        file.write('\n')
```

```
        # Calculate function value at next step
```

```
        if (ADAPTIVE):
```

```
            x,t,h=stepper(rk,x,t,f,err)
```

```

        else:
            t=h*i
            x=rk(x,t,h,f)
            i+=1

    file.close()

    return

def stepper(rk,x,t,f,err):
    """
    Computes the next step of the function f using the given Runge-Kutta method
    rk to the given accuracy 'err'. Only called if adaptively time stepping.
    """

    global h
    h0=h
    n=0

    while (1):
        x1=rk(x,t,h,f)
        x2=rk(rk(x,t,h/2,f),t+h/2,h/2,f)

        if (max(abs(x2-x1)) > err[0]):
            h/=2
            if h < MINH:
                print 'Exceeded max precision.'
                sys.exit()
        else:
            h_old=h
            if max(abs(x2-x1)) < err[0]/10.: h*=2
            return x2,t+h_old,h_old

        n+=1
        if ((MAXITER-n)<10):
            print "abs(x2-x1)={0},err={1}\n".format(abs(x2-x1),err)
            if (n==MAXITER):
                print "Failed to converge within {0} iterations.".format(MAXITER)
                print "[x={0},err={1},h0={2},hf={3},t={4}]" .format(x,abs(x2-x1),h0,h,t)
                sys.exit()

# RUNGE-KUTTA ROUTINES -----

def rk4(x,t,h,f):
    """
    Computes the function value x with derivative f at the time t + h using
    the fourth order Runge-Kutta method.
    """

    k1=h*f(x,t)
    k2=h*f(x+k1/2,t+h/2)

```

```

    k3=h*f(x+k2/2,t+h/2)
    k4=h*f(x+k3,t+h)

    return x + (k1 + 2*k2 + 2*k3 + k4)/6

def rk3(x,t,h,f):
    """
    Computes the function value x with derivative f at the time t + h using
    the third order Runge-Kutta method.
    """

    k1=h*f(x,t)
    k2=h*f(x+k1/2,t+h/2)
    k3=h*f(x-k1+2*k2,t+h)

    return x + (k1 + 4*k2 + k3)/6

def rk2(x,t,h,f):
    """
    Computes the function value x with derivative f at the time t + h using
    the second order Runge-Kutta method.
    """

    k1=h*f(x,t)
    k2=h*f(x+k1/2,t+h/2)

    return x + k2

```

C Script for Set 6: set6.py

```

# set6.py
# created 1/29/13 by stacy kim

import numpy as np, time
import matplotlib.pyplot as plt
from gaussianelimination import *
from rungekutta import *

# EXERCISE 1 -----
print 'reading in LSEs with dimensions'
m,b=[],[]
for i in range(1,6):
    b.append([float(line[1:])
               for line in open('LSE'+str(i)+'_bvec.dat').read().split('\n')[:-1]])
    m.append([[float(n) for n in line.split(' ')[1:] if n != ''] \
               for line in open('LSE'+str(i)+'_m.dat').read().split('\n')[:-1]])

print ' ',i, '\tm:',len(m[-1]), len(m[-1][0]),'\tb:',len(b[-1])

```



```

for i in range(len(m)):
    sy=[m[i][j]+[b[i][j]] for j in range(len(m[i]))]
    #t1=timeit.timeit(stmt='x1=myGauss(sy)',setup='from __main__ import myGauss, sy,x1',number=1)
    t1=time.clock()
    ans1=myGauss(sy)
    t1=time.clock()-t1

    t2=time.clock()
    ans2=np.linalg.solve(m[i],b[i])
    t2=time.clock()-t2
    print i,':',t1, t2

    if np.all([ans1[j]==ans2[j] for j in range(len(ans1))]):
        print 'Does not match for LSE',j+1,'!'

# EXERCISE 2 -----
# Stiff ODE Systems

# exact solution
t_exact =np.arange(0,4,0.01)
y1_exact=np.array([(99+math.exp(100*tt))/100 for tt in t_exact])
y2_exact=np.array([(1-math.exp(100*tt))/100 for tt in t_exact])

def plot_exact():
    plt.subplot(211)
    plt.plot(t_exact,y1_exact,'k',lw=2)
    plt.ylabel('Y1')
    plt.yscale('log')
    plt.xlim([0,4])

    plt.subplot(212)
    plt.plot(t_exact,-y2_exact,'k',lw=2)
    plt.xlabel('time')
    plt.ylabel('-Y2')
    plt.yscale('log')
    plt.xlim([0,4])

# RHS of our stiff ODE system
def rhs(x,t):
    # x = [y1, y2]
    dy1= x[0] - 99.0*x[1]
    dy2=-x[0] + 99.0*x[1]
    return np.array([dy1,dy2])

# Inputs
h=[0.1,0.01,1e-3,1e-4] # step size
x0=np.array([1.,0.]) # initial condition, x=[y1,y2]
t0=0.0 # initial time
tf=4.0 # time to integrate until
err=[1.0,1.0] # desired accuracy for each element of x

```

```

ls=[':', '-.-', '--', '-']      # line styles (one for each step size)

# explicit Euler
print 'explicit euler'
plot_exact()
for hh in h:
    x=[x0[0],x0[1]]
    y1,y2=[x[0]], [x[1]]
    t=np.arange(t0,tf,hh)
    for tt in t[1:]:
        x+=hh*rhs(x,tt)
        y1.append(x[0])
        y2.append(x[1])

    plt.subplot(211)
    plt.plot(t,y1,'r',ls=ls[h.index(hh)])
    plt.subplot(212)
    plt.plot(t,-np.array(y2),'r',ls=ls[h.index(hh)])

plt.savefig('stiff_explicit_euler.pdf')
plt.show()

# RK2 integrator
print 'rk2'
plot_exact()
for hh in h:
    fn='stiff_rk2_h{0}.dat'.format(hh)
    driver(rk2,x0,t0,tf,hh,rhs,err,fn)

    dat = np.array([[float(el) for el in line.split(' ') if el != '']
                    for line in open(fn).read().split('\n')[3:-1]])
    t,y1,y2=dat[:,0],dat[:,2],dat[:,3]

    plt.subplot(211)
    plt.plot(t,y1,'r',ls=ls[h.index(hh)])
    plt.subplot(212)
    plt.plot(t,-y2,'r',ls=ls[h.index(hh)])

plt.savefig('stiff_rk2.pdf')
plt.show()

# RK4 integrator
print 'rk4'
plot_exact()
for hh in h:
    fn='stiff_rk4_h{0}.dat'.format(hh)
    driver(rk4,x0,t0,tf,hh,rhs,err,fn)

    dat = np.array([[float(el) for el in line.split(' ') if el != '']
                    for line in open(fn).read().split('\n')[3:-1]])
    t,y1,y2=dat[:,0],dat[:,2],dat[:,3]

```

```

plt.subplot(211)
plt.plot(t,y1,'r',ls=ls[h.index(hh)])
plt.subplot(212)
plt.plot(t,-y2,'r',ls=ls[h.index(hh)])

plt.savefig('stiff_rk4.pdf')
plt.show()

# backward Euler
print 'bkwd euler'
plot_exact()
for hh in h:
    if hh==0.01: continue # will cause zero division error
    x=[x0[0],x0[1]]
    y1,y2=[x[0]], [x[1]]
    t=np.arange(t0,tf,hh)
    for tt in t[1:]:
        y1.append(-(y1[-1]-99*y1[-1]*hh-99*y2[-1]*hh)/(100*hh-1))
        y2.append(-(y2[-1]-y1[-1]*hh-y2[-1]*hh)/(100*hh-1))

plt.subplot(211)
plt.plot(t,y1,'r',ls=ls[h.index(hh)])
plt.xlim([3.9,4])
plt.ylim([1e167,1e182])
plt.subplot(212)
plt.xlim([3.9,4])
plt.ylim([1e167,1e182])
plt.plot(t,-np.array(y2),'r',ls=ls[h.index(hh)])

plt.savefig('stiff_bkwd_euler_closeup.pdf')
plt.show()

```