rkev

Exploring evolutionary approaches to Runge-Kutta (and discovering why symplectic approaches are better)

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Description

- This notebook contains two primary items:
- Implementation of a nbody Python package that simplifies the setup of a full *n*-body simulation.
- (12/14/18 01:25) IN PROGRESS An implementation of a genetic algorithm to optimize a Butcher Tableau to reduce changes in energy over the course of the simulation.
- In both of these cases, a general purpose s-stage Runge-Kutta library written in C++ is also being tested. As of (12/14/18 01:25), this appears to be working. It is wrapped up in the integration methods of the **nbody** package.

Imports

```
In [1]: import json
   import math
   import multiprocessing
   import random
   import time

   from deap import algorithms, base, creator, tools
   import matplotlib
   import matplotlib.pyplot as plt
   import numpy as np

import nbody as nb
```

```
In [2]: # Matplotlib configuration
   matplotlib.use('nbagg')
%matplotlib notebook
```

Setting up Butcher Tableaus

Here, I'm defining a dictionary of well known Runge-Kutta schemes. These can be used to show that the underlying methods work.

```
In [3]: BT = {}
        BT['RK4'] = [
            [ 0., 0., 0., 0.,
                                        0.1,
            [1/2., 1/2., 0., 0.,
                                        0.],
            [ 1/2., 0., 1/2.,
[ 1., 0., 0.,
                                0.,
                                        0.],
                                1.,
                                        0.],
                0., 1/6., 1/3., 1/3., 1/6.]
        ]
        BT['RK38'] = [
            [ 0., 0., 0., 0.,
                                        0.],
            [1/3., 1/3., 0., 0.,
                                        0.],
            [ 2/3.,-1/3., 1.,
                                  0.,
                                        0.],
              1., 1., -1., 1., 0.]
0., 1/8., 3/8., 3/8., 1/8.]
        1
        BT['zeros'] = [
            [0., 0., 0., 0., 0.]
            [0., 0., 0., 0., 0.]
            [0., 0., 0., 0., 0.]
            [0., 0., 0., 0., 0.]
            [0., 0., 0., 0., 0.]
        ]
```

Testing the rk_ext library with some simple first order ODEs

The last set of tests uses a Butcher Tableau of zeros to show that there are no hidden tableaus elsewhere in the library.

```
In [5]: def test_ode(t, x):
    return x/(1 + t)

def test_analytical(t):
    return t + 1
```

```
In [6]: RK4 = nb.rk ext.RKIntegrator(test ode, BT['RK4'], 10, 0, 2, 1, True)
        solution = RK4.run()
        error = ((solution - test analytical(2))/test analytical(2))*100
        print("solution = {}".format(solution))
        print("error = {}".format(error))
        solution = 3.00000000000000004
        error = 1.4802973661668752e-14
In [7]: RK38 = nb.rk ext.RKIntegrator(test ode, BT['RK38'], 10, 0, 2, 1, True)
        solution = RK38.run()
        error = ((solution - test analytical(2))/test analytical(2))*100
        print("solution = {}".format(solution))
        print("error = {}".format(error))
        solution = 3.00000000000000004
               = 1.4802973661668752e-14
In [8]: RKzero = nb.rk ext.RKIntegrator(test ode, BT['zeros'], 10, 0, 2, 1, Tr
        solution = RKzero.run()
        error = ((solution - test analytical(2))/test analytical(2))*100
        print("solution = {}".format(solution))
        print("error = {}".format(error))
        solution = 1.0
```

Implementation (no GA)

NOTES

• (12/14/18 00:52) The initial implementation of the nbody code was carried out step by step for readability in the Jupyter Notebook, but at this point, I am moving all of that code into a wrapper function that will be used as an evaluation function for DEAP.

Setting up bodies

```
In [9]: sun = nb.Body(mass=1.988e30,
                   position=[0, 0, 0],
                   velocity=[0, 0, 0],
                   name='sun',
                   )
        earth = nb.Body(mass=5.972e24,
                   position=[149597870700, 0, 0],
                   velocity=[0, 29.8e3*3600, 0],
                   name='earth',
                   )
        \#mars = nb.Body(mass=0.64171e24,
                    position=[227.92e9, 0, 0],
                    velocity=[0, 24.07e3*3600*24, 0],
                    name='earth',
        #
        #
                    )
        #jupiter = nb.Body(mass=1898.19e24,
                    position=[778.57e9, 0, 0],
                    velocity=[0, 13.06e3*3600*24, 0],
        #
                    name='earth',
        bodies = [sun, earth]
```

The below is a time dictionary where the first key is the unit, and the second key is a common value.

```
In [10]: times = {
               'second':{
                   'second':1,
                   'minute':60,
                   'hour':3600,
                   'day':24*3600,
                   'year':365.25*24*3600,
               },
               'minute':{
                   'second':1/60.,
                   'minute':1.,
                   'hour':60,
                   'day':24*60,
                   'year':365.25*24*60,
              },
'hour':{
'sec
                   'second':1/3600.,
                   'minute':1/60.,
                   'hour':1,
                   'day':24,
                   'year':365.25*24,
              },
'day':{
    'se
                   'second':1/(24*3600),
                   'minute':1/(24*60.),
                   'hour':1/24.,
                   'day':1,
                   'year':365.25,
               }
          }
```

Plotting Function

```
In [11]: | def plot(system, corrected, window size, time dict):
             t init = time dict['t init']
             t fin = time dict['t fin']
             steps = time dict['steps']
             if steps == int(1e4):
                 bound = list(range(steps+2))
             elif steps == int(1e5):
                 bound = list(range(steps+1))
             AU = 149597870700
             fig = plt.figure()
             ax1 = fig.add subplot(111)
             ax1.scatter(system.data['x'][0], system.data['y'][0], color='orang
         e', s=100)
             for i in range(1, len(system.body list)):
                 ax1.scatter(system.data['x'][i],
                          system.data['y'][i],
                          c=bound, cmap="inferno", s=0.2)
             ax1.set xlim([-window size*AU,window size*AU])
             ax1.set ylim([-window size*AU,window size*AU])
             \#cax = ax1.imshow()
             #cbar = fig.colorbar(cax)
             plt.title('Orbit of Bodies Around Sun, {} energy loss correction'.
         format(corrected))
             plt.savefig("decaying orbits.png", dpi=300)
             plt.show()
             E = system.energy
             dE = [((e - E[0])/abs(E[0]))*100  for e in E]
             fig = plt.figure()
             \#ax1 = fig.add subplot(111)
             plt.scatter(range(len(dE)), dE, c=bound, cmap="inferno", s=0.2)
             plt.colorbar()
             plt.title('Percent Change in Energy from Initial')
             plt.ylabel('Percentage of Initial Energy')
             plt.xlabel('Iteration')
             plt.tight_layout()
             plt.show()
```

run definition

```
In [12]: def run(bt, bodies, time dict):
            t init = time dict['t init']
            t fin = time dict['t fin']
            steps = time dict['steps']
            system = nb.System(bodies)
            system.setup integrators(bt, t init, t fin, steps)
            start = time.process time()
            system.run()
            end = time.process time()
            elapsed = end - start
            print("time elapsed = " + str(elapsed))
            print("-----")
            print("TOTAL ENERGY CHANGE")
print("----")
            print("absolute = {:15.5e}".format(system.energy change['absolut
        e']))
            print("percentage = {:15.5e}".format(system.energy change['percent
        age']))
            return system
```

```
In [13]: times['second']['year']
```

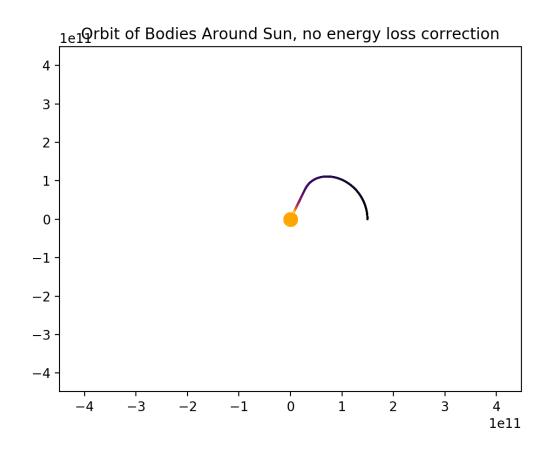
Out[13]: 31557600.0

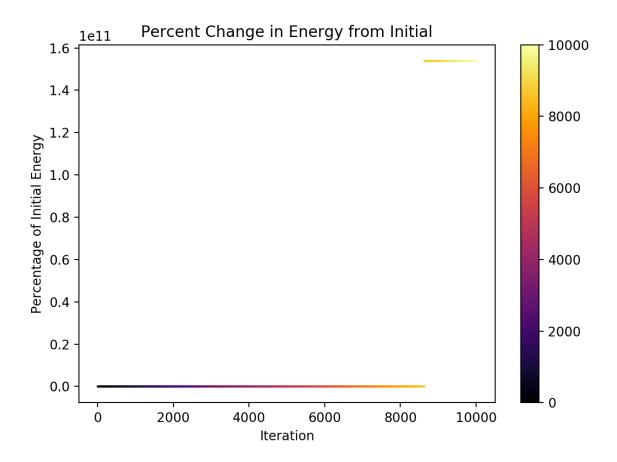
```
In [15]: time_dict = {
    't_init':0.,
    't_fin':1.5*times['hour']['year'],
    'steps':int(1e4),
}

window_size = 3
system = run(BT['RK4'], bodies, time_dict)
plot(system, 'no', window_size, time_dict)
```

TOTAL ENERGY CHANGE

absolute = 5.27282e+49 percentage = 1.53821e+11





Moving on to GA using DEAP

The standard Runge-Kutta method is undoubtedly *not* the best method for these types of problems, and we could easily arrive at a solution that conserves energy by using a symplectic integrator... but that's not what we're going to do.

In this case, we're going to attempt to use DEAP to evolve the Butcher Tableau to minimize the overall change in energy. Basically, we've got a giant, multipurpose hammer (non-symplectic Runge-Kutta), so we just need to make our problem look like a nail.

```
In [32]: def evaluate(individual, time dict):
             """This is the function that will be used to evaluate
             the individuals. To be used for other systems, all of
             the definitions need to either be made here or the
             argument list must be augmented to contend with extra
             parameters.
             t init = time dict['t init']
             t fin = time dict['t fin']
             steps = time dict['steps']
             # Initialize the system (notice the usage of "individual")
             system = nb.System(bodies)
             #print("HERE IT IS: {}".format(type(individual)))
             system.setup integrators(individual, t init, t fin, steps)
             # Run
             start = time.process time()
             system.run()
             end = time.process time()
             elapsed = end - start
             #print("time: {}".format(elapsed))
             return (system.energy change['percentage'],)
         # TEST: Make sure the above function actually works
         energy change = evaluate(BT["RK4"], time dict)
         print("energy change = {}".format(energy change))
         energy change = (-1018.5356785671061,)
In [21]: creator.create("FitnessMin", base.Fitness, weights=(-1.0,))
         creator.create("Individual", list, fitness=creator.FitnessMin)
In [33]: bts = list(BT.values())
         def init tableau(icls):
             bt = bts[random.randint(0, 1)]
```

bt = np.asarray(bt)*random.random()

bt = bt.tolist()
return icls(bt)

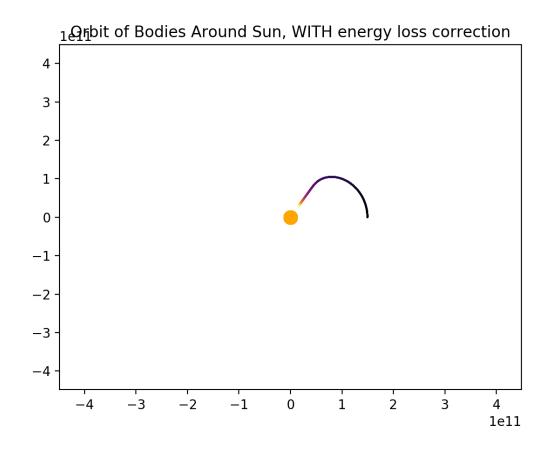
```
In [ ]: | toolbox = base.Toolbox()
        toolbox.register("init individual", init tableau)
        toolbox.register("individual", toolbox.init individual, creator.Indivi
        toolbox.register("population", tools.initRepeat, list, toolbox.individ
        ual)
        toolbox.register("evaluate", evaluate, time dict=time dict)
        toolbox.register("mate", tools.cxTwoPoint)
        toolbox.register("mutate", tools.mutGaussian, mu=0, sigma=0.3, indpb=
        0.05)
        toolbox.register("select", tools.selTournament, tournsize=3)
        pool = multiprocessing.Pool()
        toolbox.register("map", pool.map)
        pop = toolbox.population(n=50)
        hof = tools.HallOfFame(1)
        stats = tools.Statistics(lambda ind: ind.fitness.values)
        stats.register("avg", np.mean)
        stats.register("std", np.std)
        stats.register("min", np.min)
        stats.register("max", np.max)
```

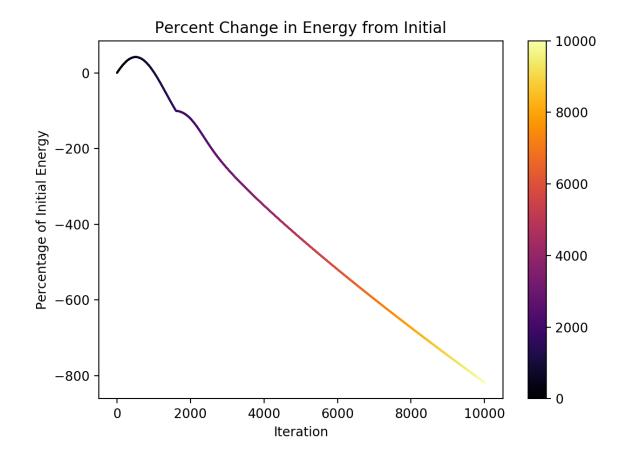
```
In [ ]: population = toolbox.population(n=20)
    NGEN=15
    for gen in range(NGEN):
        offspring = algorithms.varAnd(population, toolbox, cxpb=0.7, mutpb
=0)
        fits = toolbox.map(toolbox.evaluate, offspring)
        for fit, ind in zip(fits, offspring):
              ind.fitness.values = fit
        population = toolbox.select(offspring, k=len(population))
        top10 = tools.selBest(population, k=10)
```

```
In [19]: print('Best Remaining Individual after {} generations:'.format(NGEN))
         a = [[0.0, 0.0, 0.0, 0.0, 0.0],
          [0.3636733144010224, 0.3636733144010224, 0.0, 0.0, 0.0],
          [0.3636733144010224, 0.0, 0.3636733144010224, 0.0, 0.0],
          [0.7677566283239672,
           0.7677566283239672,
           -0.7677566283239672,
           0.7677566283239672,
           0.0],
          [0.0,
           0.0959695785404959,
           0.28790873562148767,
           0.28790873562148767,
           0.095969578540495911
         print('[')
         for row in a:
                        ' + str(row) + ',')
             print('
         print(']')
         #print(ind.fitness.values)
         Best Remaining Individual after 15 generations:
             [0.0, 0.0, 0.0, 0.0, 0.0],
             [0.3636733144010224, 0.3636733144010224, 0.0, 0.0, 0.0],
             [0.3636733144010224, 0.0, 0.3636733144010224, 0.0, 0.0],
             [0.7677566283239672, 0.7677566283239672, -0.7677566283239672, 0.76
         77566283239672, 0.0],
             [0.0, 0.0959695785404959, 0.28790873562148767, 0.2879087356214876
         7, 0.0959695785404959],
```

TOTAL ENERGY CHANGE

absolute = -2.80393e+41percentage = -8.17977e+02





Resources

• https://thesesergio.wordpress.com/2013/05/31/deap-a-self-made-tutorial-12/comment-page-1/#comment-page-1/#comment-page-1/#comment-98)