

KyotoUx-009x (/github/ryo0921/KyotoUx-009x/tree/master)
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Stochastic Processes: Data Analysis and Computer Simulation

Brownian motion 2: computer simulation

3. Simulations with on-the-fly animation

3.1. Simulation code with on-the-fly animation

Import libraries

```
In [1]: % matplotlib nbagg
import numpy as np # import numpy library as np
import matplotlib.pyplot as plt # import pyplot library as plt
import matplotlib.mlab as mlab # import mlab module to use MATLAB comman
import matplotlib.animation as animation # import animation modules from
from mpl_toolkits.mplot3d import Axes3D # import Axes3D from mpl_toolkit
plt.style.use('ggplot') # use "ggplot" style for graphs
```

Define init function for FuncAnimation

```
In [2]: def init():
    global R,V,W,RS,Vs,Ws,time
    R[:,:] = 0.0 # initialize all the variables to zero
    V[:,:] = 0.0 # initialize all the variables to zero
    W[:,:] = 0.0 # initialize all the variables to zero
    RS[:,,:] = 0.0 # initialize all the variables to zero
    Vs[:,,:] = 0.0 # initialize all the variables to zero
    Ws[:,,:] = 0.0 # initialize all the variables to zero
    time[:] = 0.0 # initialize all the variables to zero
    title.set_text(r'') # empty title
    line.set_data([],[]) # set line data to show the trajectory of parti
    line.set_3d_properties([]) # add z-data separately for 3d plot
    particles.set_data([],[]) # set position current (x,y) position data
    particles.set_3d_properties([]) # add current z data of particles to
    return particles,title,line # return listed objects that will be dra
```

Define animate function for FuncAnimation

```
In [3]: def animate(i):
    global R,V,W,Rs,Vs,Ws,time # define global variables
    time[i]=i*dt # store time in each step in an array time
    W = std*np.random.randn(nump,dim) # generate an array of random force
    V = V*(1-zeta/m*dt)+W/m # update velocity via Eq.(F9)
    R = R+V*dt # update position via Eq.(F5)
    Rs[i,:,:]=R # accumulate particle positions at each step in an array
    Vs[i,:,:]=V # accumulate particle velocities at each step in an array
    Ws[i,:,:]=W # accumulate random forces at each step in an array Ws
    title.set_text(r"t = "+str(time[i])) # set the title to display the
    line.set_data(Rs[:i+1,n,0],Rs[:i+1,n,1]) # set the line in 2D (x,y)
    line.set_3d_properties(Rs[:i+1,n,2]) # add z axis to set the line in
    particles.set_data(R[:,0],R[:,1]) # set the current position of all
    particles.set_3d_properties(R[:,2]) # add z axis to set the particle
    return particles,title,line # return listed objects that will be dra
```

Set parameters and initialize variables

```
In [4]: dim = 3 # system dimension (x,y,z)
    nump = 1000 # number of independent Brownian particles to simulate
    nums = 1024 # number of simulation steps
    dt = 0.05 # set time increment, \Delta t
    zeta = 1.0 # set friction constant, \zeta
    m = 1.0 # set particle mass, m
    kBT = 1.0 # set temperature, k_B T
    std = np.sqrt(2*kBT*zeta*dt) # calculate std for \Delta W via Eq.(F11)
    np.random.seed(0) # initialize random number generator with a seed=0
    R = np.zeros([nump,dim]) # array to store current positions and set init
    V = np.zeros([nump,dim]) # array to store current velocities and set ini
    W = np.zeros([nump,dim]) # array to store current random forces
    Rs = np.zeros([nums,nump,dim]) # array to store positions at all steps
    Vs = np.zeros([nums,nump,dim]) # array to store velocities at all steps
    Ws = np.zeros([nums,nump,dim]) # array to store random forces at all steps
    time = np.zeros([nums]) # an array to store time at all steps
```

Perform and animate the simulation using FuncAnimation

```
In [5]: fig = plt.figure(figsize=(10,10)) # set fig with its size 10 x 10 inch
ax = fig.add_subplot(111,projection='3d') # creates an additional axis t
box = 40 # set draw area as box^3
ax.set_xlim(-box/2,box/2) # set x-range
ax.set_ylim(-box/2,box/2) # set y-range
ax.set_zlim(-box/2,box/2) # set z-range
ax.set_xlabel(r"x",fontsize=20) # set x-lavel
ax.set_ylabel(r"y",fontsize=20) # set y-lavel
ax.set_zlabel(r"z",fontsize=20) # set z-lavel
ax.view_init(elev=12,azim=120) # set view point
particles, = ax.plot([],[],[],'ro',ms=8,alpha=0.5) # define object parti
title = ax.text(-180.,0.,250.,r'',transform=ax.transAxes,va='center') #
line, = ax.plot([],[],[],'b',lw=1,alpha=0.8) # define object line
n = 0 # trajectory line is plotted for the n-th particle
anim = animation.FuncAnimation(fig,func=animate,init_func=init,
                               frames=nums,interval=5,blit=True,repeat=False)
## If you have ffmpeg installed on your machine
## you can save the animation by uncomment the last line
## You may install ffmpeg by typing the following command in command prc
## conda install -c menpo ffmpeg
##
# anim.save('movie.mp4',fps=50,dpi=100)
```

