Tidynamics (CMSC6950)

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0.1 Introduction

A helpful reference for tidynamics is [**?**].

In this report I explain about **software**, scientific problems solved by the software. Also, **computational tasks** and related **visualizations** will be explained. At this report bibliography is added.

0.2 software

Tidynamics is a package to compute the dynamics of stochastic and molecular simulations with Fast Correlation Algorithm (FCA).tidynamics is designed as a library in which every routine operates directly on NumPy arrays and returns NumPy arrays The goal of tidynamics is to serve as a reference implementation with a lighter interface. This package computes the followings:

Autocorrelation (the correlation of a time series with itself) The correlation between two time-series
The mean-square displacement of a trajectory
The cross-displacement (for off-diagonal realisations of Brownian motion)

There is a lack of a self-contained implementation of the algorithm. The software nMoldyn (Hinsen, Pellegrini, Stachura, Kneller, 2012) implements it within a larger library but it has a more complex interface and more dependencies. The goal of tidynamics is to serve as a reference implementation with a lighter interface.

tidynamics is designed as a library in which every routine operates directly on NumPy arrays and returns NumPy arrays. The interface is simple and enables convenient use in interactive sessions or in teaching material.

The Fast Correlation Algorithm relies on the Fourier transform to compute correlations. For this purpose, we use NumPy's (T. E. Oliphant, 2007) FFT module np.fft. The advantage of using Fourier transforms is a reduced computational cost in comparison to a direct loop over the data. We expect a scaling of the CPU time tCPU of tCPU N log N where N is the length of the time series. We show in Figure 3 the actual CPU time and compare it favourably to the expected scaling in the example Scaling behaviour.

NumPy (T. E. Oliphant, 2007) and SciPy (Jones, Oliphant, Peterson, others, 2001) implement correlation routines as well. In the case of NumPy, the computation is based on a direct loop with a quadratic scaling of the CPU time O(N2). In SciPy, both the direct and a Fourier transform version are implemented.

The definition of np.correlate and scipy.signal.correlate differs from the definition traditionally used in dynamical systems in two ways. These routines do not correct for aperiodic signals, an issue that is addressed in the Fast Correlation Algorithm by zeropadding the signal, and they do not normalise the result by the actual number of samples. In addition to these differences, the relative complexity of building SciPy and its larger size motivated us to

rely on NumPy only. NumPy and SciPy do not provide functions to compute the mean-square displacement of trajectories. The Fast Correlation Algorithm as applied to mean-square displacements was proposed by G. R. Kneller et al. (1995) and is less known than the plain correlation algorithm. The benefits of using tidynamics originate in the implementation of the suitable definitions for the study of dynamical systems, good performance, and its ease of installation.

0.3 computational tasks

In this project, I implement two computational tasks with two different visualization.

0.3.1 tidynamics.correlation(data1, data2)

Correlation between the input data using the Fast Correlation Algorithm. It has two input signal with the same shape (N) and returns ndarray with the correlation for two inputs and the lag in units of the timestep in the input data. The correlation is given from time -N to time N.

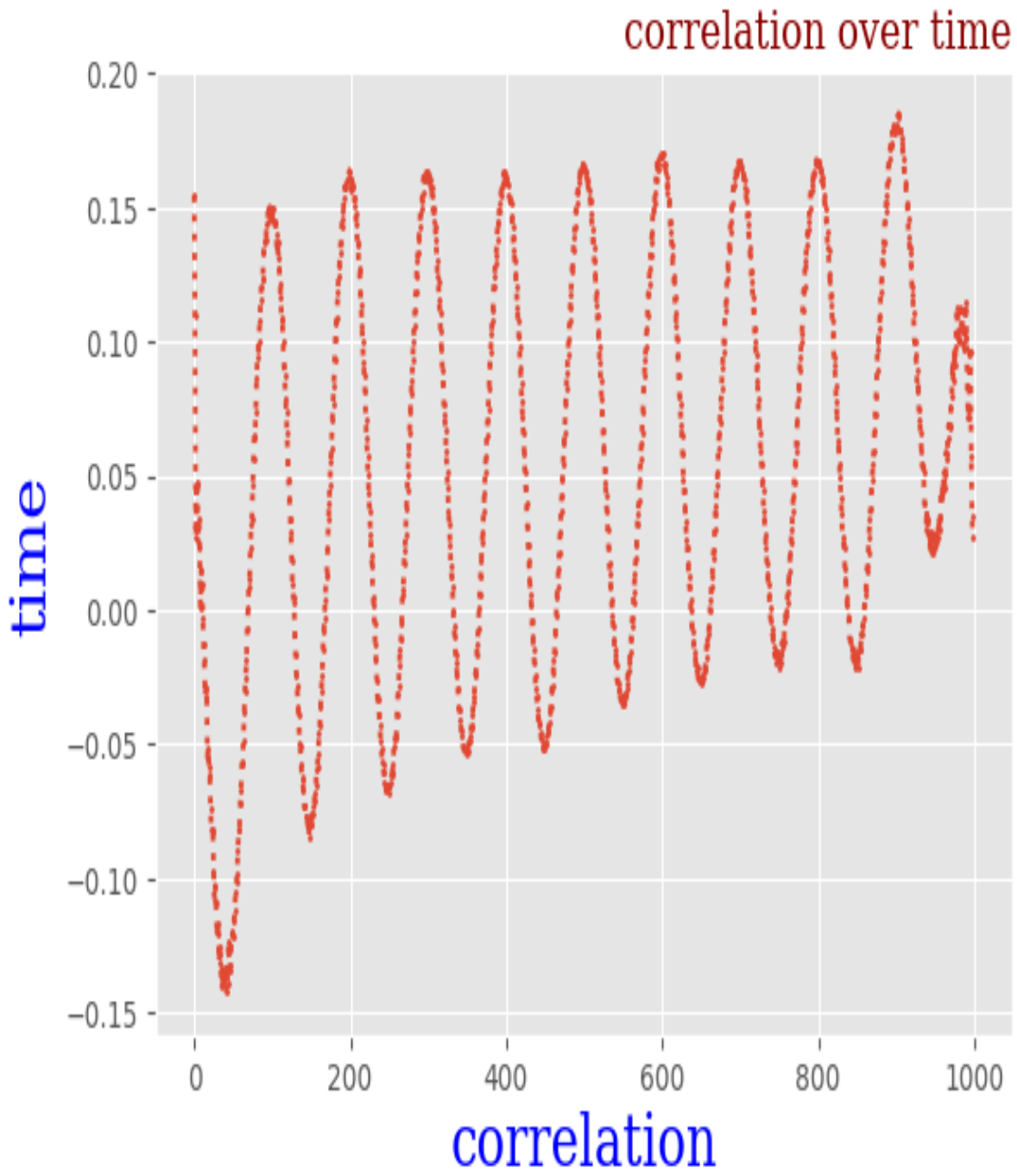
Below is the code and its visualization for tidynamics.correlation(data1, data2):

computation

```
import matplotlib.pyplot as plt
import pandas as pd
import numpy as np
import tidynamics
plt.style.use('ggplot')
font1 = ['family':'serif','color':'blue','size':20]
font2 = ['family':'serif','color':'darkred','size':15]


plt.rcParams['figure.figsize']=(10,10)


spacing = np.linspace(-5 * np.pi, 5 * np.pi, num=500)
t = np.linspace(-7 * np.pi, 7 * np.pi, num=500)
s = pd.Series(0.6 * np.random.rand(500) + 0.3 * np.sin(spacing))
t= pd.Series(0.4 * np.random.rand(500) + 0.7 * np.sin(spacing))
acf = tidynamics.correlation(s,t)


plt.plot(acf,marker='.',ms = 2, mfc = 'm',linestyle='dotted',linewidth = '2')


plt.title("correlation over time",fontdict=font2,loc = 'right')
plt.xlabel("correlation",fontdict=font1)
plt.ylabel("time",fontdict=font1)
```

plt.savefig("figure-correlaion.png", dpi=100, bbox$_inches = ' tight')$
$plt.show()$

visualization



correlation

0.3.2 tidynamics.msd(pos)

Mean-squared displacement (MSD) of the input trajectory using the Fast Correlation Algorithm. Computes the MSD for all possible time deltas in the trajectory. The numerical results for large time deltas contain fewer samples than for small time times and are less accurate. This is intrinsic to the computation and not a limitation of the algorithm.
It contains The input trajectory, of shape (N,) or (N,D) and returns ndarray of shape (N,) with the MSD for successive linearly spaced time delays.

Below is the code and its visualization for tidynamics.msd(pos):

computation

```
import array as arr
import matplotlib.pyplot as plt
import tidynamics
import random
import sys
from numpy import *


font1 = 'family':'serif','color':'blue','size':20
font2 = 'family':'serif','color':'darkred','size':15


plt.rcParams['figure.figsize']=(10,10)


plt.style.use('Solarize-Light2')


try:
N=3000
mean=linspace(0,0,N,dtype=float)
count=0
dock=range(1,100)
for i in dock:

s=[-1,1]
steps=random.choice(s, size=(N,2))
data = cumsum(steps, axis=0)
mean += tidynamics.msd(data)
count+=1
```

mean /= count
mean = mean[1:N//2]

T = arange(1,N//2)

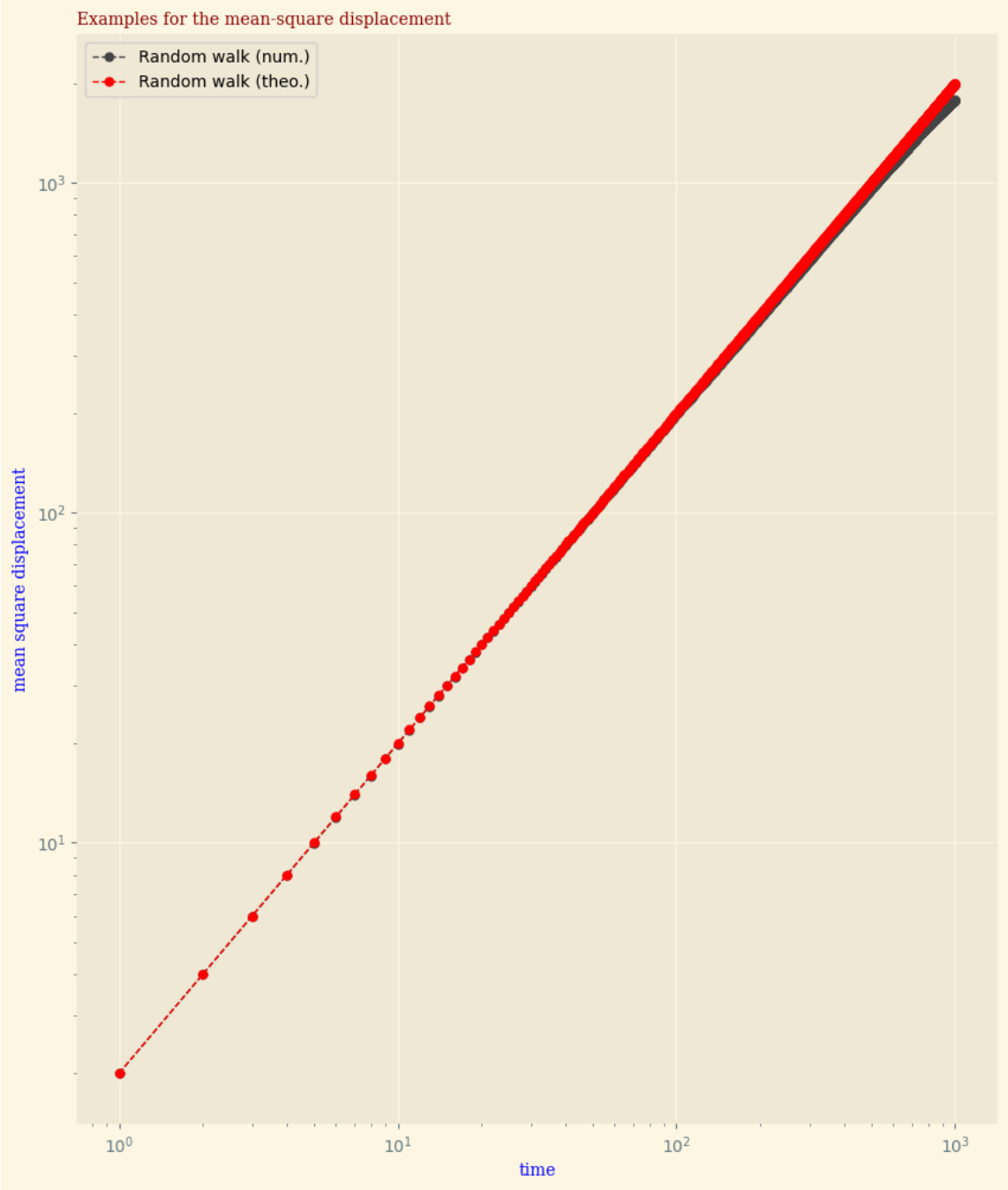
plt.plot(T, mean,color="444444",linestyle="–",marker = 'o',ms =5 ,linewidth = '1', label='Random walk (num.)')

plt.plot(T, 2*l,color="r",linestyle="–",marker = 'o',ms =5,linewidth = '1', label='Random walk (theo.)')

plt.legend()
plt.loglog()

plt.plot()
plt.xlabel('time', fontdict = font1, fontsize=10)
plt.ylabel('mean square displacement',fontdict = font1, fontsize=10)
plt.title('Examples for the mean-square displacement', fontdict = font2, fontsize=10, loc = 'left')
plt.savefig("figure$_m sd.png", dpi = 100, bbox_inches =' tight')$
$plt.show()$

visualization



correlation