Stochastic simulation for an active Brownian particle

1. Introduction

In this project, a self-propelled particle modelled by the stochastic differential equations (1) to (3) will be studied:

$$\begin{cases} \frac{dx}{dt} = v\cos\phi & (1) \\ \frac{dy}{dt} = v\sin\phi & (2) \\ \frac{d\phi}{dt} = \sqrt{2D_R}\xi & (3) \end{cases}$$

Here v is the active constant velocity,
$\mathbf{r}(t) = (x(t), y(t))$ is the position,
$\mathbf{n}(t) = \cos\phi(t)\mathbf{i} + \sin\phi(t)\mathbf{j}$ is the direction of motion,
D_R is the rotational diffusion coefficient, and
ξ is a Gaussian white noise satisfying $\langle\xi\rangle = 0$ and $\langle\xi(t_2)\xi(t_1)\rangle = \delta(t_2 - t_1)$

The autocorrelation of the direction of motion $\langle\mathbf{n}(s+t)\cdot\mathbf{n}(s)\rangle$ and the long term mean square displacement will be focused.

2. Dynamics

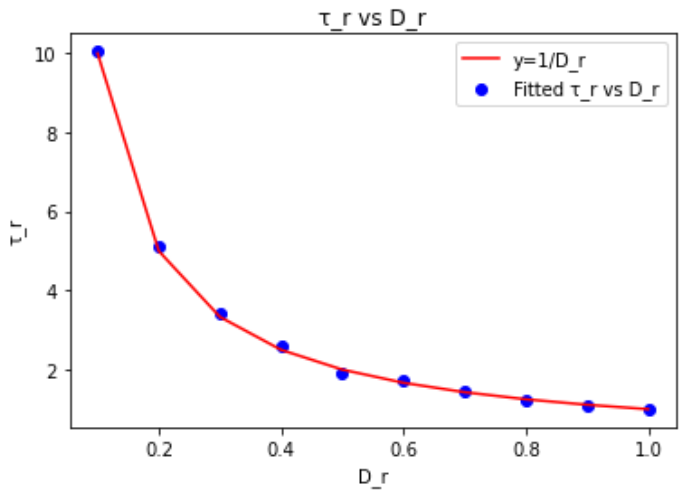
The system of stochastic differential equations (1) to (3) models a particle which propels itself with speed v while undergoing Brownian motion in orientation. In other words, its orientation undergoes free diffusion such that the direction of motion are random. This type of dynamics is referred to as rotational diffusion dynamics.

3. Autocorrelation of the direction of motion $\mathbf{n}(t)$

The autocorrelation of the direction of motion is given by:

$$\langle\mathbf{n}(s+t)\cdot\mathbf{n}(s)\rangle = \lim_{T\to\infty}\left[\frac{1}{T}\int_0^T \mathbf{n}(s+t)\cdot\mathbf{n}(s)ds\right] = \exp\left(-\frac{|t|}{\tau_R}\right) \qquad (4)$$

The autocorrelation is an exponential decay function in time, which approaches 0 when t is getting more positive or negative. It means that the dependence of the direction of motion to its lag-t direction decreases as t increases. The speed of decay is governed by τ_R which depends on the rotational diffusion coefficient D_R through the relation $\tau_R = \frac{1}{D_r}$. The smaller the τ_R, the faster the decay. The dependence of τ_R on D_R could be simulated with the code in part (A) of the Appendix and the relation could be visualized as figure below.

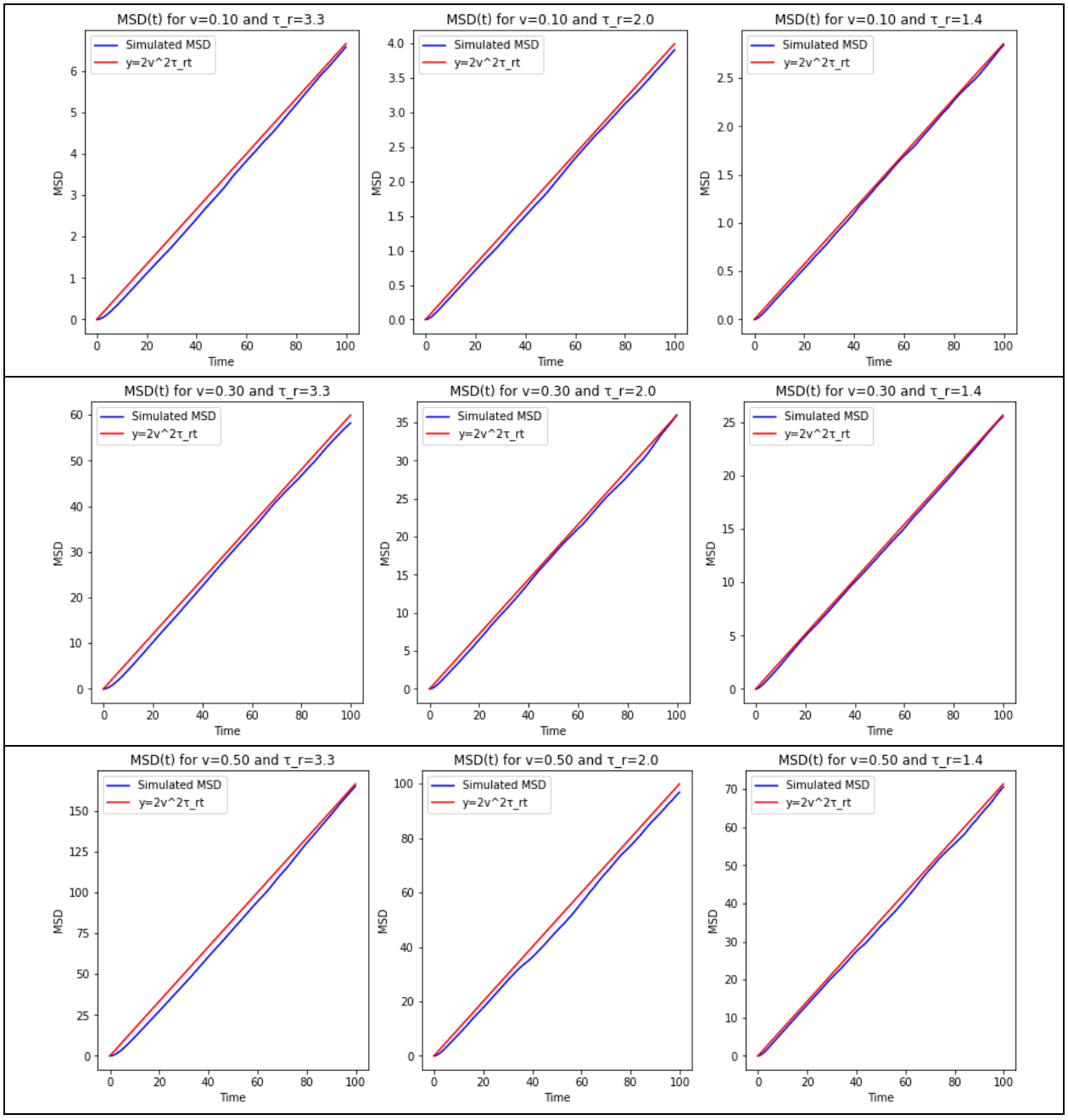


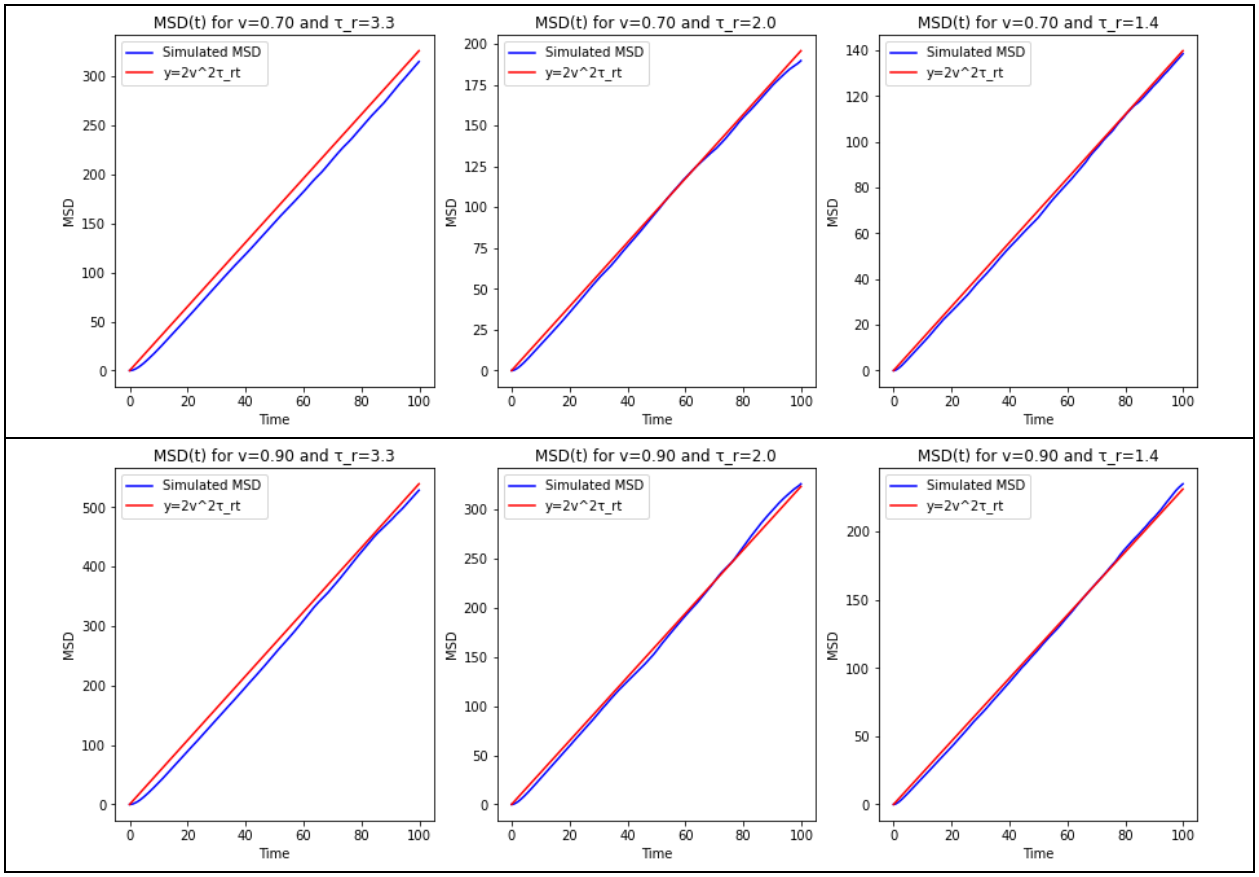
4. Mean square displacement (MSD)

The mean square displacement measures how far on average the particle is from the initial position. For the active Brownian particle described by equations (1) to (3), the theoretical MSD is given by:

$$\mathrm{MSD}(t) = 2v^2\tau_R t + 2v^2\tau_R^2\left[e^{-\frac{t}{\tau_R}} - 1\right] \qquad (5)$$

For $t \gg \tau_R$, $\mathrm{MSD}(t) = 2v^2\tau_R t - 2v^2\tau_R^2 \cong 2v^2\tau_R t$, which is a linear function of t. It means that the mean square displacement will grow linearly with rate $2v^2\tau_R$ when $t \gg \tau_R$. Such theoretical result could be verified through simulation with the code in part (B) of the Appendix and the result could be visualized as figures below.





5. Appendix (source code)

(A)Dependence of τ_R on D_R

```
import numpy as np
from numpy import sin, cos, exp, sqrt
import matplotlib.pyplot as plt
from scipy.optimize import curve_fit

np.random.seed(5003)

samples = 50
N = 1000  # number of steps
h = 0.1 # step size
Ts = np.arange(0, N*h, step=h)

phi = np.zeros(N) # array for direction of motion
Dr = np.linspace(0.1,1,10)
tau_r = np.zeros(10)

z_mu = 0
z_sd = sqrt(1/h)

def auto_corr(t, tau):
    return exp(-abs(t)/tau)
```

```
for idx, dr in enumerate(Dr):
    print(f'Dr = {dr:.1f}')
    acf = np.zeros((samples, N))
    for ns in range(samples):
        zetas = np.random.normal(z_mu, z_sd, (N-1))

        # Euler method for phi, x and y
        for i in range(1,N):
            phi[i] = phi[i-1] + h*zetas[i-1]*sqrt(2*dr)

        sinphi = sin(phi)
        cosphi = cos(phi)

        for t in range(N):
            ac = 0
            for s in range(N-t):
                ac += cosphi[s]*cosphi[s+t]+sinphi[s]*sinphi[s+t]
            acf[ns,t] = ac/(N-t)

    tau0 = 1
    macf = acf.mean(axis=0)
    c = int(1/(dr*h))
    tau_fit = curve_fit(auto_corr, Ts[:c], macf[:c], p0=[tau0])[0][0]
    print(f'tau_r = {tau_fit:.2f}')
    tau_r[idx] = tau_fit

plt.scatter(Dr, tau_r, c='b', label='Fitted \u03C4_r vs D_r')
plt.plot(Dr, 1/Dr, c='r', label='y=1/D_r')
plt.xlabel('D_r')
plt.ylabel('\u03C4_r')
plt.title('\u03C4_r vs D_r')
plt.legend()
plt.show()
```

(B) MSD with selected v and $\tau_R = \frac{1}{D_R}$

```
np.random.seed(5003)

samples = 3000
N = 1000  # number of steps
h = 0.1 # step size
Ts = np.arange(0, N*h, step=h)

phi = np.zeros(N) # array for direction of motion
x = np.zeros(N) # array for x
y = np.zeros(N) # array for y
```

```
Dr = [0.3,0.5,0.7]
V = [0.1,0.3,0.5,0.7,0.9]
msd = np.zeros((10,N))

z_mu = 0
z_sd = sqrt(1/h)

for v in V:
    plt.figure(figsize=(15,5))
    for idx, dr in enumerate(Dr):
        sd = np.zeros((samples, N))
        for ns in range(samples):
            zetas = np.random.normal(z_mu, z_sd, (N-1))
            for i in range(1,N):
                phi[i] = phi[i-1] + h*zetas[i-1]*sqrt(2*dr)
                x[i] = x[i-1] + h*v*cos(phi[i-1])
                y[i] = y[i-1] + h*v*sin(phi[i-1])
                sd[ns,i] = x[i]**2 + y[i]**2
        # Plotting
        plt.subplot(1,len(Dr),idx+1)
        plt.plot(Ts, sd.mean(axis=0), 'b', label='Simulated MSD')
        plt.plot(Ts, 2*v**2*Ts/dr, 'r', label=f'y=2v^2\u03C4_rt')
        plt.title(f'MSD(t) for v={v:.2f} and \u03C4_r={1/dr:.1f}')
        plt.xlabel('Time')
        plt.ylabel('MSD')
        plt.legend()
    plt.show()
```