Auto-correlations

May 9, 2023

1 Open TA: Auto-correlations

- Brownian particle's Langevin equation: $dV = -\gamma V dt + \sqrt{2D} dW$.
  - γ - Damping rate;
  - D - Velocity diffusion constant.

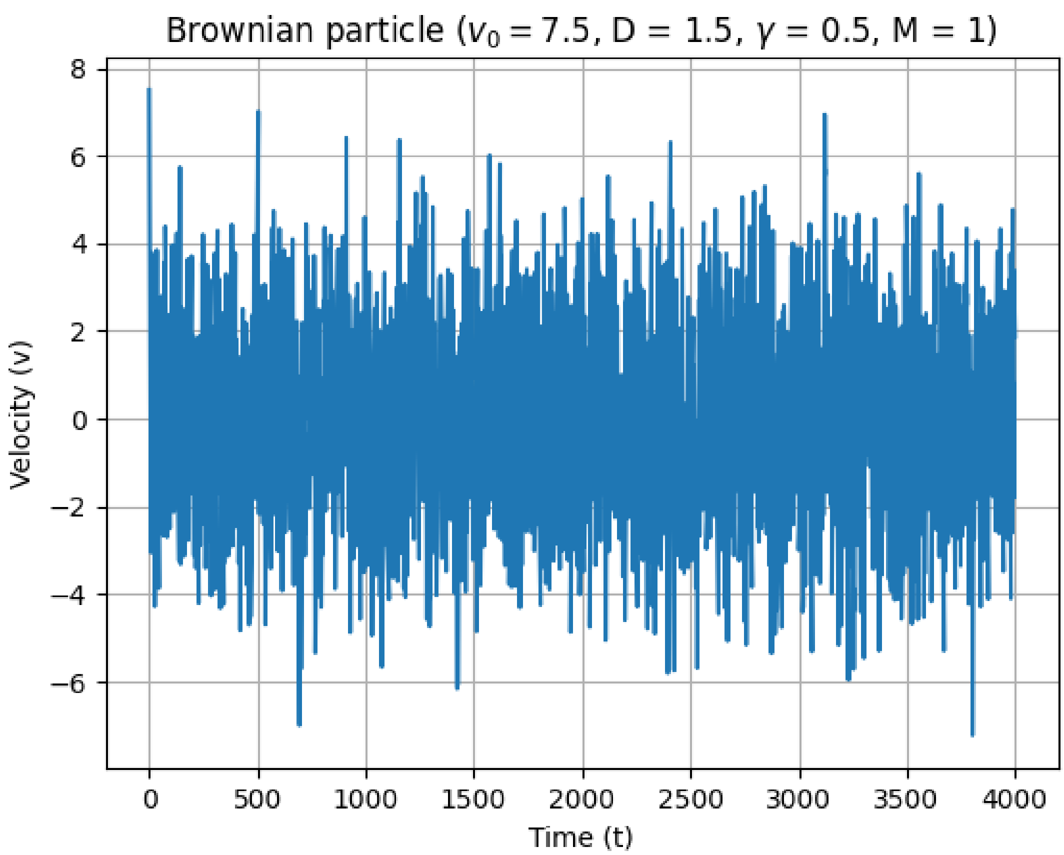
[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import trapezoid
from scipy.signal import unit_impulse
plt.style.use('fast')
```

1.1 Question a):

In this question, I choose the values of the parameters arbitrarily, since we aren't provided any concrete values. However, I do so in such a way that it is apparent how the solution decays exponentially (from $v_0 = 7.5$), initially, later arriving at a stationary state around $v = 0$ (Where the fluctuations are also clearly visible). Additionally, dt is simply chosen in a way that gives us sufficient resolution of the process. Note: dt had to be sufficiently small to be able to reliably resolve the cross(auto)-correlation plots, presented below, especially for the Dirac delta case.

[ ]:
```
v0     = 7.5    # Initial position
T      = 4_000
tSteps = 20_000 # Number of time-steps
dt     = T/tSteps
gamma  = 0.5
D      = 1.5

Trajs  = []
M      = 1      # Number of trajectories
xi     = []     # White noise vector

for m in range(M):
    vVec   = [v0]                                          # '+ 1': Just␣
↪so the dimensions match...
    dW     = np.random.normal(0., np.sqrt(dt), size = tSteps + 1) # Wiener␣
↪process: Mean = 0; Std_Dev = Sqrt(Var) = Sqrt(dt).
    xi.append(dW/dt)
```

```python
    for i in range(tSteps):
        vVec.append(vVec[i] - gamma * vVec[i] * dt + np.sqrt(2*D) * dW[i])
    Trajs.append(vVec)
    del vVec

for i in range(M):
    plt.plot(np.linspace(0., T, tSteps + 1), Trajs[i]) # Have to add +1,
                                                        # due to the initial␣
 ↪condition being included from the beginning.
plt.xlabel("Time (t)")
plt.ylabel("Velocity (v)")
plt.title(rf"Brownian particle ($v_0 = {v0}$, D = {D}, $\gamma$ = {gamma}, M =␣
 ↪{M})")
plt.grid(True)
plt.show()
```



1.2 Questions b) and c):

In this question, we attempt to extract the auto-correlation functions from the generated data. To do this, we compute the time-averages:

1. $C_{v\xi}(\tau) = \frac{1}{T}\int_{-T/2}^{T/2} dt v(t)\xi(t+\tau)$;
2. $C_{\xi\xi}(\tau) = \frac{1}{T}\int_{-T/2}^{T/2} dt \xi(t)\xi(t+\tau)$;
3. $C_{vv}(\tau) = \frac{1}{T}\int_{-T/2}^{T/2} dt v(t)v(t+\tau)$;

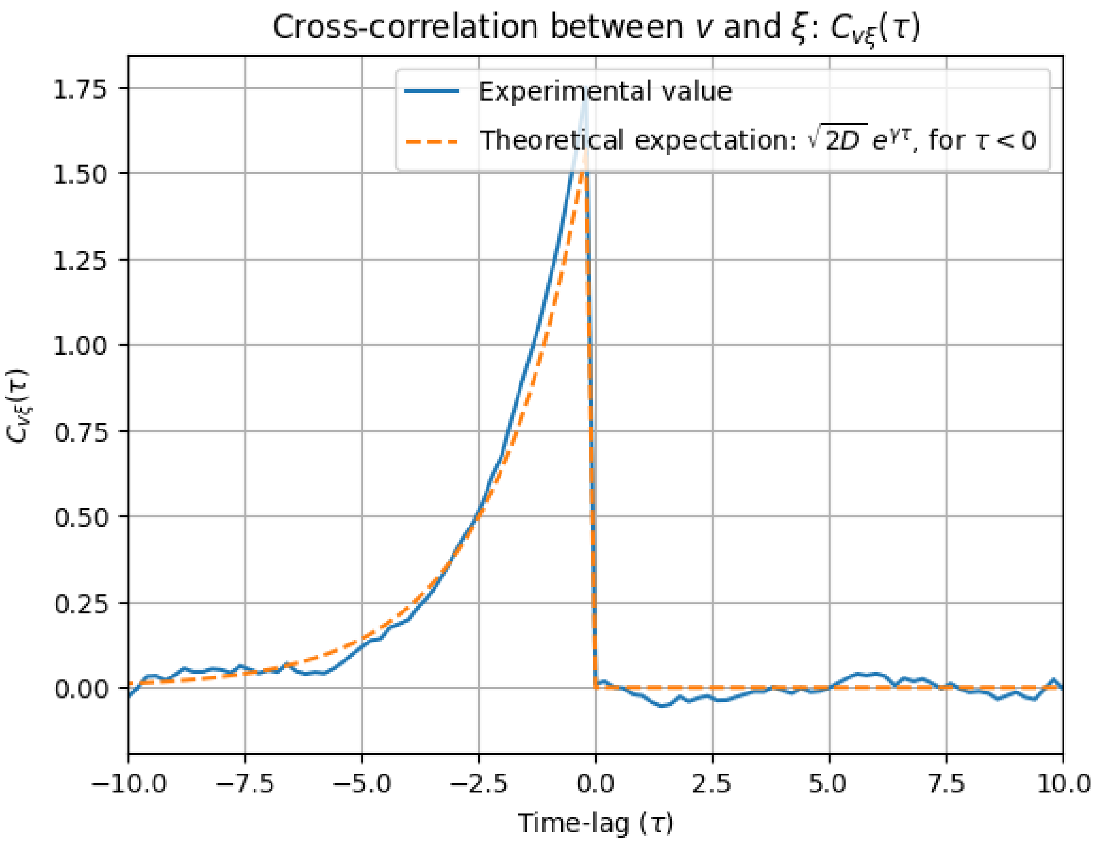
In order to do this, I shall simply compute these integrals numerically, e.g., using the trapezoidal rule.

Note that in the following I only use a **single** long trajectory! Additionally, note that these time-averages can be replaced with ensemble averages when: $\lim_{T\to\infty} \overline{X(t)}^T = \langle X \rangle$ is True, **and** the same is verified for all other moments. In this case, the process is called **ergodic**.

1.2.1 1). Cross-correlation between v and ξ: $C_{v\xi}(\tau)$

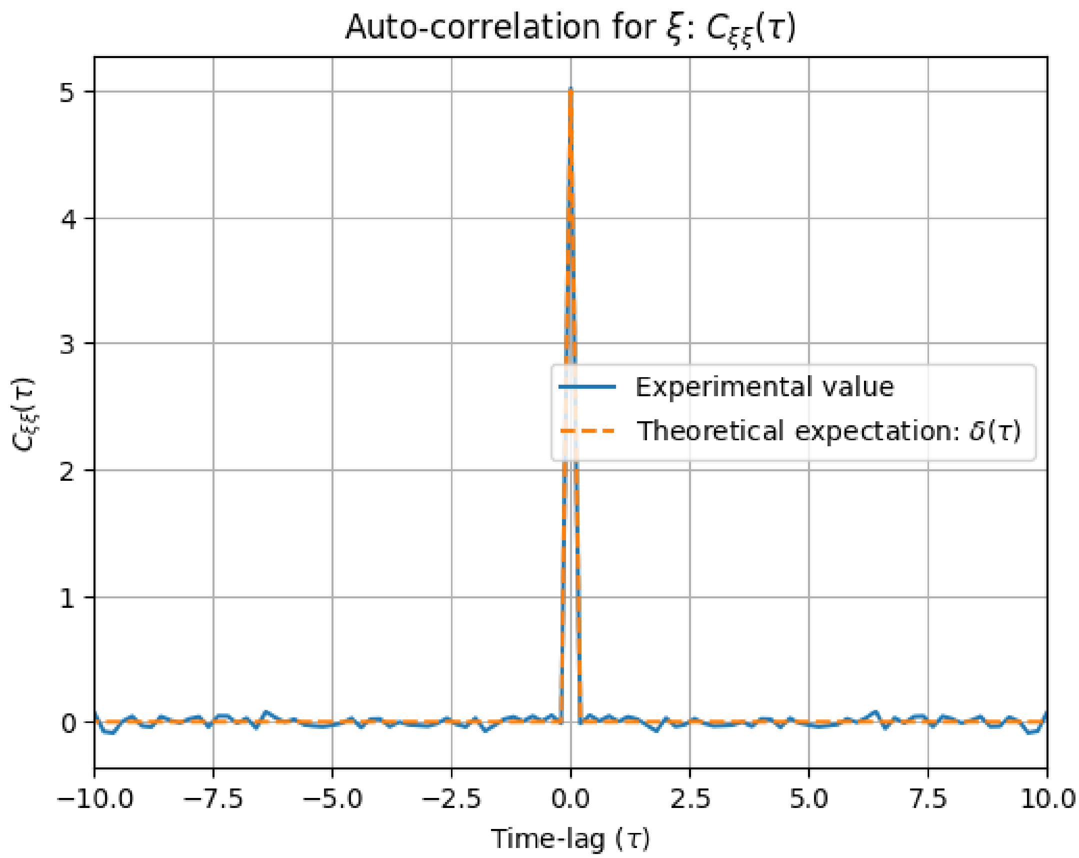
```
[ ]: # Looking for stabilized part of the signal
s_i = np.argwhere(np.array([i*dt for i in range(tSteps)]) > 100.)[0, 0]
print(f'Guaranteed to be stabilized after t[{s_i}] = {[i*dt for i in␣
 ↪range(tSteps)][s_i]}.')
T  = len(Trajs[0][s_i:-s_i]) * dt

C_vXi = np.array([1/T * trapezoid(np.array(Trajs[0][s_i:-s_i]) * xi[0][s_i+i:
 ↪-s_i+i], dx = dt) for i in range(-s_i, s_i)])
# C_vXi /= max(C_vXi)

t = np.array([i*dt for i in range(-s_i, s_i)])
plt.plot(t, C_vXi, label = 'Experimental value')
plt.plot(t, np.concatenate((np.sqrt(2*D) * np.exp(gamma*t)[:s_i], 0*t[s_i:])),
         label = r'Theoretical expectation: $\sqrt{2D}$ $e^{\gamma\tau}$, for␣
 ↪$\tau < 0$', linestyle = 'dashed')
plt.title(r'Cross-correlation between $v$ and $\xi$: $C_{v\xi}(\tau)$')
plt.xlabel(r'Time-lag ($\tau$)')
plt.ylabel(r'$C_{v\xi}(\tau)$')
plt.xlim(-10, 10)
plt.legend()
plt.grid(True)
plt.show()
# If I normalize everything, it's perfectly fine.
```

```
Guaranteed to be stabilized after t[501] = 100.2.
```



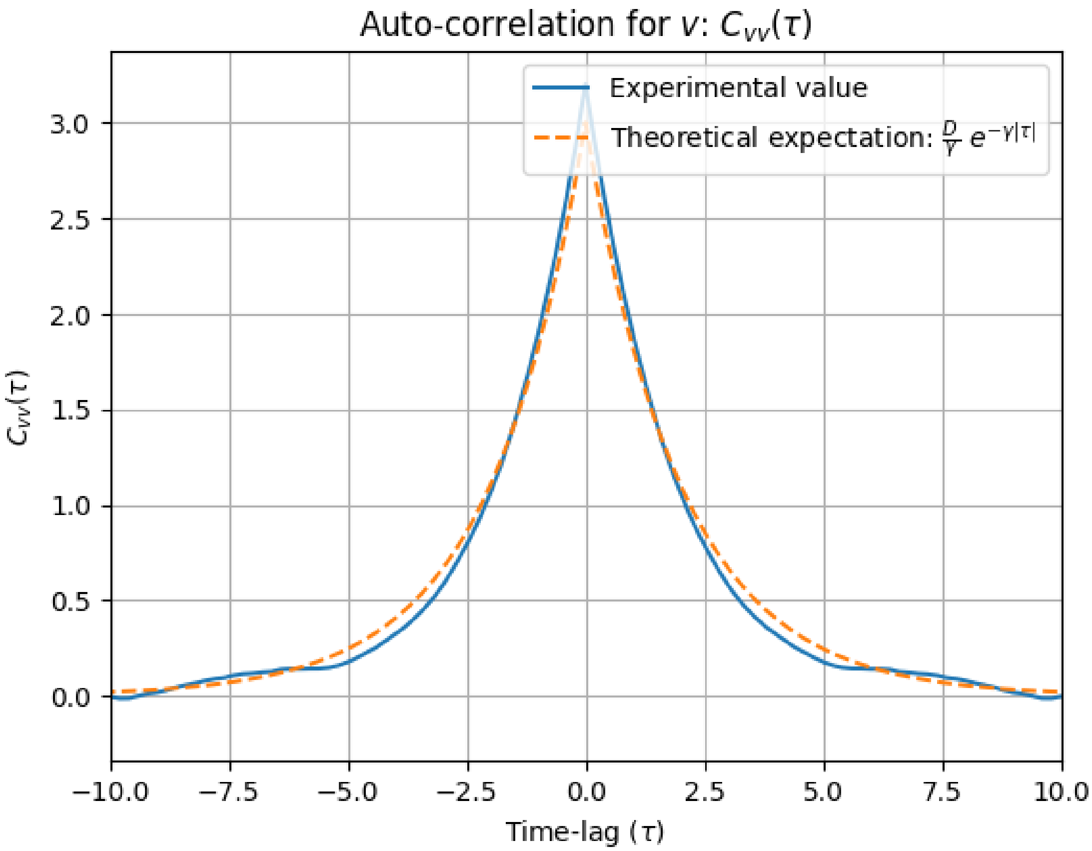
1.2.2 2). Auto-correlation for ξ: $C_{\xi\xi}(\tau)$

[ ]:
```
C_XiXi = np.array([1/T * trapezoid(np.array(xi[0][s_i:-s_i]) * xi[0][s_i+i:
  ↪-s_i+i], dx = dt) for i in range(-s_i, s_i)])
# C_XiXi /= max(C_XiXi)

t = np.array([i*dt for i in range(-s_i, s_i)])
plt.plot(t, C_XiXi, label = 'Experimental value')
plt.plot(t, 5 * unit_impulse(len(t), s_i), label = r'Theoretical expectation:␣
  ↪$\delta(\tau)$', linestyle = 'dashed')
plt.title(r'Auto-correlation for $\xi$: $C_{\xi\xi}(\tau)$')
plt.xlabel(r'Time-lag ($\tau$)')
plt.ylabel(r'$C_{\xi\xi}(\tau)$')
plt.xlim(-10, 10)
plt.legend()
plt.grid(True)
plt.show()
# If I normalize everything, it's perfectly fine.
```



1.2.3 3). Auto-correlation for v: $C_{vv}(\tau)$

[ ]:
```
C_vv = np.array([1/T * trapezoid(np.array(Trajs[0][s_i:-s_i]) * Trajs[0][s_i+i:
 ↪-s_i+i], dx = dt) for i in range(-s_i, s_i)])
# C_vv /= max(C_vv)

t = np.array([i*dt for i in range(-s_i, s_i)])
plt.plot(t, C_vv, label = 'Experimental value')
plt.plot(t, D/gamma * np.exp(-gamma * abs(t)), label = r'Theoretical␣
 ↪expectation: $\frac{D}{\gamma}$ $e^{-\gamma |\tau|}$', linestyle = 'dashed')
plt.title(r'Auto-correlation for $v$: $C_{vv}(\tau)$')
plt.xlabel(r'Time-lag ($\tau$)')
plt.ylabel(r'$C_{vv}(\tau)$')
plt.xlim(-10, 10)
plt.legend()
plt.grid(True)
plt.show()
# If I normalize everything, it's perfectly fine.
```



Finally, verifying the fluctuation-dissipation theorem (integral form):

```
[ ]: print(f'Experimental D_x = {trapezoid(C_vv[len(C_vv)//2:], dx = dt)}.')
print(f'Experimental, based on theoretical expression: D_x = {trapezoid(D/gamma␣
 ↪* np.exp(-gamma * abs(t))[len(C_vv)//2:], dx  = dt)}.')
print(f'Theoretical value: D_x = {D/gamma**2}.')
```

```
Experimental D_x = 5.412771600397436.
Experimental, based on theoretical expression: D_x = 6.00499916686503.
Theoretical value: D_x = 6.0.
```

We seem to have obtained reasonably good agreement with what was expected theoretically, for all three cases!

Notes: I saw that the cross(auto)-correlation can be defined differently for discrete objects, namely with a sum, i.e., not necessarily involving complex numerical integration techniques (Although `trapezoid` isn't that complex…). Either way, the results seem good enough.