

Math Capstone Project

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Introduction

In this article, we will explore the behavior of the damped harmonic oscillator (referred to as the particle in our discussion). Specifically, we consider the system $m\ddot{x} = -\gamma\dot{x} - Kx + \xi$, where m , γ , K , ξ denote the mass, frictional coefficient, spring constant, and noise, respectively. In part I, We will study its behavior without the noise ξ . We identified cases of overdamped, underdamped, and critical. In part II, we formally introduced the noise ξ and discussed how the spring's elastic force affects the particle's trajectory $x(t)$. In part II.1, we considered the case without the spring's presence and found the particle made a random walk. Specifically, the mean squared displacement of $x(t)$ linearly increases with the time t . In part II.2, we add back the spring and observe $x(t)$ reaches an equilibrium distribution under the spring's confine. The derivations in this article mainly used the Forward Euler Method and are all presented in the Appendix. In the end, we included all the figures and the numerical results. Python codes are also attached.

I: A Universe without the White Noise

Three Cases of the Harmonic Oscillator

Given $m\ddot{x} = -\gamma\dot{x} - Kx$ (1.1), we can set $p = \dot{x}$ (1.2), which further gives $\dot{p} = \ddot{x}$ (1.3). After specifying the initial position of the Brownian motion particle, $x(0) = x_0$ and its initial velocity, $p(0) = p_0$, we are interested in approximating the positions of the particle at different values of t . We adopted the Forward Euler Method and obtained the iterative equation,

$$x(t_{n+1}) = x(t_n) + p(t_n)h,$$

whose derivation details are presented in Appendix A. Due to the nature of the Forward Euler Method, we have already calculated the $x(t_n)$ and $p(t_n)$ from the previous steps. That makes our idea of approximating $x(t)$ for all t using Python's iterative function practicable. To set up a valid criterion to verify our numerical approximation, we will also derive the analytical solutions for (1.1). The derivation details and the physical interpretations of the ODE solutions of some special systems can be found in Appendix B.1 and B.2. The numerical results are illustrated in Figure 1.

II: A Universe with the White Noise

After setting up the basic framework, we now introduce the noise to the current system for a more realistic simulation. The governing equation, hence, turns to be

$\gamma\dot{x} = -Kx + \xi$ (3.1), where ξ represents the noise. In Physics, we regard these noises as constant kicks. These kicks guarantee the particle will never stop at a fixed point, even at its equilibrium state. We assume the noise in our model has zero mean, i.e., $\langle \xi \rangle = 0$, considering noise's mean reversion property in many real-life cases. We expect noises not to be a self-perpetuating force in favor of any specific direction but instead as a random disturbance to the system. In our model, noises oscillate with positive and negative signs and are supposed to be a neutral force in the sense that they overall cancel out each other's effect with a zero mean. We additionally assume a specified autocorrelation function to the noise. That is

$$R_\xi(t, t') = \langle \xi(t)\xi(t') \rangle = \Gamma\delta(t - t') \quad (3.2)$$

where $\Gamma = 2\gamma k_B T$ with $k_B T$ being the thermal energy. Such a setting builds a connection between the noise and the thermal energy; it reflects the physical phenomenon that particles move more vigorously and, hence, more irregularly compared to a still particle when the thermal energy increases. For example, the inks dropped into the water will spread faster under a higher temperature. In contrast, when we have an absolute zero temperature, i.e., $-273.15^\circ C$, every particle remains static, and no noise is involved.

Some properties of the modeled noise, hence, can be derived under our assumptions. We introduce a new notation $\zeta_i = \int_{(i-1)h}^{ih} \xi(t) dt$, where ζ_i is defined on the i th interval. ξ_i is an independent random noise by our assumption. ζ_i is an integration of a large number of ξ_i and each ξ_i made a minuscule contribution to its integration. We, hence, argue that ζ_i follows a normal distribution by Central Limit Theorem. The normal distribution's density function requires parameters mean μ and variance σ^2 . Since ζ_i is an integration of ξ_i , we take advantage of noise ξ_i 's mean and specified autocorrelation function to study the ones of ζ_i .

- Since $\langle \xi_i \rangle = 0$, $\langle \zeta_i \rangle = \int_{(i-1)h}^{ih} \langle \xi(t) \rangle dt$ due to the linearity of the expectation.
- We study the variance of ζ_i by considering a more general case, ζ_i 's covariance. The derivations in Appendix C gives, $\langle \zeta_i \zeta_j \rangle = 0$ if $i \neq j$; $= \Gamma h$ otherwise.

Therefore, $\zeta \sim \mathcal{N}(0, \Gamma h)$ as plotted in Figure 2.

The particle now moves consistently due to the introduction of noise. To investigate the contribution of the spring's elastic force to the system, we will separate our discussion into two cases. In case II. 1, we will first remove the spring from the model by setting $K = 0$ in the governing equation (3.1). That is, we consider a system without elastic force. Later, in case II. 2, we will add back the component involving K . That is, we resume the system with elastic force. By comparing these two contrasting systems, with and without the elastic force, we hope to understand the influence of the elastic force on the system. Specifically, we want to know how the elastic force will affect the particle's trajectory $x(t)$ throughout the time t .

II. 1 The System without the Elastic Force: - Random Walk

Under the wise of Physics, our intuition is that the elastic force confines the range of the particle's trajectory $x(t)$. Without the spring's constraint, the particle will make a random motion instead. Recall that our system becomes simpler due to the

absence of the elastic force. The governing equation, hence, becomes $\gamma\dot{x} = \xi$; a simpler system but involves ξ for us to study the particle's trajectory driven by noise. The mean squared displacement (MSD) is the standard measure of the random walk's spatial extent. We will, thus, take $x(0)$, the particle's initial position, as the reference point and study the deviation of the particle's position from its initial point over time using MSD. If the MSD grows with time, a diffusive trend can be concluded. Such a conclusion will support our expectation of the spring's functionality with more side evidence. Eventually, by contrasting the result we obtained here with the one of II. 2, we can show that the elastic force, or metaphorically, the spring, indeed, has a fixation on the particle's position.

To achieve our goal, we first need to find the expression of the particle's trajectory. The derivation is similar to the one presented in Appendix D, except $K = 0$, as we haven't introduced the elastic force. We obtained, $\Delta x_i = x_i - x_{i-1} = \zeta_i$, where i denotes at $t = ih$. Since we have already acquired some noise properties, we hope to use the noise as a bridge to establish the relationship between the trajectory x 's MSD and the time t . Eventually, using this trick, our derivation in Appendix E shows $\langle (x(t) - x(0))^2 \rangle = 2Dt$, where $D = k_B T / \gamma$. The numerical results are presented in Figures 3 and 4. The result verifies our initial conjecture about a diffusive trend of the particle's trajectory. Taking the real-life example of dropping the ink into the pond again, we can observe the contaminated ripple's radius, reflected by Root Mean Squared (RMS) Displacement, i.e., \sqrt{MSD} increases proportionally to the \sqrt{t} . Or equivalently, the area of the contaminated ripple, exhibited by MSD, expands pro rata with time t .

II. 2 The System with the Elastic Force: - Equilibrium Gaussian Distribution

Bringing back the elastic force, we resume the discussion of $\gamma\dot{x} = -Kx + \xi$ (3.1). The negative correlation between the \dot{x} and x suggests the spring will pull back the particle if it moves too far away from its equilibrium state. In a world without the noise ξ , such an equilibrium state is easy to be found as $x(t) = 0$ is an obvious solution of $\gamma\dot{x} = -Kx$. When the particle returns to position 0, both damped force and elastic force, signified by $\gamma\dot{x}$ and $-Kx$ respectively dismissed with magnitude equaling 0. However, recall that we have already abandoned such a noiseless world with a still particle with zero variance at the equilibrium state. We now shift our interest to study the *equilibrium distribution* of this particle's stochastic trajectory. Since the position $x(t) = 0$ is an equilibrium position in the world without noise, it is a natural question to ask if $x(t) = 0$ remains a critical position in a noise-filled universe. We answered this question by numerically generating $x(t)$ governed by the iterative equation.

$$x_i = x_{i-1} - \frac{K}{\gamma} x_{i-1} h + \frac{\zeta_i}{r}$$

Such an iterative equation can be obtained by applying the Forward Euler Method and generating $\zeta \sim \mathcal{N}(0, \Gamma h)$. The derivation details are shown in Appendix D. Indeed, we found the best fit normal distribution of numerically generated by $x(t)$ has a mean very close to 0 illustrated by Figure 5. That confirms our speculation. The particle attempts to return to its initial position 0, i.e., the equilibrium state

without the noise under the spring's constraint. However, due to the constant kicks by noise, the particle cannot entirely stop but oscillate around the $x(t) = 0$, contributing to the distribution's variance. We, hence, conclude that the particle will reach an *equilibrium distribution* limited by the spring's elastic force. The numerical results obtained from the Monte Carlo (MC) simulation are presented in Figure 6. Appendix F contains the corresponding MC algorithm.

III Conclusion

In this article, we have explored the particle's behavior under different settings, with and without the noise and spring, respectively. We verified the physical phenomenon by numerical simulations and concluded that the spring has a fixation on the particle's trajectory.

Figures

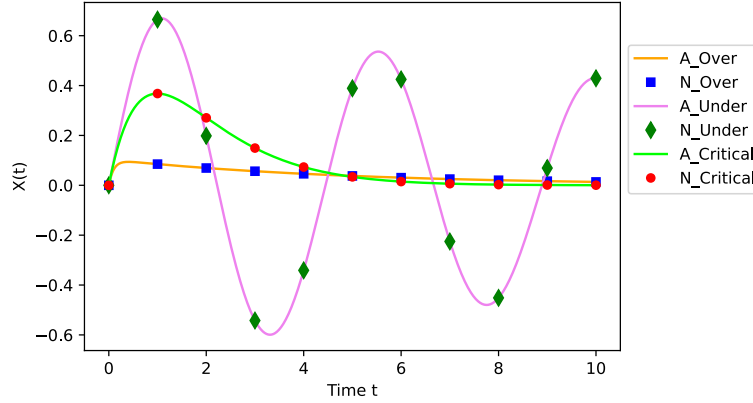


Figure 1: Comparison between the numerical and analytical results

A := analytical result, N := numerical result; lines and markers represent the analytical and the numerical values respectively; for the demonstration purpose, numerical values were drawn every 1 unit of time

the length of the interval: $t = 10$, time step: $h = 0.001$, initial position: $X(0) = 0$, initial velocity: $p(0) = 1$,

The orange line and blue squares corresponds to mass: $m = 1$, spring constant, $K = 2$, frictional coefficient $\gamma = 10$ (Overdamped)

The green line and red dots corresponds to mass: $m = 1$, spring constant, $K = 1$, frictional coefficient $\gamma = 2$ (Critical: Repeated Roots)

The purple line and green diamonds correspond to mass: $m = 10$, spring constant, $K = 20$, frictional coefficient $\gamma = 1$ (Underdamped)

The good fit between the analytical and numerical results was shown.

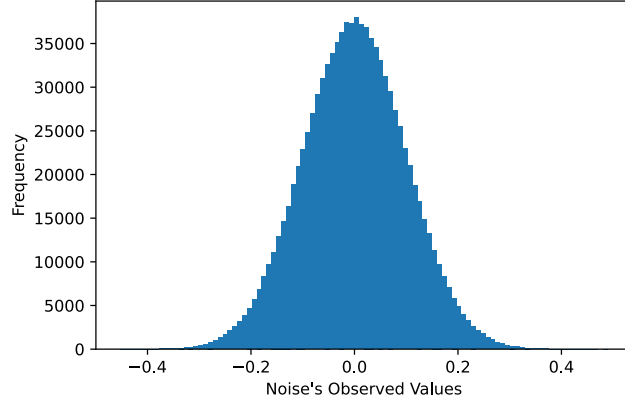


Figure 2: Noise $\sim \mathcal{N}(0, 0.1^2)$

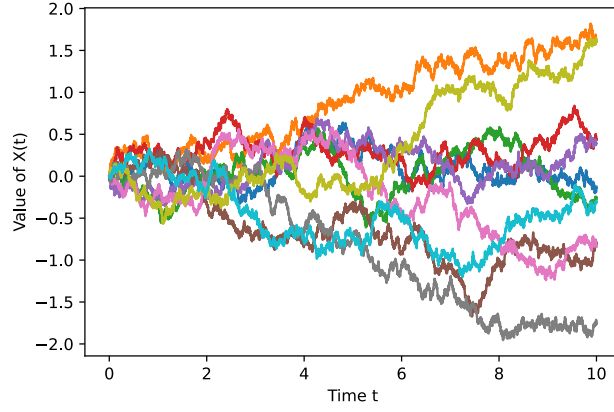


Figure 3: Trajectories of $X(t)$ generated from $x_i = x_{i-1} + \frac{\zeta_i}{r}$

10 Trajectories were drawn for the demonstration purpose. The diffusive trend of each individual trajectory diverging from the initial position is very clear.

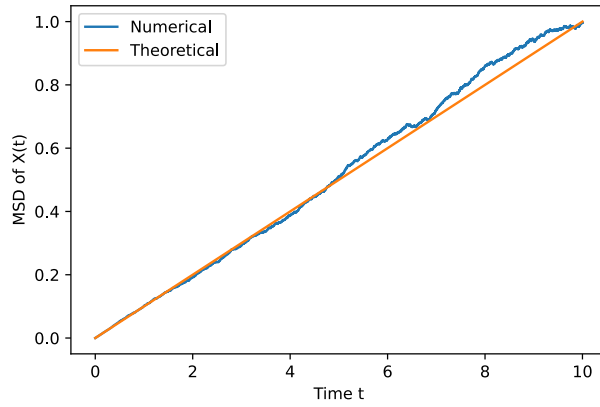


Figure 4: MSD of $x(t)$ as a function of time t

MSD is calculated every $h = 0.001$. The total number of observed points is, hence, $N = t/h = 10/0.001 = 10,000$. The theoretical line is MSD $\langle (x(t) - x(0))^2 \rangle = 2Dt$, where $2D = 2k_B T/\gamma = 2 * 0.5/10$. The best fitted single regression line has the slope $b = 0.1054$ and the intercept $a = -0.0132$

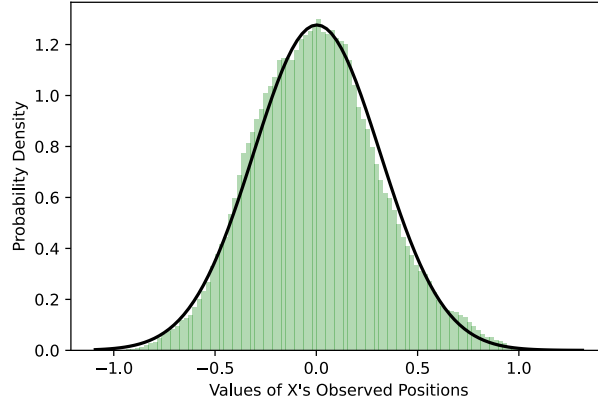


Figure 5: Estimated equilibrium distribution of $X(t)$ with noise generated from the iterative equation $x_i = x_{i-1} - \frac{K}{r}x_{i-1}h + \frac{\zeta_i}{\gamma}$ where $x_0 = 0$, $h = 0.001$, $K = 5$, $\gamma = 10$, $\zeta_i \sim \mathcal{N}(0, 0.1^2)$. The best fit normal distribution has the estimated parameters $\mu = 0.0029$, $\sigma^2 = 0.3124^2$. The theoretical distribution $X(t) \sim \mathcal{N}(0, k_B T/k = 0.5/5 = \sqrt{0.1}^2)$

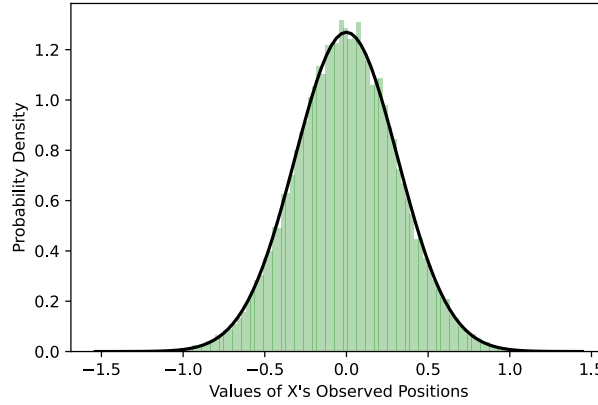


Figure 6: Estimated equilibrium distribution of $X(t)$ with noise generated from the MC simulation

The best fit normal distribution has the estimated parameters $\mu = -0.0006$, $\sigma^2 = 0.3143^2$. The theoretical distribution $X(t) \sim \mathcal{N}(0, k_B T/k = 0.5/5 = \sqrt{0.1}^2)$

Appendix

https://github.com/hyhoAlex/Math_Capstone_Project_Public

Codes: https://github.com/hyhoAlex/Math_Capstone_Project_Public

Acknowledgement

In this project, I have extensively used the materials and ideas provided by Prof. Qian Tiezheng. I deeply thank him for his supervision. All errors are mine.