Kramers–Moyal Expansion

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Abstract

In this homework I will demonstrate the conditional moments and the Kramers–Moyal (KM) expansion and specifically I calculated the KM coefficients $D^{(1)}(x,t)$ and $D^{(2)}(x,t)$. Indeed, $D^{(1)}(x,t)$ is the drift that moves the mean from x' to $(x' + \tau D^{(1)}(x',t))$, and determines where the process will go to on average. The second coefficient $D^{(2)}(x,t)$ is the diffusion coefficient and determines the strength of the stochastic influence.[1]

1 Kramers–Moyal Expansion

In stochastic process Kramers–Moyal Expansion refers to a Taylor series expansion of the master equation.[2]

The probability distributions of Markov processes satisfy a first-order partial differential equation in time and order infinity in the state variable.

The coefficients $K^{(n)}(x',t,\tau)$ can be calculated from the joint probability density functions. These joint PDFs are easily obtained from the data by counting the number $N(\bar{x},x)$ of occurrences of the two increments $\bar{x}$ and x. Then by taking the limit $\tau \to 0$, we obtain the Kramers–Moyal equation for the probability density function. [1]

The probability density $p(x,t+\tau)$,

$$p(x,t+\tau) = \int p(x,t+\tau|x',t)p(x',t)dx' \tag{1}$$

where $p(x,t+\tau|x',t)$ is the conditional probability distribution function.

We can calculate the conditional moments with Eq. 2,

$$\begin{aligned} K^{(n)}(x',t,\tau) &= \langle [x(t+\tau) - x(t)]^n \rangle |_{x(t)=x'} \\ &= \int (x-x')^n p(x,t+\tau|x',t)dx. \end{aligned} \tag{2}$$

we can write the conditional PDF as,

$$p(x,t+\tau|x',t) = \int \delta(y-x)p(y,t+\tau|x',t)dy. \tag{3}$$

Having a expansion of δ-function,

$$\begin{aligned} \delta(y-x) &= \delta(x'-x+y-x') \\ &= \sum_{n=0}^{\infty} \frac{(y-x')^n}{n!} (\frac{-\partial}{\partial x})^n \delta(x'-x). \end{aligned} \tag{4}$$

Using Eq. 3 we will obtain the following Eq. 5:

$$\begin{aligned} p(x,t+\tau|x',t) &= \sum_{n=0}^{\infty} (\frac{-\partial}{\partial x})^n \int \delta(y-x')^n p(y,t+\tau|x',t)\delta(x'-x)dy \\ &= \left[1 + \sum_{n=1}^{\infty} (\frac{-\partial}{\partial x})^n K^{(n)}(x',t,\tau)\right] \delta(x'-x) \end{aligned} \tag{5}$$

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Using Eq. 2 and Eq. 5,

$$p(x,t+\tau) - p(x,t) = \sum_{n=1}^{\infty} (\frac{-\partial}{\partial x})^n \left[\frac{K^{(n)}(x',t,\tau)}{n!} \right] p(x,t). \tag{6}$$

Finally by dividing both sides of Eq. 6 by τ and taking the limit $\tau \to 0$, we obtain the Kramers–Moyal equation,

$$\frac{\partial p}{\partial x} = \sum_{n=1}^{\infty} (\frac{-\partial}{\partial x})^n [D^{(n)}(x,t)p(x,t)] \tag{7}$$

And, the Kramers–Moyal coefficients, $D^{(n)}(x,t)$ is given in the form of the following equation,

$$D^{(n)}(x,t) = \frac{1}{n!} \lim_{\tau \to 0} \frac{1}{\tau} K^{(n)}(x,t,\tau) = \frac{1}{n!} \lim_{\tau \to 0} \frac{1}{\tau} \langle [x(t+\tau) - x(t)]^n \rangle |_{x(t)=x} \tag{8}$$

If we assume that coefficients $D^{(1)}(x,t)$ and $D^{(2)}(x,t)$ are smooth and not changing dramatically over a short time interval we can derive the conditional PDF and see that is a Gaussian distribution,(complete calculation is provided in [1], section 3.3),

$$p(x,t+\tau|x',t) = \frac{1}{2\sqrt{\pi\tau D^{(2)}(x',t)}} exp\left\{ - \frac{(x - x' - \tau D^{(1)}(x',t))^2}{4\pi D^{(2)}(x',t)} \right\} \tag{9}$$

The conditional PDF in Eq. 9 is a Gaussian distribution with mean value $(x + \tau D^{(1)}(x,t))$ and variance $2D^{(2)}(x,t)\tau$. Indeed, $D^{(1)}(x,t)$ is the drift that moves the mean from x' to $(x' + \tau D^{(1)}(x',t))$, and determines where the process will go to on average. The second coefficient $D^{(2)}(x,t)$ is the diffusion coefficient and determines the strength of the stochastic influence.[1]

2 Result

In this section, I provided the result of my python code for conditional moments and drift and diffusion coefficients.

Our dataset is a time series that included $N = 10^6$ data points. Our time step or τ for this dataset is equal to $\tau = 0.001$. In this problem, we did not consider the limit $\tau \to 0$. In Fig. 1 we can see the trajectory of our dataset, $X(t_i)$.

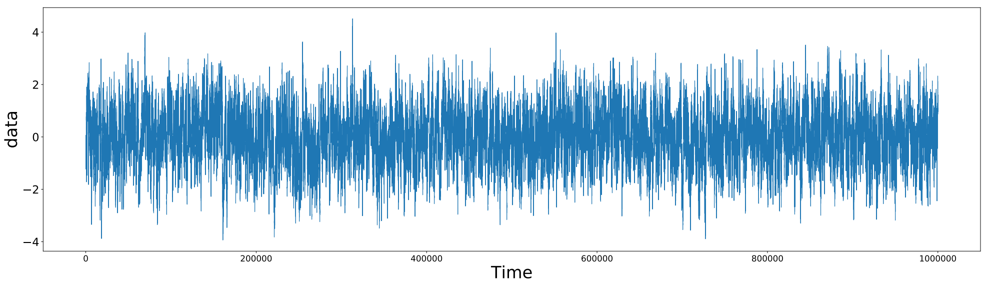

Figure 1: Time series of x(t) versus interval number t

2.1 Conditional Moments

Calculating the conditional moments or $K^{(n)}$ for this large dataset was very time-consuming, therefore to reduce the run-time I used the pandas library [6] in python, Instead of array I made a data frame format of the dataset and calculate the conditional moments.

First, with the function pd.diff, I calculated the difference between each data point and its previous data point then run this calculation for $N' = N/4$ time for each tau from 0 to $N/4$,(the NaN values is also eliminated) Also this calculation is implemented for different power $K = [0.1, 0.2, 0.3, ..., 1, 2, 3, 4, 5, 6]$.

In Fig 2, I demonstrated the S_K or the conditional moments for different Ks.

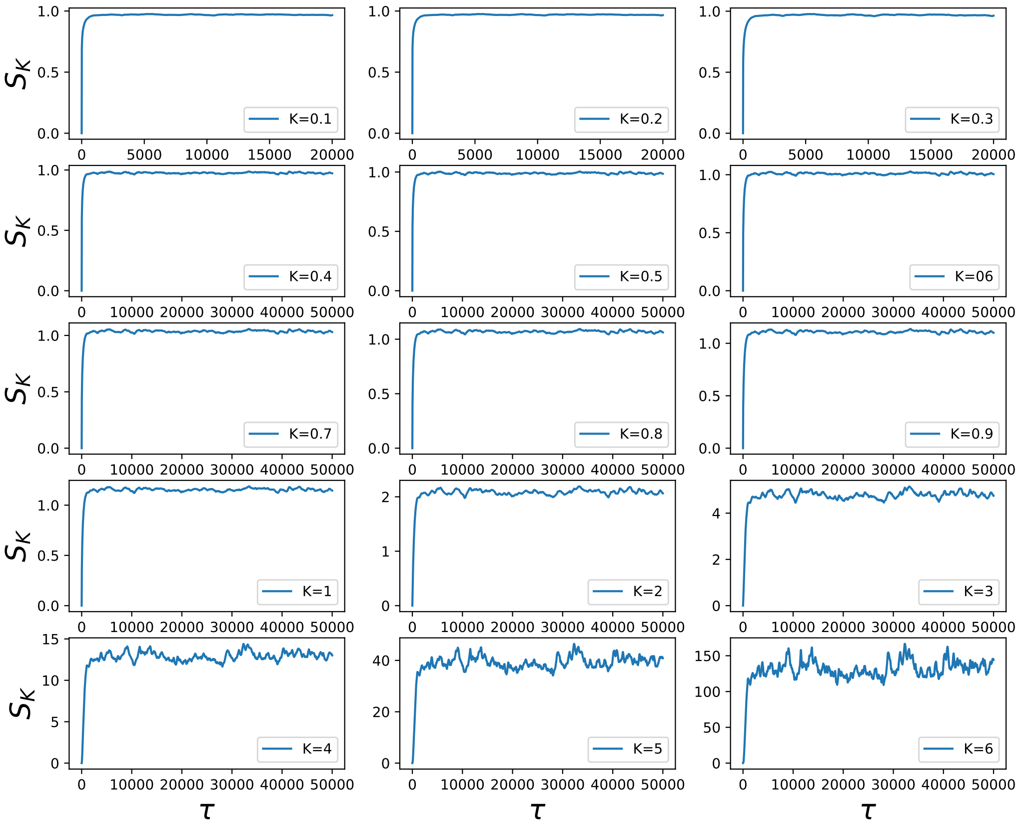

Figure 2: Conditional moments for different K.

Also, in Fig. 3 we can see the log-log plot of S_K for different Ks and the orange line is shown to represent when the S_K behave linearly in log-log plot. Also if we consider $S_K \sim \tau^{\xi_K}$, the power in this relation or ξ_K is the slope of the orange line in each plot.

In Fig. 4, I plotted the ξ_K which was derived from Fig. 3 for each K. It is obvious that for larger K, we obtain bigger ξ_K, as a result of bigger moments for bigger Ks.

2.2 "Drift" & "Diffusion"

To calculate the drift and diffusion, first we calculate the maximum and the minimum of our data. Then we can use binning to make calculation easier and faster. After we obtain max and min of data we can make an array of numbers varies from min to max with size of our bin, which in this problem we consider bins $= 51$. After binning the data we calculate the difference between $x[i+1]$ and $x[i]$ which i varies from 0 to N. Therefore now for each bin we have an array that contain the difference between each data point and its previous data point. we save this in an another array. Drift is the average of these differences for each bin and the Diffusion is the average of these difference to the power of two. So we obtain 71 points for each drift and diffusion coefficients. Also, I calculated the standard deviation for each point using the sympy library [5] in python.

In Fig. 5 and Fig. 6 we can see the drift coefficient and diffusion coefficient respectively.

both coefficient exhibit simple dependencies on the x value increment, While $D^{(1)}$ is linear in x and $D^{(2)}$ is a constant. The green line in both Fig. 5 and 6 is the line that we can fit to the 71 data points for each drift and diffusion.

$$D^{(1)}(x) = -0.003545x \tag{10}$$

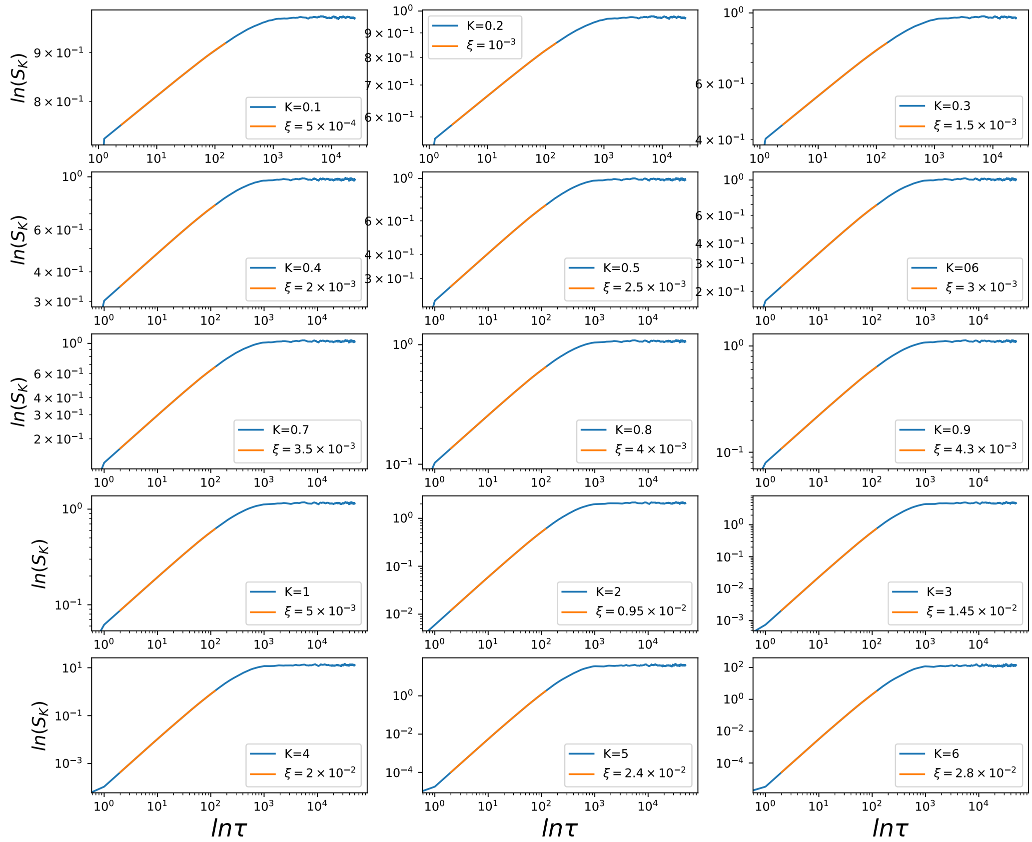

Figure 3: conditional moments in logarithmic plot.

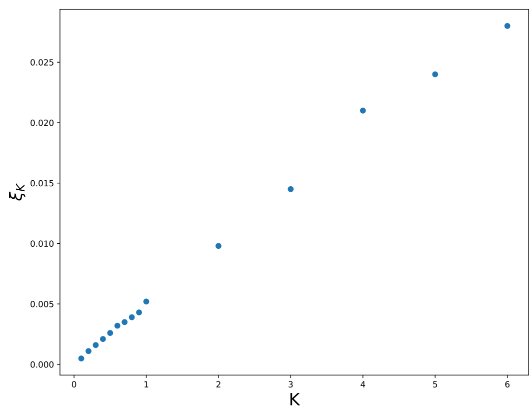

Figure 4: ξ_K for each K is plotted.

And,

$$D^{(2)}(x) = 0.006631 \tag{11}$$

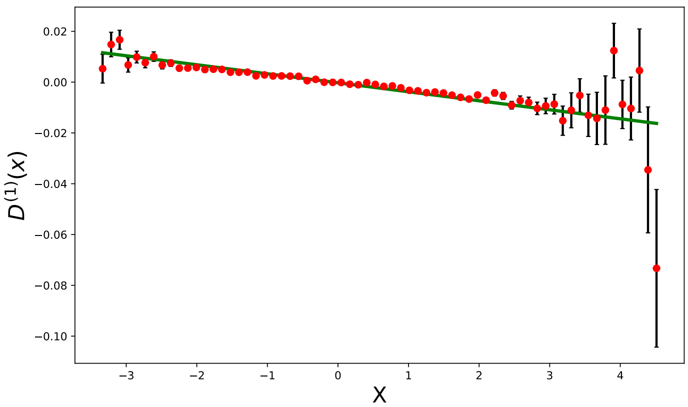

Figure 5: Drift

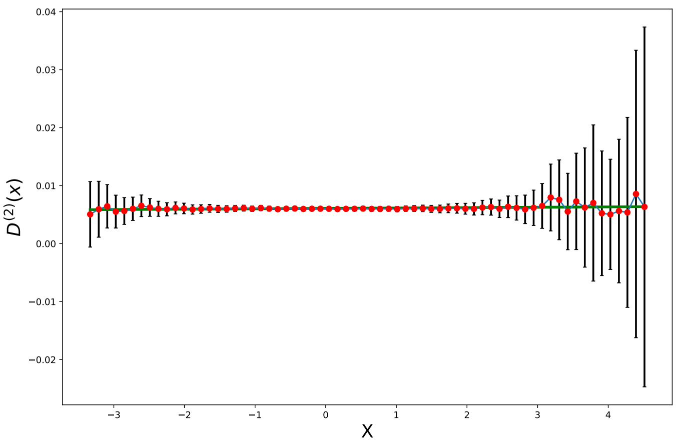

Figure 6: Diffusion

References

[1] M. R. Rahimi Tabar, Analysis and Data-Based Reconstruction of Complex Nonlinear Dynamical Systems, Understanding Complex Systems, DOI: `https://doi.org/10.1007/978-3-030-18472-8`

[2] `https://en.wikipedia.org/wiki/Kramers%E2%80%93Moyal_expansion`

[3] Anvari, M., Tabar, M. R. R., Peinke, J., & Lehnertz, K. (2016). Disentangling the stochastic behavior of complex time series. Scientific reports, 6, 35435. doi:10.1038/srep35435

[4] R. Friedrich et al. / Physics Reports 506 (2011) 87–162. doi:10.1016/j.physrep.2011.05.003

[5] `https://www.sympy.org/en/index.html`

[6] `https://pandas.pydata.org/`

Appendices

In case of ambiguity of Fig. 5 and Fig. 6, I also provided the plot of drift without the errorbars and for higher number of bins in Fig. 7 and Fig. 8.

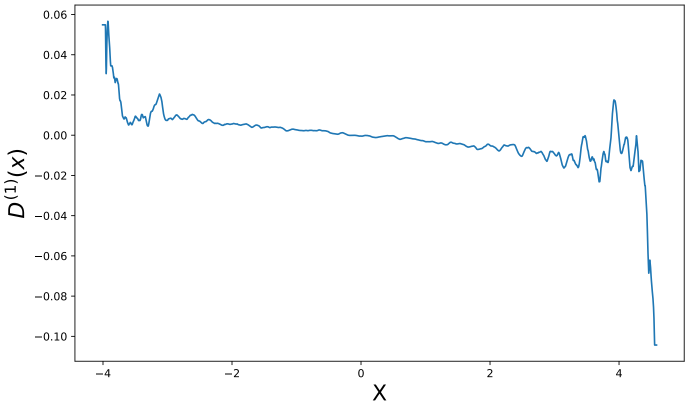

Figure 7: Drift

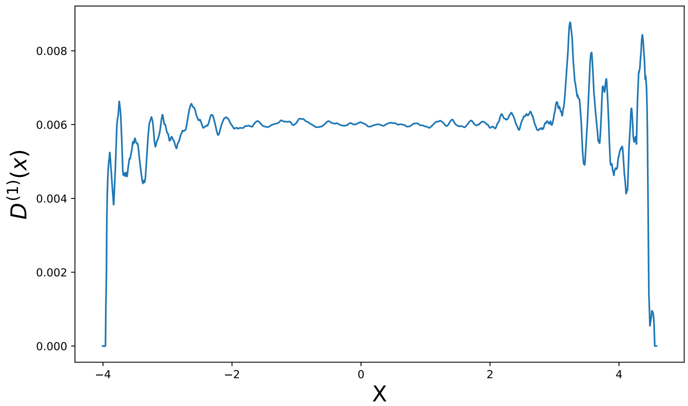

Figure 8: Diffusion