Diffusion Exercises

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January 10, 2016

Note: Based on the instructions from the file ex1.pdf

1. (i)

Examining the graph generated from the file mean_sqr.txt, it is apparent that there is a linear relationship between the n and the mean squared values generated. In particular, we observe that:

$$\frac{\langle (x(t) - x(0))^2 \rangle}{n} = 1 = 2D\Delta t \Rightarrow D = \frac{1}{2\Delta t}$$

(ii)

Given $F_X(x) = \begin{cases} 1 & x \in [0,1] \\ 0 & \text{otherwise} \end{cases}$, we will show that, for $X_i = F_X(x)$ such that each X_i is independent:

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} ((2 * X_i - 1) * \sqrt{3} * \sigma) \to N(0, \sigma)$$

Where $N(0, \sigma)$ is a normal distribution, which has the pdf:

$$\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}}$$

Proof. We first observe that since each X_i is independent and identically distributed, the central limit theorem tells us that:

$$\lim_{n\to\infty} \sqrt{n} \left(\left(\frac{1}{n} \sum_{i=1}^{n} X_i \right) - \mu \right) \to N(0, \sigma^2)$$

For our given $F_X(x), \mu = 0.5$. We can double the range of $F_X(x)$ so that $x \in [0, 2]$ by multiplying our finite sum of X_i values by two, noting that now we have $\mu = 1$, thus:

$$\lim_{n\to\infty} \sqrt{n} \left(\left(\frac{2}{n} \sum_{i=1}^{n} X_i \right) - 1 \right) \to N(0, \sigma^2)$$

We can condense this expression by observing that our two operations were equivalent to generating a new function:

$$F'_X(x) = \begin{cases} 1/2 & x \in [-1,1] \\ 0 & \text{otherwise} \end{cases}$$

Which we note is a PDF with $\mu = 0$. We will now generate X'_i values in the same manner that we generated our X_i values above, giving us that:

$$\lim_{n\to\infty} \sqrt{n} \left(\frac{1}{n} \sum_{i=1}^{n} X_i \right) = \lim_{n\to\infty} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} X_i \to N(0, \sigma^2)$$

Now from our function definition we observe that each X_i has variance:

$$\mathbb{E}[X^2] - (\mathbb{E}[X])^2 = \mathbb{E}[X^2] = \int_{-1}^{1} \frac{x^2}{2} = \sigma^2$$

This, however, only works for $\sigma = 1/\sqrt{3}$! To generalize, we realize that we can modify our variance by simply changing the bounds of $F'_X(x)$ by simply multiplying by a constant. Let us define some constant a such that:

$$F_X(x) = \begin{cases} \frac{1}{2a} & x \in [-a, a] \\ 0 & \text{otherwise} \end{cases}$$

This function has variance:

$$\mathbb{E}[X^2] = \int_{-a}^{a} \frac{x^2}{2a} = \frac{2a^3}{6a} = \frac{a^2}{3} = \sigma^2$$

Taking the square root of both sides yields that $a = \sqrt{3}\sigma$ for a given σ. Now we can put together all our described alterations to reveal that:

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} ((2 * X_i - 1) * \sqrt{3} * \sigma) \to N(0, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}}$$

□

(iii)

We will let $x(0) = 0$ and observe that other cases follow by symmetry. Then:

$$p(x,t) = \frac{e^{-x^2/4Dt}}{\sqrt{4\pi Dt}}$$

$$\frac{\partial p}{\partial t} = \frac{-e^{-x^2/4Dt}}{2t\sqrt{4\pi Dt}} + \frac{x^2 e^{-x^2/4Dt}}{4Dt^2\sqrt{4\pi Dt}}$$

$$\frac{\partial^2 p}{\partial x^2} = \frac{\partial p}{\partial x}\left(\frac{-xe^{-x^2/4Dt}}{2Dt\sqrt{4\pi Dt}}\right) = \frac{-e^{-x^2/4Dt}}{2Dt\sqrt{4\pi Dt}} + \frac{x^2 e^{-x^2/4Dt}}{4D^2t^2\sqrt{4\pi Dt}}$$

This gives us that:

$$D\frac{\partial^2 p}{\partial x^2} = \frac{-e^{-x^2/4Dt}}{2t\sqrt{4\pi Dt}} + \frac{x^2 e^{-x^2/4Dt}}{4Dt^2\sqrt{4\pi Dt}} = \frac{\partial p}{\partial t}$$

It is given that $\langle (x(t) - x(0))^2 \rangle = 2Dn\Delta t \Rightarrow D = \frac{\langle (x(t)-x(0))^2 \rangle}{2n\Delta t}$

Evaluating the data for $\sigma = 1, 2, 3$ in files sig_1.txt, sig_2.txt, and sig_3.txt respectively, it is trivial to see that:

$$\frac{\langle (x(t) - x(0))^2 \rangle}{t} = \sigma^2 \Rightarrow D = \frac{\sigma^2}{2}$$

Using this information and the given equation, data was generated for $\sigma = 1, 2, 3$ and $\Delta t = 1$ and compared with the data generated via normal probability distributions. The probability distribution appears to match well. We note that as time progresses, so does the range where the particle is likely to appear; that is, the distribution of the particle "flattens" out over time.