Life of a Particle : Assignment 2

Sam Meehan & Claire David

Due Date : 2 February 2019

2.1 - The Logistic Map on Steroids

This is the completion of what we started in the quiz. You are to work through the exercise of creating code that reproduces the results in this paper - the logistic map paper. In short, you should be demonstrating, through the use of histograms and description of what it means to be a uniform distribution or to have a pattern, whether the set of X values produced directly from the logistic map, and the sequence of Y values that are produced from the transformed logistic map. Use both one-dimensional and two-dimensional histograms to inspect the bias of both X and Y.

To summarize the main equations from that paper that we need :

$$x_{n+1} = [M * y_n * (1 - x_n) * k_1 + z_n]mod(1)$$
$$y_{n+1} = [M * y_n * sin(z_n) * k_2 + x_{n+1}]mod(1)$$
$$z_{n+1} = [M * z_n + y_{n+1} * k_3 + z_n]mod(1)$$

with : $0 <$ M < 3.99999, $k_1 > 33.5$, $k_2 > 37.9$, $k_3 > 35.7$.

2.2 - Random Number Generation

For this question, you may import the python random library. However, you may only use the random.random() function call which generates a uniformly distributed random number between [0,1.0).

Starting from a set of uniformly distributed random numbers from [0,1.0) (Don't be a hipster, use python for this!) generate a set of 10000 random numbers according to the following PDFs using the accept/reject method :

A - Quadratic Function

We started doing this in class. Generate numbers for a polynomial of degree 2 in the range $x \in [0, 3]$

$$Poly(x) = x^2$$

B - Exponential Function

Generate numbers for an exponential function which has a parameter of α in the range $x \in [0, 5]$

$$Exp(x; \alpha) = e^{\alpha x}$$

C - Gaussian Function

A Gaussian distribution of mean $\mu = 2.0$ and width $\sigma = 1.4$ in the range $x \in [-10, 10]$. As a reminder, the Gaussian distribution is also called the "normal distribution" and has the following functional form :

$$Gauss(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$$

D - Piece-wise Function

This is a bit more challenging, and will require some if statements because it is piecewise defined as follows, with two free parameters (α, β) in the range $x \in [-\beta, \beta]$

$$PieceWise(x; \alpha, \beta) = \begin{cases} \frac{\beta+x}{\beta-\alpha} & x \in [-\beta, -(\beta-\alpha)) \\ \frac{-x}{\alpha} & x \in [-(\beta-\alpha), 0) \\ \frac{x}{\alpha} & x \in [0, \beta-\alpha) \\ \frac{\beta-x}{\beta-\alpha} & x \in [\beta-\alpha, \beta] \end{cases}$$

NOTE : Wherever you see free parameters (e.g. *alpha*), these should be easily changeable parameters that are set at the top of your program. **Do not hardcode them!**.

2.2 - The Classical Particle In a Box

Before writing a simulation to describe the quantum particle in a box, it is important to be able to accurately describe the *classical* particle in a box. To do this, imagine the following experimental setup. You place a particle in a box of width a on the left side (at x =0) with some fixed velocity v that will cause it to move towards the right. You then immediately close your eyes. When the particle reaches the right hand side, you know that it will immediately reverse direction and travel back to the left. This process will continue with the particle bouncing from one side to the other for a time T (with $T >> a/v$) at which point you open your eyes and note the current position x of the particle. This measurement constitutes one experiment. Imagine that you repeat this same experiment many many times. What will

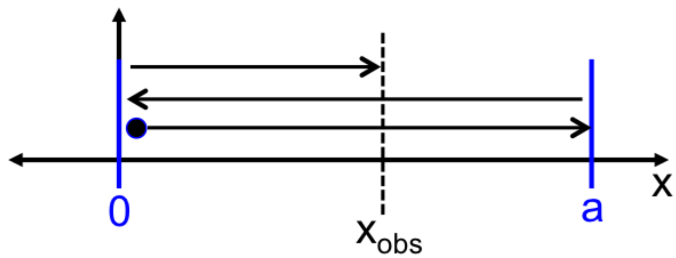

Figure 1: The experimental setup for one trial of the classical particle in a box. The ball is released, it bounces back and forth a few times and after waiting a time T, you open your eyes and observe it at $x = x_{obs}$.

be the distribution of the ensemble of x_{obs} values? Your task in this question is to design a simulation that produces this distribution.

2.3 - Modelling the Particle In a Box

We discussed at great length the solution of the Schrodinger equation for the case of a particle in a one-dimensional box with sides at x =0 and x =a (Go review Griffith's QM - Chapter 2.2 if you are not sure of how the calculation proceeds.). This is the model by which we want to describe a particle, namely the answer to the question "Where is the particle?". This will be done using the wave function $\Psi(x,t)$ of the particle, which itself may be complex valued as is composed as a linear superposition of the eigenfunctions

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \phi_n(t) \psi_n(x) = \sum_{n=0}^{\infty} c_n e^{-\frac{i}{\hbar}E_n t} sin(\frac{n\pi}{a}x)$$

However, the probability rule, which will be a function describing the PDF $P(x)$ of the location of the particle, must be a real valued function from which a single event (a single collapse of the wave function) can be viewed as the generation of a single number from this distribution $P(x)$. Therefore, we must translate this complex function into a real-valued function. Two reasonable ways to do this are :

- Square Then Sum : Take the square modulus of each of the eigenfunctions and then add these squared terms.
  - $P_A(x,t) = \sum_{n=0}^{\infty} c_n \phi_n(t) \psi_n(x) c_n^* \phi_n^*(t) \psi_n^*(x)$
- Sum Then Square : Add the individual eigenfunctions and then take the square modulus of this sum.
  - $P_B(x,t) = \sum_{n=0}^{\infty} c_n \phi_n(t) \psi_n(x) \times \sum_{m=0}^{\infty} c_m^* \phi_m^*(t) \psi_m^*(x)$

If you are feeling overwhelmed looking at these equations,its alright, we are going to deal with a simplified system. Let's imagine that we know that the particle is initially placed in the box in a state $\Psi(x,t)$ which is only composed of the E_1 and E_2 eigenstates. So the wave function is simply

$$\Psi(x,t) = c_1 \phi_1(t) \psi_1(x) + c_2 \phi_2(t) \psi_2(x)$$

First, describe how these two different possibly probability rules differ (if they do) qualitatively? Is there time dependence to one of the probability rules? What if you set t =0, meaning that the observation is made immediately after you put the particle in the box? Does the time dependence go away?

For this simplified system, you have been provided with a set of 10000 data measurements (see the course website). If you feel that you need more data points to be able to successfully carry out the assignment, please ask. Your goal is to determine which one of these two probabily rule transformations P_A or P_B is the one that really occurs in nature. To this end, you should probably start by examining the data, either by using descriptive statistics, or maybe making a histogram. Can you observe anything about the data just from this? Now try to generate a predictive set of data according to the two different models that you have for the probability, assuming that the measurements being made are performed immediately at t =0.

To fully describe the model, there are therefore two separate questions to answer

- What is the probability rule that comes from nature?
- What are the coefficients c_1 and c_2? (To make things less involved, pretend that we know that c_1 and c_2 are positive and between $[0,1]$.)

To go about this, we will need a way to compare your ensemble of predictions to that of the observations. This can be done by first casting the obervations or predictions in the form of two histograms (p and o)

and then performing a calculation of the χ^2 of these two histograms[1] where

$$\chi^2 = \sum_{i \in bins(p,o)} \frac{(p_i - o_i)^2}{\sigma_{p_i}^2 + \sigma_{o_i}^2}$$

and (p_i, o_i) is the bin content of p and o at bin i and $(\sigma_{p_i}, \sigma_{o_i})$ are the corresponding errors on these bins. When creating a histogram of the number of events in a bin (N_i), the ROOT package will automatically set the error on the bin to be the square root of this value $(\sqrt{N_i})$. This is on account of the fact that the number of events in a bin is viewed as a poisson observable. That is, if you were to run the simulation again and again, each time obtain another count of events in bin i, and you were to make a histogram of these values, then it would follow a poisson distribution of mean N and standard deviation $\sqrt{N}$ (*BONUS* points if you do this and justify the error being $\sqrt{N}$.

[1]NOTE : This is a little different than what we covered in class but more *correct* because it accounts for the statistical error on the data sample as well.