Life of a Particle : Assignment 2

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Due Date : 20 January 2017

How to Submit
This assignment should be submitted by replying to the email sent out by the tutors - **Use the online form!** - with the link to your GitHub repository. Contained within this repository should be a markdown README.md file which provides a guide to the contents of the repository, along with instructions of how to run the code, where necessary. For the full assignment, also include a well-written summary in the form of a latex document with one section per question.

You are to work with the group assigned to you by the tutors.

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 5000 data measurements (included on the assignment page). 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 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 (σ_{p_i}, σ_{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 $\sqrt{N}$.

Modelling a Real Life Particle In a Box - *Bonus*

This problem builds upon the previous problem to incorporate effects of a real particle detector. You will again be given a set of data, with the goal to measure the c_1 and c_2 coefficients. Hopefully you have discovered the probability rule from the previous question so that will not be necessary again. The challenge this time will be to properly take into account detector effects.

In the previous problem, when the wave function collapsed and produced an x position, we assumed that the measured position of this particle corresponded exactly to its *actual* position. However, in a real experiment, the manner in which the measurement of a position (or really any attribute of a particle) is imperfect. These imperfections are often caused by experimental noise within the detector that can cause the observed position to deviate slightly from the position where the particle "really" was. These imperfections are completely analagous to the imperfections which exist within the eyes of people who must wear glasses. Typically, light entering a normal eye would indicate where the object from which that light comes is located. However, if your eyesight is not 20:20, then when the light enters the eye, it becomes smeared out by these abberations and the resulting image in the eye becomes blurry. The same occurs in imperfect (read: real) particle detectors. Because of noise, when a particle enters the detector it can get shifted. If we take an ensemble of such particles all entering the same location, then they will become smeared out in a random fashion. By this, we mean that on a particle-by-particle basis, the shift which occurs is random and distributed according to what is called the "point spread function" of the detector. The point spread function can be interpreted as a PDF of the shift in the position of the measurement with respect to the actual position of the particle upon measurement. Therefore, if the true position before measurement is x_{true} then the measured position will be $x_{meas}=x_{true}+x_{shift}$ where x_{shift} is a random number drawn from the point spread function.

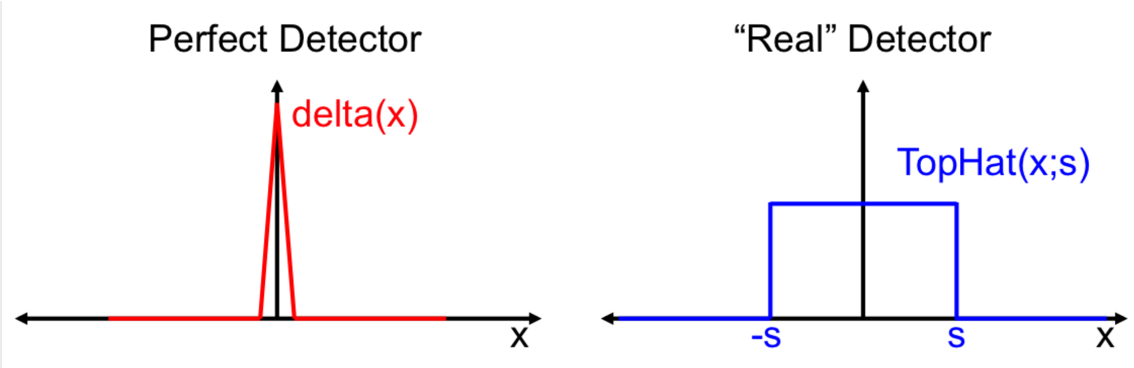

Figure 1: The point spread function for a perfect detector (left) and a real detector (right). The point spread function for the position measurement represents the PDF of the shift in the position of the measurement with respect to the actual position of the particle upon measurement.

In addition to the measurement being obscured by the smearing of the true position to the final measured position, another common effect is detector *inefficiency*. This comes about again by imperfections in the detector and also "thresholds" that must be set by the experimentalist to suppress noise. However, what these contribute to is a non-unity probability to observe a particle that enters the detector. In other words, when the wave function collapses and a particle is to be observed at some position in the detector, then there is a finite probability $\epsilon \leq 1$ that the particle is actually observed. This means that if you were to "shoot" 100 particles into the detector and $\epsilon = 0.73$ then you would only observe 73 of them.

For this question, we want to take into consideration these two effects to model the set of data coming from the real detector.

- Smearing : $x_{meas}=x_{true}+x_{shift}$ where x_{shift} is distributed according to the point spread function
- Inefficiency : There is an efficiency $\epsilon \leq 1$ for observing the particle if it enters the detector.

The detector system that we have constructed to observe our particle in the box consists of two detectors as indicated. The first detector covers the first half of the box $[0,a/2)$ and the second detector covers the second half $[a/2,a]$. Each detector has its on imperfections and may have different smearing or inefficiencies, both of which may need to be taken into account for both detectors.

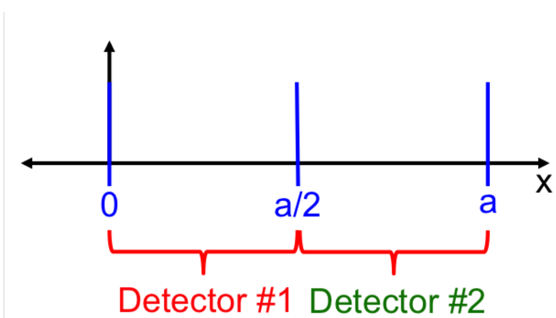

Figure 2: The setup of our particle in the box experiment.

Your challenge is to build a model which accurately describes the observed ensemble of data and measure the c_1 and c_2 coefficients using a similar technique as before (χ^2 minimization). However, in this case there are four additional free parameters

- s_1 : The magnitude of the smearing in Detector #1
- ϵ_1 : The efficiency of Detector #1
- s_2 : The magnitude of the smearing in Detector #2
- ϵ_2 : The efficiency of Detector #2

You can go about this in any way you want, by either performing a χ^2 minimization over all the parameters (might be slow), or by examining the data and trying to find an alternative way to estimate the s_i and ϵ_i parameters using a combination of qualitative and analytical arguments. There is no single approach that works better than any other, but you can be assured that the c_1 and c_2 coefficients are not the same as before.