Analysis of Experimental Data

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1 Statistical Distributions

1.1 Statistics of Experiments

A primary purpose of science is to predict the results of experiments. Consider a simple experiment with five possible outcomes which we repeat ten times. If our theoretical prediction is that each of these five outcomes is equally probable, than our prediction for a typical series of ten experiments would be for each outcome to occur two times. Now suppose we perform the experiment ten times and present the results like this:

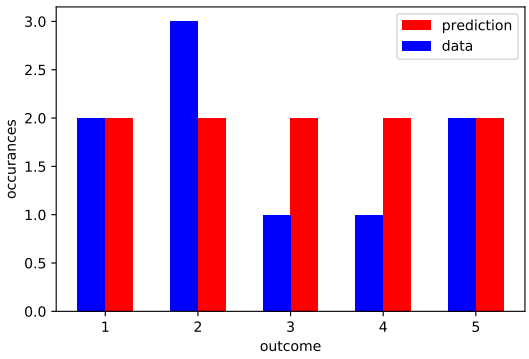


Figure 1: Comparison of experimental results with a prediction.

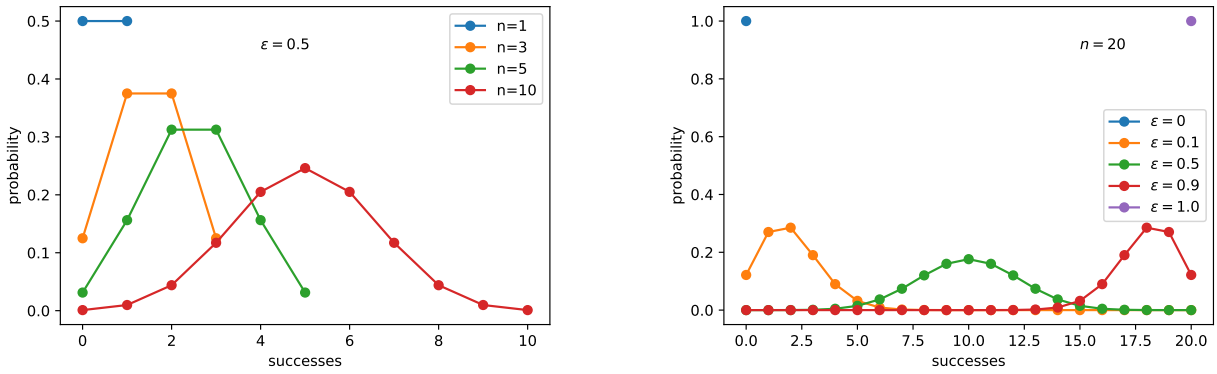
Scientist almost never display experimental data this way (as a bar graph) because it is nearly impossible to answer the crucial question *is this data consistent with this prediction?* Even if every outcome has an equal probability, the results of individual experiments experience statistical fluctuations. So even if the theory is correct, we well seldom reproduce exactly the theory prediction.

To interpret scientific experiments, it isn't enough to have a single prediction for the outcome of an experiment, instead, you need a prediction for the statistical distribution of outcomes: a probability distribution function. We'll start this discussion, therefore, by deriving three of the most frequently encountered probability distributions: the Binomial Distribution, the Poisson Distribution, and the Gaussian Distribution.

1.2 The Binomial Distribution

The Binomial Distribution is the most general of the distributions we'll consider, but it is a bit cumbersome to use in practice. The more familiar Poisson and Gaussian distributions are limiting

cases of this distribution.



(a) (b)

Figure 2: The binomial distribution for several different values of the parameters (a) n and (b) ϵ.

Suppose you repeat a particular process n times, and each time you have the same probability ϵ of a particular outcome, which, without losing generality, we'll call "success". The probability of having exactly m successes after n trials is simply given by:

$$P = \sum_i p_i$$

where i runs over all specific outcomes with m successes and p_i is the probability of each specific outcome. However, as these specific outcomes all contain exactly m successes, they share the same probability, namely:

$$p_i = \epsilon^m (1-\epsilon)^{n-m}$$

and so we are left to consider simply the total number of specific outcomes containing m successes.

The quantity we need is provided by the binomial theorem from mathematics, which states that:

$$(p+q)^n = \sum_{m=0}^{n} \binom{n}{m} p^m \, q^{n-m} \tag{1}$$

where the binomial coefficients are defined by

$$\binom{n}{m} = \frac{n!}{m!\,(n-m)!} \tag{2}$$

and are also often referred to in other contexts as n-choose-m. The binomial coefficient simply tells us how many times we can choose m instances of p instead of q, from n factors, and so it is precisely the combinatoric factor that we need.

The probability of obtaining m successes after n trials with probability ϵ is therefore given by:

$$P(m;\, n, \epsilon) = \binom{n}{m} \epsilon^m \, (1-\epsilon)^{n-m} \tag{3}$$

which is called the Binomial Distribution.

1.3 Mean and Variance

Given a probability distribution, the most urgent questions are generally "what is the mean value we can expect from this distribution?" and "how close to the mean value are most of the outcomes?" The first answer localizes the distribution while the second answer describes its width.

To calculate the mean value in answer to the first question, we simply calculate a weighted average:

$$\langle m \rangle \equiv \bar{m} \equiv \sum_m m\, P(m) \tag{4}$$

For a continuous probability distribution, we would integrate instead:

$$\langle x \rangle \equiv \bar{x} \equiv \int x\, P(x)\, dx \tag{5}$$

We usually answer the second question in terms of the variance, σ^2, of the distribution:

$$\sigma^2 \equiv \langle (x - \bar{x})^2 \rangle$$

Other answers have problems, e.g. $\langle x - \bar{x} \rangle$ can be zero or nearly so, even for wide distributions, as long as it is symmetric. You could fix this by calculating $\langle |x - \bar{x}| \rangle$ but this is generally much harder to calculate, and less useful, than the variance. For instance, it is left as an exercise to show that:

$$\langle (x - \bar{x})^2 \rangle = \langle x^2 \rangle - \bar{x}^2 \tag{6}$$

using the fact that $\bar{x}$ is simply a number, and so $\langle \bar{x} \rangle = \bar{x}$. We often write this result equivalently as:

$$\sigma^2 \equiv \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 \tag{7}$$

Which shows explicitly that we need only calculate $\langle x \rangle$ and $\langle x^2 \rangle$ in order to determine the variance of a distribution.

1.4 Mean and Variance of the Binomial Distribution

The mean value of Binomial Distribution is given by:

$$\begin{aligned} \bar{m} &= \sum_{m=0}^{n} m\, P(m) \\ &= \sum_{m=0}^{n} m \binom{n}{m} \epsilon^m (1-\epsilon)^{n-m} \end{aligned}$$

which looks rather daunting! The trick is to use the Binomial Theorem (1) and define a function of two independent variables p and q given by:

$$f(p,q) = (p+q)^n = \sum_{m=0}^{n} \binom{n}{m} p^m q^{n-m}$$

We then calculate:

$$\frac{\partial f}{\partial p} = n(p+q)^{n-1} = \sum_{m=0}^{n} m \binom{n}{m} p^{m-1} q^{n-m}$$

and multiplying by p we have:

$$np(p+q)^{n+1} = \sum_{m=0}^{n} m\binom{n}{m}p^m q^{n-m}$$

which is true for any p and q. We now substitute the particular values $p = \epsilon$ and $q = 1-\epsilon$ and find that:

$$n\epsilon = \sum_{m=0}^{n} m\binom{n}{m}\epsilon^m(1-\epsilon)^{n-m} \equiv \sum_{m=0}^{n} mP(m) = \bar{m}$$

So the mean value is given by:

$$\bar{m} = n\epsilon \tag{8}$$

or the total number of trials times the probability of success for each trial, a wholly plausible answer.

For the variance, we use a variation of the same trick, this time using the second partial derivative:

$$p^2 \cdot \frac{\partial^2 f}{\partial p^2} = n(n-1)p^2(p+q)^{n-2} = \sum_{m=0}^{n} m(m-1)\binom{n}{m}p^m q^{n-m}$$

and again putting $p = \epsilon$ and $q = 1-\epsilon$ to find that:

$$\begin{aligned} n(n-1)\epsilon^2 &= \sum_{m=0}^{n}(m^2-m)\binom{n}{m}p^m q^{n-m} \\ &= \sum_{m=0}^{n}(m^2-m)P(m) \\ &= \langle m^2-m\rangle = \langle m^2\rangle - \langle m\rangle \end{aligned}$$

and as $\langle m\rangle = n\epsilon$ we have:

$$\langle m^2\rangle = n(n-1)\epsilon^2 + n\epsilon$$

And so:

$$\sigma^2 = \langle m^2\rangle - \langle m\rangle^2 = n(n-1)\epsilon^2 + n\epsilon - n^2\epsilon^2$$

or simply:

$$\sigma^2 = n\,\epsilon\,(1-\epsilon) \tag{9}$$

Note that if $\epsilon = 0$ or $\epsilon = 1$, there is only one outcome (all failures or all success) and so the variation is zero.

1.5 The Poisson Distribution

Suppose we have some time interval over which we expect to observe a mean number of events λ. The events must be independent of one another: an event occurring at a particular time cannot affect the time at which the next event occurs. We divide the time interval over which the λ events are expected to occur into into n sub-intervals, each with an equal probability to contain an event. These intervals will be all the same size if the events are uniformly distributed in time, but if the events are not uniformly distributed, the sub-intervals are simply chosen to ensure the probability

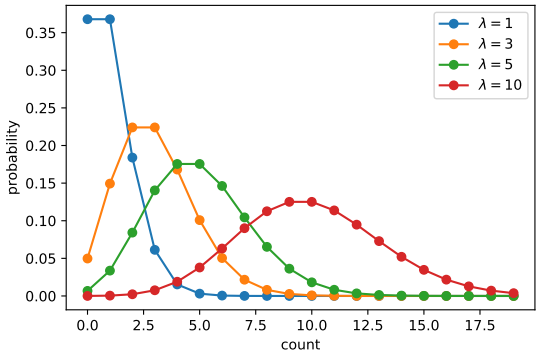


Figure 3: The Poisson distribution for several values of parameter λ.

is the same in each interval. Once cast this way, we can interpret this as a binomial distribution, with probability to contain an event, by construction, given by $\epsilon = \lambda/n$:

$$\begin{aligned} P(m) &= \binom{n}{m} \epsilon^m (1-\epsilon)^{n-m} \\ &= \frac{n!}{m!\,(n-m)!} \left(\frac{\lambda}{n}\right)^m \left(1-\frac{\lambda}{n}\right)^{n-m} \\ &= \left(\frac{\lambda^m}{m!}\right) \left(1-\frac{\lambda}{n}\right)^n \left[\frac{n!}{(n-m)!}\cdot\frac{1}{n^m}\right]_1 \left[\left(1-\frac{\lambda}{n}\right)^{-m}\right]_2 \end{aligned}$$

We obtain the Poisson distribution by considering the limit that $n \to \infty$. It is left as an exercise to show that both $[\ldots]_1 \to 1$ and $[\ldots]_2 \to 1$ as $n \to \infty$. Recalling that

$$\lim_{n\to\infty} \left(1-\frac{\lambda}{n}\right)^n = e^{-\lambda}$$

we obtain the Poisson distribution, the probability for observing m events for a mean of λ:

$$P(m\ ;\ \lambda) = \frac{\lambda^m}{m!}\, e^{-\lambda} \tag{10}$$

Notice that there is no longer a parameter n, since we took $n \to \infty$, and so m now ranges from 0 to ∞.

1.6 Mean and Variance of The Poisson Distribution

The mean of the Poisson distribution is given by:

$$\begin{aligned} \bar{m} &= \sum_{m\geq 0} m\, P(m) \\ &= \sum_{m\geq 0} m\, \frac{\lambda^m}{m!}\, e^{-\lambda} \end{aligned}$$

Since the first term ($m = 0$) is zero, we have:

$$\begin{aligned}
\bar{m} &= e^{-\lambda} \sum_{m \geq 1} \frac{\lambda^m}{(m-1)!} \\
&= \lambda e^{-\lambda} \sum_{m \geq 1} \frac{\lambda^{m-1}}{(m-1)!} \\
&= \lambda e^{-\lambda} \sum_{n \geq 0} \frac{\lambda^n}{n!} \\
&= \lambda e^{-\lambda} e^{\lambda} \\
\bar{m} &= \lambda \qquad (11)
\end{aligned}$$

which should come as no surprise, as the assumption in the derivation was the that mean number of events was λ.

For the variance, we use a similar manipulation to calculate:

$$\begin{aligned}
\langle m^2 \rangle &= \sum_{m \geq 0} m^2 \, P(m) \\
&= \sum_{m \geq 0} m^2 \, \frac{\lambda^m}{m!} \, e^{-\lambda} \\
&= \lambda \sum_{m \geq 1} m \, \frac{\lambda^{m-1}}{(m-1)!} \, e^{-\lambda} \\
&= \lambda \sum_{n \geq 0} (n+1) \, \frac{\lambda^n}{(n)!} \, e^{-\lambda} \\
&= \lambda \, \langle m+1 \rangle = \lambda \, (\lambda + 1)
\end{aligned}$$

And so:

$$\begin{aligned}
\sigma^2 &= \langle m^2 \rangle - \langle m \rangle^2 \\
&= \lambda \, (\lambda + 1) - \lambda^2 \\
\sigma^2 &= \lambda. \qquad (12)
\end{aligned}$$

That is, the variance of a Poisson distribution is simply the mean.

1.7 The Gaussian Distribution

Next, we consider the Poisson Distribution in the limit $\lambda \to \infty$. In this case, we can apply the Stirling Approximation:

$$\lim_{n \to \infty} n! = \sqrt{2\pi n} \; e^{-n} \; n^n$$

to the Poisson distribution as follows:

$$\begin{aligned}
P(m) &= \frac{\lambda^m}{m!} \, e^{-\lambda} \\
&\to \frac{\lambda^m e^{-\lambda}}{\sqrt{2\pi m} \; e^{-m} \; m^m} \\
&= \frac{e^{m-\lambda}}{\sqrt{2\pi\lambda}} \left(\frac{\lambda}{m} \right)^{m+\frac{1}{2}}
\end{aligned}$$

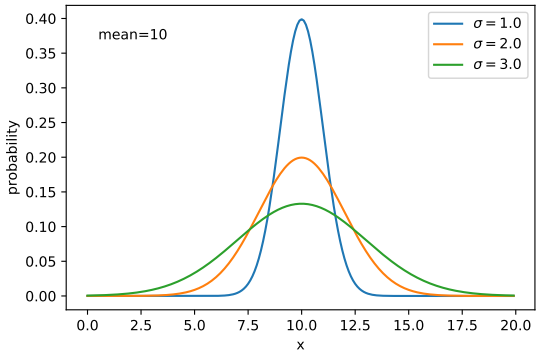


Figure 4: The Gaussian distribution for a mean of 10 and several values of parameter σ.

Now we consider a new variable δ, defined by

$$\delta \equiv \frac{m - \lambda}{\lambda}$$

which measures the difference between the observed number of events m and the mean of the distribution, as a fraction of the mean. Intuitively, the function is getting very narrow, and so we expect this to be a small quantity, but let's check this. First we have:

$$\langle \delta \rangle = \frac{\langle m \rangle - \lambda}{\lambda} = \frac{\lambda - \lambda}{\lambda} = 0$$

but also:

$$\langle \delta^2 \rangle = \frac{\langle (m - \lambda)^2 \rangle}{\lambda^2} = \frac{\lambda}{\lambda^2} = \frac{1}{\lambda}$$

where we have used the fact that the variance is given by $\langle (m - \lambda)^2 \rangle = \lambda$, and so as $\lambda \to \infty$ we have

$$\langle \delta^2 \rangle \to 0$$

So we can write:

$$m = \lambda(1 + \delta) \tag{13}$$

where we expect the approximation $\delta \to 0$ to hold as long as we require $\lambda \to \infty$. So now we can write the distribution in terms of the small quantity δ and the large quantity λ as:

$$\begin{aligned} P(\delta) &= \frac{e^{\lambda\delta}}{\sqrt{2\pi\lambda}} \left(\frac{\lambda}{\lambda(1+\delta)} \right)^{\lambda(1+\delta)+\frac{1}{2}} \\ &= \frac{e^{\lambda\delta}}{\sqrt{2\pi\lambda}} \cdot \frac{1}{X} \end{aligned} \tag{14}$$

where we define the quantity:

$$X = (1 + \delta)^{\lambda(1+\delta)+\frac{1}{2}}$$

which can be approximated as follows:

$$\begin{aligned}
\ln X &= \left(\lambda(1+\delta)+\frac{1}{2}\right)\cdot\ln(1+\delta) \\
&= \left(\lambda(1+\delta)+\frac{1}{2}\right)\cdot\left(\delta-\frac{\delta^2}{2}+\mathcal{O}(\delta^3)\right) \\
\frac{\ln X}{\lambda} &= \left(1+\delta+\frac{1}{2\lambda}\right)\cdot\left(\delta-\frac{\delta^2}{2}+\mathcal{O}(\delta^3)\right) \\
&= \left(1+\delta+\mathcal{O}\left(\delta^2\right)\right)\cdot\left(\delta-\frac{\delta^2}{2}+\mathcal{O}(\delta^3)\right) \\
&= \delta+\frac{\delta^2}{2}+\mathcal{O}(\delta^3),
\end{aligned}$$

where in the second to last step we used $\mathcal{O}\left(\frac{1}{\lambda}\right)\sim\mathcal{O}\left(\delta^2\right)$. Neglecting the small quantities, we can approximate

$$X=\exp\left(\lambda\delta+\lambda\frac{\delta^2}{2}\right)$$

which, when plugged backed into Equation 14 yields:

$$\begin{aligned}
P(\delta) &= \frac{e^{\lambda\delta}}{\sqrt{2\pi\lambda}}\cdot\frac{1}{\exp\left(\lambda\delta+\lambda\frac{\delta^2}{2}\right)} \\
&= \frac{1}{\sqrt{2\pi\lambda}}\cdot\exp\left(-\lambda\frac{\delta^2}{2}\right) \qquad (15)
\end{aligned}$$

Now notice that Equation 13 implies that m is quite large, and so may now be treated as a continuous variable, which we will rename x (since m looks like an integer value), hence we have:

$$\delta\equiv\frac{m-\lambda}{\lambda}=\frac{x-\lambda}{\lambda}$$

and likewise we know that the variance of the original Poisson distribution is given by $\sigma^2=\lambda$, and so we can rewrite Equation 15 in the (hopefully) more familiar form:

$$P(x)=\frac{1}{\sqrt{2\pi}\sigma}\cdot\exp\left(-\frac{(x-\lambda)^2}{2\sigma^2}\right) \qquad (16)$$

Which is a Gaussian distribution with mean value λ and variance σ^2. The proof that these quantities are indeed the mean and the variance is left as an exercise.

1.8 Continuous versus Discrete Distributions

The Binomial and Poisson distributions are not continuous functions: they describe the probability of outcomes which are integer quantities. The Poisson probability for having 2.31 events is either undefined or taken to be zero. The value of the Binomial and Poisson distribution function at a particular integer value is simply the probability of that particular outcome. To determine the probability that an outcome is within a range of integers, say m_1 to m_2 the probability distribution function is simply added:

$$P=\sum_{m=m_1}^{m_2}P(m).$$

The Gaussian distribution is a continuous function: it describes the probability density function of a particular value of x. The probability of any particular outcome, say $x = 1.24323$, is vanishing small. But the probability that the value lies within a range of values can be non-zero, and is determined by integrating:

$$P = \int_{x_{\min}}^{x_{\max}} P(x)\,dx$$

The probability distribution function is normalized so that:

$$\int_{-\infty}^{+\infty} P(x)\,dx = 1$$

To determine the mean value of a function $f(x)$ we likewise integrate:

$$\langle f(x) \rangle \equiv \int_{-\infty}^{+\infty} f(x)P(x)\,dx = 1$$

In particular the mean value of x is:

$$\langle x \rangle \equiv \int_{-\infty}^{+\infty} xP(x)\,dx = 1$$

and:

$$\langle x^2 \rangle \equiv \int_{-\infty}^{+\infty} x^2P(x)\,dx = 1$$

with:

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 .$$

The Gaussian distribution is a probability density function (PDF), because it reports a probability density. A discrete probability distribution is sometimes referred to as probability mass function (PMF), to draw upon an analogy with physical mass and density.

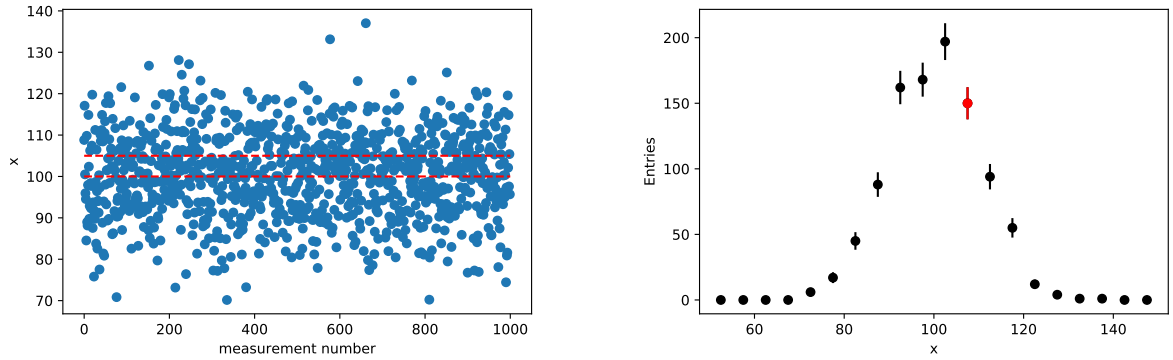
1.9 Histograms in Scientific Python

Suppose a particular variable x is measured 1000 times. One way to visualize the collected data is shown in Fig. 5a, which simply plots each measurement value above the measurement number (from 0 to 1000). In this example, the number of measurements that occur within the range from $x = 100$ to $x = 105$ is 181. This count is plotted as the red data point in Fig. 5b, 181 entries located above $x = 102.5$, the center of the range. If we repeat this exercise across a number or ranges, the resulting plot in Fig. 5b is called a histogram. A histogram reports the number of entries that occur within each of a sequence of consecutive ranges of x-values. Each range considered is called a histogram bin, and the choice of which bins to use is at the discretion of the analyzer.

The content of each bin is a single number, a count, and is therefore subject to the Poisson distribution. We can estimate the mean of the Poisson distribution by the measured value, so that $\lambda = N$. For the Poisson distribution, the variance $\sigma^2 = \lambda$, and so $\sigma = \sqrt{N}$. It is customary to draw a line of size $\sqrt{N}$ when plotting a histogram value N. This is an example of an error bar, which indicates how well our measurement has determined a particular value.

An example producing a histogram in Scientific Python is shown in Fig. 6. The data to plot is simply a sequence of 1000 values randomly and uniformly chosen in the range $[0, 20]$:

```
x = np.random.uniform(high=20.0,size=1000)
```



(a) (b)

Figure 5: The 1000 measurements of variable x in (a) are used to produce the histogram in (b). The red data point in (b) is the count of the number of entries in range indicated by the red dashed lines in (a).

To create a histogram from these 1000 values, we use the `np.histogram` function:

```
counts,edges = np.histogram(x,bins=10,range=(0,20))
```

where we have specified 10 bins, uniformly covering the range from 0 to 20. The function returns to arrays, which we save as `counts` and `edges`. The `counts` array contains the bin contents, the count of the number of values in each bin:

```
counts:   [ 92  82 123  96  85 106 105  99  99 113]
```

The edges array contains the edges of the bins:

```
edges:    [ 0.  2.  4.  6.  8. 10. 12. 14. 16. 18. 20.]
```

You'll notice that 10 consecutive bins have 11 edges. For plotting continuous data, one choice is to plot the contents at the center of each bin:

```
cbins = (edges[:-1] + edges[1:])/2.0
```

the two slices `edges[:-1]` and `edges[1:]` are all but the last and all but the first. The average of the two is the center of each bin:

```
cbins:    [ 1.  3.  5.  7.  9. 11. 13. 15. 17. 19.]
```

The error bar values are chosen as the square root of the bin values:

```
err   = counts**0.5
```

The histogram is plotted using the `plt.errorbar` function:

```
plt.errorbar(cbins,counts,yerr=err,fmt="ko")
```

which plots the bin contents `counts` at the bin center values `cbins` using the square root error bars in the array `err`, using the format `"ko"` for black circles.

```
x = np.random.uniform(high=20.0,size=1000)
counts,edges = np.histogram(x,bins=10,range=(0,20))
print("counts:  ", counts)
print("edges:   ", edges)
cbins = (edges[:-1] + edges[1:])/2.0
err   = counts**0.5
print("cbins:   ", cbins)
plt.errorbar(cbins,counts,yerr=err,fmt="ko")
plt.xlabel("x")
plt.ylabel("Entries")
```

```
counts:   [ 81  96 104 108 104  99 102 110  98  98]
edges:    [ 0.  2.  4.  6.  8. 10. 12. 14. 16. 18. 20.]
cbins:    [ 1.  3.  5.  7.  9. 11. 13. 15. 17. 19.]
```

```
Text(0,0.5,'Entries')
```

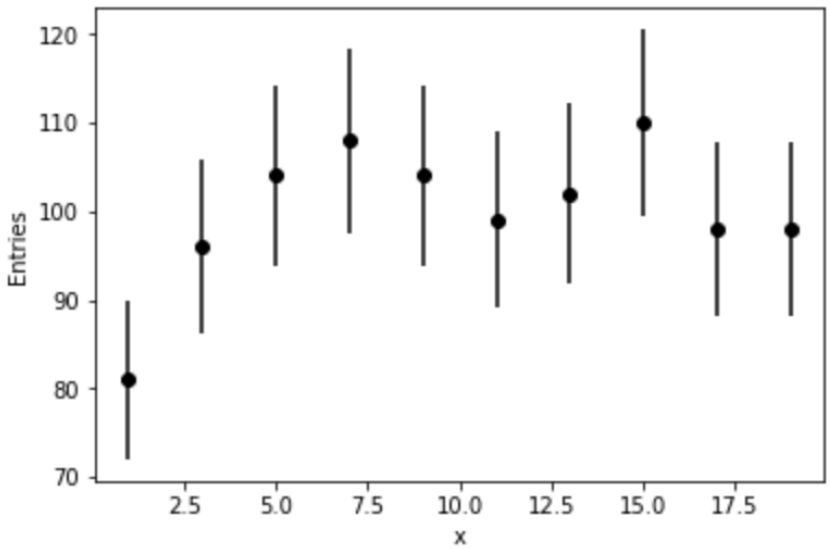


Figure 6: Example producing a histogram in Scientific Python.

1.10 Comparing a Histogram to a Probability Distribution Function

Our theoretical models often predict a PDF for some observable variable x. As experimentalists, we are often therefore concerned with the question as to whether our collected data for an observable x is consistent with the theoretical PDF. A visual approach to answering this question is to plot the data in a histogram, and to draw the PDF as a curve normalized to the histogram.

To predict the number of events in a bin with edges x_{lower} and x_{upper}, in principle we need to integrate the PDF and normalize to the number of experiments:

$$N_{\text{pred}} = N_{\text{meas}} \int_{x_{\text{lower}}}^{x_{\text{upper}}} p(x)\, dx$$

In practice, we generally choose the bin sizes small enough that the PDF is approximately constant during the entire bin, and in this case, the prediction can be taken as:

$$N_{\text{pred}} = N_{\text{meas}}\ \Delta x\ p(x)$$

where Δx is the width of each bin. This scale factor $N_{\text{meas}}\ \Delta x$ allows us to compare a continuous function to data collected in discrete bins, as shown in Fig. 7.

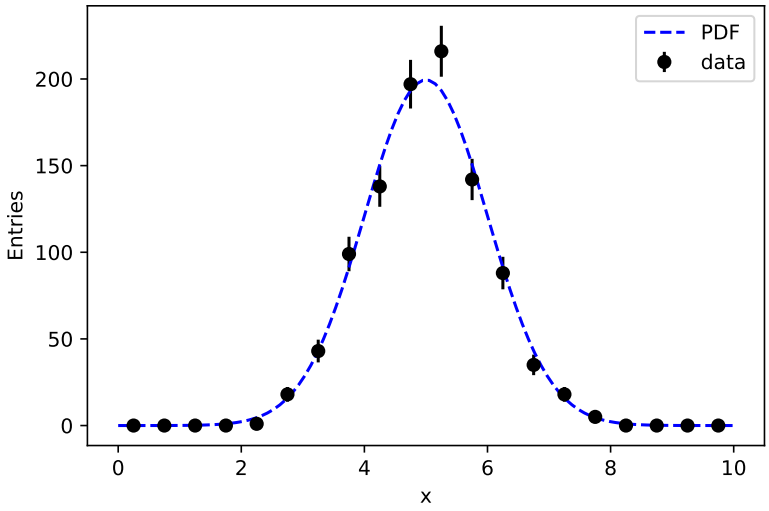


Figure 7: The Gaussian PDF scaled to compare to data from a Gaussian distribution. In this case, there are 1000 total entries in the histogram and the bin size is 0.5, for a scale factor of 500.

1.11 Homework Exercises for Distributions

Problem 1: Show that the Binomial distribution, $P(m)$, in Equation 3 is properly normalized:

$$\sum_{m=0}^{n} P(m) = 1$$

as a consequence of the Binomial Theorem (Equation 1).

Problem 2: Show that Equation 6 is correct.

Problem 3: Show that the Poisson distribution, $P(m)$, in Equation 10 is properly normalized:

$$\sum_{m \geq 0} P(m) = 1.$$

Hint: recall the Taylor series expansion for e^{λ}.

Problem 4: Show that the Gaussian distribution, $P(x)$, in Equation 16 is properly normalized:

$$\int_{-\infty}^{\infty} P(x)dx = 1.$$

Problem 5: Show that the mean of the Gaussian distribution has been correctly identified in Equation 16. That is, show explicitly that:

$$\int_{-\infty}^{\infty} xP(x)dx = \lambda$$

Problem 6: Show that the variance of the Gaussian distribution has been correctly identified in Equation 16. That is, show explicitly that:

$$\int_{-\infty}^{\infty} x^2 P(x)dx = \sigma^2$$

when we take $\lambda = 0$ (which is equivalent to simply changing variables $y = x - \lambda$.)