Python for Scientific Data Analysis

SciPy

Section 3: Statistics, Part 1

“There are three kinds of lies: Lies, Damned Lies, and Statistics”

Mark Twain (or was it Benjamin Disraeli?)

The `scipy.stats` subpackage contains different a large number of functions dedicated to the latter: frequentists statistics, probability, distributions, correlation, functions, different statistical tests, etc. Want to generate a distribution with a known functional form? this subpackage has it? Is one distribution different than another? How different? This subpackage has it.

In previous generations, a lot of these topics were covered in the venerable "Numerical Recipes" textbook (er, phonebook) for code in C and FORTRAN. Your instructor and his advisor (and his advisor before him, most likely) learned numerical techniques from this source. We are no longer in the dark ages of dial-up Internet and cellphones the size of books, but this text (written *before* such an era) IS the authority on this topic, in my opinion. And the value of that text to highlight what is important even in Python remains.

Therefore, some of my discussion will basically look like a "*Numerical Recipes in SciPy*" (someone should write this textbook).

The key topics we want to cover are as follows:

- *Statistical Properties of Data* - You have some data, how do you describe it?
- *Distributions of Data* - You have some data, how is the data-as-an-aggregate intelligible? What patterns do it fit into?
- *Statistical Tests of Data* - You have some data, how sure are you that it differs from some other data, how sure are you that something you think is interesting is actually significant vs noise, etc.

Similar to before, our key start-up commands are to import relevant libraries: numpy, matplotlib, and the stats subpackage of SciPy:

```
import numpy as np
import matplotlib.pyplot as plt
from scipy import stats
```

Properties of Data

We have some data. How would you describe it? Well, let's then start with some data:

```
A = np.array([[10, 14, 11, 7, 9.5], [8, 9, 17, 14.5, 12],
              [15, 7, 11.5, 10, 10.5], [11, 11, 9, 12, 14]])

print(A.shape) #this is a (4,5) array
```

Basic Properties

Key properties of the data include the mean, median, standard deviation, and variance.

- mean -- The mean of an array is $\Sigma_i A_i/N$, where N is the number of elements of A. Note, that if you call the program without any axis keyword, then the mean is calculated over the entire array. Whereas the axis keyword specifies that the mean is calculated over a specific dimension. E.g. `mean=scipy.stats.mean(A,axis=1)`.

- median -- the median of an array x of length n equals $x_{(n+1)/2}$ if n is odd and $0.5 \times (x_{n/2} + x_{(n/2)+1})$ if n is even.

- variance -- By "variance" here we usually mean the "average of the squared deviations from the mean": $S^2 = \Sigma_i (x_i - \bar{x})^2/N$, where N equals the total population size. This is also known as the *population variance*. There is also the *sample variance*, where $S^2 = \Sigma_i (x_i - \bar{x})^2/n - 1$.

  The best way to think about the latter is that we are picking out a sample of n from the larger population of N. As such, we have an additional correction factor (the "Bessell correction", which is responsible for the $n - 1$ in the denominator. You can also think of this as a "degree of freedom": i.e. you estimate the variance from a random sample of n independent measurements, so the dof equals n minus the number of parameters estimated (i.e. the sample mean).

- standard deviation -- The standard deviation of a random variable, σ, is equal to the square

root of its variance. e.g. for a population standard deviation, $\sigma = \sqrt{\Sigma_i (x_i - \bar{x})^2 / N}$. Similarly, the sample standard deviation includes a $n - 1$ factor in the denomintor, not N: $\sigma = \sqrt{\Sigma_i (x_i - \bar{x})^2 / (n - 1)}$

We can call these from SciPy as follows:

- `mean=scipy.mean(A,axis=axis)`
- `median=scipy.ndimage.median(A)` . I.e. Within SciPy, the function to compute the median is (confusingly) found in the `ndimage` subpackage, not stats.
- `variance = scipy.stats.tvar(A,ddof=ddof)` .
- `standard_deviation = scipy.stats.tstd(A,ddof=ddof,axis=axis)`

Note here that the weirdness with the function calls. The "mean" call is understandable (though why is it not in stats?) but median lives in another subpackage. Similarly, the variance and standard deviation are actually computed from the *trimmed [variance/standard deviation]* functions. What this does is allow you to select a subset of the sample range in computing the variance or standard deviation, though of course if you do not put anything for this keyword, then the full range is considered.

For these and probably a bunch of other reasons, most often you want to use equivalent NumPy functions for these operations. Here I list the functions with the major keywords and their default values. So in NumPy ...

- `mean=np.mean(A,axis=None,ddof=0)`
- `median=np.median(A,axis=None)`
- `variance=np.var(A,axis=None,ddof=0)`
- `standard_deviation = np.std(A,axis=None,ddof=0)`

`axis=None` says "compute ___ over entire array", whereas `axis=[not None/some number]` says compute over a specific axis. Also, the ddof keyword refers to "delta degrees of freedom": the divisor in the calculations use $n - ddof$. By default, ddof=0 (i.e. this is a maximum likelihood estimate of the variance for normally distributed variables.

Anyway, this all seems rather silly (who cares so long as you know which version you are using, right?). Except that the default assumptions about what is *actually* being computed varies from programming language to language and package to package.

E.g. take the array `[2. , 3. , 4. , 2.1, 2.2, 3.3]`

Here's what you get if you just ask NumPy what the mean, standard deviation and variance are without any keywords:

```
#NumPy

a=np.array([2. , 3. , 4. , 2.1, 2.2, 3.3])
print(np.mean(a))
2.766666666666667

print(np.std(a))
0.7318166133366716

print(np.var(a))
#0.5355555555555555
```

and SciPy

```
#SciPy
print(scipy.mean)
#2.766666666666667

print(scipy.stats.tstd(a))
#0.8016649341630621   #uh oh!

print(scipy.stats.tvar(a))
#0.6426666666666666  #oh no!
```

Okay, maybe this is just some weirdness with SciPy vs NumPy ... nope! Here are the equivalent commands in IDL

```
IDL> print,mean(a)
#2.76667

IDL> print,stdev(a)
#0.801665 #SciPy-like

IDL> print,variance(a)
#0.64266670 #SciPy-like again
```

So yeah, the NumPy implementations of these basic statistical properties are pretty user friendly ... but be very careful that you understand **exactly** what you are computing.

Dealing with NaNs

Now, if you have NaNs in your array these simple NumPy functions are probably going to crash when you try to compute the mean, median, variance or standard deviation. Thankfully, NumPy

has thought ahead and created functions that compute these statistical values *while ignoring* NaNs:

`np.nanmean`, `np.nanmedian`, `np.nanvar`, `np.nanstd`.

More Advanced Properties

The above statistics can be done with either NumPy (recommended, provided you understand caveats) or SciPy (works but "Rube-Goldberg machine"-ish?). For more advanced characteristics, SciPy -- in particular `scipy.stats` -- becomes more useful and is the preferred option.

Some more complicated properties include

- skew -- `scipy.stats.skew` -- Gives the relative weight to the right or left tail of a distribution. For normally distributed data, the skewness should be about zero. For unimodal continuous distributions, a skewness value greater than zero means that there is more weight in the right tail of the distribution. The sample skewness is computed as the Fisher-Pearson coefficient of skewness: $g_1 = m_3/m_2^{1.5}$, where $m_i = \Sigma_{n=1}^{N}(x[n] - \bar{x})^i/N$

- kurtosis -- `scipy.stats.kurtosis` -- is the measure of the "tailed-ness" of a given distribution (i.e. how often outliers occur). It equals the "fourth central moment" divided by the square of the variance (i.e. $\mu_4/S^2 = \mu_4/\sigma^4$). For a normal distribution the value of the kurtosis is 0.

- interquartile range -- `scipy.stats.iqr` -- The interquartile range is the difference between the 75th and 25th percentile of the data. It is an outlier-resistant measure of the dispersion of data.

  Now this is great but what if you actually want the values for the 75th or 25th percentile? I'm sure there is a scipy function to do this, but the simpler route is to just use NumPy. E.g. `np.nanpercentile([array],25)` gives the 25th percentile value of an array.

Distributions of Data

SciPy's stats subpackage contains a lot of ways to compute probability distributions. We subdivide these distributions up into two: continuous distributions and discrete distributions.

Continuous Distributions

Some examples of continuous distributions are `norm` (normal distribution), `gamma` (gamma distribution), `uniform` (uniform distribution). Each object of continuous distributions comes

with many useful methods, such as its PDF (probability density function), its CDF (cumulative distribution function), etc.

What do we mean by these terms?

Normal (Gaussian) -- A normal distribution (aka a Gaussian distribution) is a bell-shaped distribution with a sharp drop in the "tails" of the distribution (i.e. outside the "bell"). It can be represented by the functional form

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-0.5((x-\mu)/\sigma)^2},$$

where μ is the mean of the distribution, σ is the standard deviation, and the variance is σ^2. The width of the bell is described usually as the "full width at half-maximum" (FWHM) which is $FWHM = 2\sqrt{2ln2}\ \sigma \approx 2.36\ \sigma$.

Log-Normal (Gaussian)

This distribution is similar, with a probability density distribution of $f(x) = \frac{1}{x\sigma\sqrt{2\pi}} e^{-0.5((lnx-\mu)/\sigma)^2}$.

Here, instead of the value of a variable is not normally distributed but the log of that value is normally distributed.

Density Functions

The "Probability Density Function" (PDF) is the probability per unit length of a continuous random variable, giving a *relative* likelihood of some value. I.e. since values for the variable are continuous, not discrete, the probability of any one value is vanishingly small, but probably over some δlength can be large.

The "Cumulative Density Function" (CDF) of a function f with a range of values X, evaluated at value x, is the probabilty that X will have a value less than or equal to x: $f_X(x) = P(X \leq x)$.

Example

Below is an example of a normal distribution with a mean of π and a standard deviation of 2π.

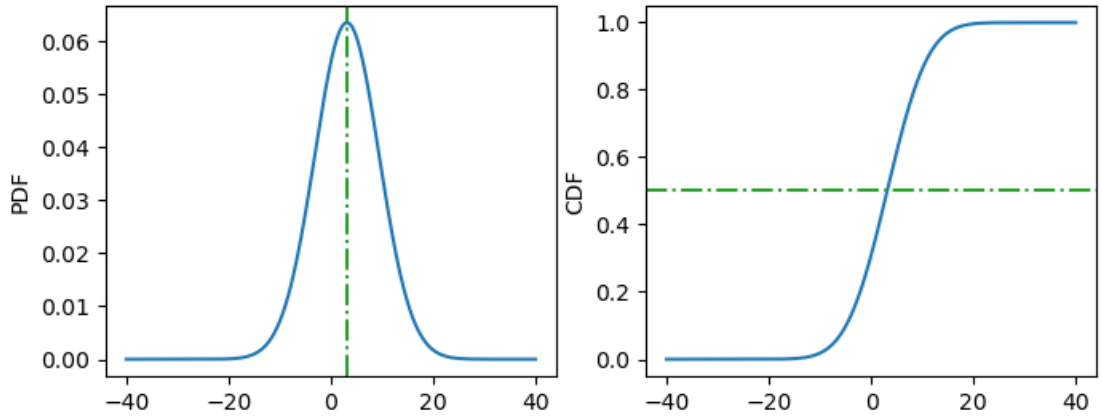
```
from scipy.stats import norm
import numpy as np

bins=np.arange(-40,40,0.01)
PDF=norm.pdf(bins,loc=np.pi,scale=2*np.pi) #generates PDF in bins
CDF=norm.cdf(bins,loc=np.pi,scale=2*np.pi) #generates CDF in bins
```

Now we plot the results

```
fig, ax  = plt.subplots(1,2,figsize=(8,3))
ax[0].plot(bins,PDF)
ax[0].set_ylabel("PDF")
ax[0].axvline(np.pi,ls='-.',color='tab:green')
ax[1].plot(bins,CDF)
ax[1].axhline(0.5,ls='-.',color='tab:green')
ax[1].set_ylabel("CDF")
plt.show()
```

Which produces the following plot:



Here we notice that the peak of the PDF equals the mean value of π (denoted by vertical green line) and the value of where CDF = 0.5 also equals π (horizontal green line).

One common practice is to fit a dataset into a distribution. That is, we have some data and then say "let's fit it with a normal distribution" or "let's fit it with a gamma distribution", etc.

This can be accessed through the `fit` function. E.g. `scipy.stats.norm.fit`.

To demonstrate this idea, we generate some pseudo data through the `rvs` function (`norm.rvs`) which generates random numbers that follow a given distribution.

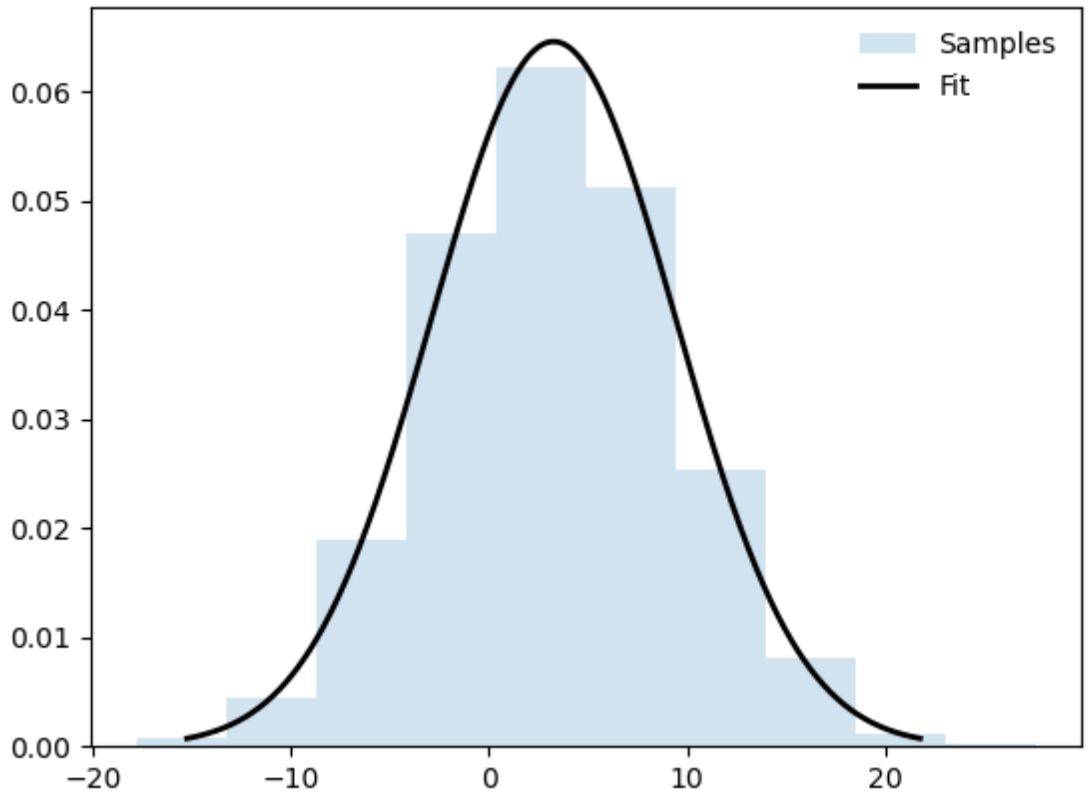
Here's an example:

```
samples = norm.rvs(loc=np.pi, scale=2*np.pi, size=5000)  # random data set

mu, sigma = norm.fit(samples, method="MLE")  # do a maximum-likelihood fit
print(mu, sigma)

# Plot figure
bins = np.arange(mu - 3 * sigma, mu + 3 * sigma, 0.005)
plt.hist(samples, density=True, histtype='stepfilled',
         alpha=0.2, label='Samples')
plt.plot(bins, norm.pdf(bins, loc=mu, scale=sigma),
         'k-', lw=2, label='Fit')
plt.legend(loc='best', frameon=False)
plt.show()
```

This particular iterations produces a fitted mean of 3.267 and standard deviation of 6.17, which are very close to a mean of π and standard deviation of 2π. Repeating this simulation will give slightly different answers each time (since we are selecting random numbers *drawn from* some distribution but we should expect qualitatively the same answer.



Discrete Distributions

Discrete distributions describe the rate of occurances of discrete (countable) outcomes. They contrast with continuous distributions, whcih can have outcomes that fall anywhere on a continuum.

SciPy contains several examples of discrete distributions, including `bernoulli` (Bernoulli distribution), `binom` (binomial distribution), `poisson` (Poisson distribution). As with continous distributions, each call to a discrete distribution comes with some key functions, e.g. its PMF (probability mass function) and its CDF (cumulative distribution function).

Binomial

A binomial distribution describes the number of successes in a series of n independent draws, each with an outcome probability p ("success" or "positive result") or probability q ("failure" or "null result"). A single draw follows a Bernoulli distribution. The binomial distribution provides the basis for the binomial statistical significance test.

In any case, with a binomial distribution, the probability p of k "successful"/"positive result" outcomes given n independent draws is:

$$f(prob(k, n, p)) = \frac{n!}{k!(n-k)!} p^k (1-p)^{n-k}$$

Poisson

The Poisson distribution is a simpler discrete distribution, measuring the probability of a given number of events happening in a specified time period.

It has a functional form of

$$f(prob(k, \lambda)) = \frac{\lambda^k e^{-\lambda}}{k!}$$

In the simplest possible terms, you can think of a Poisson distribution as a binomial distribution the limit of an infinite number of draws and where the expected number of "successes" is constant with time.

Bernoulli

This is the discrete probability distribution of a random variable which takes the value 1 with probability p and the value 0 with probability $q = 1 - p$. It can be thought of as a binomial distribution where $n = 1$ (i.e. a single draw).

Confidence Intervals

In frequentist statistics (i.e. what we are dealing with), a confidence interval (CI) describes the likelihood that some measurement will fall within some range a certain fraction/percentage of the time.

E.g. you make some measurement x with value y. What if you measure the same thing again but with a differetn sample? and again? and again? The "95% confidence interval" then means "you will measure x to be y within [some range] 95% of the time". The concept is intertwined with measurement uncertainties in physics and astronomy (e.g. the brightness of a star in a given passband), so you will hear this term thrown around a lot. And there are deep misunderstandings about what these terms mean and even deeper confusion about how to calculate them in Python.

Poisson statistics

For Poisson distribution statistics, the confidence intervals are symmetric about the mean, p (k/n). E.g. a 1-σ (68%) interval has upper and lower ranges about the mean (measured) value of $1 + q$ and $1 - q$, where $q = \sqrt{1/k + 1/n}$. In other words:

(upper bound) = p(1+q)

(lower bound) = p(1-q)

In the limit that k is small compared to n, this further reduces to the symmetrical limits of $\sqrt{k}/n$.

The limitations of Poisson statistics seems straightforward but in practice even professional researchers can ignore them. For example, see this example where the author (Adam Burgasser, UCSD) lectures the field on using Poisson statistics for samples that are tens in size (!!!!), which is obviously from the above a no-go.

https://arxiv.org/pdf/astro-ph/0211470.pdf

Since they are invalid, we have to use more appropriate statistics: binomial statistics.

Binomial statistics

And ... here's where things get complicated and documentation you may find gives wildly different impressions of the "right" approach (and where your instructor went down a *MASSIVE* rabbit hole the past week looking over).

So if you have a probability distribution (i.e. a curve with some area) x fraction of that area will lie within two numbers. Here's an example from the Burgasser et al paper I mentioned above:

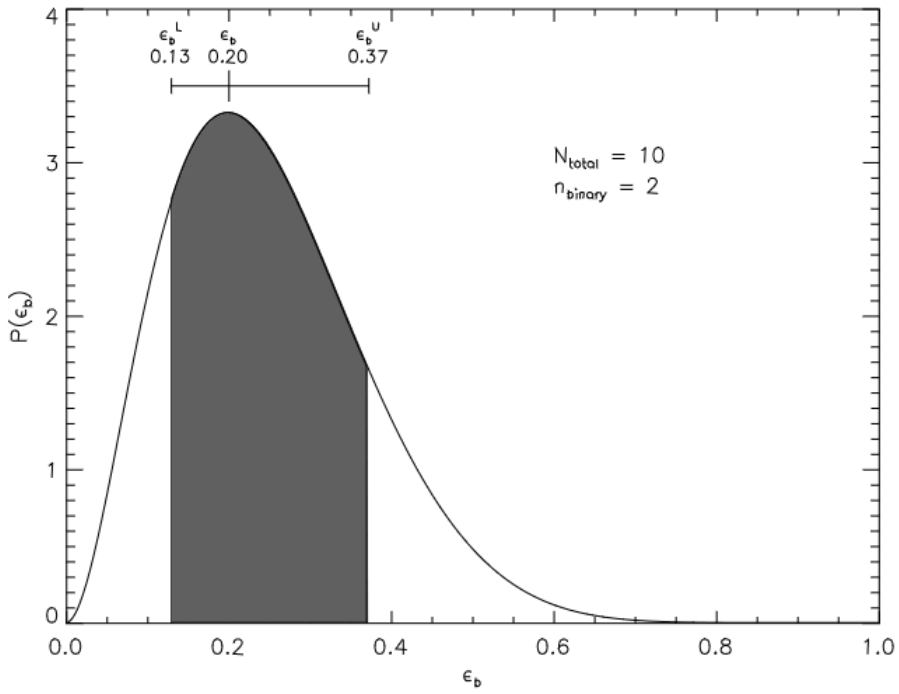


FIG. A10.— Probability distribution for ϵ_b constructed for a sample size $N = 10$ and number of binaries $n = 2$. The shaded region gives the $\pm 1\sigma$ range of acceptable values, whose limits are defined in the Appendix. The integrated probability in this region, 68%, is equivalent to 1σ Gaussian limits.

The simple interpretation of, say, a 68% confidence interval is "shaded region about the mean comprising 68% of the total area". And that would be exactly true in the case of a *flat prior* (uniform prior) on the distribution. The reality is that the exact confidence interval calculated in a binomial distribution is a non-trivial calculation. In fact this widely-cited paper has a long, blunt discussion (er rant) about confidence intervals): https://core.ac.uk/download/pdf/132271468.pdf

The key is to know *what* you are calculating and understand the limitations/assumptions.

Here are your options and how to calculate them in SciPy:

- **Flat Prior** -- A flat (uniform) prior on the binomial proportion over the range 0 to 1. The posterior density function is a Beta distribution: β(k + 1, n - k + 1). In SciPy upper and lower bounds are computed by the inverse β function, which is this horrendous-looking thing ...

Computes x such that:

$$y = I_x(a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \int_0^x t^{a-1}(1-t)^{b-1}dt,$$

The implementation SciPy is less horrendous ...

```
from scipy.special import betaincinv

alpha=1-confidence_interval #e.g. 0.68 for 68% CI

lowerbound = betaincinv(k + 1, n - k + 1, 0.5 * alpha)
upperbound = betaincinv(k + 1, n - k + 1, 1.0 - 0.5 * alpha)
```

Here, we can recover Burgasser's quoted confidence interval:

```
k=2
n=10
confidence_interval=0.682 #exact val for 1-sigma CI
alpha=1-confidence_interval #e.g. 0.68 for 68% CI

lowerbound = betaincinv(k + 1, n - k + 1, 0.5 * alpha)
upperbound = betaincinv(k + 1, n - k + 1, 1.0 - 0.5 * alpha)

print(lowerbound)
#0.12845821647659547
print(upperbound)
#0.373010124833298
```

This understanding of a confidence interval is what I "grew up" with in pre-Python (IDL) days.

- **Jeffrys Interval** -- This interval is derived by applying Bayes' theorem to the binomial distribution with the noninformative Jeffreys prior. The noninformative Jeffreys prior is the Beta distribution, Beta(1/2, 1/2), which has the density function. The posterior density function is a Beta distribution: β(k + 1/2, n - k + 1/2).

The general "expert" consensus is that the Jeffreys Prior is "better".

```
k=2
n=10
confidence_interval=0.682 #exact val for 1-sigma CI
alpha=1-confidence_interval #e.g. 0.68 for 68% CI

lowerbound = betaincinv(k + 1/2, n - k + 1/2, 0.5 * alpha)
upperbound = betaincinv(k + 1/2, n - k + 1/2, 1.0 - 0.5 * alpha)

print(lowerbound)
#0.10563168409670065
print(upperbound)
#0.350859220932479
```

As you see, the answers are *slightly* different than a flat prior.

- **Wilson Interval**

This interval, attributed to Wilson [2], is given by
$CI_{\text{Wilson}} = \frac{k+\kappa^2/2}{n+\kappa^2} \pm \frac{\kappa n^{1/2}}{n+\kappa^2}((\hat{\epsilon}(1-\hat{\epsilon}) + \kappa^2/(4n))^{1/2},$

where $\hat{\epsilon} = k/n$ and κ is the number of standard deviations corresponding to the desired confidence interval for a *normal* distribution (for example, 1.0 for a confidence interval of 68.269%). For a confidence interval of 100(1 - α)%, $\kappa = \Phi^{-1}(1-\alpha/2) = \sqrt{2}\text{erf}^{-1}(1-\alpha)$.

Now, this looks truly "involved". Thankfully SciPy has decided to have a canned function especially for it, using the `binomtest.proportion_ci` function. The call is pretty simple:

`from scipy.stats import binomtest`

then

`binomtest(k,n).proportion_ci(method='wilson',confidence_level=[confidence level]`

E.g. for a 1-σ confidence interval (68.2% or 0.682) for our example of $k = 2$ and $n = 10$

```
from scipy.stats import binomtest
binomtest(2,10).proportion_ci(method='wilson',confidence_level=0.682)
#ConfidenceInterval(low=0.10372027242788966, high=0.3506840498201643)

#you can access the specific values by calling the "low" and "high" proper
ties

#result=binomtest(2,10).proportion_ci(method='wilson',confidence_level=0.6
82)
#print(result.low)
#0.10372027242788966
#print(result.high)
#0.3506840498201643
```

This value gets *really* close to a Jeffreys prior.

- **exact** (aka Clopper-Pearson method) - calling this an "exact" method may be a bit questionable (particularly to the authors of the paper listed above) but I include it for completeness since the function call is pretty straightforward (like Wilson except just a slightly different keyword)

```
from scipy.stats import binomtest
binomtest(2,10).proportion_ci(method='exact',confidence_level=0.682)
#ConfidenceInterval(low=0.07205052578034218, high=0.405232091711883)
```

So which to use? Depends. The Wilson and Jeffreys prior are recommended by that paper. My advice (which is true for code in general): just understand clearly which method you are using and clearly communicate that to others.

Statistical Tests of Data

Chi-Squared Test and Goodness of Fit

Chi-Squared

Warning/Note -- In preparing this section, I discovered that SciPy's presentation is a bit "wonky" (to be very charitable). So we will proceed in full-on, first-principles "Numerical Recipes" style.

With that said ...

When comparing data and models we are typically doing one of two things:

• *Hypothesis testing* : we have a set of N measurements with individual measurements i. These measurements have values x_i and uncertainties σ_i. We compare the data to some model, which says that these measurements should have values μ_i.

How probable is it that these measurements would have been obtained, if the model is correct?

• *Parameter estimation* : we have a parameterized model which describes the data, such as $y = mx + b$, and we want to determine the best-fitting parameters and errors (er, confidence intervals) in those parameters.

The chi-squared statistic (χ^2) is our answer. It is a quantitative measure of the goodness-of-fit of the data to the model. In its simple form -- assuming that the measurments and their errors are independent (more on this later) -- of the following:

$\chi^2 = \sum_{i=1}^{N} \frac{(x_i - \mu_i)^2}{\sigma^2}$.

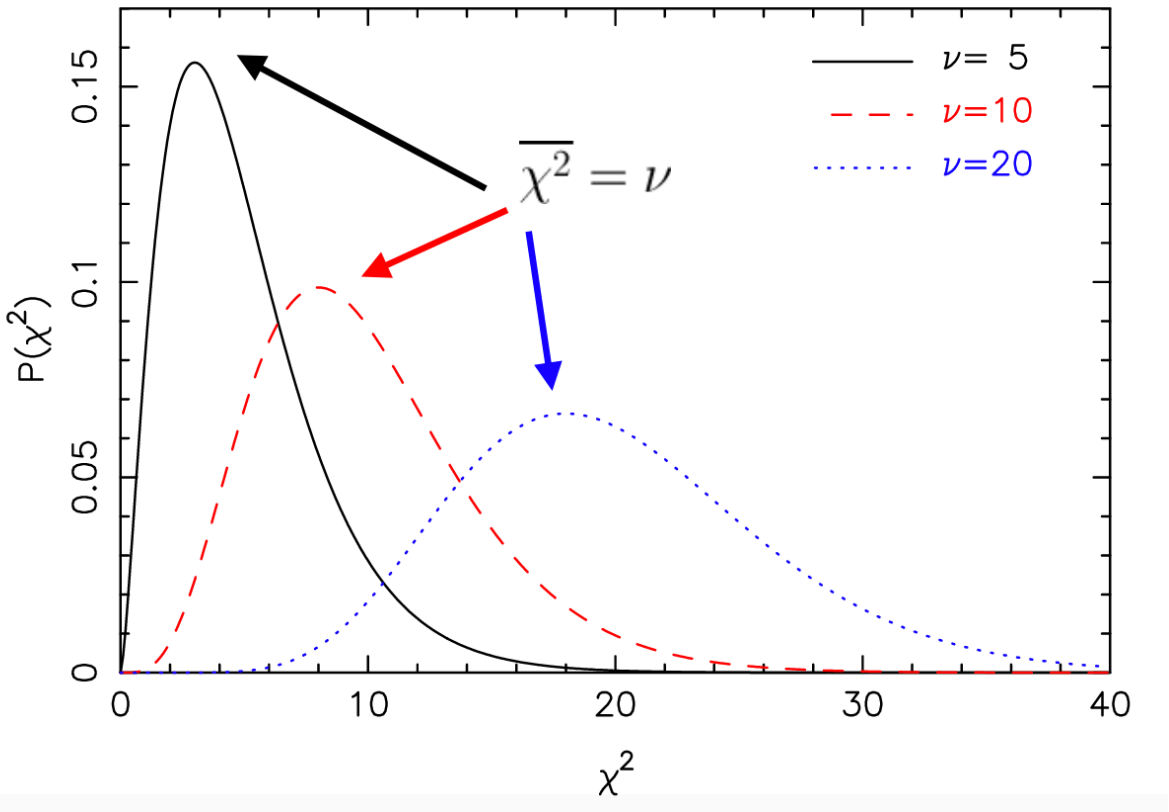
Note that this is a different thing than the Pearson chi-square statistic which is $\sum_{i=1}^{N} \frac{(x_i - \mu_i)^2}{\mu_i^2}$, which does not consider measurement error (and isn't useful in our context).

Anyway, the chi-squared statistic (χ^2) penalizes the model according to how many standard deviations each data point lies from the model. E.g. if the measurement i is x_i = 2 and σ_i = 0.5

(so the measurement is 2± 0.5) and the model predicts 3, then this is a 2-σ-discrepant prediction for i and the χ^2 contribution from that data point is equal to 4.

For Gaussian-distributed variables, the chi-squared statistic has a probability distribution of $P(\chi^2) \propto (\chi^2)^{(\nu-2)/2} e^{-\chi^2/2}$.

Here, ν equals "degrees of freedom". If the model has no free parameters then $\nu = N$. But if we are fitting a model with p free parameters, then we can “force the model to exactly agree with p data points”, and so $\nu = N - p$. Note we almost always have at least one free parameter when we do model fitting.



In each case, the mean of the distribution is related to the number of degrees of freedom ... and by related I mean equal: $\bar{\chi}^2 = \nu = N - p$. The variance is also related: $Var(\chi^2) = 2\nu$.

Thus, if the model is correct and if our measurement errors are accurate (i.e. they are not underestimated or inflated), we would expect:

$$\chi^2 \sim \nu \pm \sqrt{2\nu}$$

One can understand this intuitively. Each data point should contribute about ~1-σ from the model and hence ~ 1 to the χ^2 statistic.

p-values

If the model is correct [our hypothesis], what is the probability that this value of chi-squared, or a larger one, could arise by chance? This probability is called the p-value and may be calculated from the chi-squared distribution.

If the p-value is not low, then the data are consistent with being drawn from the model, which is “ruled in”. If the p-value is low, then the data are not consistent with being drawn from the model. The model is “ruled out” in some sense.

We will continue this discussion next week.