<u>Lecture 1:</u> <u>Chi-Squared & Some Basics</u>

D. Jason Koskinen koskinen@nbi.ku.dk

Advanced Methods in Applied Statistics Feb - Apr 2018

Photo by Howard Jackman University of Copenhagen

Niels Bohr Institute

Variance

Because it's something we all should know

$$\sigma^2 \equiv \langle (X - \mu)^2 \rangle \qquad \qquad \sigma^2 = \frac{1}{N} \sum_{i=0}^N (x_i - \bar{x})^2$$

 σ^2 is the variance

- μ is the mean, which can sometimes also be the expected value
- N is the number of data points
- x_i is the individual observed data points

Unbiased Variance

• Just because it's something we all should know

$$S_{N-1} \equiv \frac{1}{N-1} \sum_{i=0}^{N} (x_i - \bar{x})^2$$

 S_{N-1} is the 'unbiased' estimator of the variance

- $ar{x}$ is the mean calculated from the data itself
- N is the number of data points
- x_i is the individual observed data points

For further information on 1/(N-1) see Bessel's correction wikipedia

Probability Distribution Function

 Probability Distribution Functions (PDF), where sometimes the "D" is density, is the probability of an outcome or value given a certain variable range



• The PDF does not have be nicely described by a single continuous equation

Probability Distribution Function

 The PDF does not have be nicely described w/ equations, and sometimes cannot be

PDFs

- They can be F
 discrete, continuous,
 or a combination
- They often have an implied conditionality
 - "What is the energy of an outgoing electron F(x) from nuclear betadecay?" implies betadecay
 - PDF should be normalized to 'one'

 Let's imagine an experiment which has two identical electron traps (A & B) separated by a finite barrier. An electron w/ energy below the barrier threshold is deposited in trap A. Sketch out the PDF of the x position after a very short time.

time $\approx \frac{1}{\infty}$

- Sketch out the PDF of the x position after a very short time.
 - My trap has a potential which keeps it mostly in the middle of the trap, and it's mostly in trap A because it hasn't had time to tunnel.

• Sketch out the PDF of the x position after a near infinitely long time.

time $\approx \infty$

- Sketch out the PDF of the x position after a near infinitely long time.
 - Same distribution shape as before, but now the probability of being in trap A and trap B are equal.
 - Had to renormalize the PDF

time $\approx \infty$

• Notice that there are discontinuities in the PDF, which is not uncommon in experimental PDFs due to boundary conditions. How many discontinuities as a function of x?

time $\approx \infty$

Some PDF Remarks

- Previous examples are univariate PDFs, i.e. probability only as a function of a single variable (x), but the PDF comes from a multivariate situation
 - Multivariate, because the PDF doesn't just depend on x, but also the time of the measurement, energy of the electron, barrier height, etc.
 - We'll stick with univariate (or at least 1-dimensional unchanging PDFs) initially, before moving onto more complex situations later in the course
- Probability distribution functions can be used to not only derive the most likely outcome, but having recorded the outcome, i.e. get data, figure out the mostly likely situation. For example, if we record a single electron at a position in trap B, it is more likely that the data was taken at t=∞ versus t=1/∞

Cumulative Distribution Function

- The Cumulative Distribution Function (CDF) is related to the PDF and gives the probability that a variable (x) is less than some value x₀
- Basically, the integral or sum from -infinity to x_0

$$CDF = F(x) = \int_{-\infty}^{x_0} f(x)dx$$

where f(x) is the PDF

Cumulative Distribution Function

• The Cumulative Distribution Function (CDF) is related to the PDF and gives the probability that a variable (x) is less than some value x₀

Empirical Distribution Function

- The Empirical Distribution Function (EDF) is similar to the CDF, but constructed from data
 - Used in methods we'll cover later, e.g. the Kolmogrov-Smirnov test
 - Much less common than the CDF or PDF

Gaussian PDF

• Gaussian Probability Distribution Function (PDF) only relies on the mean (µ) and the standard deviation (σ) of a sample

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

Gaussian PDF

• Gaussian is one of the single most common PDFs, in part because of the Central Limit Theorem (CLT)

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

Central Limit Theorem

- Because the central aim is the practical application of analyses techniques, we will not be overly concerned with theorems, math-stuff, and theoretical derivations. This is an *applied* methods course after all.
- In loose terms, the CLT says that for a large number of measurements of continuous variables (or combinations thereof) the outcome approaches a gaussian distribution.
 - Even if the underlying PDF (or joint PDFs) are not themselves gaussian

Statistical Tests

• Pearson's Chi-squared test

$$\chi^{2} = \sum \frac{(Observed - Expected)^{2}}{Expected}$$

• Many different permutations for a Figure of Merit (FOM), and a quick modification of χ^2 is a nice tool to have when seeing new results

$$\chi^{2} = \sum \frac{(Observed - Expected)^{2}}{Expected + \sigma_{systematics}^{2}}$$

Gaussian/Poisson Uncertainty is Everywhere

- Thanks to basic statistics, and Siméon Poisson, an estimate of the uncertainty on data points is generically sqrt(number of events). It works because almost all data is at some level a collection of discrete events.
 - Does not include the impact of systematic uncertainties
 - Does not include the impact of any biases either
 - Works better for larger number of events than smaller
- When in doubt, take the square root of something

Exercise 1

- Read in data from "FranksNumbers.txt"
 - There is some non-numeric text in the file, so data parsing is important
 - Use any methods and/or combinations of coding languages which work(s) for you
 - Parse data in python, analyze in MatLab
 - Parse data and analyze in R
 - Parse data in C, analyze in Fortran (not recommended, but possible)
 - Copy/paste using spreadsheets (Excel, OpenOffice, etc.) is discouraged because the data is already in .txt files, and reading in .txt files is a very important skill
 - Note that a future data set has 1.28M entries, which will kill a spreadsheet
- Calculate the mean and variance for each data set in the file
 - There should be 5 unique data sets

Exercise 1 pt.2

- Using the eq. y=x*0.48 + 3.02, calculate the Pearson's χ^2 for each data set
 - Write your own method
 - Bonus: use a class or external package to get value
- Using the same eq. calculate a χ^2 where the uncertainty on each data point is ± 1.22
- From the two χ^2 , what is a better reflection of the uncertainty?
 - ±1.22 or sqrt(events)?

Some chi-squared Remarks

- A chi-squared distribution is based on gaussian 'errors', so beware when errors/uncertainties are not gaussian
 - Low statistics
 - Biases in the data or x can also produce non-gaussianity
- The concept that a reduced chi-squared near 1 is 'good' depends strongly on the degrees of freedom (DoF) and/or data
 - A reduced chi-squared of 1.2 w/ 20 DoF has a pretty good p-value
 - 1.2 w/ 1000 DoF has a very bad p-value

Conclusion

- Know your distribution functions (probability, cumulative, and empirical)
- Central Limit Theorem says most variables will produce a gaussian distribution at large numbers of measurements
- Chi-square(d) calculation is a frequent metric for goodnessof-fit and quantitative data/hypothesis matching
- Light load this week, so try and get your software working
 - If you have problems ask classmates who have similar computer setups
 - If you have solutions help your classmates
- First problem set is online
- Read "Not Normal: the uncertainties of scientific measurements", there will be a discussion next class

Extra

Distribution Functions

- Many nice illustrations for different functions at <u>https://</u> <u>commons.wikimedia.org/wiki/Probability_distribution</u>
- Many of the plots used in the lecture notes come from wikipedia (because it's awesome)