Lecture 1:
Chi-Squared & Some Basics

D. Jason Koskinen
koskinen@nbi.ku.dk

Advanced Methods in Applied Statistics
Feb - Apr 2025

Photo by Howard Jackman

Variance

- Because it's something we all should know

$$\sigma^2 \equiv \langle (X-\mu)^2 \rangle$$

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

σ^2 is the variance

μ is the expected value, which can sometimes also be the mean

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

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

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

$\bar{x}$ is the mean calculated from the data itself

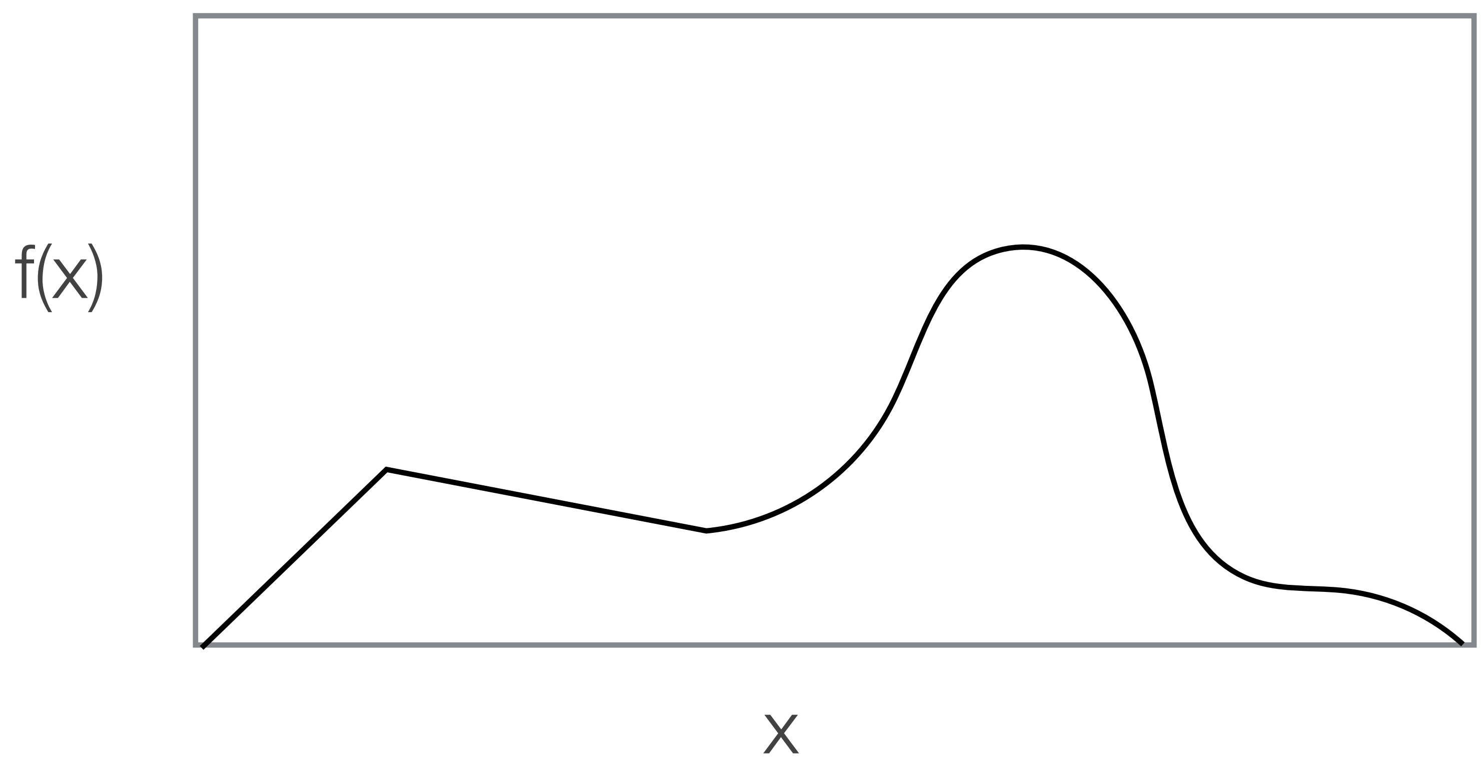
N is the number of data points

x_i is the individual observed data points

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

Probability Distribution Function

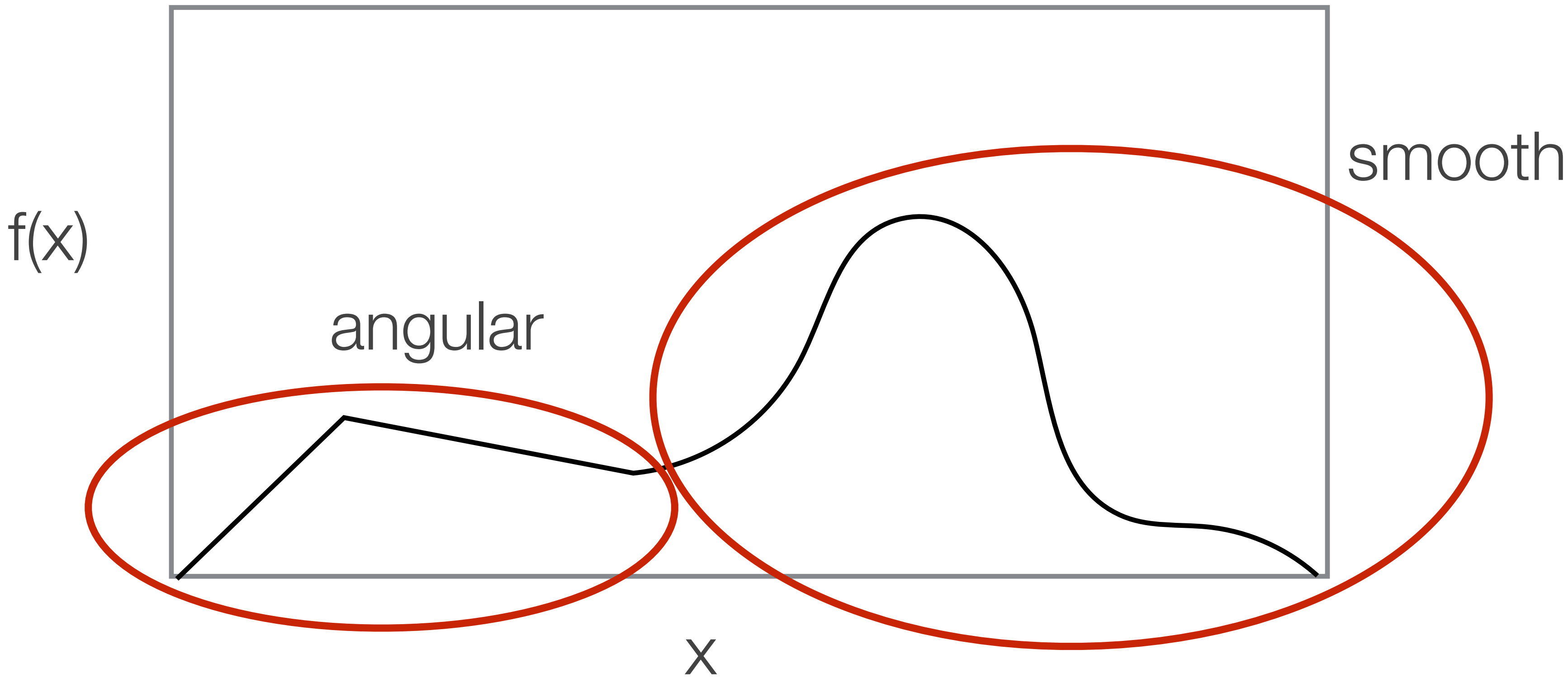
- **P**robability **D**istribution **F**unctions (PDF), where sometimes the "D" is density, is the probability of an outcome or value given a certain variable range



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

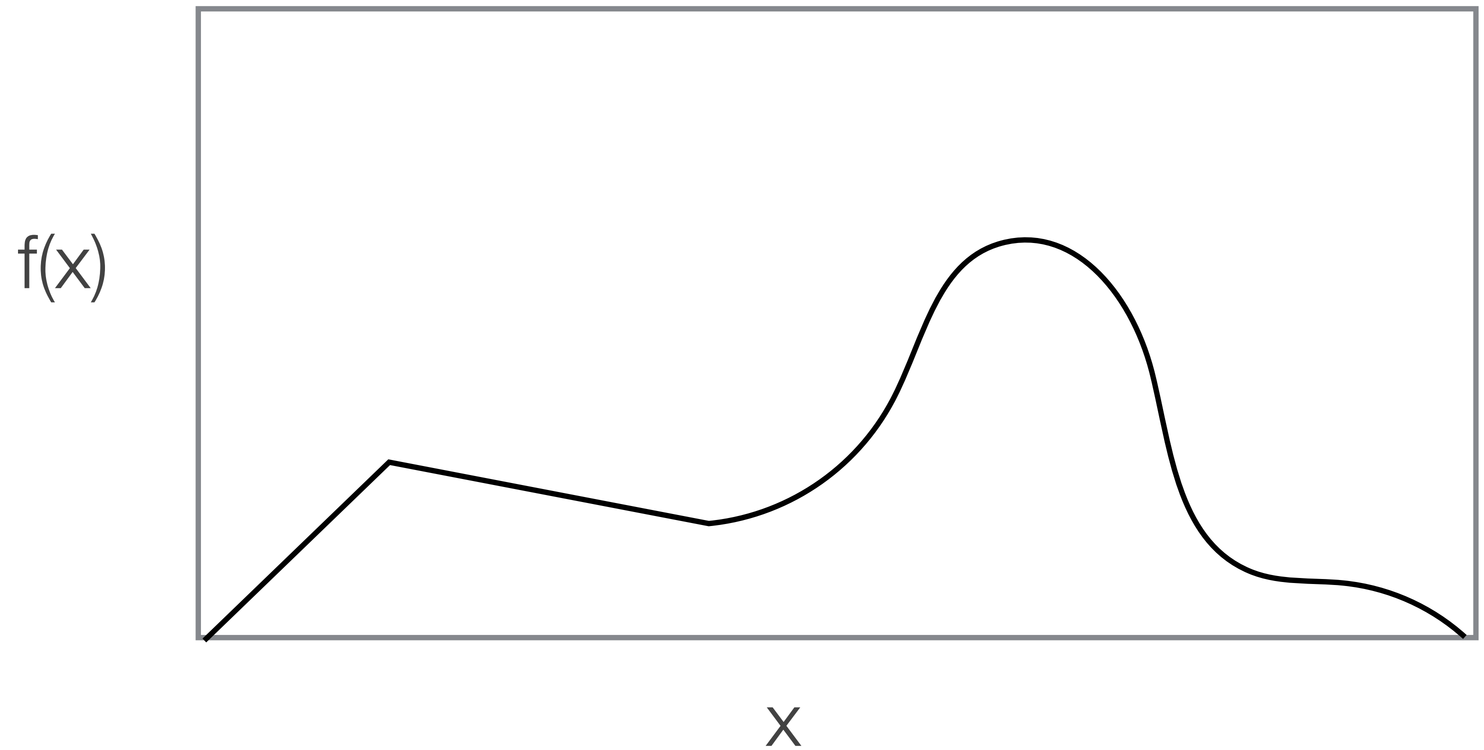
Probability Distribution Function

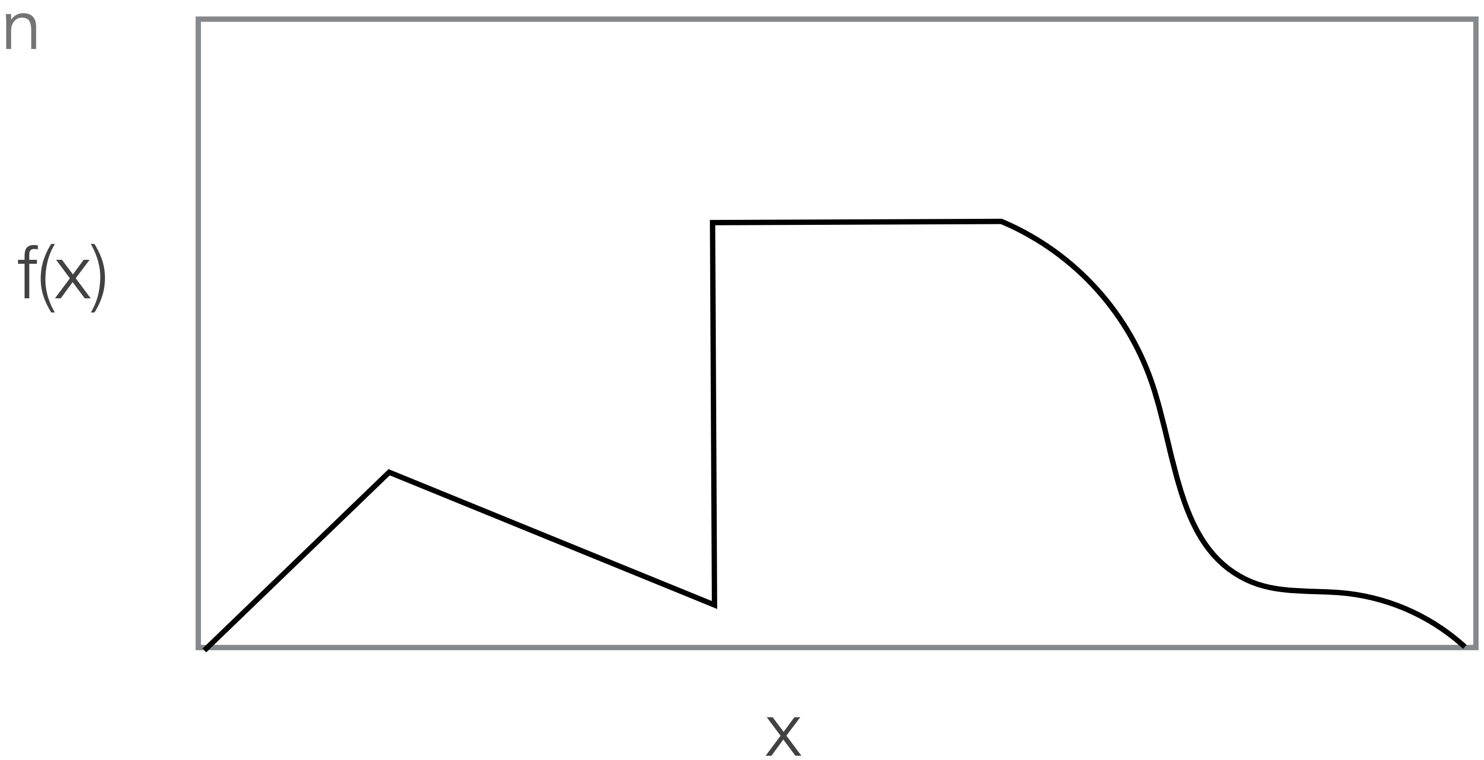
- The PDF does not have be nicely described w/ equations, and sometimes cannot be



PDFs

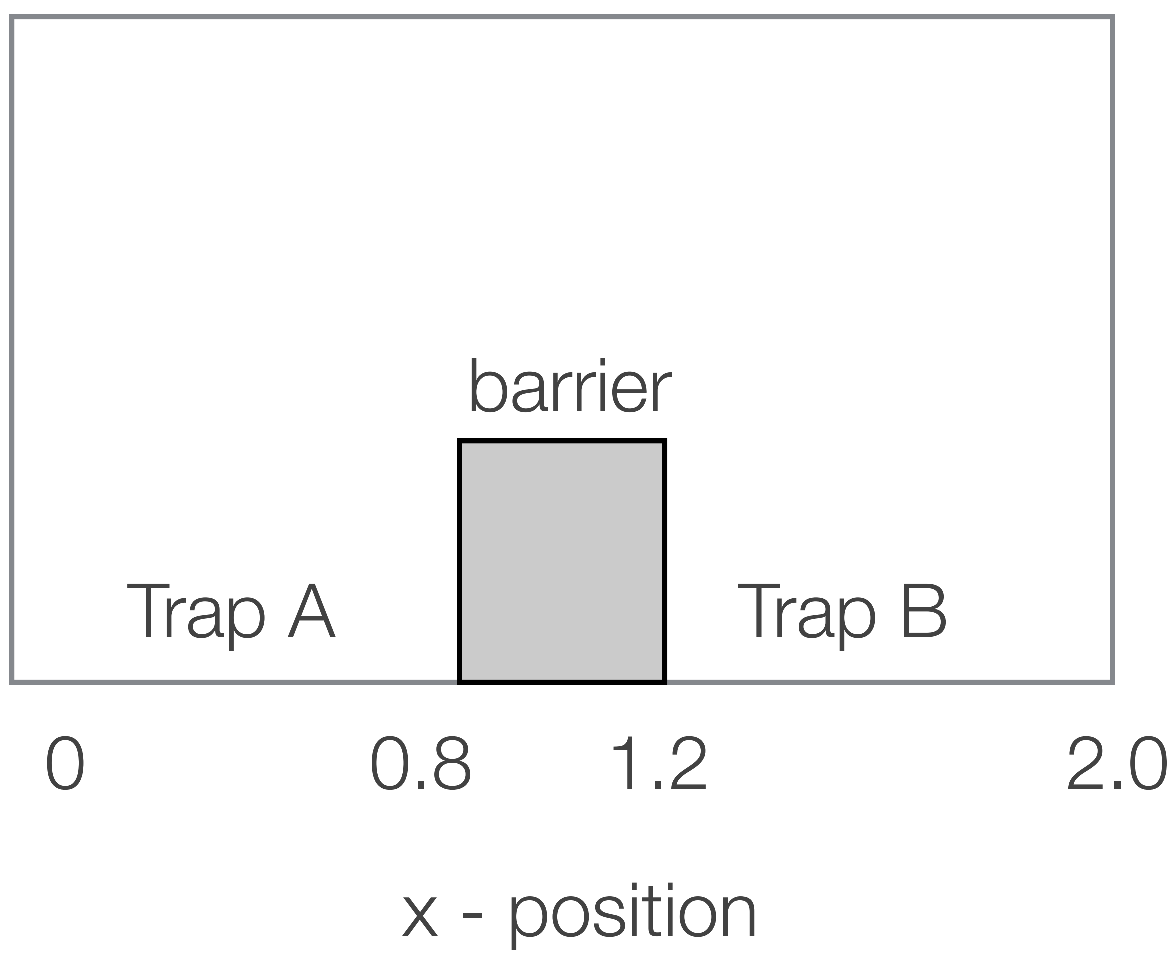
- They can be discrete, continuous, or a combination
- They often have an implied conditionality
  - "What is the energy of an outgoing electron from nuclear beta-decay?" implies beta-decay
  - PDF must always be normalized to **one**





PDF Possibility

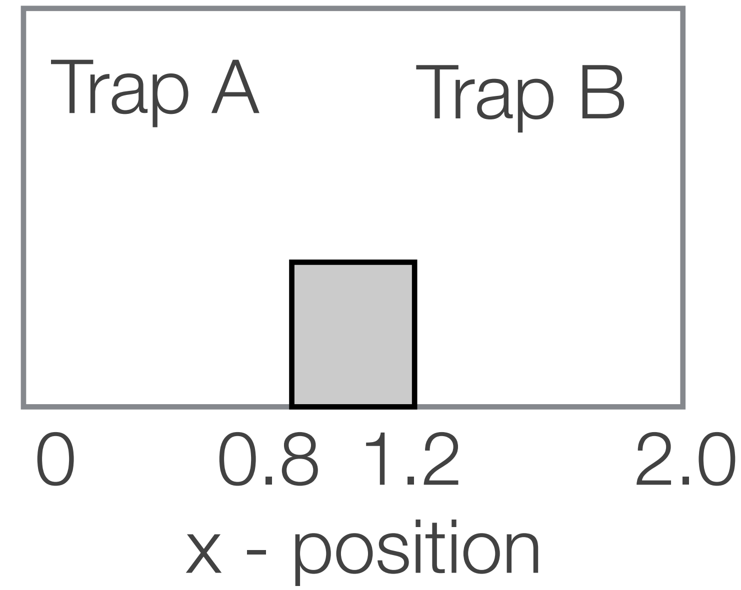
- Let's imagine an experiment which has two identical electron traps (A & B) separated by a finite barrier. An electron w/ energy below the barrier threshold is deposited in trap A. Sketch* out the PDF of the x position after a very short time.



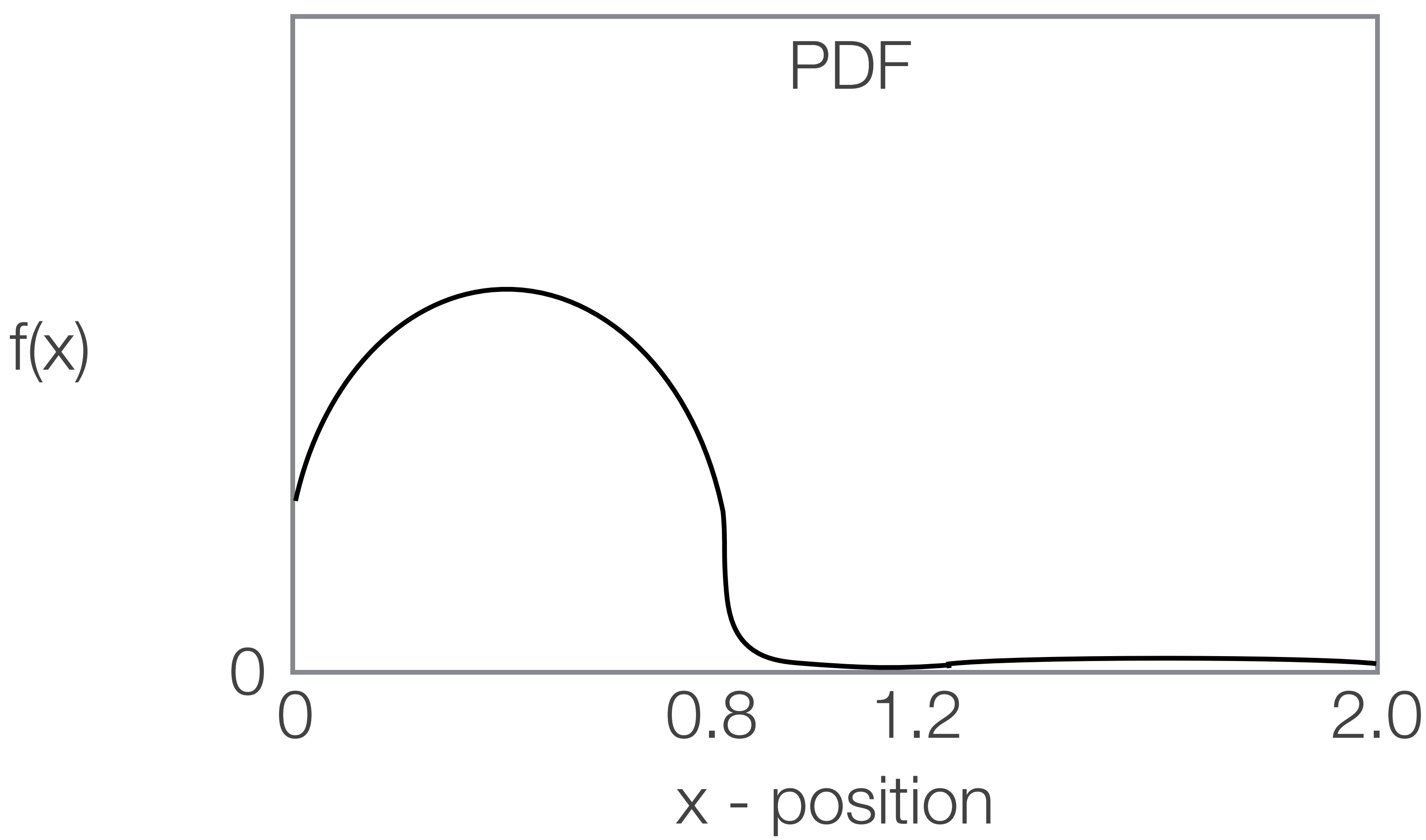
$$\mathrm{time} \approx \frac{1}{\infty}$$

*rough sketch, don't take it too literal

PDF Possibility



- 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.



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

*rough sketch, don’t take it too literal

PDF Possibility

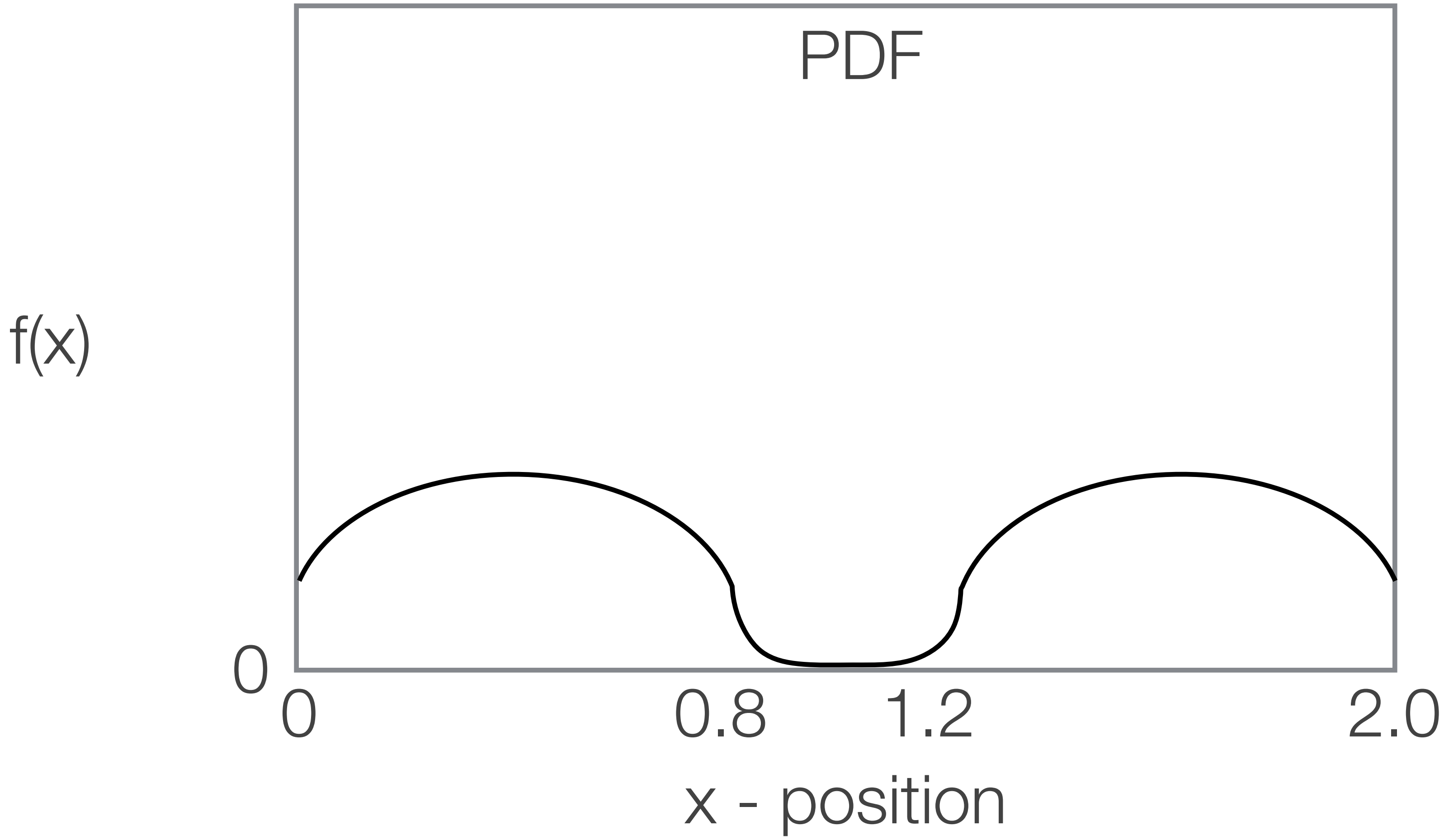
- Sketch out the PDF of the x position after a near infinitely long time.

$$\text{time} \approx \infty$$

PDF Possibility

- 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.
  - The PDF is still normalized

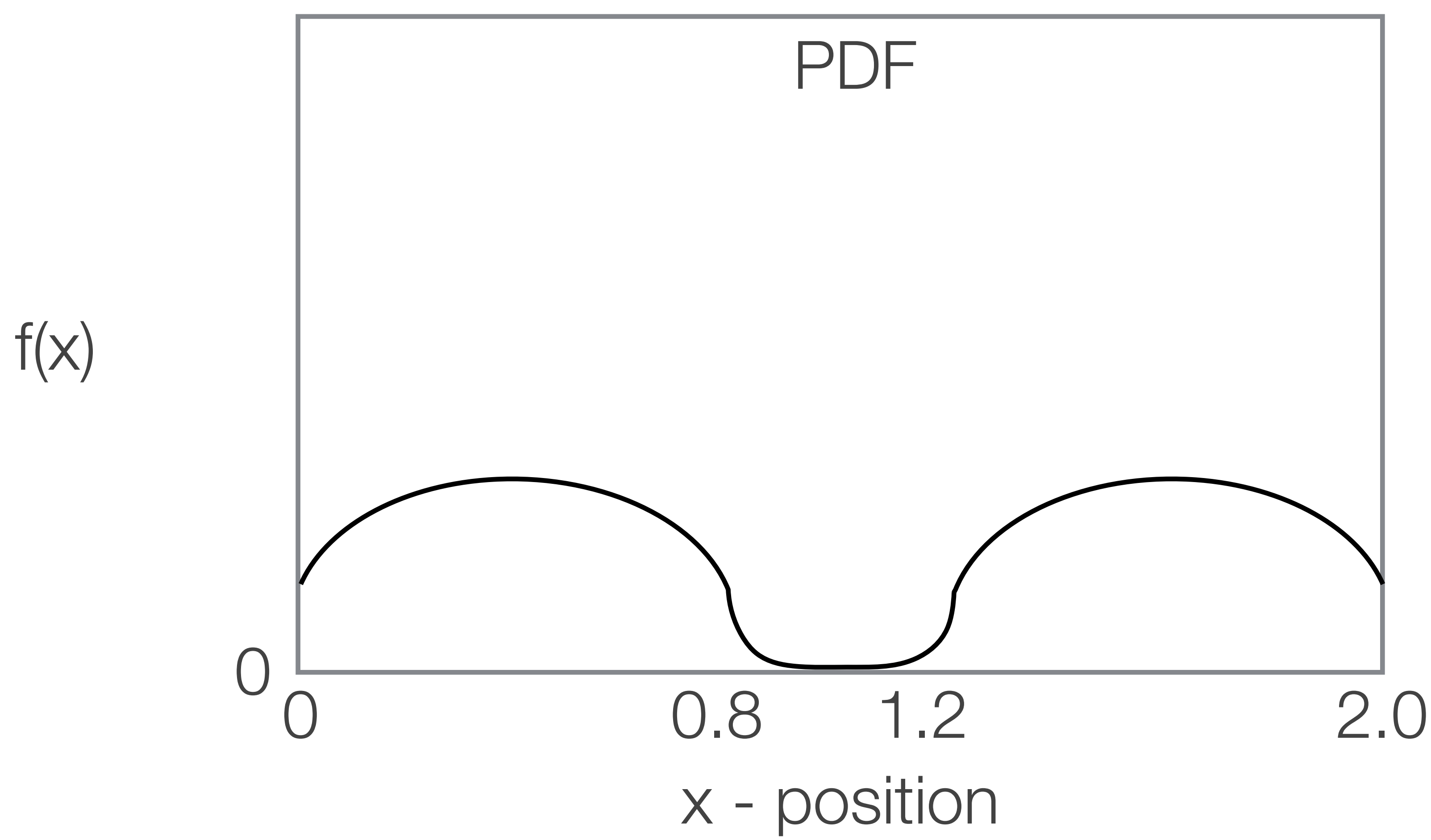
$$\mathrm{time} \approx \infty$$



PDF Possibility

- 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?

$$\text{time} \approx \infty$$



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, 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 $t = \infty$ versus $t = 1/\infty$

Cumulative Distribution Function

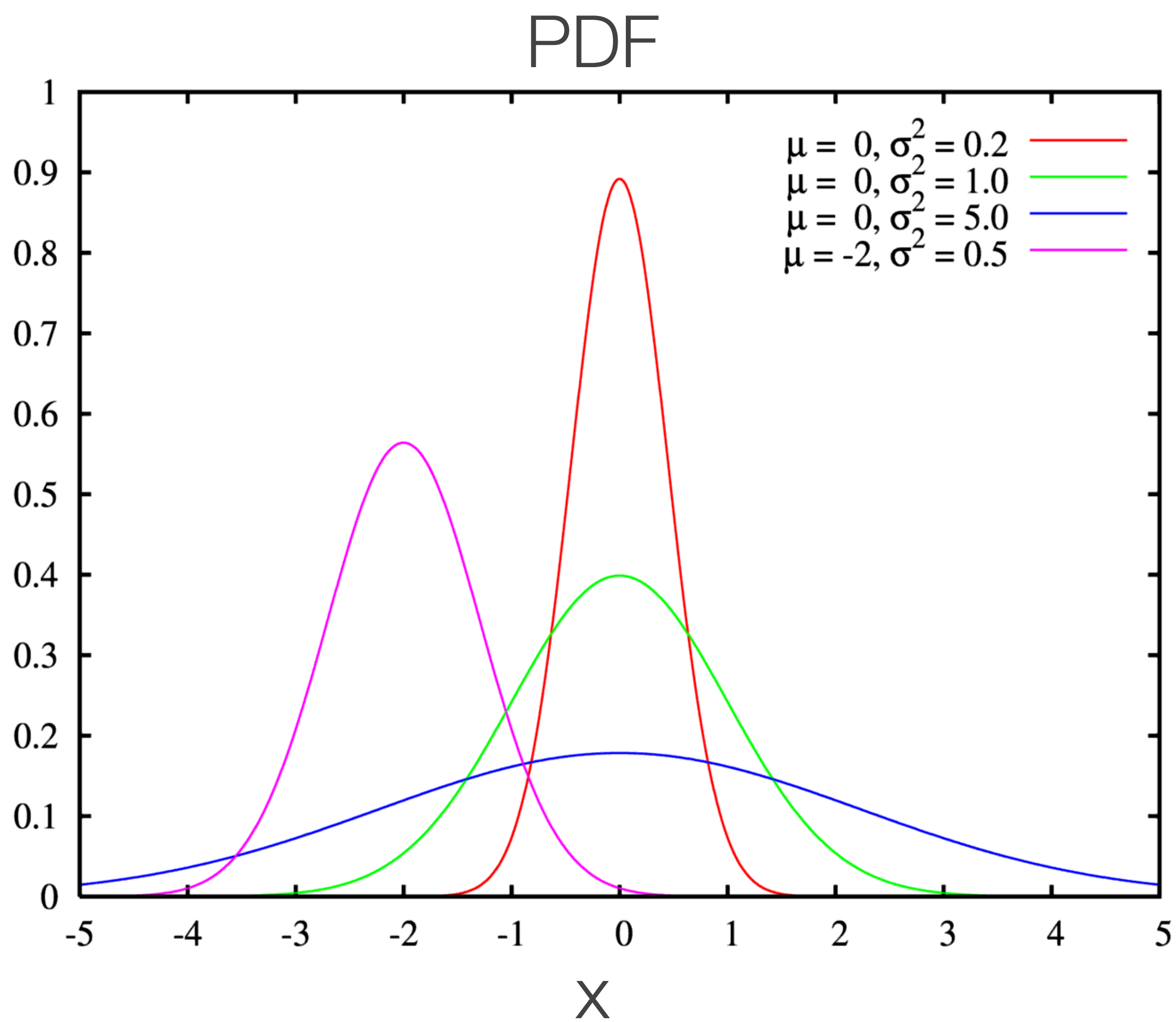
- The Cumulative Distribution Function (CDF) is related to the PDF and gives the probability that a variable (x) is less than some value x_0
- Basically, the integral or sum from -infinity to x_0

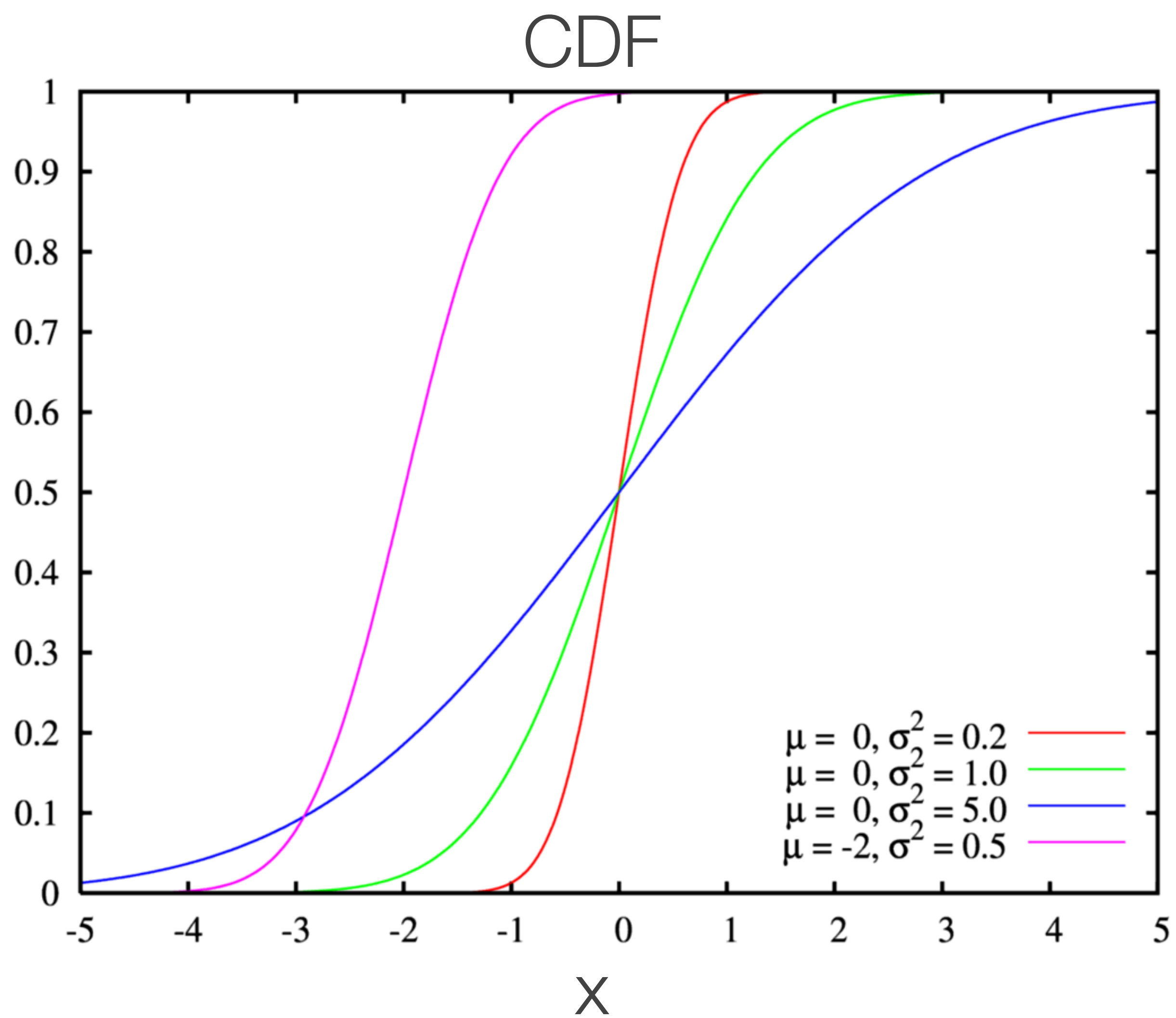
$$CDF(x_0) = F(x_0) = \int_{-\infty}^{x_0} f(x)dx$$

where $f(x)$ is the PDF

Cumulative Distribution Function

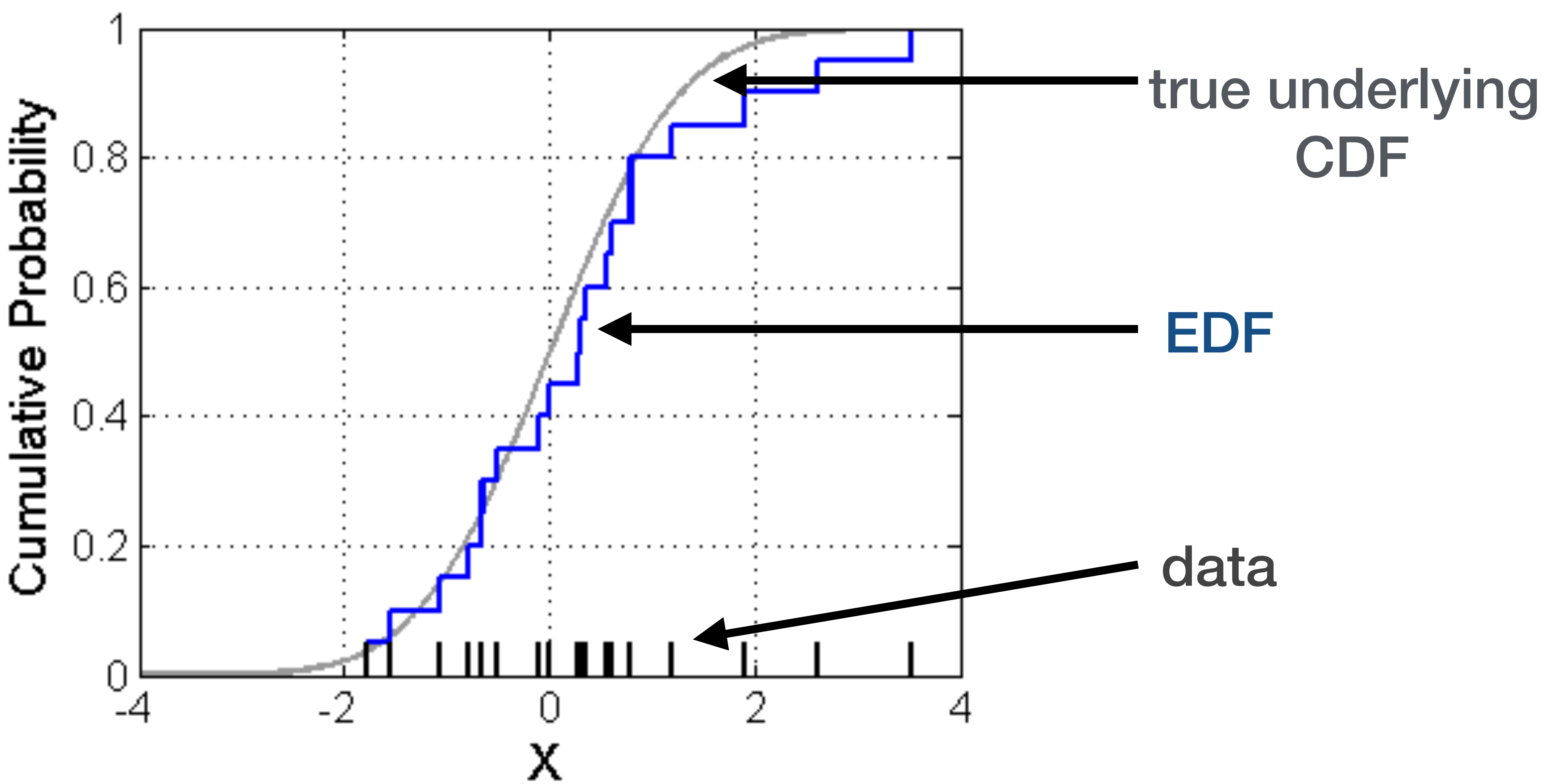
- The Cumulative Distribution Function (CDF) is related to the PDF and gives the probability that a variable (x) is less than some value x_0





Empirical Distribution Function

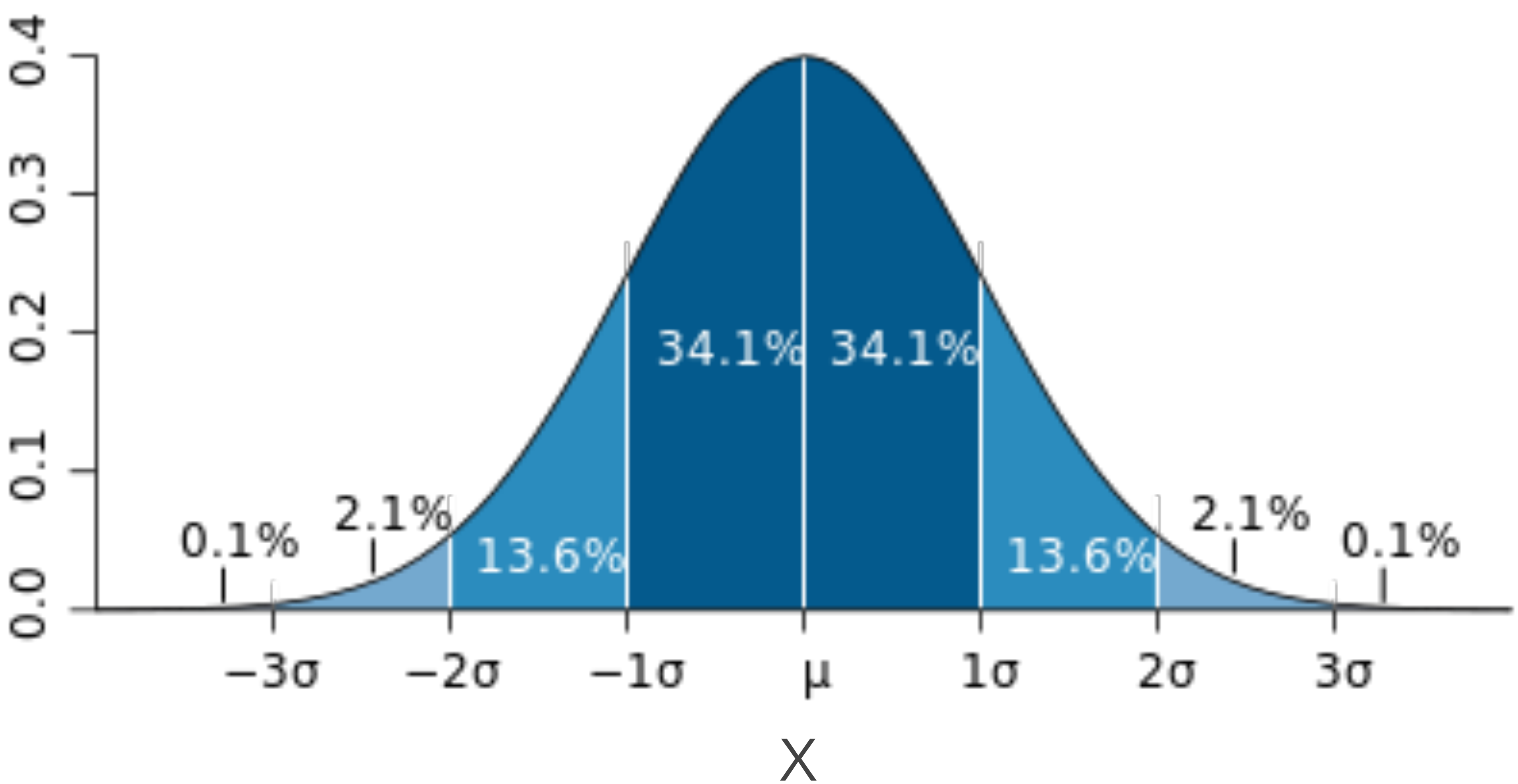
- The Empirical Distribution Function (EDF) is similar to the CDF, but constructed from data
  - Used in methods we'll cover later, e.g. the Kolmogrov-Smirnov test
  - Much less common than the CDF or PDF



Gaussian PDF

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

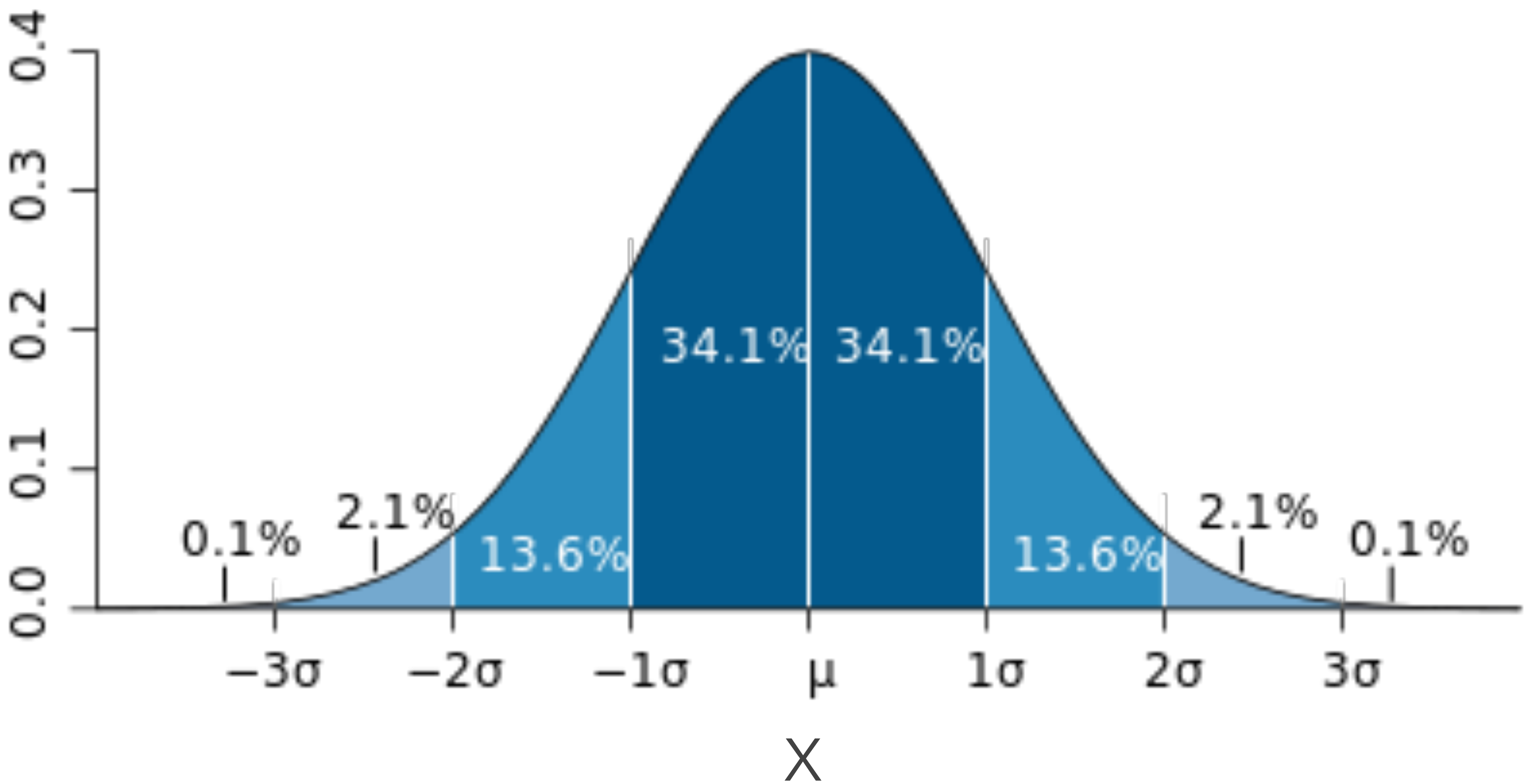
$$f(X;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(X-\mu)^2}{2\sigma^2}}$$



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 focused on theorems, math proofs, and theoretical derivations. This is an ***applied*** methods course.
- In loose terms, the CLT says that for a large number of measurements of a continuous variable X done in batches*, **the distribution of the batch mean average(s) $\bar{X}$ will be approximately gaussian**.
  - Even if the underlying PDF (or joint PDFs) of X are not themselves gaussian

*As a rule of thumb, the batch size should be ≥30

Statistical Tests

- Chi-squared test

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

- Often, the χ^2 is shown assuming N observations across some range of values (i), for example

$$\chi^2 = \sum_i \frac{(N_{i,obs} - N_{i,exp})^2}{\sigma^2_{i,exp}}$$

- If the uncertainties are only statistical, and N is large enough that $\sigma_{i,exp} = \sqrt{N_{i,exp}}$, then we get the conventional

$$\chi^2 = \sum_i \frac{(N_{i,obs} - N_{i,exp})^2}{N_{i,exp}}$$

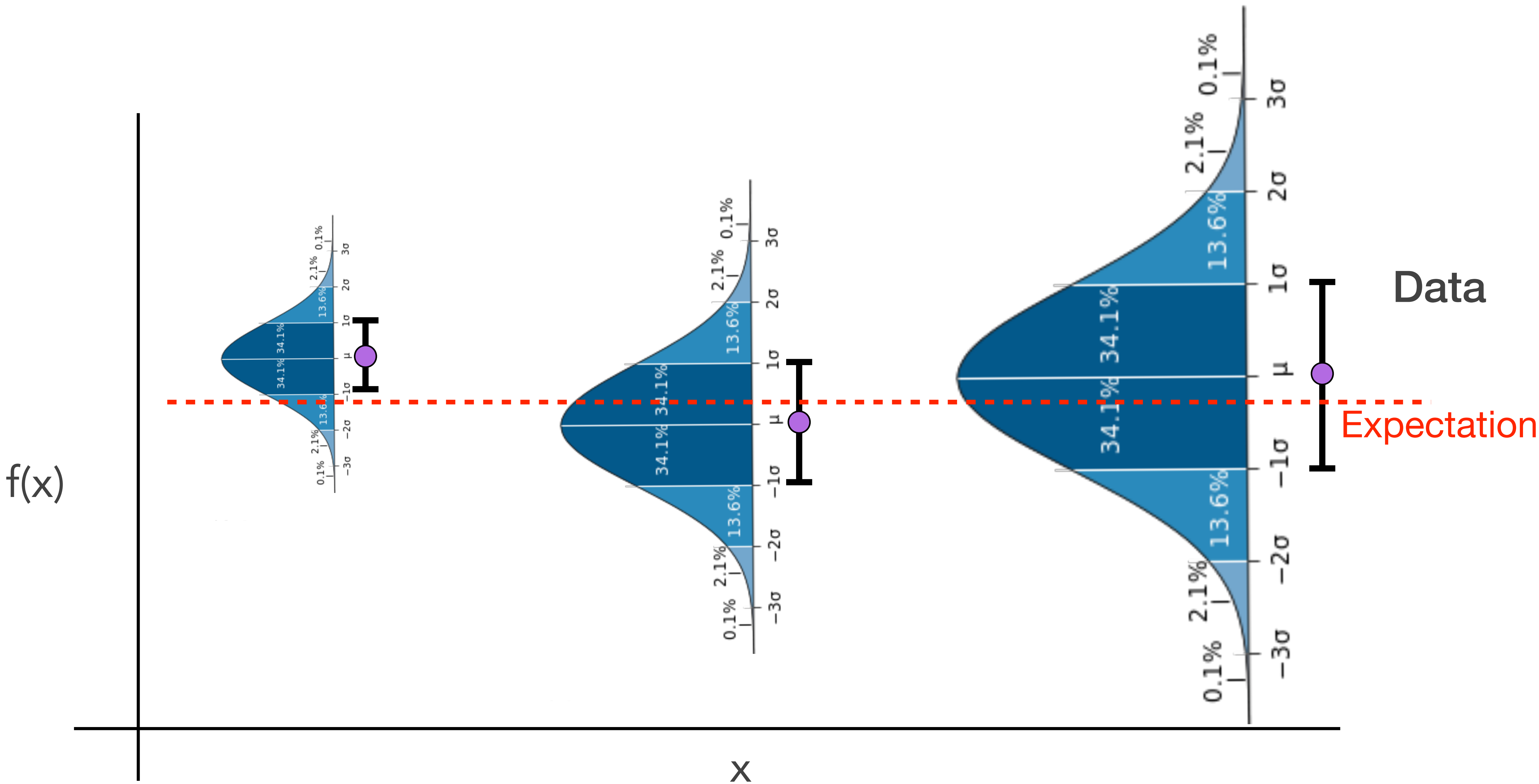
Chi-Squared

- The Chi-squared lets us know how far away our observed data is from our expectation(s)
  - The denominator is the $uncertainty^2$, so the entire χ^2 is always calculated relative to the total uncertainty
  - The total uncertainty is a combination of the statistical uncertainty **AND** any systematic uncertainty

Basic Reduced Chi-Square

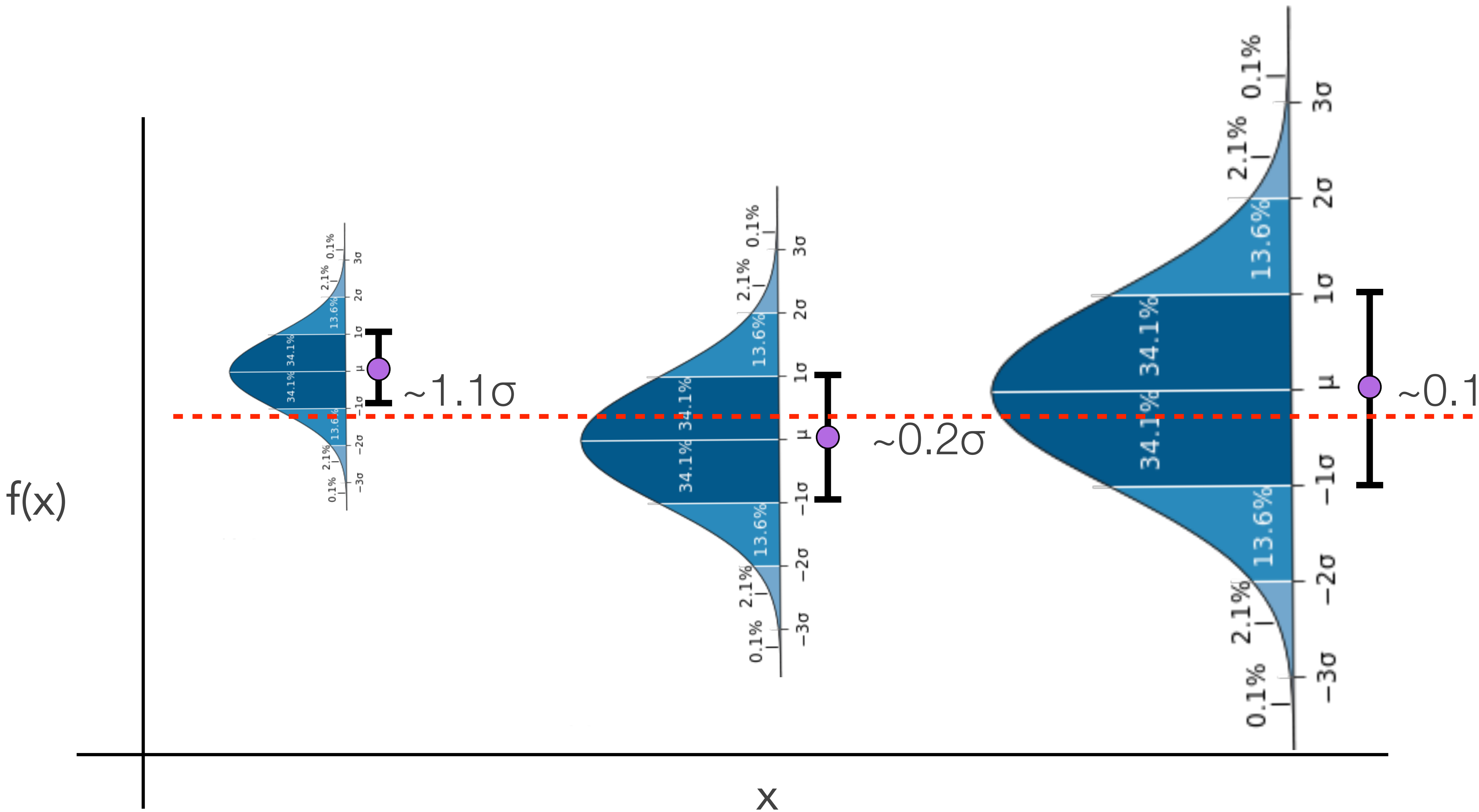
$$\chi^2_{reduced} \ll 1$$
$$\chi^2_{reduced} \approx 1$$
$$\chi^2_{reduced} \gg 1$$

$$\chi^2_{reduced} = \chi^2 / D.O.F.$$

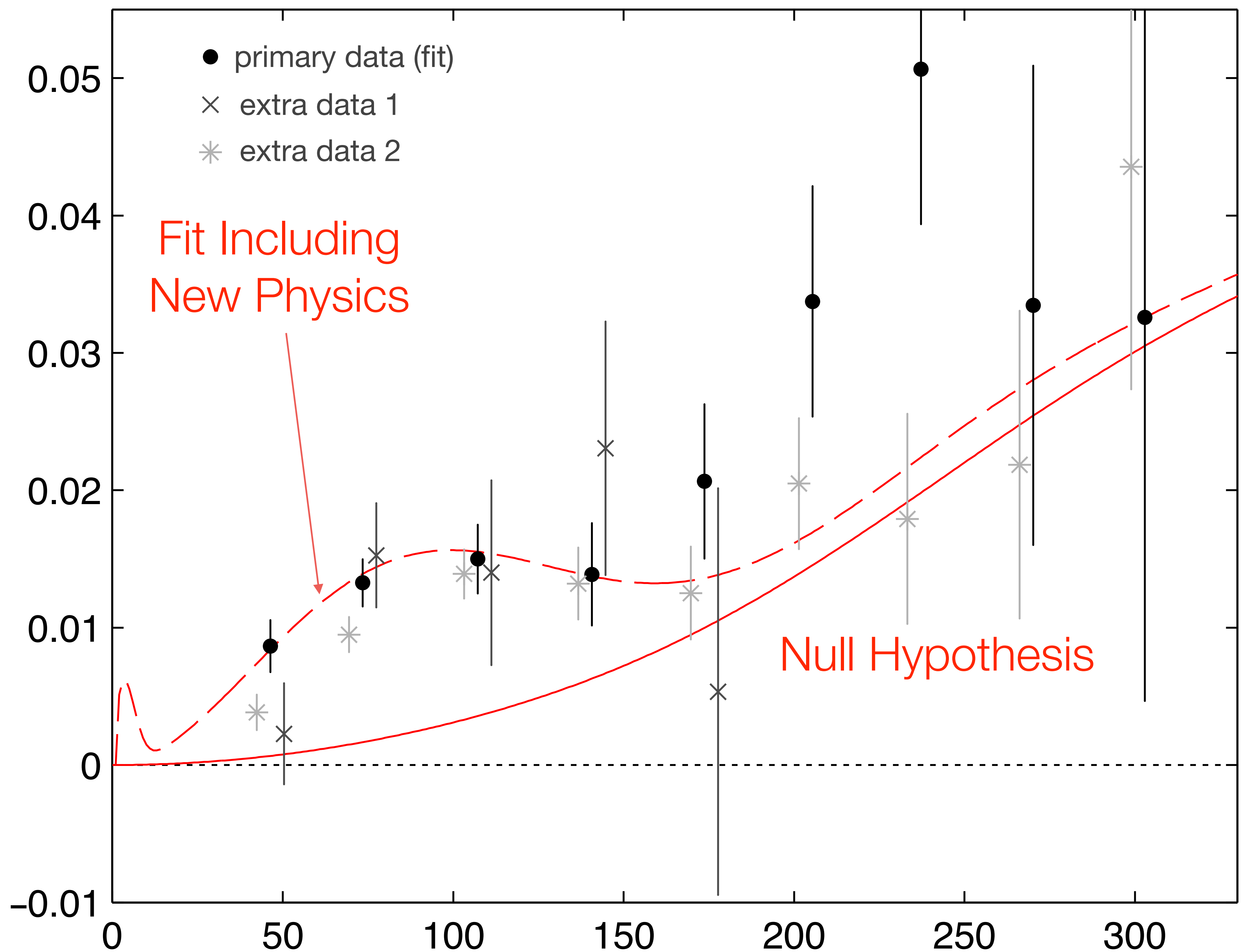


Basic Reduced Chi-Square

- Each data point has an associated approximate difference to the expectation of: 1.1σ, 0.25σ, and 0.1σ. So the total is 1.35 and with 3 data points, we get an approximate reduced chi-square of ~0.4-0.5.



Chi-By-Eye



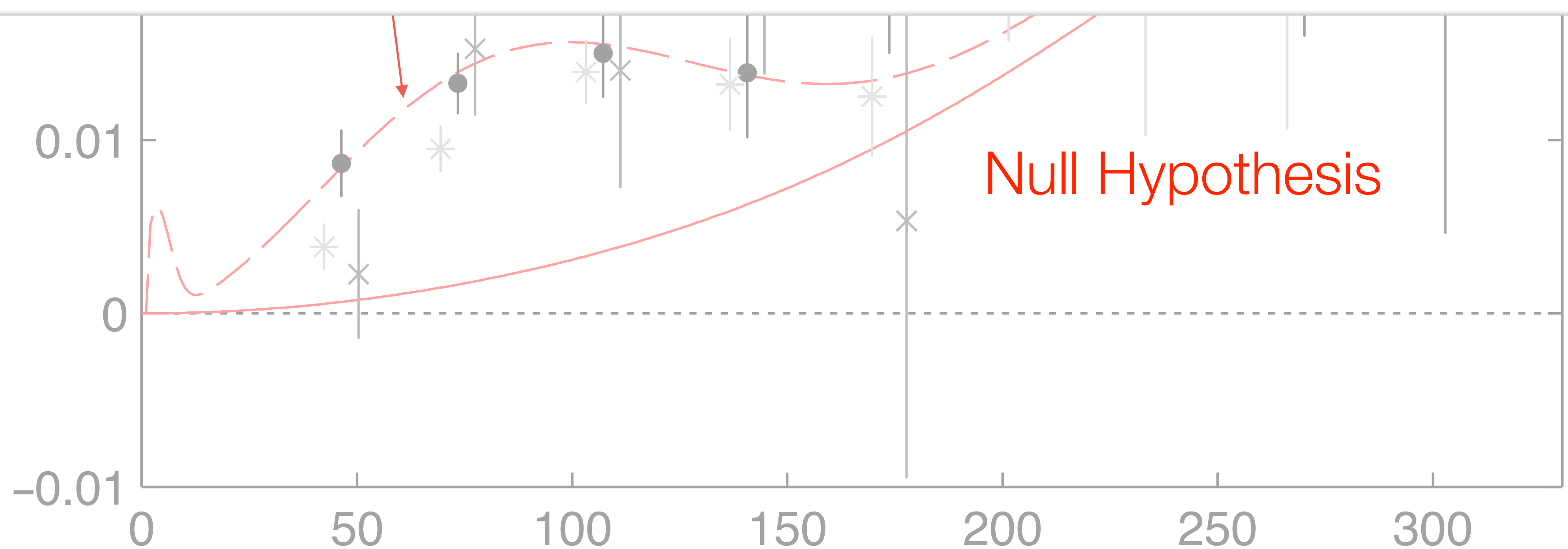
primary data (fit)
extra data 1
extra data 2
Fit Including
New Physics
Null Hypothesis
0.05
0.04
0.03
0.02
0.01
0
−0.01
0
50
100
150
200
250
300

Chi-By-Eye

doi:10.1103/PhysRevLett.112.241101

Detection of *B*-Mode Polarization at Degree Angular Scales by BICEP2

P. A. R. Ade,[1] R. W. Aikin,[2] D. Barkats,[3] S. J. Benton,[4] C. A. Bischoff,[5] J. J. Bock,[2,6] J. A. Brevik,[2] I. Buder,[5] E. Bullock,[7] C. D. Dowell,[6] L. Duband,[8] J. P. Filippini,[2] S. Fliescher,[9] S. R. Golwala,[2] M. Halpern,[10] M. Hasselfield,[10] S. R. Hildebrandt,[2,6] G. C. Hilton,[11] V. V. Hristov,[2] K. D. Irwin,[12,13,11] K. S. Karkare,[5] J. P. Kaufman,[14] B. G. Keating,[14] S. A. Kernasovskiy,[12] J. M. Kovac,[5,*] C. L. Kuo,[12,13] E. M. Leitch,[15] M. Lueker,[2] P. Mason,[2] C. B. Netterfield,[4,16] H. T. Nguyen,[6] R. O'Brient,[6] R. W. Ogburn IV,[12,13] A. Orlando,[14] C. Pryke,[9,7,†] C. D. Reintsema,[11] S. Richter,[5] R. Schwarz,[9] C. D. Sheehy,[9,15] Z. K. Staniszewski,[2,6] R. V. Sudiwala,[1] G. P. Teply,[2] J. E. Tolan,[12] A. D. Turner,[6] A. G. Vieregg,[5,15] C. L. Wong,[5] and K. W. Yoon[12,13]
(BICEP2 Collaboration)



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

Exercise 1

- Read in data from "FranksNumbers.txt"
  - Link is on the course webpage
  - 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 Rust or 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 up to 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 (Extra)

- If you have extra time or want more to do, I have also included an additional data set on the webpage "aruj.txt"
  - There should be 4 data sets
  - File format is different, so you can modify and improve your data handling skills

Exercise 1 pt.2

- Using the eq. y=x*0.48 + 3.02, calculate the Pearson's χ^2 for each of the 5 data sets in FranksNumbers.txt, assuming that the uncertainty on the 'y-value' is $\sqrt{value}$
  - Write your own method
  - Bonus: use a class or external package to get value
- Using the same equation, calculate a χ^2 where the uncertainty on each data point is ±1.22
- From the two χ^2, which uncertainty shows better agreement with the data?
  - ±1.22 or sqrt(events)?

Discussion/Comments

- What values did people get for the χ^2?

- Note: do **<u>not</u>** use a test statistic, such as the χ^2, to estimate or assign statical uncertainties or systematic uncertainties on experimental derived data

Some chi-squared Remarks

- A chi-squared distribution is based on gaussian uncertainties, so beware when errors/uncertainties are not gaussian. For example:
  - Low statistics
  - Biases in the data 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 is not a cause for concern
  - A reduced chi-squared of 1.2 w/ 1000 DoF is very, very bad and incredibly unlikely

Conclusion

- Know your distribution functions (probability, cumulative, and empirical)
- Central Limit Theorem says that means of most variables will produce a gaussian distribution of the mean value for a large numbers of measurements
- Chi-square(d) calculation is a frequent metric for goodness-of-fit and quantitative data/hypothesis matching
- Very 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 should be available now in Absalon
- Read "Not Normal: the uncertainties of scientific measurements", there will be a discussion this Thursday afternoon

Extra

Distribution Functions

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