

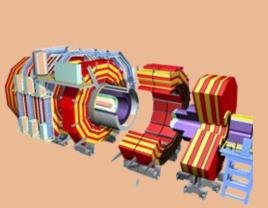
Data analysis and Statistics at the LHC

Dr. Nicholas Wardle



VSOP Quy Nhon, Vietnam 15-26 July 2024



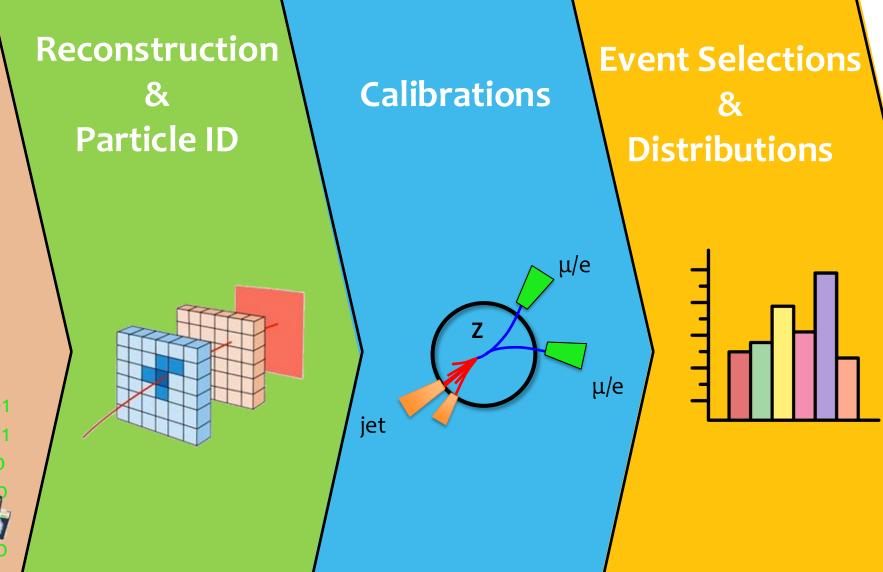


Data

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Nicholas Wardle

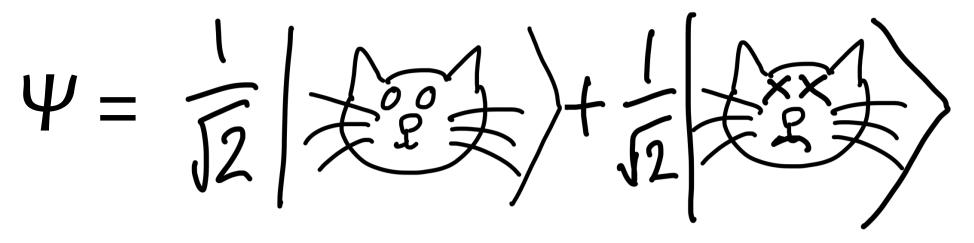


RESULTS

Statistical Analysis at the LHC

In particle physics,

- 1. Physical laws (and the observations we make) are **probabilistic in nature** due to quantum mechanics
- 2. The way we perform experiments (e.g collider experiments) means that *events are statistically independent*

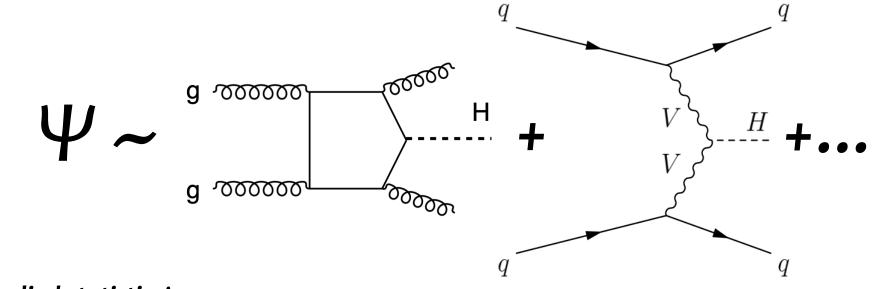


 \rightarrow ideal scenario for applied statistics!

Statistical Analysis at the LHC

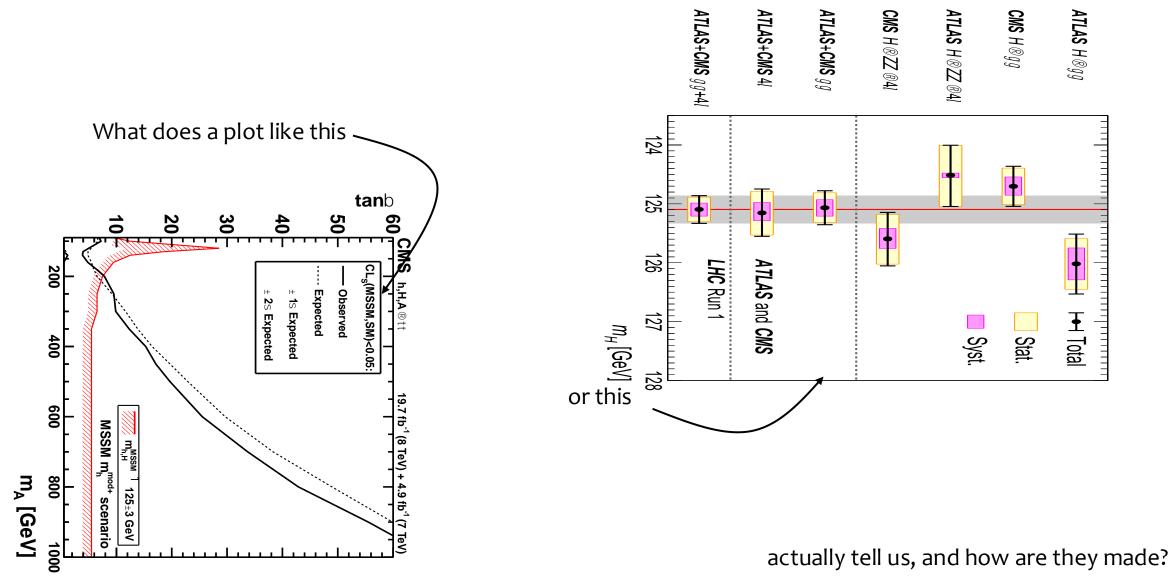
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Statistical Analysis at the LHC



Probability

We all have an intuitive sense of what *probability* means. The mathematics developed in 1933 by Kolmogorov treats probability as something which satisfies three axioms, and therefore no specific definition is given. The Kolmogorov axioms are,

•
$$P(X_i) \ge 0$$
 for all i

•
$$P(X_i \text{ or } X_j) = P(X_i) + P(X_j)$$
 if X_i and X_j are exclusive

• $\sum_{\Omega} P(X_i) = 1$,

Where $P(X_i)$ are **probabilities** that events/outcomes X_i occur and Ω is the set of all possible outcomes \rightarrow E.G. when rolling an unbiased 6-sided die, $\Omega = \{1, 2, 3, 4, 5, 6\}$

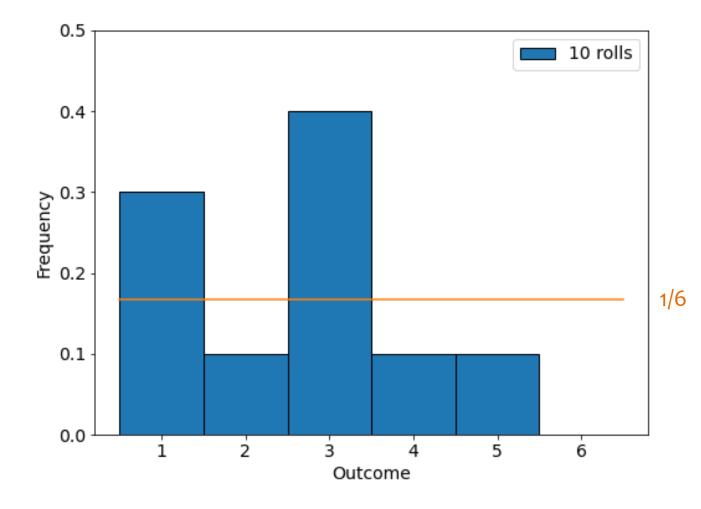
Frequentist probability

Frequentist (or classical) probability is the definition that you are most likely familiar with.

As the name suggests, this definition of probability is related to the frequency with which an event (say the roll of a die) occurs in **repeated trials**.

The number of times *n* that an event *X* occurs in *N* trials yields the probability as *N* gets large

$$P(X) = \lim_{N \to \infty} \frac{n}{N}.$$



Bayesian Probability

Bayesians think differently about the interpretation of probability.

If I asked you what you think the probability it will rain tomorrow is, answering that you'd need to repeat "tomorrow" to give me a frequency is not very helpful!

Bayesians avoid this by interpreting probability in terms of a *degree of belief* something will occur.



In these lectures, I'll avoid discussing Bayes' vs Frequentist interpretation of probability too much \rightarrow usually for particle physicists we **choose the one which is most useful** for a given analysis

Bayes Rule

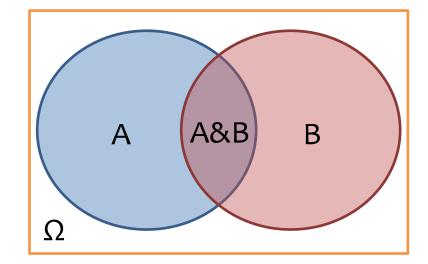
The probability that two events **A** and **B** occur is given by

$$P(A \text{ and } B) = P(A|B)P(B) = P(B|A)P(A)$$

Probability that A occurs / given that B has occurred

Rearranging gives us Bayes' rule!

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

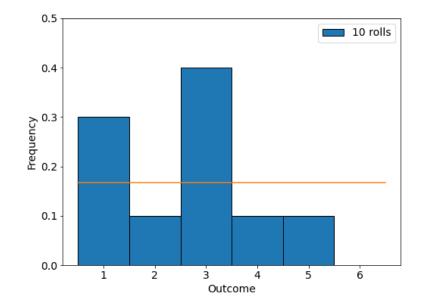


Probability Distributions

For a sequence of events X1, X2, X3..., we will often use vector notation **X**. Note however that **X** can also refer to a repeated set of experiments and each experiment will have a single observation

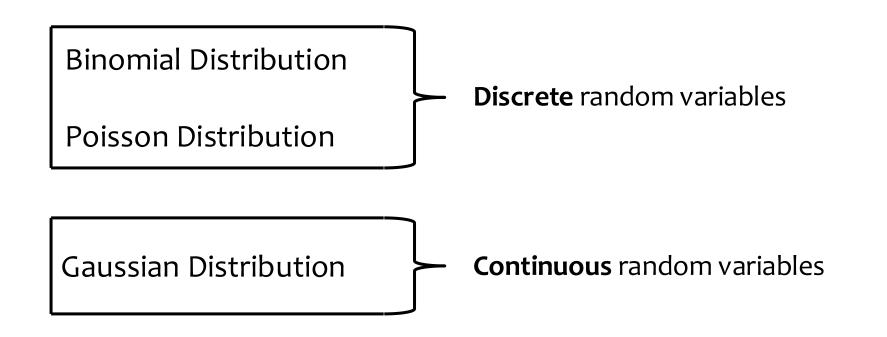
The corresponding probabilities $P(X)\Omega$ over all possible values of $X \in \Omega$ form a probability distribution. As an example, if X is the outcome of a single die roll, then $\Omega = \{X = 1, X = 2, X = 3, X = 4, X = 5\}$ and P(X) = 1/6 for every possible value of X, meaning the **probability distribution is uniform**.

A single event (roll) can be then thought of a random draw from such a probability distribution, and successive rolls of the die will yield a distribution of values whose frequency converges to a uniform distribution (U). We will write this as $X \sim U(1, 6)$



Most important Probability distributions

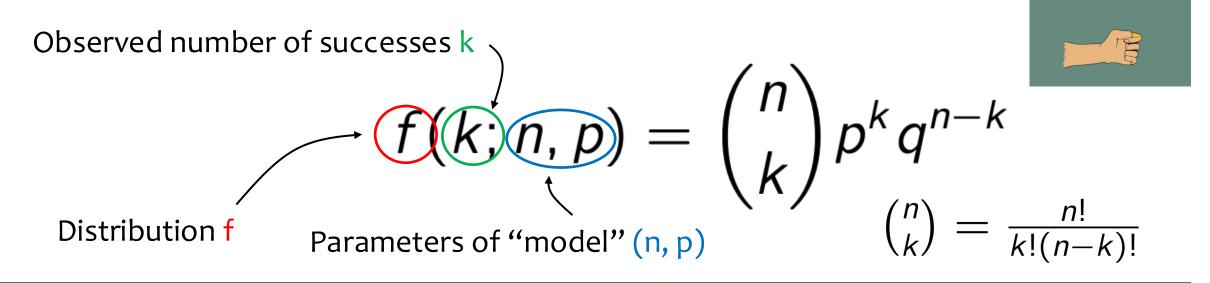
We'll take a look at a few common probability distributions (they're common at least to me but let me know if any of them sound completely off-topic)



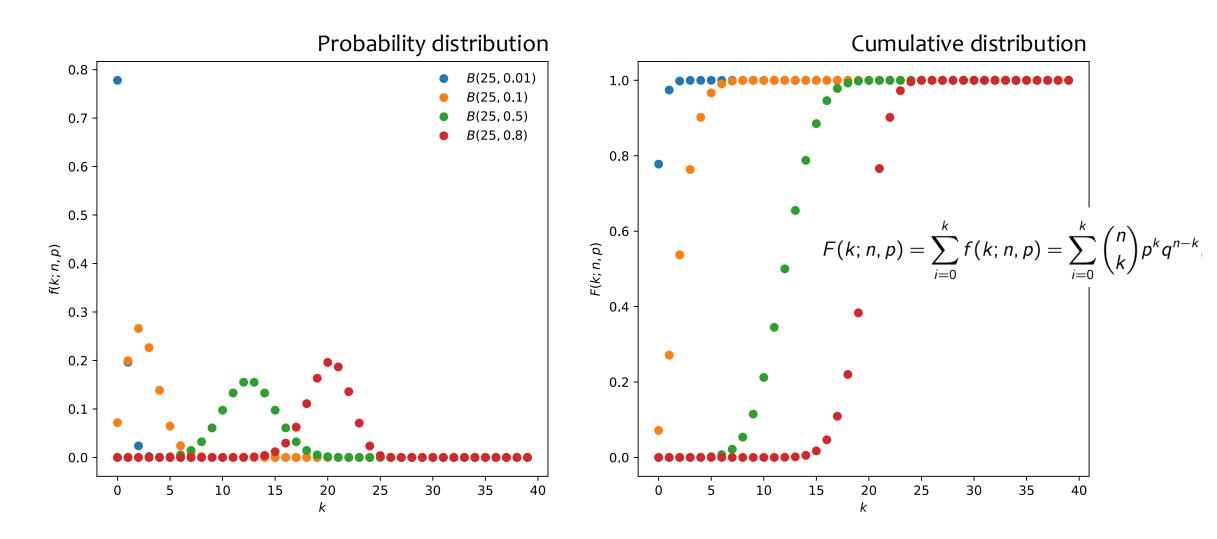
Binomial Distribution

The binomial distribution describes the distribution of the number of successes (k) in a sequence of **n** independent trials, where the probability of success in any trial is **p**.

More generally, any sequence of experiments, each of which results in a yes/no, 1/0 or other binary result with probabilities p and q = (1 - p) assigned to each outcome will be described by the binomial distribution,



Binomial Distribution

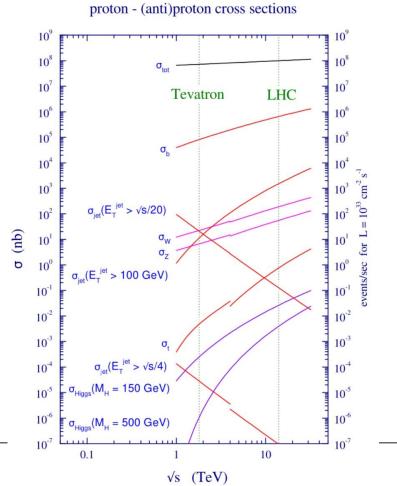


Poisson Distribution

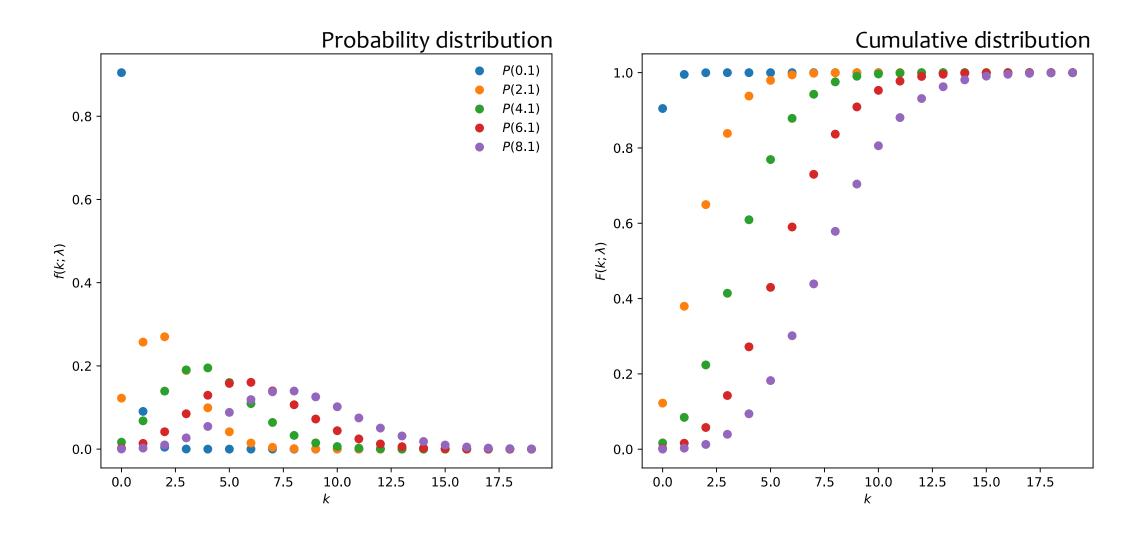
The Poisson distribution is a limit case of the binomial distribution where $n \rightarrow \infty$, and $p \rightarrow 0$ such that the product $\lambda = np$ is constant.

In particle physics, this is a very common distribution since it models processes that are rare $(p \rightarrow 0)$ in data sets that are very large $(n \rightarrow \infty)$.

$$f(k; n, p) \rightarrow f(k; \lambda) = \frac{\lambda^{k}}{k!} e^{-\lambda}$$



Poisson Distribution



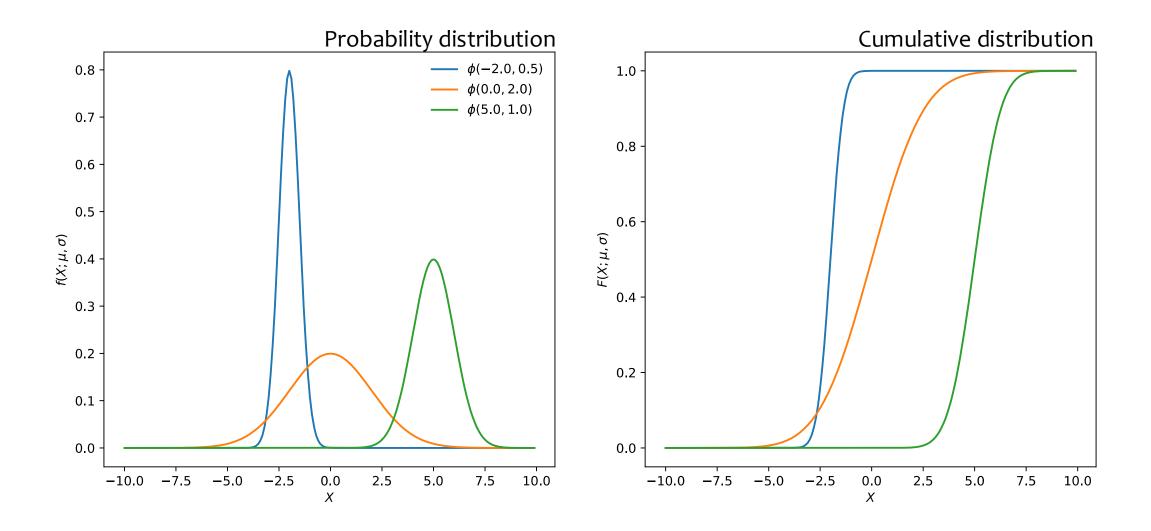
Gaussian Distribution

The Gaussian (or Normal) distribution is the most common probability distribution used in statistics. There is a good reason for this but for now, just to refresh our memories about the Gaussian distribution.

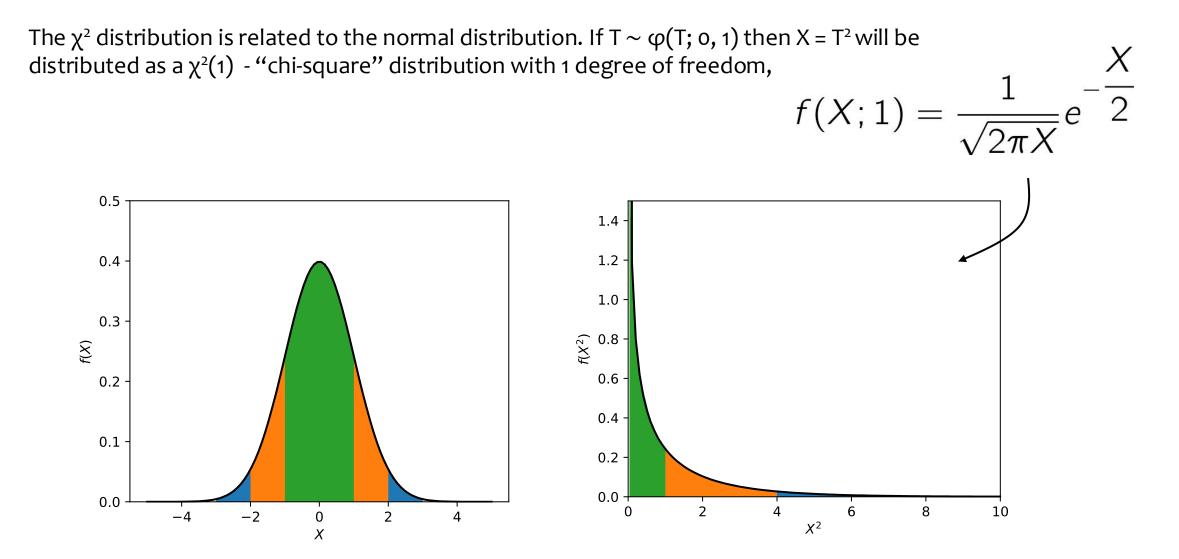
If a continuous random variable X is distributed as a Normal distribution then,

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

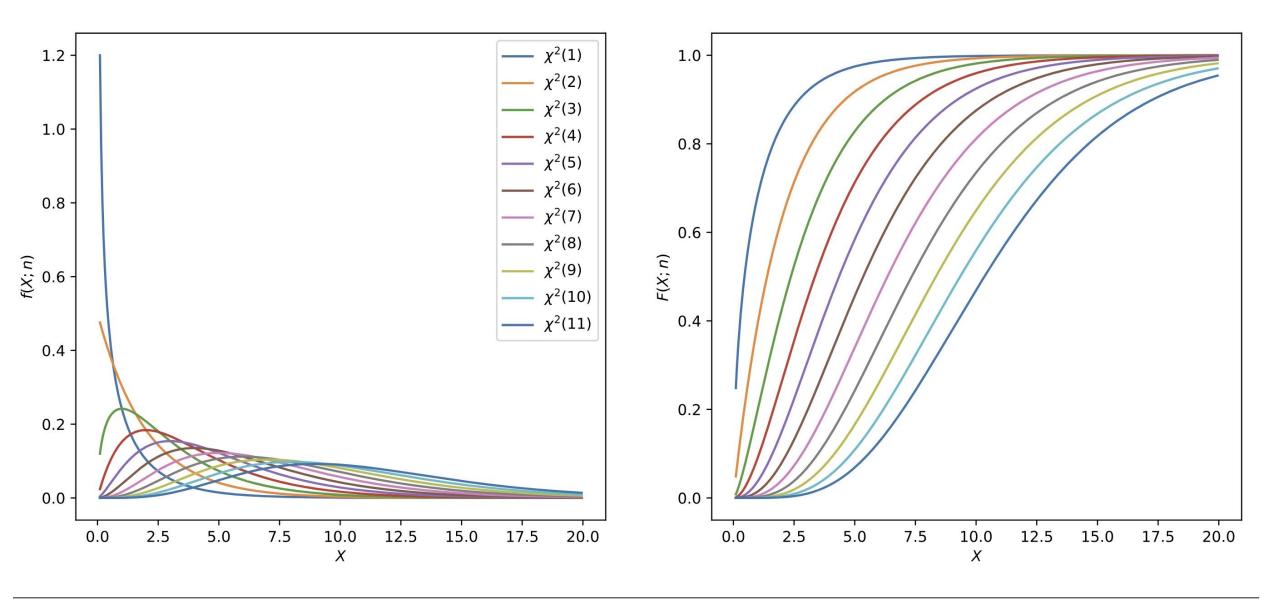
Gaussian Distribution



χ^2 distribution



χ^2 distribution



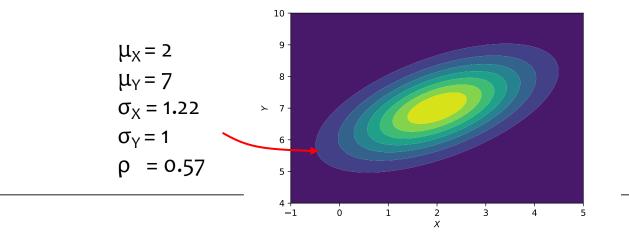
Multi-variate distributions

The multivariate Gaussian probability density can be written as,

$$f(\boldsymbol{X};\boldsymbol{\mu},\boldsymbol{V}) = \frac{1}{\sqrt{(2\pi)^N \det(\boldsymbol{V})}} e^{-\frac{1}{2}(\boldsymbol{X}-\boldsymbol{\mu})^T(\boldsymbol{V}^{-1})(\boldsymbol{X}-\boldsymbol{\mu})}$$

Where $\mathbf{X} = (X_1, X_2, X_3, ..., X_N)$ is a vector of random variables (not to be confused with a sequence of random outcomes of X), and V is a N × N symmetric matrix of co-variances $V_{ij} = \text{covariance}(X_i, X_j)$.

In the special case where
$$f(X,Y;\mu_X,\mu_Y,\sigma_X,\sigma_Y,\rho) = \frac{1}{2\pi\sigma_X\sigma_Y\sqrt{1-\rho^2}} \exp\left(-\frac{1}{2(1-\rho^2)}\left[\left(\frac{X-\mu_X}{\sigma_X}\right)^2 + \left(\frac{Y-\mu_Y}{\sigma_Y}\right)^2 - 2\rho\left(\frac{X-\mu_X}{\sigma_X}\right)\left(\frac{Y-\mu_Y}{\sigma_Y}\right)\right]\right)$$



Multivariate distributions quickly become complicated and difficult to estimate (more about this later)

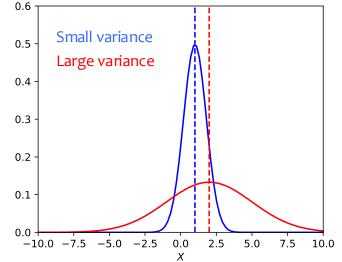
Moments

Probability density distributions can be used to obtain useful information about a particular random variable, or functions of random variables. For example, the mean value of a random variable X (or its *expectation value* under f (X)) is given by,

$$E[X] = \int_{\Omega} Xf(X)dX_{A}$$

Similarly, any function of X, g(X) has an expectation value E[g] under f (X) of

$$E[g] = \int_{\Omega} g(X)f(X)dX$$



The expectation is a linear operator $\longrightarrow E[a \cdot g(X) + b \cdot h(Y)] = a \cdot E[g(X)] + b \cdot E[h(Y)]$

The expectation value (mean) is often referred to as the first moment of the distribution of X, but of course we can define higher moments too. For example, the expectation of the function $g(X) = (X - E[X])^2$ is called the *variance** of X under f (X),

$$V(X) = E[(X - E[X])^{2}] = \int_{\Omega} (X - E[X])^{2} f(X) dX$$

With the properties V(X + a) = V(X) and $V(aX) = a^2V(X)$ for a constant value *a*

Nicholas Wardle

Moments

Moments of probability distributions are **not the same** as sample moments. For a finite sample of a random variable, it is always possible to determine sample moments (unlike in the case of some probability densities) \rightarrow they are a property of the specific data set.

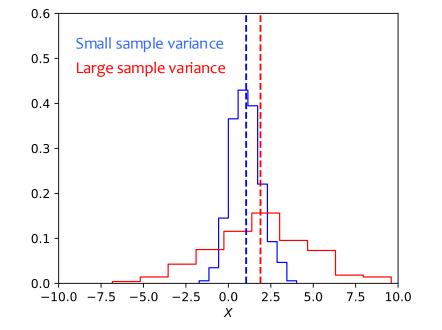
For a sequence of a random variable ($X_1, X_2, ..., X_N$) of size N, we can define the n-th sample moment as,

You'll be familiar with the 1st such moment, which is the sample mean,

$$m_1 = \bar{X} = \frac{1}{n} \sum_{i}^{N} X_i,$$

and the second central moment, which is the sample variance,

$$\bar{V} = \frac{1}{n} \sum_{i}^{N} (X_i - \bar{X})^2.$$

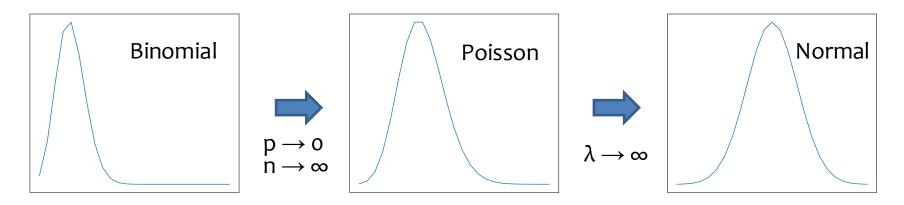


Moments

Probability distribution	$E[\cdot]$	$Var[\cdot]$
$f(k; n, p) = \binom{n}{k} p^k q^{n-k}$	np	np(1-p)
$f(k;\lambda) = \frac{\lambda^k}{k!} e^{-\lambda}$	k	\sqrt{k}
$f(X;\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{X-\mu}{\sigma}\right)^2}$	μ	σ

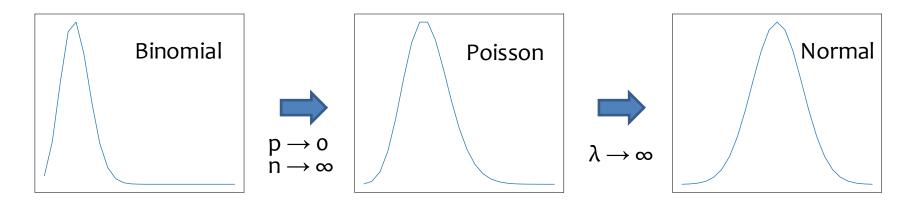
In certain limiting cases, distributions of random variables can be well approximated by other (often more convenient) distributions.

E.G ...



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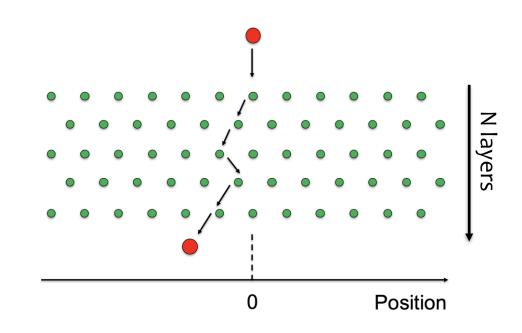
E.G ...



Theorem: Suppose we have a sequence of independent random variables X_i , each from a distribution with mean μ_1^i and variance ν_2^i . Define,

$$T_N = \frac{\bar{X}N - \sum_{i=1}^N \mu_1^i}{\sqrt{\sum_{i=1}^N \nu_2^i}}.$$

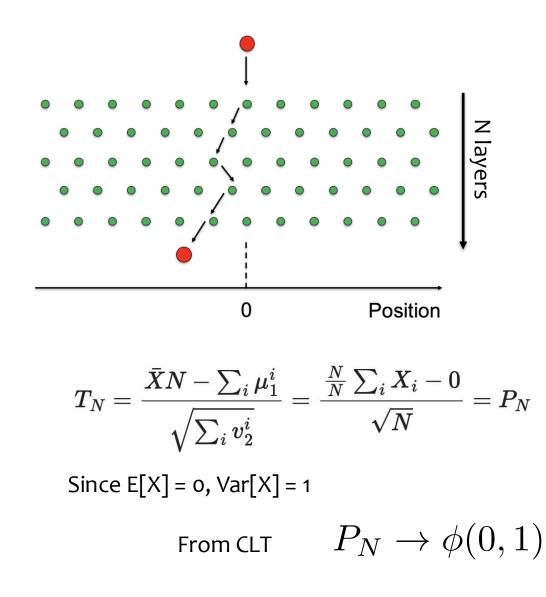
Then for T = $\lim_{N\to\infty} T_N$, we have that T ~ $\phi(T;0,1) \rightarrow T_N$ converges in distribution to a standard normal distribution



Example: a Galton board with N layers

The change in position after each layer X_i can be thought of as a uniform random variable $X_i \in [-1, 1]$

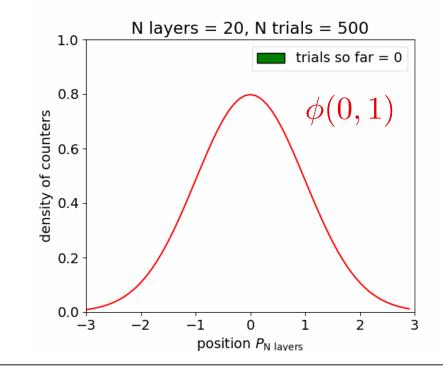
Define:
$$P_N = rac{1}{\sqrt{N}}\sum_i X_i.$$



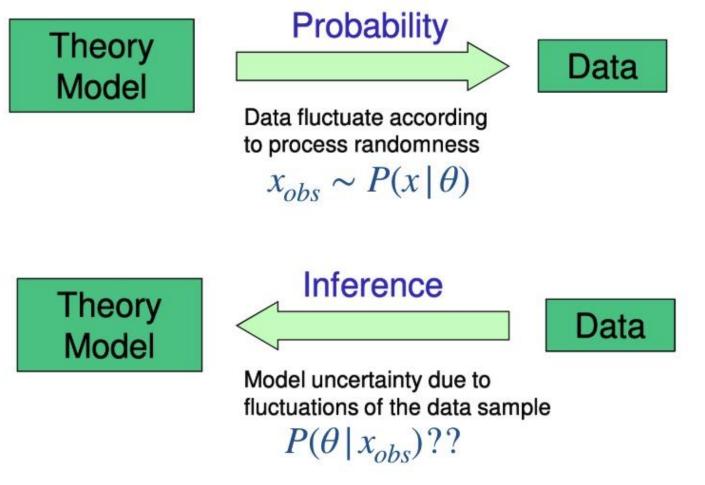
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Statistical Inference



N. Smith

Estimators

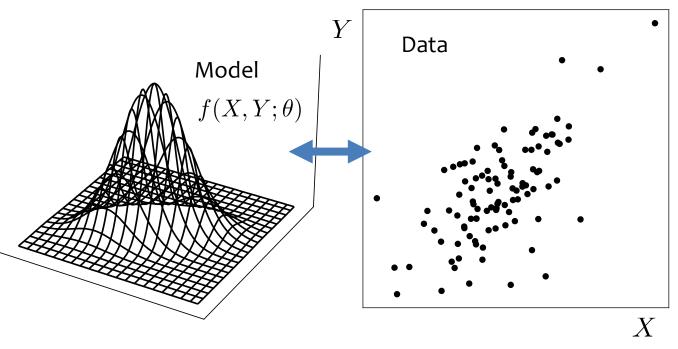
So far, we only talked about probability distributions \rightarrow Where does the data come in?

Typically, we want to learn something about our model using the data \rightarrow estimators is the first thing we can use the data for

An estimator $\hat{\theta}$ for a quantity $\hat{\theta}$ is a function of the observed data.

- θ usually a parameter of a **model**
- θ is a property of a specific set of observations → its value depends on the data observed and it is itself a random variable

There are many different estimators, but we will focus on the most common one used at the LHC → the maximum likelihood estimator



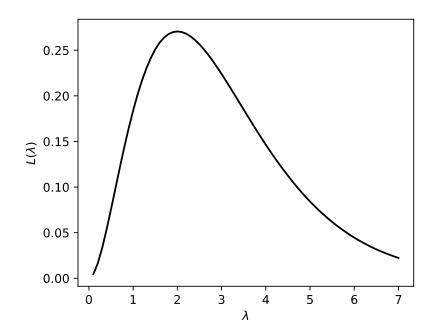
Likelihoods

The likelihood is a function of the model parameters $\boldsymbol{\theta}$ at a fixed value for the data \mathbf{X}

The likelihood function is proportional to the probability density P

 $L(\theta) \propto P(X|\theta).$

Example: For the Poisson distribution, let's suppose we observe the number of events k=2



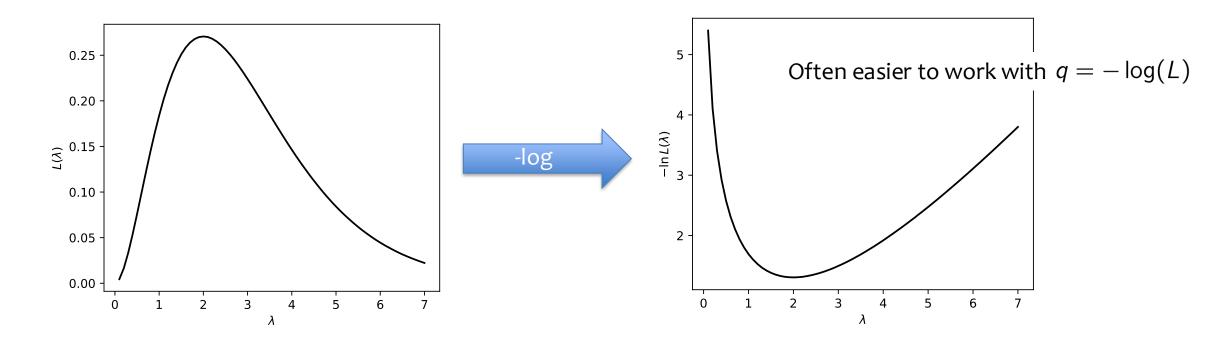
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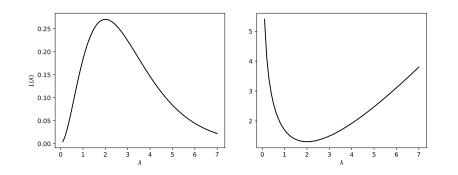


Maximum likelihood estimator

Maximum likelihood estimators (MLE) are given by the values of θ for which

 $rac{\partial q}{\partial heta}|_{ heta = \hat{ heta}} = 0$

Maximum likelihood $\leftarrow \rightarrow$ Minimum –ve log likelihood



Example: For the Poisson distribution

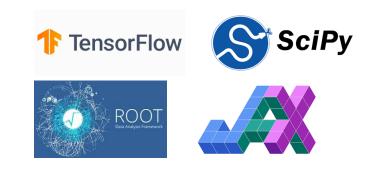
$$q = \lambda - k \ln \lambda - \ln(k!)$$
$$\frac{dq}{d\lambda} = 1 - \frac{k}{\lambda} \implies \hat{\lambda} = k$$

Numerical minimization (Gradient Descent)

We use many different computational tools for finding the MLE. Many of these different tools use a common algorithm \rightarrow gradient descent

 $\frac{\partial q}{\partial \theta_1}$ $abla (q)|_{oldsymbol{ heta}_{init}} = egin{bmatrix} rac{\partial q}{\partial heta_2} \ dots \ rac{\partial q}{\partial heta_2} \ dots \ rac{\partial q}{\partial heta_2} \end{pmatrix}$ 50 $rac{\partial q}{\partial heta_n}$ 40 $\theta = \theta_{init}$ 30 20 10 0 3.0 2.5 1.0 2.0 07 1.5 2.0 *O*1 1.5 2.5 3.0

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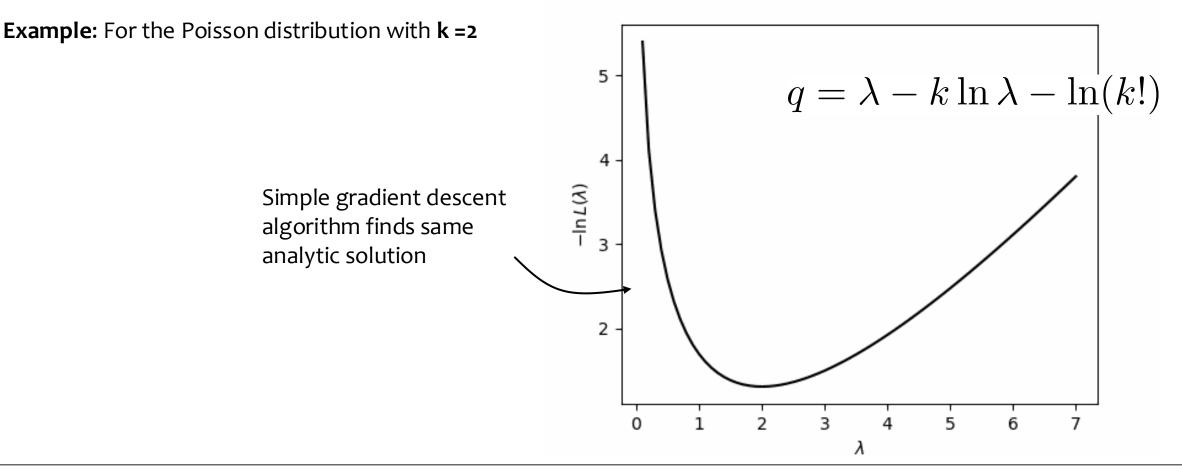
Iterative process

$$oldsymbol{ heta}_k = oldsymbol{ heta}_{init} - oldsymbol{k} imes oldsymbol{h}
onumber \
on$$

Stop when $|\nabla(q)|_{\theta} = \sqrt{\left(\frac{\partial q}{\partial \theta_1}\right)^2 + \left(\frac{\partial q}{\partial \theta_2}\right)^2 + \ldots + \left(\frac{\partial q}{\partial \theta_n}\right)^2} < \epsilon$

Numerical minimization (Gradient Descent)

We typically use numerical minimization algorithms since often calculating these analytically is not possible \rightarrow there's lots of these tools available for you to use in common HEP software



Properties of MLE

MLEs have **very nice properties**, which is why they are common in LHC analyses

1. Maximum likelihood estimators are invariant under **bijective transformations of variables**

$$f_Y(Y)dY = f_X(X)dX \implies f_Y(Y) = \frac{f_X(X)}{|g'(X)|}$$

Since the likelihood is equal to the probability density for a random variable, the maximum of it (or minimum of its log) will not change when multiplying (adding) by a **constant**!

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2. Relationships between parameter estimates are **preserved**

Suppose $\hat{\theta}$ is the maximum likelihood estimate for θ and $\alpha = g(\theta)$ is some function of θ , then the maximum likelihood estimator of α will be, $\hat{\alpha} = g(\hat{\theta})$.

This is obvious since

$$0 = \frac{\partial L}{\partial \theta}|_{\theta = \hat{\theta}} = \frac{\partial L}{\partial \alpha} \frac{dg}{d\theta}|_{\alpha = \hat{\alpha}} = \frac{\partial L}{\partial \alpha} g'(\alpha)|_{\alpha = \hat{\alpha}} \implies \frac{\partial L}{\partial \alpha}|_{\alpha = \hat{\alpha}} = 0$$

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3. MLEs are **consistent estimators** i.e the value of the **estimator converges to the true value** as more data are included $(n \rightarrow \infty)$

$$P(|\hat{\theta}_n - \theta| > \epsilon) \to 0$$
 for any $\epsilon > 0$

Variance of the Poisson estimator

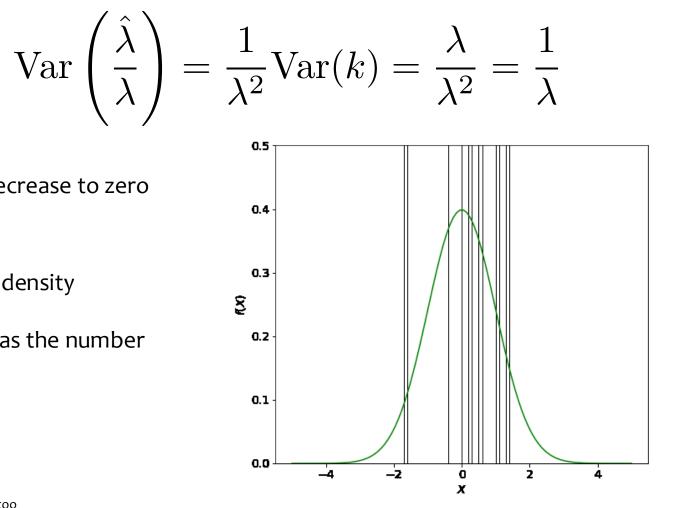
From the 3rd property, we know that the variance of the MLE* converges to zero as $k \rightarrow \infty$

Example, Poisson random variable

Which means for larger samples, this will decrease to zero

A **histogram** is an estimate of a probability density

The density in each bin is better estimated as the number of observations in each bin gets large!



* Generally, the law of large numbers tells us this is true for other estimators too

(Co)variance of Gaussian estimators

If we had a random variable that was distributed as a Gaussian with $\theta \sim \varphi(\theta, \sigma)$, we would find that the twice the negative log-likelihood would be,

$$2\left(q(\theta) - q(\hat{\theta})\right) = -2\left(\ln(\phi(\theta, \sigma)) - \ln(\phi(\hat{\theta}, \sigma))\right) = -2\left(-\frac{1}{2}\left(\frac{\theta - \hat{\theta}}{\sigma}\right)^2 + \frac{1}{2}\left(\frac{\hat{\theta} - \hat{\theta}}{\sigma}\right)^2\right) = \left(\frac{\theta - \hat{\theta}}{\sigma}\right)^2$$

But if instead we Taylor expand

$$2\left(q(\theta) - q(\hat{\theta})\right) = 2\left(q'/\hat{\theta}) \cdot (\theta - \hat{\theta}) + \frac{1}{2}q''(\hat{\theta})(\theta - \hat{\theta})^2\right)$$

-0

We must have

 $\frac{1}{\sigma^2} = q''(\hat{\theta})$

So the variance can be estimated from the second derivative of q!

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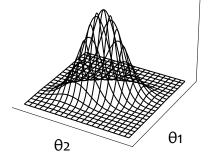
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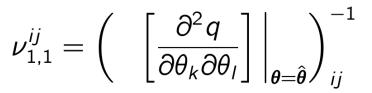
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We must have $\ \ \frac{1}{\sigma^2} = q^{\prime\prime}(\hat{ heta})$

So the variance can be estimated from the second derivative of q!



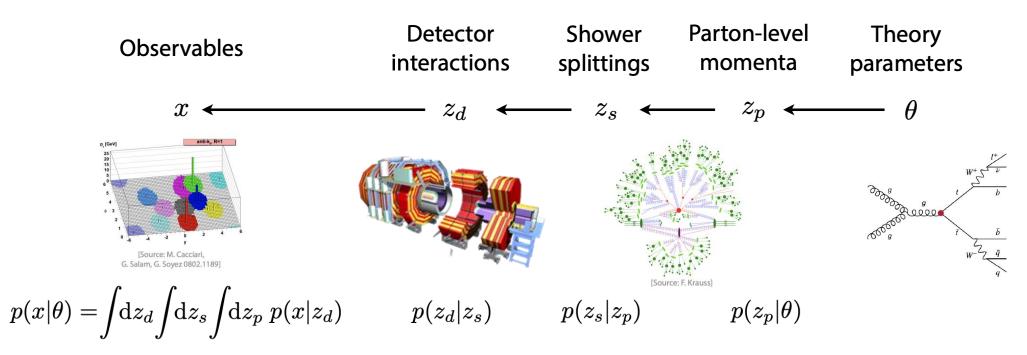
More generally



Combined likelihoods

Our data at the LHC is much richer than a single Poisson random variable

(Example from K. Cranmer)



Evaluating this integral is essentially impossible \rightarrow reduce the dataset x \rightarrow x' and use simulation to estimate p(x'| θ)

Combined likelihoods

For N independent observations $X = \{X_1, X_2, ..., X_N\}$, the likelihood function is,

$$L(\theta) := \prod_{i=1}^{N} f_i(X_i; \theta),$$

where f_i are the p.d.f for each observation X_i

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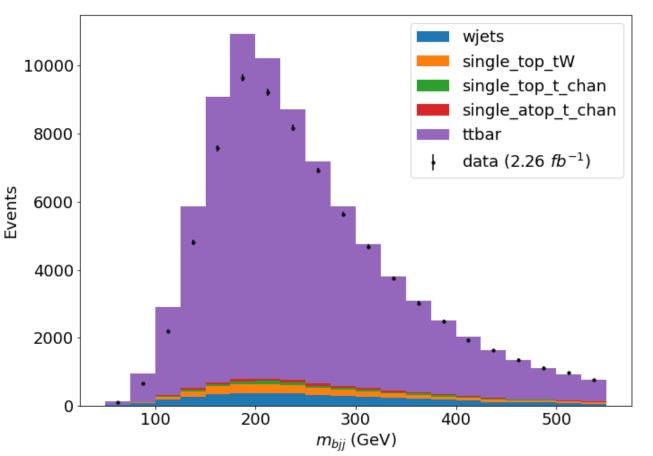
A histogram can be treated as a set of N independent Poisson random variables where N = number of bins!

$$f_i(k_i;\lambda_i) = \frac{\lambda_i^{k_i}}{k_i!} e^{-\lambda_i}$$

At the LHC, we split the contributions into **signal (S)** and **backgrounds (B)**

$$\lambda_i = rS_i + B_i$$

And L \rightarrow L(r) is a function of the **signal strength**

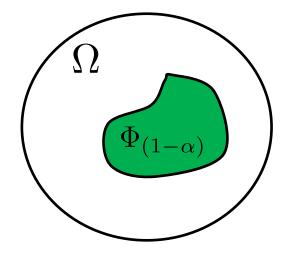


An estimator is only part of making a measurement at the LHC \rightarrow we also report **uncertainties.** In **frequentist statistics**, we use the concept of a <u>confidence interval</u>

A confidence interval (or region) is a set of parameter values $\theta \in \Phi_{(1-\alpha)}$ at a specified confidence level 100 x (1- α)

The confidence region at a confidence level 100 x (1- α) is a region which is constructed such that the true values of the true parameters θ_0 is contained in the region with a probability (1- α)

Example: a 68% confidence interval in θ will contain the true value θ_0 in 68% of the outcomes in data



The **Neyman construction** of frequentist intervals is an elegant way to achieve intervals with exactly that property

We use the ratio of likelihoods

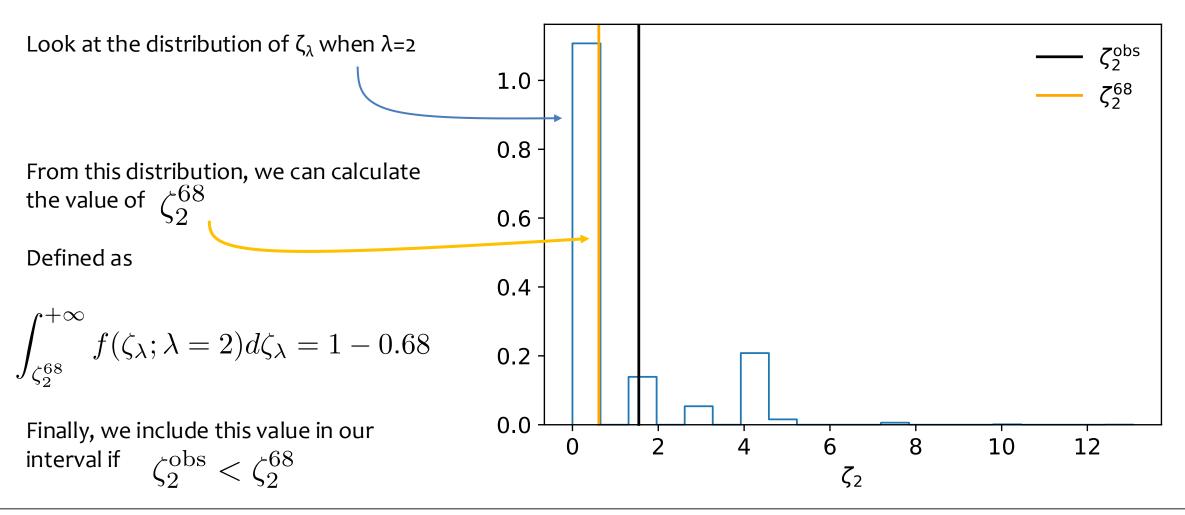
$$f_{\theta} = -2 \ln \frac{L(\theta)}{L(\hat{\theta})} = q(\theta) - q(\hat{\theta})$$

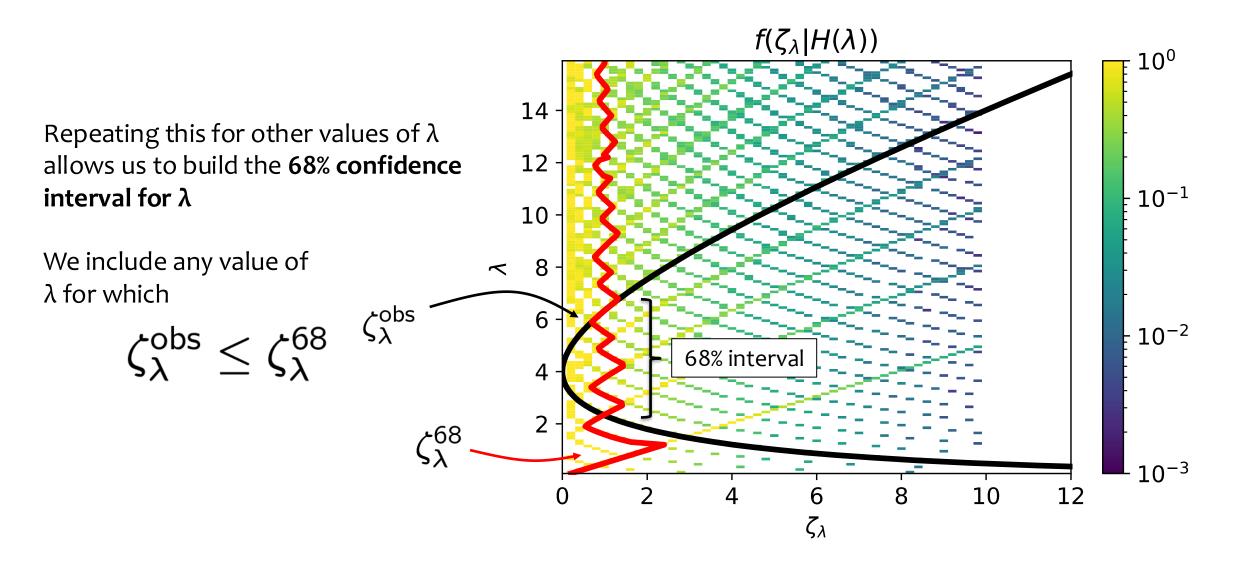
Note the extra factor of 2 now

Let's look at what this looks like for our Poisson random variable where n = 4

Remember the MLE for λ is given by $\frac{dq}{d\lambda}|_{\lambda=\hat{\lambda}} = 0 \implies \hat{\lambda} = n$

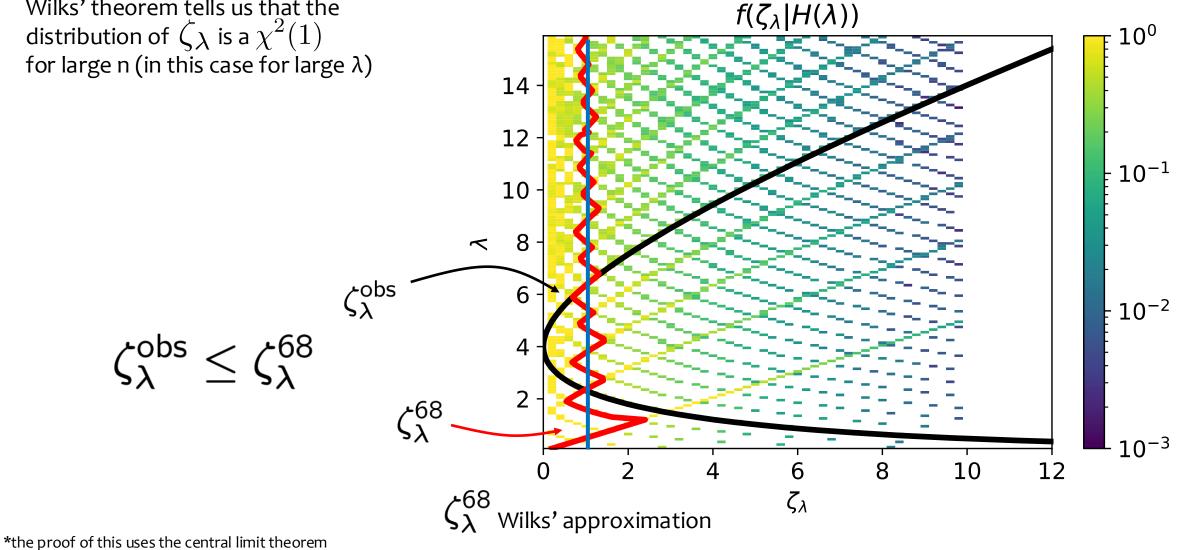
 $\zeta_{\lambda} = q(\lambda) - q(\hat{\lambda}) = -2\left(\ln(\lambda) - \lambda\right) + 2\left(\ln(n) + n\right)$





Wilks' theorem

Wilks' theorem tells us that the distribution of ζ_{λ} is a $\chi^2(1)$ for large n (in this case for large λ)

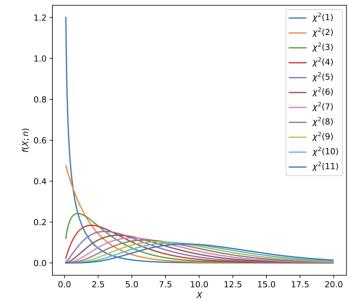


Wilks' theorem

In general, Wilks' theorem gives us the result for any number of degrees of freedom.

The result is that for a log-likelihood difference with n parameters θ_1 , θ_2 , ..., θ_n , the test statistic $\zeta_{\theta_1,...,\theta_n}$ will be distributed under H(θ_1 , ..., θ_n) (the null hypothesis) as,

$$f(\zeta_{\theta_1,\ldots,\theta_n}|H(\theta_1,\ldots,\theta_n)) = \chi^2(\zeta_{\theta_1,\ldots,\theta_n};n)$$



Read off values for where to apply threshold for different confidence intervals, for different number of parameters

n	1	2	3	4	5
68.3%	1.00	2.30	3.53	4.72	5.89
95.5%	4.02	6.20	8.05	9.74	11.34
99.74%	9.07	11.90	14.24	16.34	18.29

Coverage

Frequentists care about the **coverage of confidence intervals** \rightarrow check the fraction of intervals that contain the true value of λ (λ_0) for different values of λ_0

We can check for our Poisson case using

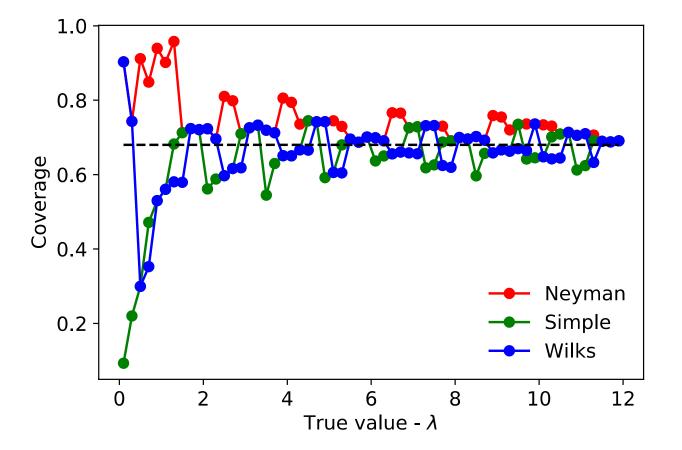
Full frequentist construction slow but only over covers

$$n_{\rm obs} - \sqrt{n_{\rm obs}} < \lambda < n_{\rm obs} + \sqrt{n_{\rm obs}}$$

Variance on n

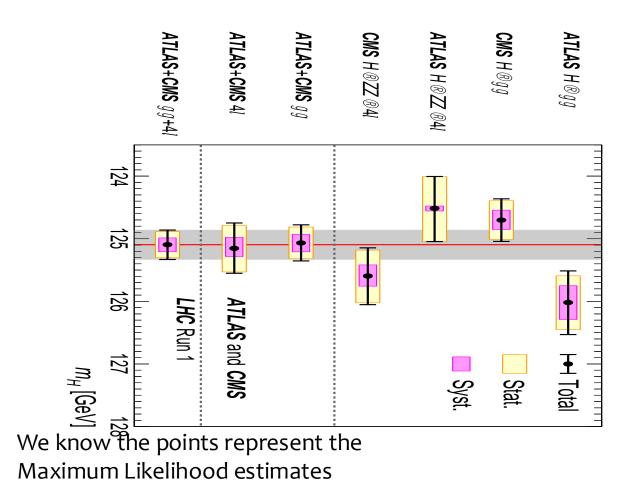
Very fast but can seriously undercover

Use Wilks' theorem - somewhere in between the others



Uncertainties @ the LHC

When we see a plot like this...



Uncertainties @ the LHC

And we know that the error bars are derived When we see a plot like this... from the region for which $\zeta_{m_H}^{\rm obs} < 1$ ATLAS+CMS gg CMS H®gg ATLAS H®gg ATLAS+CMS gg+4 CMS H®ZZ @4 ATLAS+CMS 4 ATLAS H®ZZ ®4. -2In ∟(*m_µ*) С 124 LHC Run 1 ATLAS and CMS 124.5 124 -obs I Will 125 - Combined gg+4l 126 · H®gg · H®ZZ ®4l Stat. only uncert 125.5 LHC Run 1 ATLAS and CMS m_H [GeV] H Total ひ m_H [GeV] Syst Stat. প্র We know the points represent the Tomorrow, we'll see what the Maximum Likelihood estimates dashed vs solid lines means

Now it's your turn!

In this afternoon's exercises, you will use the histograms that you produced yesterday and calculate the MLE for the signal strength for the *tt* process – in HEP we call this "*fitting*" to the data

For this exercise, you will be using the software package Combine, that is used in almost every CMS statistical analysis

Make sure you have obtained the cms combine container

Exercise 2 - Maximum Likelihood Fits

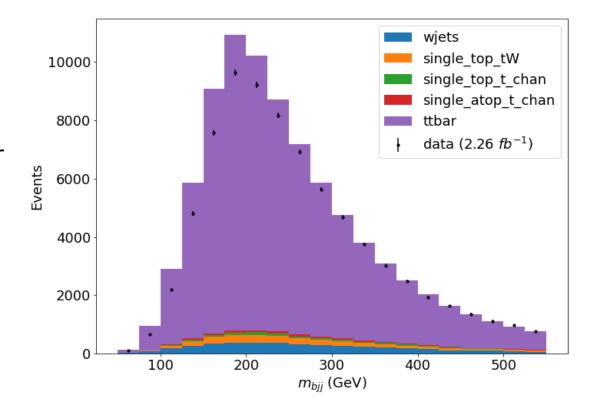
From yesterday's exercise, we now have a set of histograms, from data and simulation, in our .csv file. Don't worry if you didn't manage to run over all of the samples from yesterday, you can use the pre-prepared file ttbarAnalysis/exercise1solutions/signalregion_mbjj.csv.

In today's exercises, we're going to use the CMS statistics software tool combine to extract statistical results from the data (and simulation) that we processed yesterday. combine is a software package that is designed with a command line interface that uses simple .txt files as inputs. You can find out lots more about the tool at the online documentation pages here.

We'll begin by starting the container that has combine compiled for us. If you didn't download the container already, go back to the Getting started pages before continuing.

To do this, type the following into a terminal on your laptop (or by clicking the play button next to the cms_combine container in the Docker desktop application and using the terminal there).

Bash	
docker start -i cms_combine	



Don't worry if you didn't complete the previous exercise, all of the solutions can be found in ttbarAnalysis/exercise1solutions