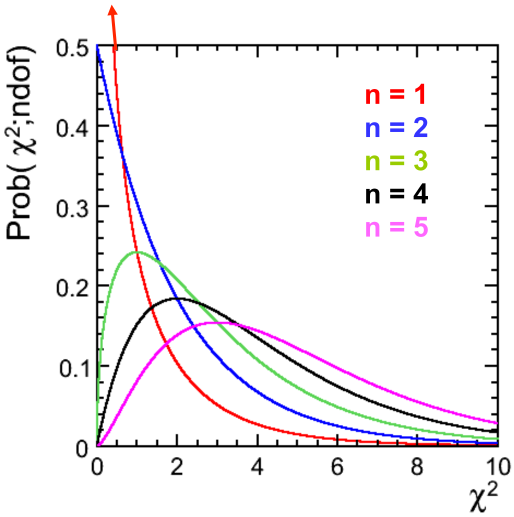
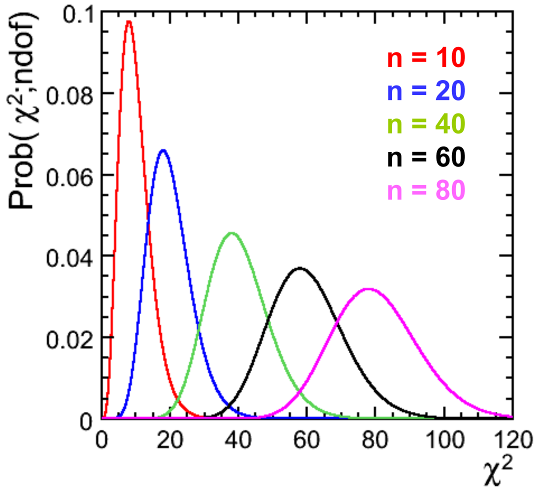
Statistics

Lent Term 2015
Prof. Mark Thomson





Lecture 3 : Fitting and Hypothesis testing

Lecture 1: Back to basics
Introduction, Probability distribution functions, Binomial distributions, Poisson distribution

Lecture 2: The Gaussian Limit
The central limit theorem, Gaussian errors, Error propagation, Combination of measurements, Multi-dimensional Gaussian errors, Error Matrix

Lecture 3: Fitting and Hypothesis Testing
The χ^2 test, Likelihood functions, Fitting, Binned maximum likelihood, Unbinned maximum likelihood

Lecture 4: The Dark Arts Part I
Bayesian Inference, Credible Intervals

Lecture 5: The Dark Arts II
The Frequentist approach, Confidence Intervals, Limits near physical boundaries, Systematic Uncertainties .

Introduction

★ Given some **data** (event counts, distributions) and a **particular theoretical** model
- are the data consistent with the model:
  - hypothesis testing
  - goodness of fit
- in the context of the model, what are our best estimates of its parameters:
  - fitting

★ In both cases, need a measure of consistency of data with our model

★ Start with a discussion of χ^2

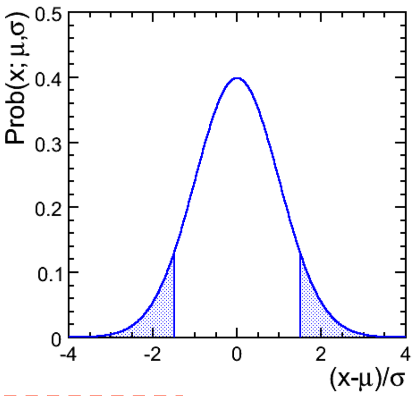
The Chi-Squared Statistic

★ Suppose we measure a parameter, $x \pm \sigma$, which a theorist says should have the value μ

★ Within this simple model, we can write down the prior probability of obtaining the value $x \pm \sigma$ given the prediction

$$P(\text{data};\text{prediction}) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

★ To express the consistency of the data, ask the question **"if the model is correct what is the probability of obtaining result at least far as far from the prediction as the observed value"**



★ This is simply the fraction of the area under the Gaussian with $|x-\mu| > |x_{obs}-\mu|$

★ e.g. if **1.5σ** from the prediction: $\boxed{13\,\%}$

★ Only care about degree of consistency, not whether we are on the +ve or –ve side, so equivalently want the probability

$$P(\chi^2 > \chi^2_{obs}) \quad \text{where} \quad \boxed{\chi^2 = \frac{(x-\mu)^2}{\sigma^2}}$$

★ For Gaussian distributed variables, χ^2 , forms the basis of our consistency test

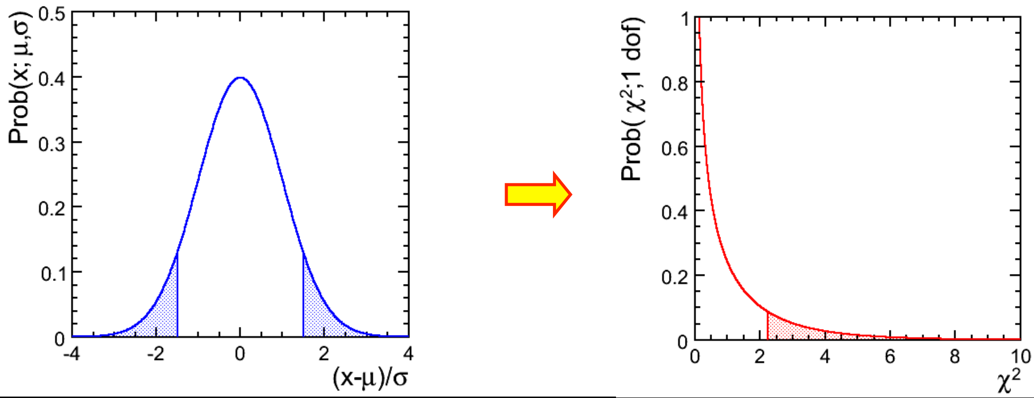
★ The probability distribution for, χ^2, can be obtained easily from the ID distribution

$$P(\chi^2)\mathrm{d}(\chi^2) = G(x)\mathrm{d}x \qquad \text{and} \qquad \frac{\mathrm{d}\chi^2}{\mathrm{d}x} = 2\frac{(x-\mu)}{\sigma^2} = 2\frac{\sqrt{\chi^2}}{\sigma}$$

$$P(\chi^2) = 2 \times \frac{1}{\sqrt{2\pi}\sigma}\frac{\sigma}{2\sqrt{\chi^2}}\exp\left\{-\frac{\chi^2}{2}\right\}$$

Factor of two from +ve and –ve parts of Gaussian

$$\boxed{P(\chi^2) = \frac{1}{\sqrt{2\pi}}(\chi^2)^{-\frac{1}{2}}\exp\left\{-\frac{\chi^2}{2}\right\}}$$



The Chi-Squared Statistic in higher dimensions

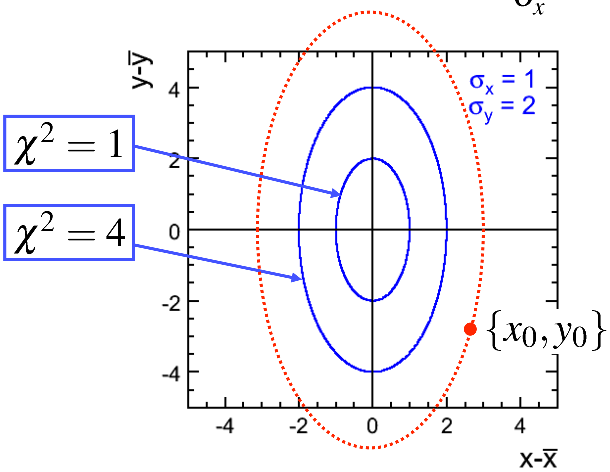
★ So far, this isn't particularly useful…

★ But now extend this to two dimensions (ignoring correlations for the moment, although we now know how to include them)

$$P(x,y) = \frac{1}{2\pi\sigma_x\sigma_y}\exp\left\{-\frac{1}{2}\left[\frac{(x-\mu_x)^2}{\sigma_x^2} + \frac{(y-\mu_y)^2}{\sigma_y^2}\right]\right\}$$

★ Lines of equal probability are equivalent to lines of equal χ^2

$$\chi^2 = \chi_x^2 + \chi_y^2 = \frac{(x-\mu_x)^2}{\sigma_x^2} + \frac{(y-\mu_y)^2}{\sigma_y^2}$$



★ What if I measure $\{x_0, y_0\}$

★ How consistent is this with expected values ?

★ ANSWER: the probability of obtaining smaller probability then observed

- i.e. integrate 2D PDF over region where $\chi^2 > \chi^2_{obs}$

★ It is worth seeing how this works mathematically…

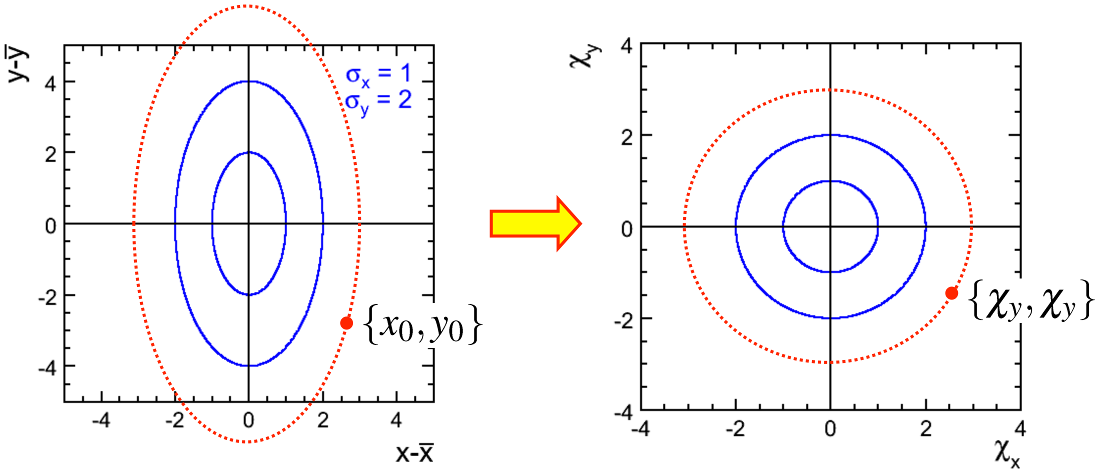
- First transform error ellipse into circular contours

$$\{x,y\} \Rightarrow \{\chi_x,\chi_y\} \qquad \chi_x^2 = \frac{(x-\mu_x)^2}{\sigma_x^2} \qquad \chi_y^2 = \frac{(y-\mu_y)^2}{\sigma_y^2}$$

$$P(\chi_x,\chi_y)\mathrm{d}\chi_x\mathrm{d}\chi_y = P(x,y)\mathrm{d}x\mathrm{d}y$$

- Therefore

$$P(\chi_x,\chi_y) = \frac{1}{2\pi}\exp\left\{-\frac{1}{2}\left[\chi_x^2+\chi_y^2\right]\right\}$$



★ Only interested in "radius" i.e. χ^2

- so transform $\{\chi_x,\chi_y\} \Rightarrow \{\chi,\phi\}$

with $\delta\chi_x\delta\chi_y = \chi\delta\chi\delta\phi$

$$\begin{aligned} P(\chi,\phi)\delta\chi\delta\phi &= P(\chi_x,\chi_y)\delta\chi_x\delta\chi_y \\ &= \chi P(\chi_x,\chi_y)\delta\chi\delta\phi \\ P(\chi)\delta\chi &= 2\pi\chi P(\chi_x,\chi_y)\delta\chi \\ P(\chi) &= \chi\exp\left(-\frac{\chi^2}{2}\right) \end{aligned}$$

★ Therefore, probability distribution in chi-squared:

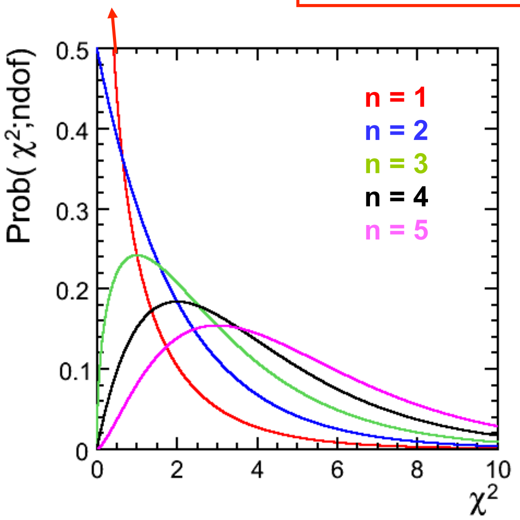
$$\boxed{P(\chi^2;n=2) = \frac{1}{2}\exp\left(-\frac{\chi^2}{2}\right)} \qquad \boxed{\delta(\chi^2) = 2\chi\delta\chi}$$

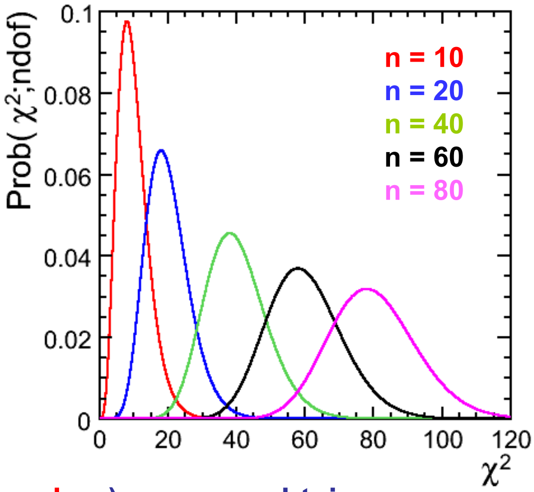
★ For two Gaussian distributed variables, we now have an expression for the chi-squared probability distribution !

Problem: Show that:

$$P(\chi^2;n=3) = \frac{1}{2\pi}(\chi^2)^{\frac{1}{2}}\exp\left(-\frac{\chi^2}{2}\right) \quad \text{and} \quad \boxed{P(\chi^2;n) \propto (\chi^2)^{\frac{(n-2)}{2}}\exp\left(-\frac{\chi^2}{2}\right)}$$

$$P(\chi^2;n) \;\propto\; (\chi^2)^{\frac{(n-2)}{2}} \exp\left(-\frac{\chi^2}{2}\right)$$





★ **For any number of variables (degrees of freedom) can now obtain**

$$P(\chi^2 > \chi^2_{obs}) = \int_{\chi^2_{obs}}^{\infty} P(\chi^2, n)\,\mathrm{d}\chi^2$$

★ **Already done for you, e.g. tables or more convenient** TMath::Prob(χ^2,n)

Properties of chi-squared

★ **For n degrees of freedom** $\boxed{\langle\chi^2\rangle = n}$

Proof:

$$\begin{aligned}\langle\chi^2\rangle &= \left\langle \sum_{i=1}^{n} \chi_i^2 \right\rangle \\ &= \sum_{i=1}^{n} \left\langle \frac{(x_i-\mu_i)^2}{\sigma_i^2} \right\rangle \\ &= \sum_{i=1}^{n} 1 = n\end{aligned}$$

or

$$\begin{aligned}\langle\chi^2\rangle &= \frac{\int \chi^2 P(\chi^2;n)\mathrm{d}(\chi^2)}{\int P(\chi^2;n)\mathrm{d}(\chi^2)} \\ &= \frac{\int \chi^2 (\chi^2)^{\frac{(n-2)}{2}} e^{-\frac{\chi^2}{2}} 2\chi \mathrm{d}\chi}{\int (\chi^2)^{\frac{(n-2)}{2}} e^{-\frac{\chi^2}{2}} 2\chi \mathrm{d}\chi} \\ &= \frac{\int x^{n+1} e^{-\frac{x^2}{2}} \mathrm{d}x}{\int x^{n-1} e^{-\frac{x^2}{2}} \mathrm{d}x} \\ &= n\end{aligned}$$

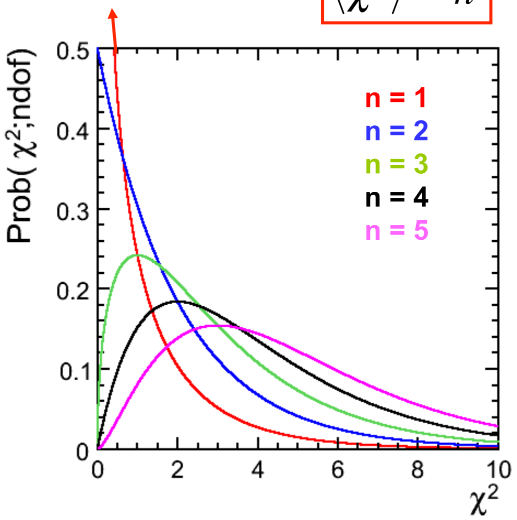
★ **For n degrees of freedom** $\boxed{Var(\chi^2) = 2n}$

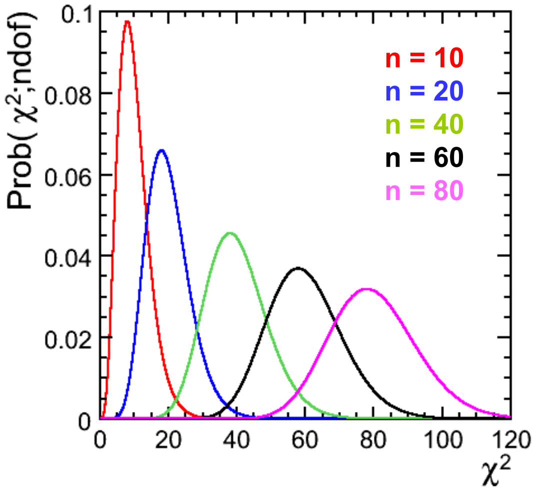
Proof:

$$\begin{aligned}Var(\chi^2) &= \langle\chi^2\chi^2\rangle - \langle\chi^2\rangle^2 \\ &= n\langle\chi_i^4\rangle + n(n-1) - n^2 \\ &= 3n + n^2 - n - n^2 \\ &= 2n\end{aligned}$$

$$\begin{aligned}\langle\chi^4\rangle &= \frac{\int x^{n+3} e^{-\frac{x^2}{2}} \mathrm{d}x}{\int x^{n-1} e^{-\frac{x^2}{2}} \mathrm{d}x} \\ &= I_{n+3}/I_{n-1} \\ &= (n+2)n \\ Var(\chi^2) &= \langle\chi^4\rangle - \langle\chi^2\rangle^2 \\ &= n^2 + 2n - n^2 = 2n\end{aligned}$$

$\langle \chi^2 \rangle = n$ $\qquad$ $Var(\chi^2) = 2n$





★ **For large n; the distribution tends to a Gaussian** **(large ~ 40)**

Useful for quick estimates…

Example

★ **Suppose we have an absolute prediction for a distribution, e.g. a differential cross section and we can account perfectly for experimental effects (efficiency, background, bin-bin migration)**

★ **Measure number of events in bins of cosθ, n_i , and compare to prediction μ_i**

★ **If prediction is correct, expect the observed number of events in a given bin to to follow a Poisson distribution of mean μ_i**

★ **If the expectations in all bins are sufficiently large, the Poisson distribution can be approximated as a Gaussian with mean μ_i and variance μ_i**

★ **In this limit can use chi-squared for consistency with hypothesis**

$$\chi_i^2 = \frac{(n_i - \mu_i)^2}{\mu_i}$$

Expected fluctuations around mean

★ **For N bins, have N independent (approximately) Gaussian distributed variables**

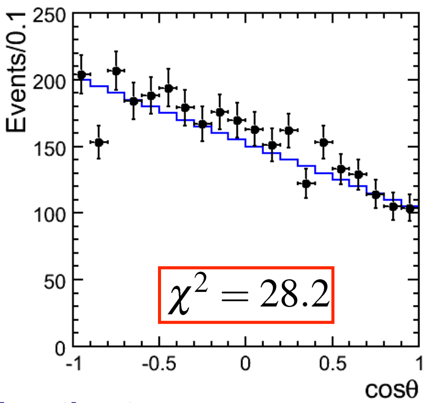
★ **Overall consistency of data with prediction assessed using**

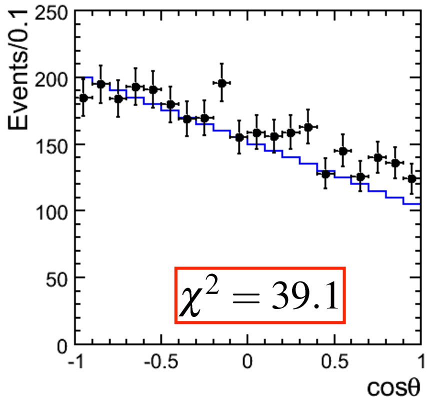
$$\chi^2 = \sum_i \chi_i^2$$

★ **If hypothesis (prediction) is correct expect**

$$\boxed{\langle \chi^2 \rangle = n} \qquad \boxed{Var(\chi^2) = 2n}$$

$$\langle\chi^2\rangle = 20 \qquad \sigma_{\chi^2} = \sqrt{40} = 6.3$$





- **Quick estimates:**

$$\approx 8.2/6.3\sigma = 1.3\sigma \qquad \approx 19.1/6.3\sigma = 3.0\sigma$$

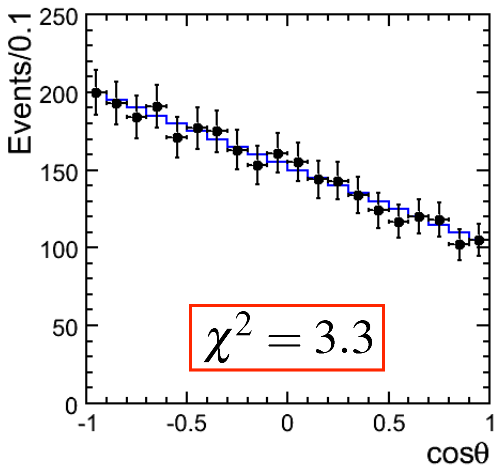
- **But N=20, not very large, these estimates only give an indication of the agreement.**
- **Correct numbers (integral of expected χ^2 distribution)** TMath::Prob(χ^2,20)

$$P(\chi^2 > 28.2; N=20) = 10.4\,\% \qquad P(\chi^2 > 39.1; N=20) = 0.6\,\%$$

Perfectly consistent: 10 % probability of getting a χ^2 worse than observed value by chance

A bit dodgy: only 1 % probability of getting a χ^2 worse than observed value by chance

- **What about a very small value of chi-squared, e.g.**

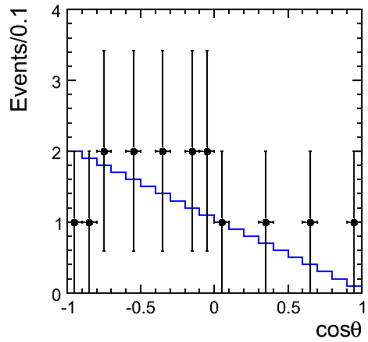


- **Expected** $\langle\chi^2\rangle = 20$
- **Observed value is much smaller**
- $P(\chi^2 > 3.3; N=20) = 99.999\,\%$
- $P(\chi^2 < 3.3; N=20) = 0.00001$
- **Conclude 1/1000000 chance of getting such a small value: highly suspicious…**
- **What could be wrong:**
  - **Errors not estimated correctly**
  - **…**

Log-Likelihood

★ The chi-squared-n distribution is just a re-expression of a Gaussian for N-variables

★ If the expected numbers of events are low, have to base consistency of data and prediction on Poisson statistics



▪ For the ith bin:

$$P_i(n_i;\mu_i) = \frac{\mu_i^{n_i} e^{-\mu_i}}{n_i}$$

▪ Therefore the joint probability of obtaining **exactly** the observed $\{n_i\}$, i.e. the likelihood L

$$L = \prod_i P_i = \prod_i \frac{\mu_i^{n_i} e^{-\mu_i}}{n_i!}$$

▪ Convenient to take the **natural logarithm** (hence log-likelihood)

$$\boxed{\ln L = \sum_i \ln\left(\frac{\mu_i^{n_i} e^{-\mu_i}}{n_i!}\right)}$$

Poisson distributed variables

★ The likelihood is often **very small**. It is the probability of obtaining **exactly** the observed numbers of events in each bin

▪ For above distribution $L = 2\times 10^{-10}$ $(\ln L = -22.4)$

★ What constitutes a good value of log-likelihood ?

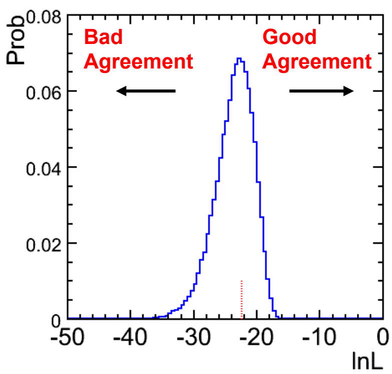
▪ i.e. for the distribution shown, does $\ln L = -22.4$ imply good agreement ?

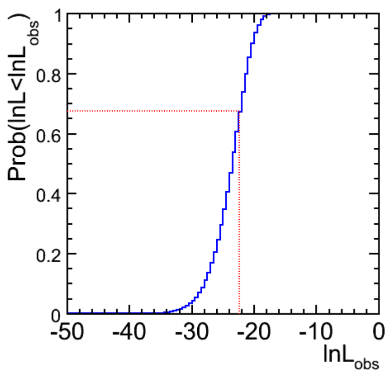
★ There is no simple answer to this question

★ Unlike for the chi-squared distribution, there is **no general analytic form**

★ One practical way of assessing the consistency, is to generate many "**toy MC**" distributions according to expected distributions

```
Float_t LogLikelihood = 1.0;
TRandom2* r = new TRandom2();
for( Int_t i=1; i<= nbins;  i++){
    Float_t expected = hist->GetBinContent(i);
    Int_t nObs = r->Poisson(expected);
    Double_t  prob = TMath::PoissonI(nObs,expected);
    LogLikelihood += log(prob);
}
```





★ Hence have obtain expected lnL distribution for particular problem

Relationship between chi-squared and likelihood

★ **For Gaussian distributed variables**

$$L(\{x_i\}) \propto e^{-\frac{\chi^2}{2}} \propto \prod_i \exp\left\{-\frac{1}{2}\left[\frac{(x_i-\mu_i)^2}{\sigma_i^2}\right]\right\}$$

$$-\ln L = \frac{\chi^2}{2} + k$$

$$\boxed{\chi^2 = -2\ln L + \kappa}$$

Chi-squared × ½ is lnL for Gaussian distributed variables

Chi-Squared Fitting: Gaussian Errors

★ **Given some data and a prediction which depends on a set of parameters, we want to determine our best estimate for the parameters.**

★ **Construct the probability:** $P(\text{data};\{x_i\})$

★ **Best estimate is the set of parameters that maximises** $P(\text{data};\{x_i\})$

Simple Example:

- **Two measurements of a quantity, x, using different methods**

$$x = x_1 \pm \sigma_1 = 5.1 \pm 0.5 \qquad x = x_2 \pm \sigma_2 = 6.0 \pm 0.3$$

(assume independent Gaussian errors)

- **What is our best estimate of the true value of x ?**

$$P(\text{data};x) = \frac{1}{2\pi\sigma_1\sigma_2}\exp\left\{-\frac{1}{2}\left[\frac{(x_1-x)^2}{\sigma_1^2}+\frac{(x_2-x)^2}{\sigma_2^2}\right]\right\} = Ae^{-\frac{\chi^2}{2}}$$

$$-\ln P = \frac{\chi^2}{2}$$

- **Maximum probability corresponds to minimum chi-squared**
- **For Gaussian distributed variables: fitting ⇨ minimising chi-squared**
- **Here require**

$$\boxed{\frac{\mathrm{d}\chi^2}{\mathrm{d}x} = 0}$$

$$\frac{d\chi^2}{dx}=0 \quad \Rightarrow \quad \frac{d\chi^2}{dx} - 2\frac{(x_1-\bar{x})}{\sigma_1^2} - 2\frac{(x_2-\bar{x})}{\sigma_2^2} = 0$$

$$\boxed{\bar{x} = \frac{\frac{x_1}{\sigma_1^2}+\frac{x_2}{\sigma_2^2}}{\frac{1}{\sigma_1^2}+\frac{1}{\sigma_2^2}}}$$

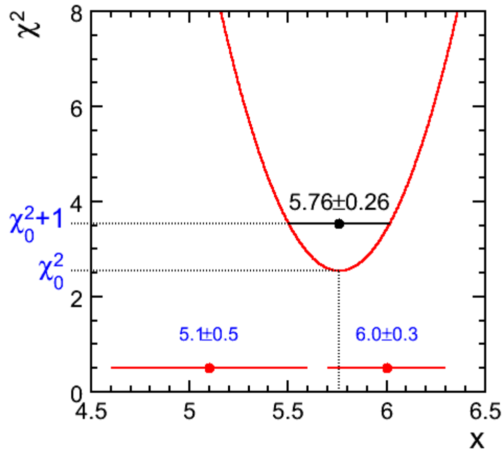
- Which is the formula we found previously for averaging two measurements
- **Note:** chi-squared is a quadratic function of the parameter x
- Taylor expansion about minimum with

$$\frac{d^2\chi^2}{dx} = 2\left(\frac{1}{\sigma_1^2}+\frac{1}{\sigma_2^2}\right) \quad \text{and} \quad \frac{d^3\chi^2}{dx}=0$$

gives $\chi^2(x-\bar{x}) = \chi_0^2 + \frac{1}{2!}\frac{d^2\chi^2}{dx^2}(x-\bar{x})^2$

$$P(x) \propto e^{-\frac{\chi^2}{2}} = e^{-\frac{\chi_0^2}{2}} e^{-\frac{(x-\bar{x})^2}{2\sigma_x^2}}$$

therefore $\sigma_x^2 = \left(\frac{1}{2}\left[\frac{d^2\chi^2}{dx^2}\right]_{x=\bar{x}}\right)^{-1}$



Goodness of Fit

- Started with two measurements of a quantity, x

$$x = x_1 \pm \sigma_1 = 5.1 \pm 0.5 \qquad x = x_2 \pm \sigma_2 = 6.0 \pm 0.3$$

- Best estimate of the true value of x, is that which maximises the likelihood, i.e. minimises chi-squared, giving a chi-squared at the minimum of:

$$\chi_0^2 = \left[\frac{(x_1-\bar{x})^2}{\sigma_1^2} + \frac{(x_2-\bar{x})^2}{\sigma_2^2}\right]$$

- What is the probability that our data are consistent with a common mean? i.e. how do we interpret this chi-squared minimum
- Expanding and substituting for $\bar{x}$

$$\chi_0^2 = \frac{x_1^2}{\sigma_1^2}+\frac{x_2^2}{\sigma_2^2} - \bar{x}^2\left(\frac{1}{\sigma_1^2}+\frac{1}{\sigma_2^2}\right)$$

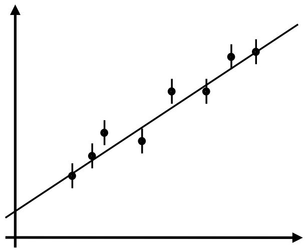
$$= \frac{(x_1-x_2)^2}{\sigma_1^2+\sigma_2^2} = \frac{(\Delta x)^2}{\sigma_{\Delta x}^2} \quad \text{with} \quad \left\{\begin{array}{l}\Delta x = x_1 - x_2 \\ \sigma_{\Delta x}^2 = \sigma_1^2+\sigma_2^2\end{array}\right.$$

- Here the minimum chi-squared corresponds is distributed as chi-squared for a single Gaussian measurement, i.e. 1 degree of freedom

In general, the fitted minimum chi-squared is distributed as chi-squared for (**number of measurements – number of fitted parameters**) degrees of freedom

Example: Straight line fitting

★ Given a set of points $\{x_i, y_i \pm \sigma_i\}$ find the best fit straight line and the uncertainties



★ First define the chi-squared: $\chi^2 = \sum_{i=0}^{n} \frac{(y_i - mx_i - c)^2}{\sigma_i^2}$

★ Minimise chi-squared with respect to the 2 parameters describing the model

$$\frac{\partial \chi^2}{\partial m} = \sum_{i=0}^{n} -2x_i \frac{(y_i - mx_i - c)}{\sigma_i^2} = 0 \qquad \frac{\partial \chi^2}{\partial c} = \sum_{i=0}^{n} -2 \frac{(y_i - mx_i - c)}{\sigma_i^2} = 0$$

$$\Rightarrow \quad \overline{m}\sum_{i=0}^{n} \frac{x_i^2}{\sigma_i^2} + \overline{c}\sum_{i=0}^{n} \frac{x_i}{\sigma_i^2} = \sum_{i=0}^{n} \frac{x_i y_i}{\sigma_i^2} \qquad \overline{m}\sum_{i=0}^{n} \frac{x_i}{\sigma_i^2} + \overline{c}\sum_{i=0}^{n} \frac{1}{\sigma_i^2} = \sum_{i=0}^{n} \frac{y_i}{\sigma_i^2}$$

$$\Rightarrow \quad \boxed{\begin{pmatrix} s_{x^2} & s_x \\ s_x & s \end{pmatrix} \begin{pmatrix} \overline{m} \\ \overline{c} \end{pmatrix} = \begin{pmatrix} s_{xy} \\ s_y \end{pmatrix}}$$

Where the sums are represented by $\boxed{s_x = \sum_{i=1}^{n} \frac{x_i}{\sigma_i^2}}$ etc.

★ For the errors first make Taylor expansion around the minimum chi-squared:

$$\chi^2(m,c) = \chi^2(\overline{m},\overline{c}) + \frac{1}{2!}\frac{\partial^2 \chi^2}{\partial m^2}(m-\overline{m})^2 + \frac{1}{2!}\frac{\partial^2 \chi^2}{\partial m^2}(c-\overline{c})^2 + 2\frac{1}{2!}\frac{\partial^2 \chi^2}{\partial m \partial c}(m-\overline{m})(c-\overline{c})^2$$

(since the function is quadratic there are no other terms)

which gives an elliptical contours

★ In terms of the inverse error matrix

$$\boxed{\chi^2 = \mathbf{x}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{x}} \quad \text{with} \quad \mathbf{x} = \begin{pmatrix} m - \overline{m} \\ c - \overline{c} \end{pmatrix}$$

★ Hence

$$\mathbf{M}^{-1} = \begin{pmatrix} \frac{1}{2}\frac{\partial^2 \chi^2}{\partial m^2} & \frac{1}{2}\frac{\partial^2 \chi^2}{\partial m \partial c} \\ \frac{1}{2}\frac{\partial^2 \chi^2}{\partial m \partial c} & \frac{1}{2}\frac{\partial^2 \chi^2}{\partial c^2} \end{pmatrix} \qquad \boxed{(\mathbf{M}^{-1})_{ij} = \frac{1}{2}\frac{\partial^2 \chi^2}{\partial a_i \partial a_j}}$$

★ Here

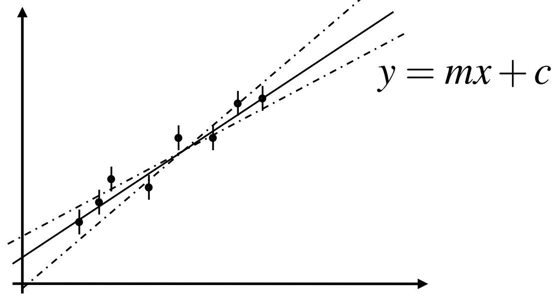
$$\mathbf{M}^{-1} = \begin{pmatrix} s_{x^2} & s_x \\ s_x & s \end{pmatrix}$$

$$\mathbf{M} = \frac{1}{s_{x^2}s - s_x^2} \begin{pmatrix} s & -s_x \\ -s_x & s_{x^2} \end{pmatrix} = \begin{pmatrix} \sigma_m^2 & \rho\sigma_m\sigma_c \\ \rho\sigma_m\sigma_c & \sigma_c^2 \end{pmatrix}$$

★ Giving

$$\boxed{\rho = \frac{-s_x}{(ss_{x^2})^{\frac{1}{2}}} = -\frac{\sum \frac{x_i}{\sigma_i^2}}{\left(\sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2}\right)^{\frac{1}{2}}}}$$

$$\rho = \frac{-s_x}{(s s_{x^2})^{\frac{1}{2}}} = -\frac{\sum \frac{x_i}{\sigma_i^2}}{\left(\sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2}\right)^{\frac{1}{2}}}$$



★ Suppose we want to calculate the error on y as a function of x based on our fit:

$$\sigma_y^2 = (x, 1)\begin{pmatrix} \sigma_m^2 & \rho\sigma_m\sigma_c \\ \rho\sigma_m\sigma_c & \sigma_c^2 \end{pmatrix}\begin{pmatrix} x \\ 1 \end{pmatrix}$$
$$= \sigma_m^2 x^2 + 2\rho x \sigma_m \sigma_c + \sigma_c^2$$

$\frac{\partial y}{\partial m}$

$\frac{\partial y}{\partial c}$

★ It is worth noting that the correlation coefficient is proportional to $\sum \frac{x_i}{\sigma_i^2}$, hence one could fit after making the transformation $x' = x - \overline{x}$ such that $\sum \frac{x_i'}{\sigma_i^2} = 0$

and the uncertainties on the new intercept and gradient become uncorrelated

Binned Maximum Likelihood Fits

★ So far only considered chi-squared fitting (i.e. assumes Gaussian errors)

★ In particle physics often dealing with low numbers of events and need to account for the Poisson nature of the data

★ In general can write down the joint probability

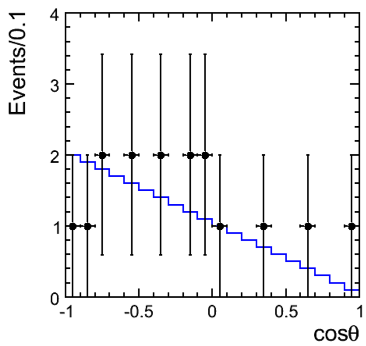
$$P(\text{data}; \text{parameters}) \equiv P(\{x_i\}; \{a_i\})$$

- e.g. if we predict a distribution should follow a first order polynomial

$$\mu_i = a_1 \cos\theta_i + a_0$$

- and measure events in bins of $\cos\theta_i$
- define likelihood based on Poisson statistics

$$L = \prod_i P_i = \prod_i \frac{\mu_i^{n_i} e^{-\mu_i}}{n_i!}$$



- best estimates of parameters, defined by maximum likelihood or, equivalently, the minimum of -log-likelihood

$$\mathscr{L} = -\ln L = \sum_i -\ln\left(\frac{\mu_i^{n_i} e^{-\mu_i}}{n_i!}\right) = \sum_i \ln(n_i!) + \mu_i - n_i \ln\mu_i$$

★ Maximising the likelihood corresponds to solving the set of linear equations

$$\frac{\partial \mathscr{L}}{\partial a_i} = 0$$

★ To estimate the errors on the parameters, expand –lnL, about its minimum

$$\mathscr{L} = \mathscr{L}(\bar{a}_i) + \frac{1}{2!}\sum_i (a_i - \bar{a}_i)^2 \frac{\partial^2 \mathscr{L}}{\partial a_i^2} + \frac{1}{2!}\sum_{i \neq j}(a_i - \bar{a}_i)(a_j - \bar{a}_j)\frac{\partial^2 \mathscr{L}}{\partial a_i \partial a_j} + O((a-\bar{a})^3)$$

★ Unlike the case of Gaussian errors, the

$$\frac{\partial^3 \mathscr{L}}{\partial a^3} \neq 0$$

- hence the resulting likelihood surface will not have a quadratic form

★ For the moment, restrict the discussion to a single variable

$$-\ln L = \mathscr{L} = \mathscr{L}(\bar{a}) + \frac{1}{2!}(a-\bar{a})^2 \frac{\partial^2 \mathscr{L}}{\partial a^2} + O((a-\bar{a})^3)$$

$$L = e^{-\mathscr{L}} = e^{-\mathscr{L}(\bar{a})} \times \underbrace{e^{-\frac{1}{2!}(a-\bar{a})^2 \frac{\partial^2 \mathscr{L}}{\partial a^2}}}_{\text{Gaussian}} \times \underbrace{e^{-O((a-\bar{a})^3)}}_{\text{Higher Order}}$$

★ If resulting likelihood distribution is "sufficiently Gaussian" could assign an estimate of the error on our measurement as:

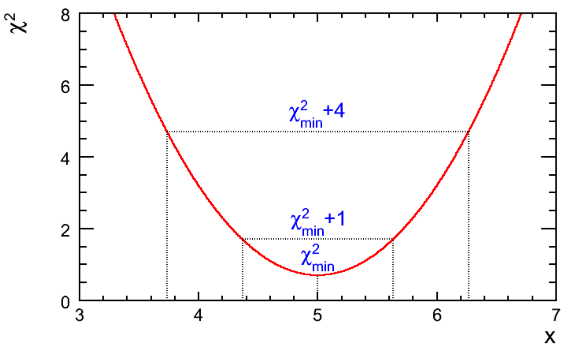
$$\sigma^2 = \left(\frac{\partial^2 \mathscr{L}}{\partial a^2}\right)^{-1}$$

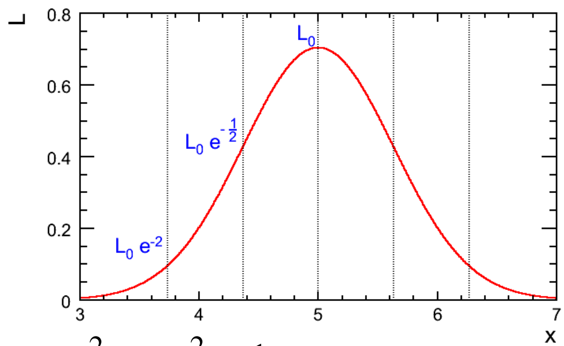
★ This is **OK in the Gaussian limit**, but in general it is not very useful

★ Usually adopt a Gaussian inspired procedure…

★ For Gaussian distributed variables, have a parabolic chi-squared curve which gives a Gaussian likelihood

$$L = L_0 e^{-\frac{\chi^2}{2}} \quad \text{with} \quad L_0 = e^{-\frac{\chi^2_{min}}{2}}$$



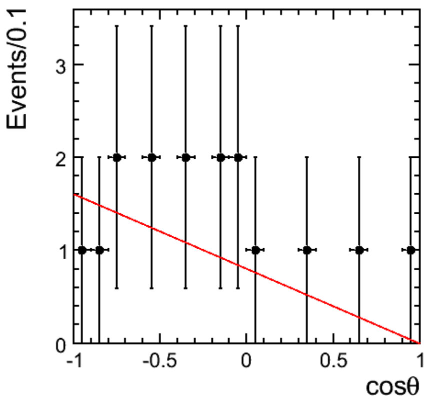


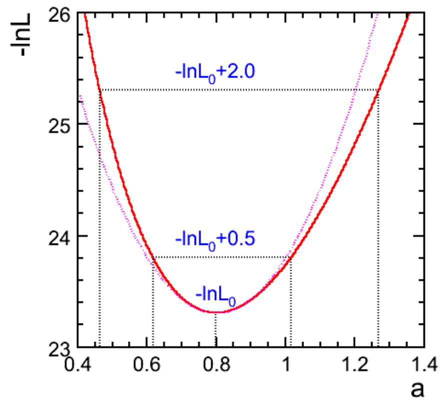
★ "1 sigma errors" defined the points where $\chi^2 \rightarrow \chi^2 + 1$

★ Or, **EQUIVALENTLY**, where the Relative Likelihood compared to the maximum likelihood decreases by $e^{-1/2}$

Example

e.g. assume a form $\mu_i = a(1 - \cos\theta_i)$





★ Not unreasonable to use estimate of "1 sigma" uncertainty as the values:

$$-\ln L \to -\ln L + 0.5$$

Similarly for the "2 sigma" uncertainty:

$$-\ln L \to -\ln L + 2$$

★ At these points, have probabilities of $e^{-1/2}$ and e^{-2} relative to maximum

★ **BUT:** no guarantee that 68 % of PDF lies within $\pm 1\sigma$

Interpretation requires some care – a dark art (see later)

Binned Maximum Likelihood: Goodness of Fit

★ Safest way is to generate toy MC experiments, perform the fit, and thus obtain the expected lnL distribution

★ However, there is an invaluable trick

- For Poisson errors, we minimised the function

$$\mathscr{L} = -\ln L = -\sum_i \ln\left(\frac{\mu_i^{n_i} e^{-\mu_i}}{n_i!}\right) = \sum_i \ln(n_i!) + \mu_i - n_i \ln \mu_i$$

- Free to add a constant to this – doesn't affect the result
- Here the data are fixed and we vary the expectation
- Add the lnL of observing n_i given an expectation of n_i

Likelihood ratio

$$\begin{aligned}
\mathscr{L} \to \mathscr{L} &= -\sum_i \ln\left(\frac{\mu_i^{n_i} e^{-\mu_i}}{n_i!}\right) + \boxed{\sum_i \ln\left(\frac{n_i^{n_i} e^{-n_i}}{n_i!}\right)} \equiv -\ln\left[\frac{L(n_i;\mu_i)}{L(n_i;n_i)}\right] \\
&= \sum_i \ln n_i! + \mu_i - n_i \ln \mu_i - \ln n_i! - n_i + n_i \ln n_i \\
&= \sum_i \mu_i - n_i + n_i \ln \frac{n_i}{\mu_i} \\
&= \sum_i \frac{\mu_i^2 - \mu_i n_i}{\mu_i} + n_i \ln\left(1 + \frac{n_i - \mu_i}{\mu_i}\right)
\end{aligned}$$

★ In the limit where the μ_i are "not too small, in region of best fit $\frac{n_i-\mu_i}{\mu_i}$ is small

$$\begin{aligned}
\mathscr{L} &= \sum_i \frac{\mu_i^2-\mu_i n_i}{\mu_i} + n_i \ln\left[1+\left(\frac{n_i-\mu_i}{\mu_i}\right)\right] \\
&= \sum_i \frac{\mu_i^2-\mu_i n_i}{\mu_i} + n_i\left(\frac{n_i-\mu_i}{\mu_i}\right) - \frac{n_i}{2}\left(\frac{n_i-\mu_i}{\mu_i}\right)^2 + O\left\{n_i\left(\frac{n_i-\mu_i}{\mu_i}\right)^3\right\} \\
&\approx \sum_i \frac{\mu_i^2-\mu_i n_i+n_i^2-\mu_i n_i}{\mu_i} - \frac{n_i}{2}\left(\frac{n_i-\mu_i}{\mu_i}\right)^2 \\
&= \sum_i \frac{(n_i-\mu_i)^2}{\mu_i} - \frac{n_i}{2}\left(\frac{n_i-\mu_i}{\mu_i}\right)^2 \\
&= \sum_i \frac{(n_i-\mu_i)^2}{\mu_i}\left(1-\frac{n_i}{2\mu_i}\right) \\
&\approx \frac{1}{2}\sum_i \frac{(n_i-\mu_i)^2}{\mu_i}
\end{aligned}$$

with $\langle n_i \rangle = \mu_i$

For Poisson distributed variables $\sigma_i^2 = \mu_i$

$$\mathscr{L} = -\ln\lambda = \frac{\chi^2}{2} \quad \text{with} \quad \lambda = \frac{L(n_i;\mu_i)}{L(n_i;n_i)}$$

★ Hence $-2\ln\lambda$ is distributed as χ^2 in the limit of "large" n

★ This is a very useful trick.

★ When fitting a histogram with Poisson errors

ALWAYS

- Perform a maximum likelihood, not a chi-squared fit
- Use the likelihood ratio

$$-2\ln\lambda = \sum_i \mu_i - n_i + n_i \ln\frac{n_i}{\mu_i}$$

NOTE

- Best fit parameters determined by

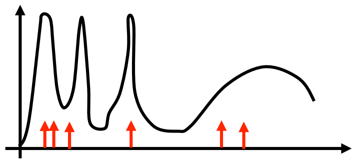
$$\frac{\partial[-2\ln\lambda]}{\partial a_i} = \sum_i \left(1-\frac{n_i}{\mu_i}\right)\frac{\partial\mu_i}{\partial a_i} = 0 \qquad \mu_i(\{a_i\})$$

- At the best fit point $-2\ln\lambda$ tends to a chi-squared distribution for n-m d.o.f.

Unbinned Maximum Likelihood Fits

★ For some applications, binning data results in a loss of precision

- e.g. sparse data and a rapidly varying prediction



★ In other cases there is simply no need to bin data: unbinned maximum likelihood

NOTE: this is a "shape-only" fit: normalisation doesn't enter

★ Suppose we can construct the predicted PDF for the data as a function of the parameter of interest

- e.g. make N measurements of decay time, $\{t_i\}$, and want to estimate lifetime τ
  - Write down NORMALISED PDF

$$P(t) = \frac{1}{\tau}e^{-\frac{t}{\tau}}$$

  - We can now write down the likelihood of obtaining our set of data

$$L(\{t_i\}) = \prod_i \frac{1}{\tau}e^{-\frac{t_i}{\tau}}$$

  - Obtain lifetime by maximising likelihood (or equivalently lnL)

$$\begin{aligned} \ln L &= -\sum_i \frac{t_i}{\tau} + \ln\tau \\ \frac{\partial \ln L}{\partial \tau} &= \frac{\sum_i t_i}{\tau^2} - \frac{N}{\tau} \\ \Rightarrow \quad \tau &= \frac{1}{N}\sum_i t_i \end{aligned}$$

i.e. the expected, but not entirely obvious result

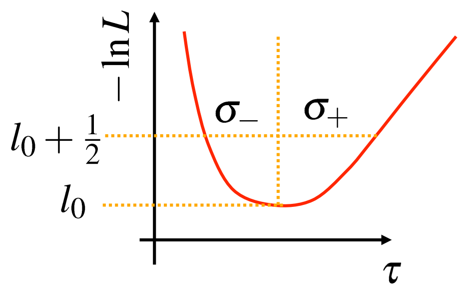
- For the error estimate take the second derivative

$$\begin{aligned} \frac{\partial^2 \ln L}{\partial \tau^2} &= -\frac{2}{\tau^3}\sum_i t_i + \frac{N}{\tau^2} \\ &= -\frac{N}{\tau^2} \\ \sigma_\tau &= \left(-\frac{\partial^2 \ln L}{\partial \tau^2}\right)^{-1} \\ &= \frac{\tau}{N^{\frac{1}{2}}} \end{aligned}$$

- Since we now know what we are doing, it is immediately obvious that the error is not symmetric

$$\frac{\partial^3 \ln L}{\partial \tau^3} \neq 0$$

- The likelihood function is



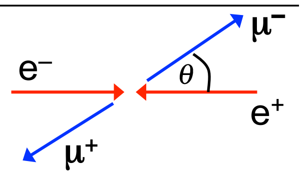
- Usual to quote with asymmetric errors, e.g.

$$\tau = 1.0^{+0.6}_{-0.4}$$

Another Example

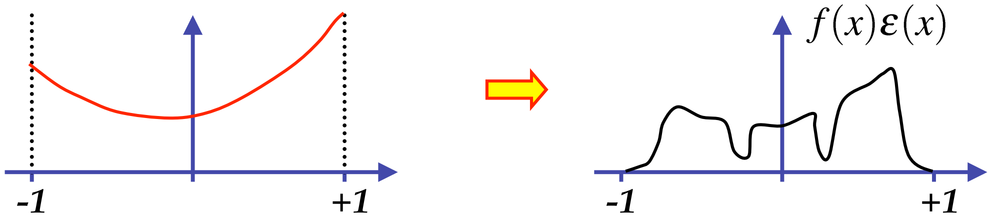
★ **Forward-Backward asymmetry at LEP**

- **Expected angular distribution of form**



$$f(x) \propto (1 + x^2 + \tfrac{3}{4}Ax) \qquad\qquad x = \cos\theta$$

- **But measured angular distribution depends on efficiency** $\varepsilon(x)$



- **However** $\varepsilon(x)$ **is not known (at least not precisely)**
- **But it is known to be symmetric**
- **Sufficient to construct an unbinned maximum likelihood fit**
- **First write down the PDF in terms of the unknown efficiency**

$$P(x) \propto f(x)\varepsilon(x) \propto \varepsilon(x)(1 + x^2 + \tfrac{3}{4}Ax)$$

- **For unbinned maximum likelihood fit PDF must be normalised**

$$\int_{1-}^{+1} f(x)\varepsilon(x)\mathrm{d}x = 1$$

- **Since** $\varepsilon(x)$ **is symmetric normalisation gives**

$$\int_{1-}^{+1} (1 + x^2)\varepsilon(x)\mathrm{d}x = 1 \qquad\qquad \text{i.e. independent of } A$$

- **Hence the normalised PDF is of the form**

$$P(x) = \kappa\varepsilon(x)(1 + x^2 + \tfrac{3}{4}Ax)$$

- **For the N observed values** $\{x_i\}$ **the log-likelihood function becomes:**

$$\ln L = \sum_i \ln\kappa + \ln\varepsilon(x_i) + \ln\left(1 + x_i^2 + \frac{3}{4}Ax_i\right)$$

- **For a maximum** $$\frac{\partial \ln L}{\partial A} = \frac{3}{4}\sum_i \frac{x_i}{1 + x_i^2 + \frac{3}{4}Ax_i} = 0$$

- **Which can be solved (preferably minimised by MINUIT) despite the fact we don't know the precise form of the PDF**

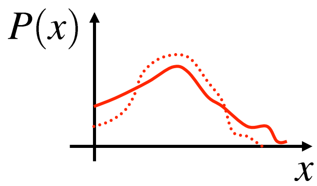
Extended Maximum Likelihood Fits

★ **Unbinned maximum likelihood** uses only shape information

★ In the **extended maximum likelihood fit** include normalisation

★ Suppose you observe n events with x_i and expect a total of μ with **PDF** which is a function of some parameter you wish to measure $P(x)$

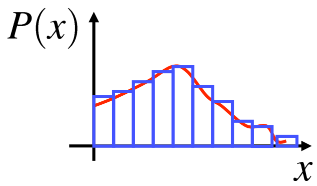
$$L(\{x_i\}) = \underbrace{\frac{e^{-\mu}\mu^n}{n!}}_{\text{Poisson}} \times \underbrace{\prod_i P(x_i)}_{\text{Unbinned ML}}$$



$$\ln L = -\mu + n\ln\mu - \ln n! + \sum_i \ln P(x_i)$$

★ Just for fun… suppose our PDF is binned with an expectation of μ_j/μ in each bin

$$\begin{aligned}
\ln L &= -\mu + n\ln\mu - \ln n! + \sum_i \ln\frac{\mu_j}{\mu} \\
&= -\mu + n\ln\mu - \ln n! - \sum_i \ln\mu + \sum_i \ln\mu_j \\
&= -\mu - \ln n! + \sum_i \ln\mu_j
\end{aligned}$$



• if there are n_j events observed in each bin

$$\ln L = -\mu - \ln\mu! + \sum_j n_j \ln\mu_j$$

$$\begin{aligned}
\ln L &= -\mu - \ln n! + \sum_j n_j \ln\mu_j \\
&= \sum_j \mu_j - \ln n! + \sum_j n_j \ln\mu_j \\
&= \underbrace{\sum_j \ln\left(\frac{e^{-\mu_j}\mu_j^{n_j}}{n_j!}\right)}_{\text{Binned Poisson Likelihood}} - \underbrace{\ln\frac{n!}{\sum_j n_j!}}_{\text{Can you see where this comes from ?}}
\end{aligned}$$

For a given data set this is a constant

Hence our previous expression for "Binned Maximum likelihood" is just an Extended Maximum Likelihood fit with a binned PDF

Fitting Summary

★ **Have covered main fitting/goodness of fit issues:**
- **definition of chi-squared**
- **chi-squared fitting**
- **definition of likelihood functions and relation to chi-squared**
- **likelihood fitting techniques**

★ **Next time we will consider more carefully the interpretation**

Appendix The Error Function

★ **For a single variable the Chi-Squared Probability**

$$P(\chi^2 < \chi_0^2) = \frac{1}{\sqrt{2\pi}\sigma}\int_{-x_-}^{+x_+} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\} \mathrm{d}x \qquad x_\pm = \mu \pm \chi_0\sigma$$

★ **Change variable** $\chi = \dfrac{x-\mu}{\sigma}$

$$P(\chi^2 < \chi_0^2) = \frac{1}{\sqrt{2\pi}}\int_{-\chi_0}^{+\chi_0} \exp\left\{-\frac{\chi^2}{2}\right\} \mathrm{d}\chi$$

★ **Change variable again** $t^2 = \chi^2/2$ **and integrate over positive values only**

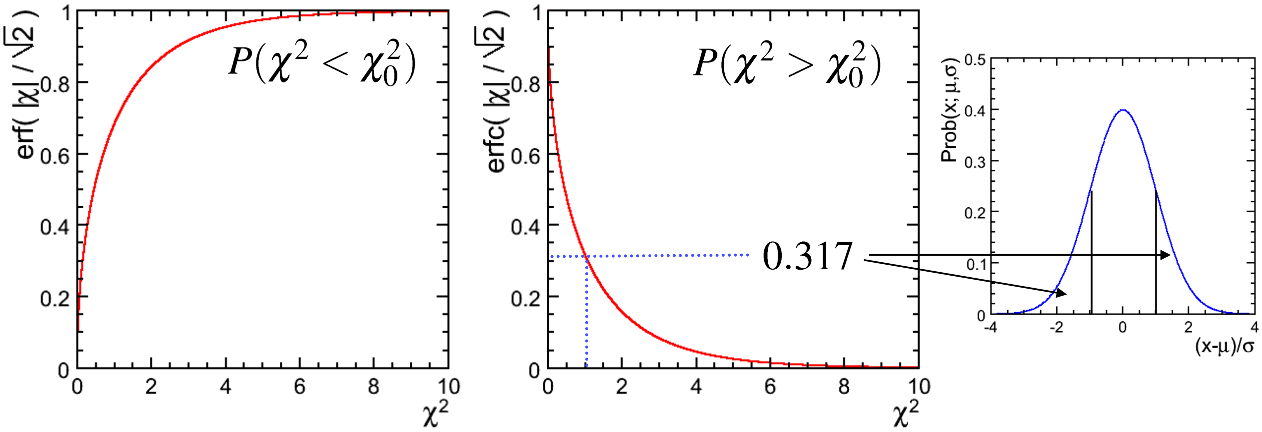
$$\begin{aligned} P(\chi^2 < \chi_0^2) &= \frac{\sqrt{2}}{\sqrt{\pi}}\int_0^{\chi_0} e^{-\frac{\chi^2}{2}} \mathrm{d}\chi \\ &= \frac{2}{\sqrt{\pi}}\int_0^{\chi_0/\sqrt{2}} e^{-t^2} \mathrm{d}t \\ &= \boxed{\mathrm{erf}\left(\frac{\chi}{\sqrt{2}}\right)} \end{aligned}$$

Error function

★ The probability of obtaining a value of $\chi^2 > \chi_0^2$ by chance is:

$$P(\chi^2 > \chi_0^2) = 1 - \frac{2}{\sqrt{\pi}} \int_0^{\chi_0/\sqrt{2}} e^{-t^2} \mathrm{d}t = \mathrm{erfc}\left(\frac{\chi}{\sqrt{2}}\right)$$

Complement of the Error Function



★ This is nothing more than a different way of expressing a 1D Gaussian distribution (or more correctly its two-sided integral)