The Poisson counting experiment

Suppose we do a counting experiment and observe *n* events.

Events could be from *signal* process or from *background* – we only count the total number.

Poisson model:

$$P(n|s,b) = \frac{(s+b)^n}{n!}e^{-(s+b)}$$

s = mean (i.e., expected) # of signal events

b = mean # of background events

Goal is to make inference about *s*, e.g.,

test s = 0 (rejecting  $H_0 \approx$  "discovery of signal process")

test all non-zero *s* (values not rejected = confidence interval)

In both cases need to ask what is relevant alternative hypothesis.

Poisson counting experiment: discovery *p*-value Suppose b = 0.5 (known), and we observe  $n_{obs} = 5$ . Should we claim evidence for a new discovery?

Give *p*-value for hypothesis *s* = 0:

p-value =  $P(n \ge 5; b = 0.5, s = 0)$ 



Poisson counting experiment: discovery significance Equivalent significance for  $p = 1.7 \times 10^{-4}$ :  $Z = \Phi^{-1}(1-p) = 3.6$ Often claim discovery if Z > 5 ( $p < 2.9 \times 10^{-7}$ , i.e., a "5-sigma effect")



In fact this tradition should be revisited: *p*-value intended to quantify probability of a signallike fluctuation assuming background only; not intended to cover, e.g., hidden systematics, plausibility signal model, compatibility of data with signal, "look-elsewhere effect" (~multiple testing), etc.

#### Significance from *p*-value

Often define significance Z as the number of standard deviations that a Gaussian variable would fluctuate in one direction to give the same p-value.



$$p=\int_Z^\infty rac{1}{\sqrt{2\pi}}e^{-x^2/2}\,dx=1-\Phi(Z)$$
 1 - TMath::Freq

$$Z=\Phi^{-1}(1-p)$$
 the two terms of the terms of term

TMath::NormQuantile

#### The significance of a peak

Suppose we measure a value *x* for each event and find:

Each bin (observed) is a Poisson r.v., means are given by dashed lines.



In the two bins with the peak, 11 entries found with b = 3.2. The *p*-value for the s = 0 hypothesis is:

$$P(n \ge 11; b = 3.2, s = 0) = 5.0 \times 10^{-4}$$

The significance of a peak (2)

But... did we know where to look for the peak?

→ "look-elsewhere effect";
 want probability to find peak at least as significant as the one seen anywhere in the histogram.

How many bins × distributions have we looked at?

 $\rightarrow$  look at a thousand of them, you'll find a 10<sup>-3</sup> effect

Is the observed width consistent with the expected *x* resolution?

 $\rightarrow$  take x window several times the expected resolution

Did we adjust the cuts to 'enhance' the peak?

→ freeze cuts, repeat analysis with new data Should we publish????

But one should also consider the degree to which the data are compatible with the new phenomenon, not only the level of disagreement with the null hypothesis; *p*-value is only first step!

The primary role of the *p*-value is to quantify the probability that the background-only model gives a statistical fluctuation as big as the one seen or bigger.

It is not intended as a means to protect against hidden systematics or the high standard required for a claim of an important discovery.

In the processes of establishing a discovery there comes a point where it is clear that the observation is not simply a fluctuation, but an "effect", and the focus shifts to whether this is new physics or a systematic. Proposed exercise

Extract N random numbers distributed as an exponential function with lifetime  $\boldsymbol{\tau}$ 

Fill an histogram

Write the likelihood  $L(t|\tau)$  in the binned and unbinned cases

N=100; x<-runif(N) ; x

[1] 0.405059710 0.028044254 0.758571449 0.382914253 0.231949128 0.457176317 [7] 0.736658152 0.038088207 0.104203774 0.513283288 0.742335360 0.368812945 [13] 0.898926650 0.884993284 0.029905424 0.510855547 0.976764989 0.163296696 [19] 0.312905139 0.172199152 0.789298260 0.518792378 0.076755612 0.187093519 [25] 0.613189997 0.007589616 0.476067148 0.091391122 0.254679165 0.642145047 [31] 0.068187724 0.213190998 0.284391620 0.652574104 0.375936000 0.938753973 [37] 0.768648992 0.934079373 0.576549295 0.822300084 0.963397188 0.677318145 [43] 0.804149516 0.278122875 0.918408046 0.161690666 0.816283114 0.219679127 [49] 0.247514679 0.144359027 0.238819577 0.499138632 0.801599954 0.882881265 [55] 0.817341159 0.484859340 0.865183191 0.866059658 0.375084123 0.287952191 [61] 0.832247817 0.392507337 0.292606502 0.018239798 0.980023583 0.892270450 [67] 0.843237637 0.927634800 0.204098272 0.763523759 0.545941953 0.600462520 [73] 0.078878091 0.445519178 0.375912647 0.614324038 0.194723071 0.839467755 [79] 0.265073122 0.870599505 0.696728359 0.085964346 0.004559065 0.710412472 [85] 0.824518329 0.868817609 0.730170102 0.016328960 0.087571226 0.173662371 [91] 0.367700928 0.491316323 0.085512807 0.738371863 0.977629644 0.378448315 [97] 0.194459494 0.754219429 0.376693783 0.939928670

Histogram of -log((1 - x))



## Likelihood is NOT a PDF

A Poisson distribution describes a discrete event count n for a real valued  $Me_{\mu}$ .

$$Pois(n|\mu) = \mu^n \frac{e^{-\mu}}{n!}$$

Say, we observe  $n_o$  events What is the likelihood of  $\mu$ ? The likelihood of  $\mu$  is given by  $L(\mu) = Pois(n_o | \mu)$ It is a continues function of  $\mu$  but it is NOT a PDF

as a function of  $\boldsymbol{\mu}$  it is not a pdf

原始の 「「「」」



Figure from R. Cousins, Am. J. Phys. 63 398 (1995)

## Testing an Hypothesis (wikipedia...)

- The first step in any hypothesis test is to state the relevant null,  $H_0$  and alternative hypotheses, say,  $H_1$
- The next step is to define a test statistic, q, under the null hypothesis
- $_{\bullet}$  Compute from the observations the observed value  $q_{obs}$  of the test statistic q.
- Decide (based on q<sub>obs</sub>) to either
   fail to reject the null hypothesis or
   reject it in favor of an alternative hypothesis
- next: How to construct a test statistic, how to decide?

### Basic Definitions: type I-II errors

- By defining α you determine your tolerance towards mistakes... (accepted mistakes frequency)
- type-I error: the probability to reject the tested (null) hypothesi: (H<sub>o</sub>) when it is true

• 
$$\alpha = \Pr{ob(reject H_0 | H_0)}$$
  
 $\alpha = typeI error$ 

• Type II: The probability to accept null hypothesis when it is wrong  $\beta = \Pr ob(accept H_0 | \overline{H}_0) \longrightarrow$  $\beta = typeII \ error$  The pdf of q....



### **Basic Definitions: POWER**

- $\alpha = \Pr{ob(reject H_0 | H_0)}$
- The POWER of an hypothesis test is the probability to reject the null hypothesis when it is indeed
   (the alternate analysis is true)
- $POWER = \Pr ob(reject H_0 | \overline{H}_0)$   $\beta = Prob(accept H_0 | \overline{H}_0)$   $1 - \beta = Prob(reject H_0 | \overline{H}_0)$   $\overline{H}_0 = H_1$  $1 - \beta = Prob(reject H_0 | H_1)$
- The power of a test increases as the rate of type II error decreases



#### **Basic Definitions: POWER**

- $\alpha = \Pr{ob(rej ect H_0 \mid H_0)}$
- The POWER of an hypothesis test is the probability to reject the null hypothesis when the alternate analysis is true!

• 
$$POWER = Prob(reject H_0 | H_1)$$
  
 $\beta = Pr ob(rej ect H_1 | H_1) \Rightarrow$   
 $1 - \beta = Pr ob(accept H_1 | H_1) \Rightarrow$   
 $1 - \beta = Pr ob(rej ect H_0 | H_1) \Rightarrow$   
 $POWER = 1 - \beta$ 

• The power of a test increases as the rate of type II error decreases



### p-Value

- The observed p-value is a measure of the compatibility of the data with the tested hypothesis.
- It is the probability, under assumption of the null hypothesis  $H_{null,}$  of finding data of equal or greater incompatibility with the predictions of  $H_{null}$
- An important property of a test statistic is that its sampling distribution under the null hypothesis be calculable, either exactly or approximately, which allows p-values to be calculated. (Wiki)

#### PDF of a test statistic









# Spin Ovs Spin 1 Hypotheses



### The Neyman-Pearson Lemma

- Define a test statistic  $\lambda = \frac{L(H_1)}{L(H_0)}$
- When performing a hypothesis test between two simple hypotheses,  $H_o$  and  $H_1$ , the Likelihood Ratio test,  $\lambda = \frac{L(H_1)}{L(H_0)}$

which rejects  $H_0$  in favor of  $H_1$ , is the **most powerful test** for a given significance level  $\alpha = prob(\lambda \le \eta)$ with a threshold  $\eta$ 

### Building PDF

#### Build the pdf of the test statistic

$$q_{NP} = q_{NP}(x) = -2 \ln \frac{L(H_0 | x)}{L(H_1 | x)}$$





### Building PDF

#### **Build the pdf of the test statistic**

$$q_{NP} = q_{NP}(x) = -2 \ln \frac{L(H_0 | x)}{L(H_1 | x)}$$





### Power and Luminosity

For a given significance the power increases with increased luminosity

Luminosity ~ Total number of events in an experiment

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For a given significance the power increases with increased luminosity

Luminosity ~ Total number of events in an experiment















Best estimate of parameters to fit theory to data  $\hat{ heta}_i$ 

It is obtained maximizing the likelihood

We get 
$$t^*(\hat{ heta})$$

Problem of finding the maxima of a K-dimensional function

• Analytically, by doing the derivatives of the function (of the logarithm of the function to simplify the calculations) with respect to the parameters and putting them equal to 0.

 $L(x/\underline{\theta}) = L(\underline{\theta})$ 

$$\frac{\partial \ln L}{\partial \theta_k} = 0$$

system of M equations with M unknowns

• Numerically, in all cases. The "hystorical" program MINUIT developed at CERN in the '70s is still now the most used package for this kind of problems.

ML estimators properties:

- (1) **Unbiasness**: the mean of the estimator should be equal to the "true" value of the parameter  $E[\hat{\theta}] = \theta_{true}$ .
- (2) **Consistency**: the estimator should converge to the "true" value once the number of measurements increases  $Var[\hat{\theta}] \to 0$  for  $N \to \infty$ .
- (3) **Efficiency**: the estimator variance should be the minimum, any other estimator of the same parameter should have a larger variance.

$$oldsymbol{\hat{ heta}}$$
 Is a random variable with its own pdf's:  $ext{E}[\hat{ heta}] \; ext{Var}[\hat{ heta}]$ 

Central values of the parameter estimation  $\hat{ heta}\pm\sigma_{\hat{ heta}}$  and interval estimation

(for the moment with probability content in the frequentist approach)

In general maximizing :

We get central values :

$$L(x|\underline{\theta})$$

with covariance matrix : 
$$V_{jk} = cov[\hat{ heta}_j,\hat{ heta}_k]$$

 $\theta$ 

$$oldsymbol{\hat{ heta}}$$
 Is a random variable with its own pdf's:  $ext{E}[\hat{ heta}] \; ext{Var}[\hat{ heta}]$ 

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$$L(x|\underline{\theta})$$

with covariance matrix : 
$$V_{jk} = cov[\hat{ heta}_j,\hat{ heta}_k]$$

 $\theta$ 

#### Parameter estimation: Cramer-Rao inequality

(K=1). The variance of an unbiassed estimator  $\hat{\theta}$  obeys the following inequality:

$$Var[\hat{\theta}] \ge \frac{1}{E\left[-\frac{\partial^2 \ln L}{\partial \theta^2}\right]}$$

the denominator is also called **Fisher information** factor, and is usually indicated as  $I(\theta)$ .

(K > 1). Given the "Fisher information" matrix

$$I(\underline{\theta})_{jk} = E\left[-\frac{\partial^2 \ln L}{\partial \theta_j \theta_k}\right]$$

each term of the covariance matrix  $V_{jk}$  obeys the following inequality

$$V_{jk} \ge I^{-1}(\underline{\theta})_{jk}$$

The Fisher information matrix is also called Hessian matrix of the function L

The Cramer-Rao inequality states that the inverse of the Fisher information is the minimum variance attainable for an estimator. When the inequality becomes an equality, the estimator is said to be **fully efficient**.

 $I^{-1}(\underline{\theta})_{jk}$  is the inverse of the Hessian matrix.

#### ML Parameter estimators:

Theorems:

- If, for a given parameter, at least a fully efficient estimators exists, such an estimator is the ML estimator.
- For estimators based on a large number of observation  $N \to \infty$ , ML estimators are fully efficient.
- In case of fully efficient estimators, it is possible to replace the mean of the second derivative with the second derivative evaluated at the estimator central value:

$$E\left[-\frac{\partial^2 \ln L}{\partial \theta^2}\right] = -\frac{\partial^2 \ln L}{\partial \theta^2}\Big|_{\theta=\hat{\theta}}$$

The last two theorems are particularly important in practice. Second derivatives evaluated at the central values allow to get the covariance matrix for all ML estimators with a reasonably large number of observations. This method is extensively used to get the covariance matrix of the parameters.

#### **ML** Parameter estimators:

1-dimensional example:

 $f(\theta) = -\ln L(x | \theta)$ 

Taylor expansion around the minimum  $\, heta\,=\,\hat{ heta}\,$ 

$$f(\theta) = f(\hat{\theta}) + \frac{df}{d\theta} \bigg|_{\theta = \hat{\theta}} (\theta - \hat{\theta}) + \frac{1}{2} \frac{d^2 f}{d\theta^2} \bigg|_{\theta = \hat{\theta}} (\theta - \hat{\theta})^2 + \dots$$

The first order term vanishes, the second order coefficient (~ 1/width of the parabola), according to ML estimators and Cramer-Rao inequality:

$$\begin{aligned} \operatorname{Var}[\hat{\theta}] &\geq \frac{1}{E\left[-\frac{\partial^2 \ln L}{\partial \theta^2}\right]} &\qquad \qquad \left| \frac{d^2 f}{d\theta^2} \right|_{\theta = \hat{\theta}} = \frac{1}{\sigma_{\theta}^2} \\ & E\left[-\frac{\partial^2 \ln L}{\partial \theta^2}\right] = -\frac{\partial^2 \ln L}{\partial \theta^2} \Big|_{\theta = \hat{\theta}} \end{aligned}$$

#### ML Parameter estimators: profile likelihood method

(graphical method)

1-dimensional example:

$$f(\theta) = -\ln L(\mathbf{x} | \theta) \qquad \qquad f(\theta) = f(\hat{\theta}) + \frac{df}{d\theta} \Big|_{\theta = \hat{\theta}} (\theta - \hat{\theta}) + \frac{1}{2} \frac{d^2 f}{d\theta^2} \Big|_{\theta = \hat{\theta}} (\theta - \hat{\theta})^2 + \dots$$

**Profile Likelihood** 



 $\hat{\theta} \pm n\sigma_{\theta}$ 

FIGURE 11. Scheme of principle of a profile likelihood method. A  $-\ln L$  with parabolic shape is shown for a given variable X. Horizontal lines are shown for  $-\ln L_{max} + \frac{1}{2}n^2$  for n = 0, 1, 2, 3 and a  $\pm 1 \sigma$  is shown for the X variable.

#### ML Parameter estimators: profile likelihood method

(graphical method)

1-dimensional example:

$$f(\theta) = -\ln L(\mathbf{x} | \theta) \qquad \qquad f(\theta) = f(\hat{\theta}) + \frac{df}{d\theta} \Big|_{\theta = \hat{\theta}} (\theta - \hat{\theta}) + \frac{1}{2} \frac{d^2 f}{d\theta^2} \Big|_{\theta = \hat{\theta}} (\theta - \hat{\theta})^2 + \dots$$

**Profile Likelihood** 



 $\hat{\theta} \pm n\sigma_{\theta}$ 

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#### ML Parameter estimators: profile likelihood method



1-dimensional example:

FIGURE 11. Scheme of principle of a profile likelihood method. A  $-\ln L$  with parabolic shape is shown for a given variable X. Horizontal lines are shown for  $-\ln L_{max} + \frac{1}{2}n^2$  for n = 0, 1, 2, 3 and a  $\pm 1 \sigma$  is shown for the X variable.

$$\hat{\theta} \pm n\sigma_{\theta}$$

If 2<sup>nd</sup> order terms can be neglected => gaussian limit => confidence intervals with gaussian probability content (n=1,2,3 => 68%, 95%, 99.7%) (Notice that log of a gaussian function -> parabola)

#### ML Parameter estimators: profile likelihood method 1-dimensional example:

If we are not in the gaussian limit, the profile likelihood method can be used as well, and the probability content remains to a good approximation the same of the gaussian case. In this case, as shown in the example of fig.12, the intervals can be asymmetric and the result will be written as



FIGURE 12. Example of a profile likelihood method when  $-\ln L$  has not a parabolic shape. As in fig.11, horizontal lines are shown for  $-\ln L_{max} + \frac{1}{2}n^2$  for n = 0, 1, 2, 3. A "2sigma" interval is shown for X clearly asymmetric.

ML Parameter estimators: profile likelihood method 1-dimensional example:



FIGURE 13. 1-dimensional  $\chi^2$  of the Standard Model fit to get an interval for the unknown Higgs boson mass. Notice that the horizontal axis is in logarithmic scale, so that the minimum is strongly asymmetric. (very "popular" plot, taken e.g. from www.zfitter.com).

ML Parameter estimators: profile likelihood method 1-dimensional example:



FIGURE 13. 1-dimensional  $\chi^2$  of the Standard Model fit to get an interval for the unknown Higgs boson mass. Notice that the horizontal axis is in logarithmic scale, so that the minimum is strongly asymmetric. (very "popular" plot, taken e.g. from www.zfitter.com).

### ML Parameter estimators: contour likelihood method 2-dimensional example:

5.5.4. Contour Likelihood. The Profile Likelihood method described above can be applied to the single parameter case only. However when K = 2 a graphical method is also available providing an interesting insight into the fit result: the so called **contour likelihood method**. The function  $-\ln L$  is, in this case, a 2D function  $f(\theta_1, \theta_2)$  that, around the minimum  $\hat{\theta}_1, \hat{\theta}_2$  has a 2-D paraboloid shape. For a given probability content  $\beta$ , regions  $S_\beta$  can be defined in the  $\theta_1 - \theta_2$  plane with the property:

(134) 
$$p([\theta_1, \theta_2] \subset S_\beta) = \beta$$

that is regions containing the point  $\theta_1, \theta_2$  with probability  $\beta$ . Such regions can be obtained by intersecting the surface  $f(\theta_1, \theta_2)$ , with planes of constant  $-\ln L$  at values (compare to eq.130)

(135) 
$$-\ln L_{max} + \Delta \ln L_{\beta}$$

The equivalent of eq.128 for the two parameters case, is, in the gaussian limit

(136) 
$$-\ln L = -\ln L_{max} + \frac{1}{2}(\theta - \hat{\theta})^T V^{-1}(\theta - \hat{\theta})$$

where we have used directly the matrix formalism (T means transposed). By comparing eq.136 with eq.117 we see that  $-\ln L + \ln L_{max}$  has a  $\chi^2$  distribution with 2 degrees of freedom. This allows to evaluate the values of  $\Delta \ln L_{\beta}$  of eq.135. Table 2 gives the values of  $\Delta \ln L_{\beta}$  for K = 1, 2 and 3 for three different values of  $\beta$ . For K = 3 or more, the graphical contour representation is not available, but regions  $S_{\beta}$  can be built with the same method.

#### ML Parameter estimators: contour likelihood method 2-dimensional example:

TABLE 2. For 3 different values of probability levels (corresponding to the usual 1,2 and 3 gaussian std.deviations) the values of  $\Delta \ln L_{\beta}$  are given for one-parameter (K=1) and two or three-parameters fits.

$\beta$ (%)	$2\Delta \ln L_{\beta} \ (K=1)$	$2\Delta \ln L_{\beta} \ (K=2)$	$2\Delta \ln L_{\beta} \ (K=3)$
68.3	1	2.30	3.53
95.4	4	6.18	8.03
99.7	9	11.83	14.16

#### contour

$_{\sim}$ 10 <b>Table 9.4</b> The $n = 1, 2, 3, 4, 5$ fitte	values ed para	of the co meters.	onfidence	level 1 —	: $\gamma$ for diff	ferent valı	ies of $Q_{\gamma}$ and for	
	0			$1 - \gamma$				
	<i>Ψ</i> γ	n = 1	n = 2	n = 3	n = 4	n = 5		
	1.0	0.683	0.393	0.199	0.090	0.037		
	2.0	0.843	0.632	0.428	0.264	0.151		
	4.0	0.954	0.865	<b>0</b> .7 <b>3</b> 9	0.594	0.451		
	9.0	0.997	0.989	0.971	0.939	0.891		

From Cowan:

**Table 9.5** The values of the quantile  $Q_{\gamma}$  for different values of the confidence level  $1 - \gamma$  for n = 1, 2, 3, 4, 5 fitted parameters.

$1-\gamma$	$Q_{\gamma}$					
	n = 1	n = 2	n = 3	n = 4	n = 5	
0.683	1.00	2.30	3.53	4.72	5.89	
0.90	2.71	4.61	6.25	7.78	9.24	
0.95	3.84	5.99	7.82	9.49	11.1	
0.99	6.63	9.21	11.3	13.3	15.1	

\_\_\_\_\_ 10 θ,



inclination of the two axis being a measure of the correlation between  $\theta_1$  and  $\theta_2$ .

An important point to notice is the following: the probability content  $\beta$  of an ellipse, corresponds to the probability that both parameters are in the region. On the other side, the projection of the ellipse on each single axis (e.g. on the  $\theta_1$  axis see fig.14) corresponds to the probability that  $\theta_1$  is in the range whatever is the value of  $\theta_2$ . Such probability is of course larger than  $\beta$ . To give the size of this effect we quote the following numbers: an interval for  $\theta_1$  built as a projection from a 2D ellipse with  $\beta$ =68.3% has a probability content of 97%. On the other hand if the projection has a probability content of 68.3%, the  $\beta$  of the corresponding ellipse is 39.3%.



FIGURE 14. Contour plot of two correlated parameters in the gaussian limit. The ellipse shown in yellow, is the  $S_{\beta}$  region described in the text. The horizontal and vertical bands allow to get 1-dimensional intervals for the two variables. The probability contents of these intervals is different from  $\beta$ .

Finally, non-elliptical contours are built when the gaussian limit is not reached. Examples of highly non-elliptical 2D contours are shown in fig.15.



FIGURE 15. From the ATLAS experiment. Results of the fits of 3 different Higgs decay channels (namely  $\gamma\gamma$ , ZZ and WW) in a 2-dimensional plane, mass vs. signal strength. For each fit, both 68% and 95% probability regions are shown. Notice that in all the cases apart from the  $\gamma\gamma$ , we are very far from the gaussian limit. (taken from ATLAS collaboration, Phys.Lett. B716 (2012) 1-29).