# PRACTICAL STATISTICS FOR PARTICLE PHYSICISTS

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## LECTURES

- Likelihood: Parameter determination and L-ratio
   Chi-squared: Param determination & Goodness of Fit
- 2) Bayes & Frequentist Approaches
- 2) and 3) Searches for New Physics: Discovery and Limits

Possible 4) Learning to love the Covariance Matrix

Plus: Discussions Problems Working on statistical issues

# Omitting introductory material

- Why spend time on understanding Statistics?
- Relation of Statistics to Probability Theory
- Random and systematic uncertainties
- Binomial distribution
- Poisson distribution
- Relationships among Binomial, Poisson & Gaussian
- Types of Statistical Procedures:

Parameter determination

- Goodness of Fit
- Hypothesis Testing
- **Decision Theory**

**Likelihoods** 1) Brief Introduction 2) Do's & Dont's

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# Topics

- What it is
- How it works: Resonance
- **Uncertainty estimates**
- **Detailed example: Lifetime**
- **Several Parameters**
- Extended maximum  $\mathcal{L}$

## Do's and Dont's with $\boldsymbol{\mathcal{L}}$

## DO'S AND DONT'S WITH *L*

- NORMALISATION FOR LIKELIHOOD
- JUST QUOTE UPPER LIMIT
- $\Delta(\ln \mathcal{L}) = 0.5 \text{ RULE}$  \*\*\*\*
- $\mathcal{L}_{max}$  AND GOODNESS OF FIT \*\*\*\*\*\*
- $\bullet \int_{p_L}^{p_u} \mathcal{L} \, \mathrm{d}p = 0.90$
- BAYESIAN SMEARING OF  $\mathcal L$
- USE CORRECT  $\mathcal{L}$  (PUNZI EFFECT)

### Simple example: Angular distribution

Data =  $\theta_1 \ \theta_2 \ \theta_3 \ \dots \ \theta_n$ 

 $y = N (1 + \beta \cos^2 \theta)$  {RULE 1: Write down pdf}  $y_i = N (1 + \beta \cos^2 \theta_i)$ = probability density of observing  $\theta_i$ , given  $\beta$  $\mathcal{L}(\beta) = \prod y_i$ = probability density of observing the data set  $y_i$ , given  $\beta$ Best estimate of  $\beta$  is that which maximises  $\mathcal{L}$ Values of  $\beta$  for which  $\mathcal{L}$  is very small are ruled out Uncertainty of estimate for  $\beta$  comes from width of  $\mathcal{L}$  distribution

**RULE 2: CRUCIAL** to normalise y  $N = 1/\{2(1 + \beta/3)\}$ 

(Information about parameter  $\beta$  comes from **shape** of exptl distribution of  $\cos\theta$ )







н.

## Maximum likelihood uncertainty

Range of likely values of param  $\mu$  from width of  $\mathcal{L}$  or  $\ell$  dists. If  $\mathcal{L}(\mu)$  is Gaussian, following definitions of  $\sigma$  are equivalent: 1) RMS of  $\mathcal{L}(\mu)$ 

2)  $1/\sqrt{(-d^2 \ln \mathcal{L} / d\mu^2)}$  (Mnemonic)

3)  $\ln(\mathcal{L}(\mu_0 \pm \sigma) = \ln(\mathcal{L}(\mu_0)) - 1/2$ 

If  $\mathcal{L}(\mu)$  is non-Gaussian, these are no longer the same

"Procedure 3) above still gives interval that contains the true value of parameter µ with 68% probability"

Uncertainties from 3) usually asymmetric, and asym uncertainties are messy. So choose param sensibly

e.g 1/p rather than p;  $\tau \text{ or } \lambda$ 

### Lifetime Determination

Realistic analyses are more complicated than this

$$\frac{d}{dt} = \frac{1}{2} e^{-\frac{t}{2}/t}$$

$$\frac{d}{dt} = \frac{1}{2} (-\frac{t}{2}/t) = \frac{1}{2} e^{-\frac{t}{2}/t}$$

$$\frac{d}{dt} = \frac{1}{2} (-\frac{t}{2}/t) = -\frac{1}{2} e^{-\frac{t}{2}/t}$$

$$\frac{d}{dt} = \frac{1}{2} (+\frac{t}{2}/t) = -\frac{1}{2} e^{-\frac{t}{2}/t}$$

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$$\frac{d}{dt} = \frac{1}{2} e^{-\frac{t}{2}/t}$$

$$\frac{d}{dt} = \frac{1}{2$$

12

#### Several Parameters



#### PROFILE $\mathcal{L}$

 $\mathcal{L}_{prof} = \mathcal{L}(\beta, v_{best}(\beta)), \text{ where } \beta = param of interest } v = nuisance param(s) Uncertainty on <math>\beta$  from decrease in  $ln(\mathcal{L}_{prof})$  by 0.5

a) May line  
Prob for fixed N = Binomial  
Prob for fixed N = 
$$F = F(1-f)^{n} \frac{N!}{F!B!}$$
  
Maximise  $lnP_{n}$  with  $f \Rightarrow f = F/N$   
Error  $n f : 1/\sigma^{2} = -\frac{\partial^{2} ln P_{n}}{\partial f^{2}}$   
 $= \frac{N}{f(1-f)}$   $f = f$   
 $\Rightarrow Estimate of  $F = NF = F \pm \sqrt{FF/N} = Conflictly$   
 $= N(1-f) = B \pm [FB/N] = anti-corr$   
b) EML  $P_{i} = P_{n} \times \frac{d}{N!}$  Prism for orall rate  
Maximize  $ln P_{i}(v, f)$   
 $\Rightarrow S = N \pm \sqrt{N}$  Prism for orall rate  
Maximize  $ln P_{i}(v, f)$   
 $\Rightarrow F = F_{i} \pm \sqrt{F(1-f)}$  uncorrelated  
For  $F = R^{2}$ , eiter projegate errors for  $F = \hat{v}f$   
 $f = F_{i} \pm \sqrt{F(1-f)}$   
 $f = F \pm \sqrt{F}$   
 $B = B \pm \sqrt{F}$$ 

## DO'S AND DONT'S WITH *L*

- COMBINING PROFILE  $\mathcal{L}_{S}$
- NORMALISATION FOR LIKELIHOOD
- JUST QUOTE UPPER LIMIT
- $\Delta(\ln L) = 0.5 \text{ RULE } ******$
- $\mathcal{L}_{max}$  AND GOODNESS OF FIT \*\*\*\*\*\*
- $\int_{p_L}^{p_u} \mathcal{L} dp = 0.90$
- BAYESIAN SMEARING OF  $\boldsymbol{\mathcal{L}}$
- USE CORRECT  $\mathcal{L}$  (PUNZI EFFECT)

# Danger of combining profile *L*s

Experiments quote *£*ikelihood, profiled over nuisance parameters, so that combinations can be performed.

Very simple 'tracking' example:

- \* No magnetic field
- \* 2-D fit of straight line y = a + bx

a = parameter of interest, b = nuisance param

\* Track hits in 2 subdetectors, each of 3 planes





(a) Hits in 2 sub-detectors, each with 3 planes

(b) Covariance ellipses for separate fits  $L_1$  In and  $L_2$ , and combined  $L_{comb}$ 

(c)  $\ln \mathcal{L}_{prof}$  as function of a, for all 3 lines (d)  $b_{best}$  as a function of a

N.B.  $b_{best}$  for L<sub>1</sub> and L<sub>2</sub> are the same

\*\*\* Combining  $\mathcal{L}_{prof}$  for L<sub>1</sub> and L<sub>2</sub> loses a lot of information, and a<sub>best</sub> wrong \*\*\*\*



#### COSMOLOGY EXAMPLE

Plot of dark energy fraction v dark matter fraction by various methods. Each determines dark energy fraction poorly, but combination is fine, because of different correlations.

Combining Profile Likelihoods would give very large uncertainty on dark energy fraction.



## $\Delta \ln \mathcal{L} = -1/2$ rule

If  $\mathcal{L}(\mu)$  is Gaussian, following definitions of  $\sigma$  are equivalent:

1) RMS of  $\mathcal{L}(\mu)$ 

2)  $1/\sqrt{(-d^2 \mathcal{L}/d\mu^2)}$ 

3)  $ln(\mathcal{L}(\mu_0 \pm \sigma) = ln(\mathcal{L}(\mu_0)) - 1/2$ 

If  $\mathcal{L}(\mu)$  is non-Gaussian, these are no longer the same "Procedure 3) above still gives interval that contains the true value of parameter  $\mu$  with 68% probability"

Heinrich: CDF note 6438 (see CDF Statistics Committee Web-page) Barlow: Phystat05





← 68%

μ

Ideal coverage

plot

IC(µ)

\* What it is:

For given statistical method applied to many sets of data to extract confidence intervals for param  $\mu$ , coverage C is fraction of ranges that contain true value of param. Can vary with  $\mu$ 

#### \* Does not apply to **your** data:

It is a property of the **statistical method** used It is **NOT** a probability statement about whether  $\mu_{true}$  lies in your confidence range for  $\mu$ 

\* Coverage plot for Poisson counting expt Observe n counts

Estimate  $\mu_{\text{best}}$  from maximum of likelihood

 $\begin{aligned} \mathcal{L}(\mu) &= e^{-\mu} \, \mu^n / n! \quad \text{and range of } \mu \text{ from } \ln\{\mathcal{L}(\mu_{\text{best}}) / \mathcal{L}(\mu)\} < 0.5 \\ \text{For each } \mu_{\text{true}} \text{ calculate coverage } C(\mu_{\text{true}}), \text{ and compare with nominal } 6\% \end{aligned}$ 

#### COVERAGE

How often does quoted range for parameter include param's true value?

N.B. Coverage is a property of METHOD, not of a particular exptl result

Coverage can vary with  $\mu$ 

Study coverage of different methods of Poisson parameter  $\mu$ , from observation of number of events n



## **COVERAGE**

If true for all  $\mu$ : "correct coverage"

- $P < \alpha$  for some  $\mu$  "undercoverage" (this is serious !)
  - $P > \alpha$  for some  $\mathcal{L}$  "overcoverage" Conservative
    - Loss of rejection power

### Coverage : *L* approach (Not Neyman construction)

 $P(n,\mu) = e^{-\mu}\mu^{n}/n!$  (Joel Heinrich CDF note 6438)

-2  $\ln\lambda < 1$   $\lambda = P(n,\mu)/P(n,\mu_{best})$  UNDERCOVERS



### Neyman central intervals, NEVER undercover

(Conservative at both ends)



## **Feldman-Cousins Unified intervals**



## **Probability ordering**





#### NOT Neyman : Coverage = $0\% \rightarrow 100\%$



## Unbinned $\mathcal{L}_{max}$ and Goodness of Fit?

Find params by maximising  $\mathcal L$ 

So larger  $\mathcal L$  better than smaller  $\mathcal L$ 

So  $\mathcal{L}_{max}$  gives Goodness of Fit??









#### Example 1

Fit exponential to times  $t_1, t_2, t_3$  ..... [Joel Heinrich, CDF 5639]

 $\mathcal{L} = \mathbf{\pi} \lambda \exp(-\lambda t_i)$ 

 $ln \mathcal{L}_{max} = -N(1 + ln t_{av})$  (Follows from slide 12)

i.e. Depends only on AVERAGE t, but is

**INDEPENDENT OF DISTRIBUTION OF t** (except for.....)

(Average t is a 'sufficient statistic')

Variation of  $\mathcal{L}_{max}$  in Monte Carlo is due to variations in samples' average t , but NOT TO BETTER OR WORSE FIT





Example 2

$$\frac{dN}{d\cos\theta} = \frac{1 + \alpha\cos^2\theta}{1 + \alpha/3}$$
$$\mathcal{L} = \prod_{j} \frac{1 + \alpha\cos^2\theta_j}{1 + \alpha/3}$$



pdf (and likelihood) depends only on  $\cos^2\theta_i$ 

Insensitive to sign of  $\cos\theta_i$ 

So data can be in very bad agreement with expected distribution

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e.g. all data with \cos\theta < 0
```

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and \mathcal{L}_{max} does not know about it.
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#### **Example of general principle**

### $\boldsymbol{\ell}_{\text{max}}$ and Goodness of Fit?

Conclusion:

 $\mathcal{L}$  has sensible properties with respect to parameters NOT with respect to data

# $\mathcal{L}_{max}$ within Monte Carlo peak is NECESSARY not SUFFICIENT

('Necessary' doesn't mean that you have to do it!)

### Binned data and Goodness of Fit using *L*-ratio



 $ln[\mathcal{L}-ratio] = ln[\mathcal{L}/\mathcal{L}_{best}]$ 

 $\overrightarrow{large \mu_i}$  -0.5 $\chi^2$  i.e. Goodness of Fit  $\mathcal{L}_{best}$  is independent of parameters of fit, and so same parameter values from  $\mathcal{L}$  or  $\mathcal{L}$ -ratio

Baker and Cousins, NIM A221 (1984) 437

# For comparing 2 hypotheses

e.g. Does data favour 'Just SM' or 'SM + New Physics'. (Much more later in Lecture 2) If hypotheses are "simple", then Neyman-Peason

lemma says that  $\mathcal{L}$ -ratio is "best" for separating them.

"simple" = no free parameters

"best" = minimum contamination for fixed efficiency.

Even when hypotheses are not simple,  $\mathcal{L}$ -ratio may still be useful.

## **L** and pdf

## Example 1: Poisson

pdf = Probability density function for observing n, given  $\mu$   $P(n;\mu) = e^{-\mu} \mu^n/n!$ From this, construct  $\mathcal{L}$  as  $\mathcal{L}(\mu;n) = e^{-\mu} \mu^n/n!$ i.e. use same function of  $\mu$  and n, but for pdf,  $\mu$  is fixed, but for  $\mathcal{L}$ , n is fixed  $\mu$  $\mathcal{L}$ 

N.B.  $P(n;\mu)$  exists only at integer non-negative n  $\mathcal{L}(\mu;n)$  exists only as continuous function of non-negative  $\mu$  Example 2 Lifetime distribution

pdf  $p(t;\lambda) = \lambda e^{-\lambda t}$ 

So  $\mathcal{L}(\lambda;t) = \lambda e^{-\lambda t}$  (single observed t)

Here both t and  $\lambda$  are continuous

pdf maximises at t = 0

 $\mathcal{L}$  maximises at  $\lambda = t$ 

N.B. Functional form of p(t) and  $\mathcal{L}(\lambda)$  are different



Example 3: Gaussian

$$pdf(x;\mu) = exp\{-(x-\mu)^2/2\sigma^2\} / (\sigma\sqrt{2\pi})$$

### $\mathcal{L}(\mu; \mathbf{x}) = \exp\{-(\mathbf{x} - \mu)^2 / 2\sigma^2\} / (\sigma \sqrt{2\pi})$

N.B. In this case, same functional form for pdf and  $\boldsymbol{\pounds}$ 

So if you consider just Gaussians, can be confused between pdf and  $\mathcal{L}$ 

So examples 1 and 2 are useful

## Transformation properties of pdf and $\mathcal{L}$

Lifetime example:  $dn/dt = \lambda e^{-\lambda t}$ 

Change observable from t to y =  $\sqrt{t}$  $\frac{dn}{dy} = \frac{dn}{dt}\frac{dt}{dy} = 2y\lambda e^{-\lambda y^2}$ 

So (a) pdf changes, BUT

(b) 
$$\int_{t_0}^{\infty} \frac{dn}{dt} dt = \int_{\sqrt{t_0}}^{\infty} \frac{dn}{dy} dy$$

i.e. corresponding integrals of pdf are INVARIANT

Now for  $\mathcal{L}$ ikelihood

When parameter changes from  $\lambda$  to  $\tau=1/\lambda$ 

(a')  $\boldsymbol{\mathcal{L}}$  does not change

 $dn/dt = (1/\tau) \exp\{-t/\tau\}$ 

and so  $\mathcal{L}(\tau;t) = \mathcal{L}(\lambda=1/\tau;t)$ 

because identical numbers occur in evaluations of the two  $\mathcal{L}$ 's

BUT 
$$\int_{0}^{\lambda_{0}} L(\lambda;t) d\lambda \neq \int_{\tau_{0}}^{\infty} L(\tau;t) d\tau$$

So it is NOT meaningful to integrate  $\boldsymbol{\mathcal{L}}$ 

(However,.....)

	pdf(t;λ)	<b>£</b> (λ;t)
Value of function	Changes when observable is transformed	INVARIANT wrt transformation of parameter
Integral of function	INVARIANT wrt transformation of observable	Changes when param is transformed
Conclusion	Max prob density not very sensible	Integrating £ not very sensible 48

#### CONCLUSION:

$$\int_{p_l}^{p_u} L dp = \alpha \quad \text{NOT recognised statistical procedure}$$

[Metric dependent:

 $\tau$  range agrees with  $\tau_{pred}$  $\lambda$  range inconsistent with  $1/\tau_{pred}$  ]

#### BUT

- Could regard as "black box" 1)
- Make respectable by  $\mathcal{L}$   $\square$  Bayes' posterior 2)

Posterior( $\lambda$ ) ~  $\mathcal{L}(\lambda)$ \* Prior( $\lambda$ ) [and Prior( $\lambda$ ) can be constant]

6) BAYESIAN SHEARING OF X  
"USE la I FOR 
$$\beta + \delta_{\beta}$$
  
SHEAR IT TO INCORORATE  
SYSTEMATIC UNCERTAINTIES  
SLEAARIO:  
M = POISSON ( $\mu = se + b$ )  
PARAM OF INTEREST I BACKGROUND  
GFPIC/ACCEPTANCE//X  
UNCERTAINTIES  
MERSURED IN SUBSIDIARY EXPT  
P(s, e | n) =  $n(n|s, e) T(s, e)$   
N : SUBSIDIARY EXPT  
P(s | n) =  $\int P(s, e| n) de$   
=  $\int X T(s) T(e) Ae$   
 $I = \int P(s, e| n) de$   
I : SHEAR X (not but) by prior for e

# Getting *L* wrong: Punzi effect

Giovanni Punzi @ PHYSTAT2003 "Comments on  $\mathcal{L}$  fits with variable resolution"

Separate two close signals, when resolution  $\sigma$  varies event by event, and is different for 2 signals e.g. 1) Signal 1 1+cos<sup>2</sup> $\theta$ Signal 2 Isotropic and different parts of detector give different  $\sigma$ 

2) M (or  $\tau$ ) Different numbers of tracks  $\rightarrow$  different  $\sigma_{M}$  (or  $\sigma_{\tau}$ ) Events characterised by  $x_i$  and  $\sigma_i$ 

#### A events centred on x = 0

B events centred on x = 1

$$\mathcal{L}(f)_{wrong} = \Pi [f * G(x_i, 0, \sigma_i) + (1-f) * G(x_i, 1, \sigma_i)]$$
  
$$\mathcal{L}(f)_{right} = \Pi [f^* p(x_i, \sigma_i; A) + (1-f) * p(x_i, \sigma_i; B)]$$

$$p(S,T) = p(S|T) * p(T)$$
$$p(x_i,\sigma_i|A) = p(x_i|\sigma_i,A) * p(\sigma_i|A)$$
$$= G(x_i,0,\sigma_i) * p(\sigma_i|A)$$

So

 $\boldsymbol{\mathcal{L}}(f)_{right} = \Pi[f \ast G(x_i, 0, \sigma_i) \ast p(\sigma_i | A) + (1 - f) \ast G(x_i, 1, \sigma_i) \ast p(\sigma_i | B)]$ 

If  $p(\sigma|A) = p(\sigma|B)$ ,  $\mathcal{L}_{right} = \mathcal{L}_{wrong}$ 

but NOT otherwise

Punzi's Monte Carlo for		A: G(x,0,σ	<u>д</u> )			
		B: G(x,1,σ <sub>1</sub>	<sub>3</sub> )			
		$f_{A} = 1/3$				
		$\mathcal{L}_{wror}$	$\mathcal{L}_{wrong}$		$\mathcal{L}_{right}$	
$\sigma_{\rm A}$	$\sigma_{\rm B}$	f <sub>A</sub>	$\sigma_{\rm f}$	f <sub>A</sub>	$\sigma_{f}$	
1.0	1.0	0.336(3)	0.08	Same		
1.0	1.1	0.374(4)	0.08	0.333(0)	0	
1.0	2.0	0.645(6)	0.12	0.333(0)	0	
1 → 2	1.5 →3	0.514(7)	0 <sup>.</sup> 14	0.335(2)	0.03	
1.0	1 <del>→</del> 2	0.482(9)	0.09	0.333(0)	0	
				0055		

1)  $\mathcal{L}_{wrong}$  OK for  $p(\sigma_A) = p(\sigma_B)$ , but otherwise BIASSED

- 2)  $\mathcal{L}_{right}$  unbiassed, but  $\mathcal{L}_{wrong}$  biassed (enormously)!
- 3)  $\mathcal{L}_{right}$  gives smaller  $\sigma_{f}$  than  $\mathcal{L}_{wrong}$



Fit gives upward bias for  $N_A/N_B$  because (i) that is much better for A events; and (ii) it does not hurt too much for B events



Originally:

Positions of peaks = constant

K-peak  $\rightarrow \pi$ -peak at large momentum

 $\sigma_i \text{ variable, } (\sigma_i)_A \neq (\sigma_i)_B \qquad \sigma_i \sim \text{ constant, } p_K \neq p_{\pi}$ 

COMMON FEATURE: Separation/Error  $\neq$  Constant

Where else??

MORAL: Beware of event-by-event variables whose pdf's do not appear in  $\mathcal{L}$ 

# Avoiding Punzi Bias

### BASIC RULE:

Write pdf for ALL observables, in terms of parameters

 Include p(σ|A) and p(σ|B) in fit (But then, for example, particle identification may be determined more by momentum distribution than by PID)

#### OR

• Fit each range of  $\sigma_i$  separately, and add  $(N_A)_i \rightarrow (N_A)_{total}$ , and similarly for B

Incorrect method using  $\mathcal{L}_{wrong}$  uses weighted average of  $(f_A)_j$ , assumed to be independent of j

Talk by Catastini at PHYSTAT05

## Conclusions

- How it works, and how to estimate uncertainties
- $\Delta(\ln \mathcal{L}) = 0.5$  rule and coverage
- **Several Parameters**
- Likelihood does not guarantee coverage
- Unbinned  $\mathcal{L}_{max}$  and Goodness of Fit
- Use correct  $\mathcal{L}$  (Punzi effect)