PRACTICAL STATISTICS FOR PARTICLE PHYSICISTS

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LECTURES

- 1) Likelihood: Parameter determination
- 2) Chi-squared: Param determination & Goodness of Fit
- 3) Learning to love the Covariance Matrix
- 4) (a) Combining results
 - (b) Understanding Neural Networks
- 5) Searches for New Physics: Discovery and Limits
- 6) What is Probability? Bayes & Frequentist Approaches

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

Likelihoods

Brief Introduction
 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 £

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 θ_i , given β

$$\mathcal{L}(\beta) = \prod y_i$$

= probability density of observing the data set y_i , given β

Best estimate of β is that which maximises \mathcal{L}

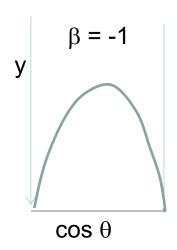
Values of β for which \mathcal{L} is very small are ruled out

Uncertainty of estimate for β comes from width of \mathcal{L} distribution

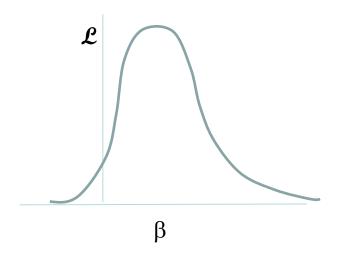
CRUCIAL to normalise y
$$N = 1/\{2(1 + \beta/3)\}$$

$$N = 1/\{2(1 + \beta/3)\}$$

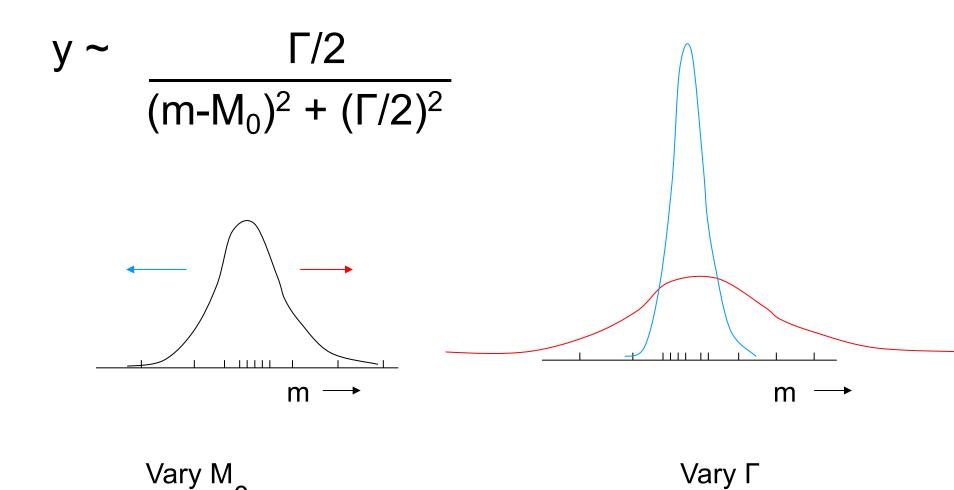
(Information about parameter β comes from **shape** of exptl distribution of $\cos\theta$)







How it works: Resonance



Conventional to consider

$$\ell = \ln(\mathcal{L}) = \sum \ln(y_i)$$

For large N, $\mathcal{L} \rightarrow$ Gaussian

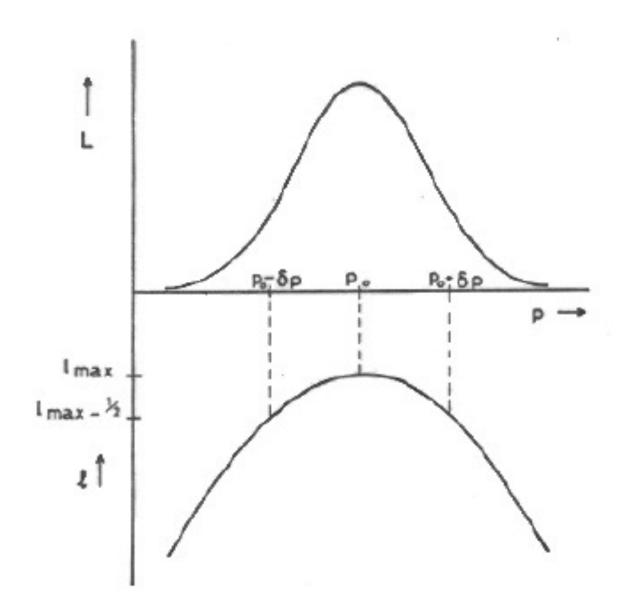
Proof"

Taylor aspard I char it maximum

$$l = l_{max} + \frac{1}{2!} l'' \left[\delta \left(\frac{6}{a} \right) \right]^2 + \cdots$$

$$= l_{max} - \frac{1}{2c} \delta^2 + \cdots \qquad c=-1/l''$$

$$\Rightarrow l' \sim exp \left(-\frac{\delta^2}{2c} \right)$$



Maximum likelihood uncertainty

Range of likely values of param μ from width of \mathcal{L} or 1 dists. If $\mathcal{L}(\mu)$ is Gaussian, following definitions of σ 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

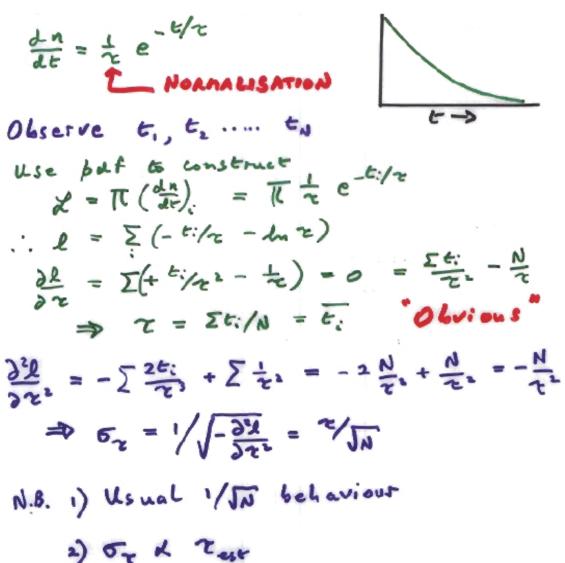
"Procedure 3) above still gives interval that contains the true value of parameter μ with 68% probability"

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

e.g 1/p rather than p; τ or λ

Lifetime Determination

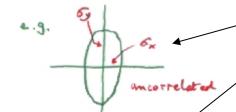
Realistic analyses are more complicated than this



Several Parameters

1 farm b

from
$$\frac{\partial L}{\partial p} = 0$$
 $\sigma_p^2 = \frac{1}{(-\frac{\partial^2 L}{\partial p^2})}$



Contours of $In \mathcal{L}$

PROFILE \mathcal{L}

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

Extended Maximum Likelihood

Maximum Likelihood uses shape → parameters

Extended Maximum Likelihood uses shape and normalisation
i.e. EML uses prob of observing:

- a) sample of N events; and
- b) given data distribution in x,.....
 - → shape parameters and normalisation.

```
Example: Angular distribution

Observe N events total e.g 100

F forward 96

B backward 4

Rate estimates ML EML

Total --- 100±10

Forward 96±2 96±10

Backward 4+2 4+2
```

ML and EML

ML uses fixed (data) normalisation EML has normalisation as parameter

```
Example 1: Cosmic ray experiment
             See 96 protons and
```

ML estimate 96 ± 2% protons 4 ±2% heavy nuclei EML estimate 96 ± 10 protons 4 ± 2 heavy nuclei

4 heavy nuclei

Example 2: Decay of resonance Use ML for Branching Ratios Use EML for Partial Decay Rates

a) Mar Like Prob for fixed N = Binomial

Prob for fixed N = Binomial

Fill 1

FIB! Maximise LP STE f = F/N Error a f: 1/62 = - 32 lm Pa $\approx \frac{N}{\hat{a}(1-\hat{a})}$ $f = \hat{f}$ => Estimate of F = NF = F± (FE/N = Conflicted) B = N(1-4) = B = [FB/N anti-corr b) EML P = P x = x Priss for overall rate Maxing ise In P. (v, f) $\hat{f} = N \pm \sqrt{N} = uncorrelated$ $\hat{f} = \sqrt{f(1-f)} = uncorrelated$ For $\hat{F} = \hat{g}$, eiter propagate errors for $\hat{F} = \hat{y}\hat{f}$ or reside eqn ϕ as product $\hat{g} = \hat{g}(1-\hat{f})$ $\hat{F} = F \pm JF$ $A = B \pm JB$

DO'S AND DONT'S WITH £

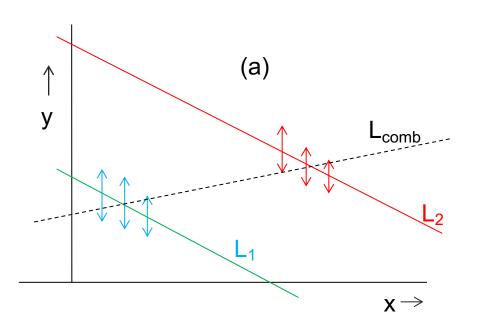
- COMBINING PROFILE Ls
- NORMALISATION FOR LIKELIHOOD
- JUST QUOTE UPPER LIMIT
- $\Delta(\ln \mathcal{L}) = 0.5 \text{ RULE}$
- L_{max} AND GOODNESS OF FIT
- BAYESIAN SMEARING OF £
- USE CORRECT £ (PUNZI EFFECT)

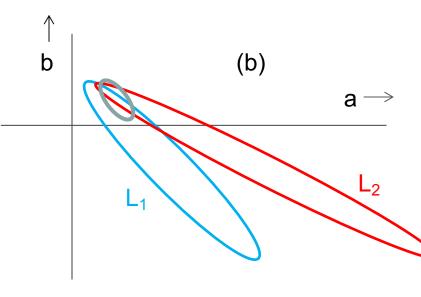
Danger of combining profile Ls

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



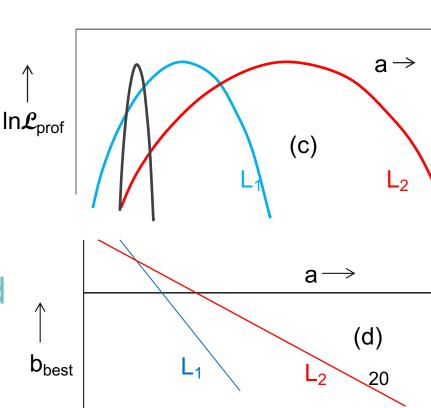


(a) Hits in 2 sub-detectors, each with 3 planes

(b) Covariance ellipses for separate fits L_1 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 L₁ and L₂ are the same

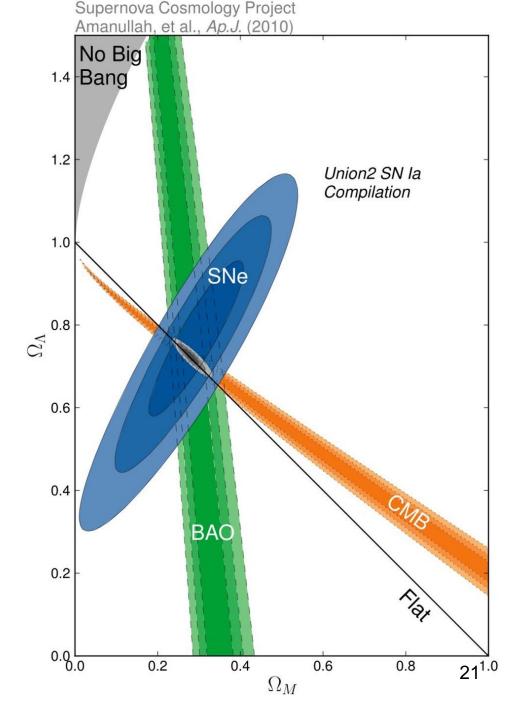
*** Combining \mathcal{L}_{prof} for L_1 and L_2 loses a lot of information, and a_{best} wrong *****



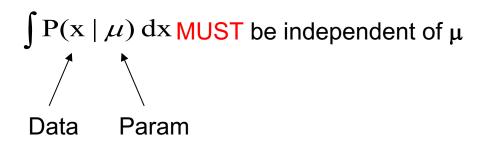
COSMOLOGY EXAMPLE

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.



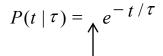
NORMALISATION FOR LIKELIHOOD



$$[\tau = \sum t_i / N]$$

Exponential Distribution





Missing $1/\tau$

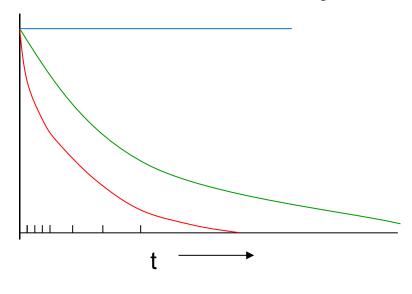
---- τ infinite



τ too large



 τ about right



QUOTING UPPER LIMIT

"We observed no significant signal, and our 90% confupper limit is"

Need to specify method e.g.

L

Chi-squared (data or theory error)

Frequentist (Central or upper limit)

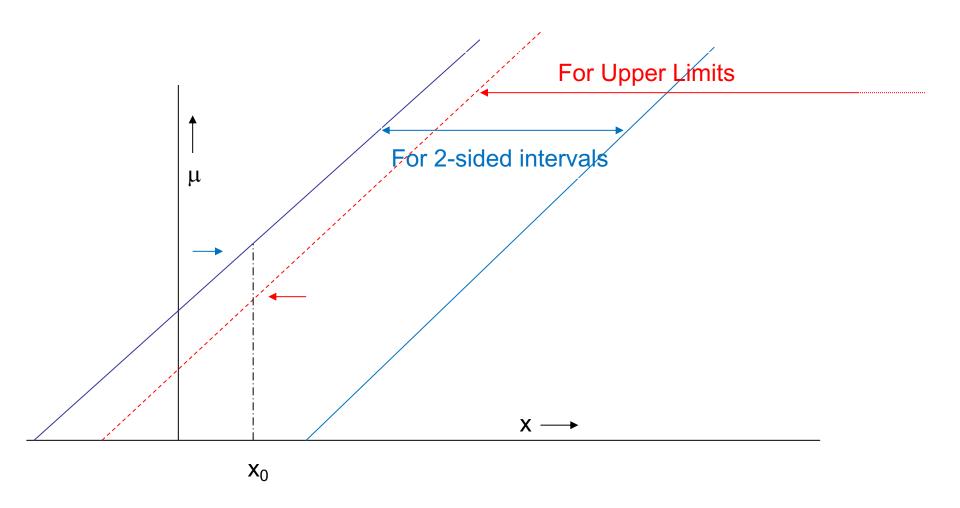
Feldman-Cousins

Bayes with prior = const,

"Show your £"

- 1) Not always practical
- 2) Not sufficient for frequentist methods

90% C.L. Upper Limits



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

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

- 1) RMS of $\mathcal{L}(\mu)$
- 2) $1/\sqrt{(-d^2 \mathcal{L}/d\mu^2)}$
- 3) $ln(\mathcal{L}(\mu_0 \pm \sigma) = ln(\mathcal{L}(\mu_0)) 1/2$

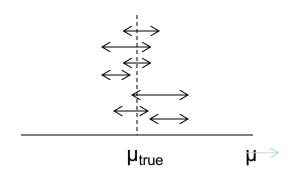
If $\mathcal{L}(\mu)$ is non-Gaussian, these are no longer the same

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

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

Barlow: Phystat05

Coverage



* What it is:

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

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

It is a property of the **statistical method** used

It is **NOT** a probability statement about whether μ_{true} lies in your confidence range for μ

* Coverage plot for Poisson counting expt Observe n counts

Estimate μ_{best} from maximum of likelihood

 $\boldsymbol{\mathcal{L}}(\mu) = e^{-\mu} \, \mu^n/n! \quad \text{ and range of } \mu \text{ from } \ln\{\boldsymbol{\mathcal{L}}(\mu_{best})/\boldsymbol{\mathcal{L}}(\mu)\} < 0.5$

For each μ_{true} calculate coverage C(μ_{true}), and compare with nominal 68%



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 µ

Study coverage of different methods of Poisson parameter μ , from observation of number of events n

COVERAGE

If true for all μ : "correct coverage"

P< α for some μ "undercoverage" (this is serious!)

 $P>\alpha$ for some μ "overcoverage"

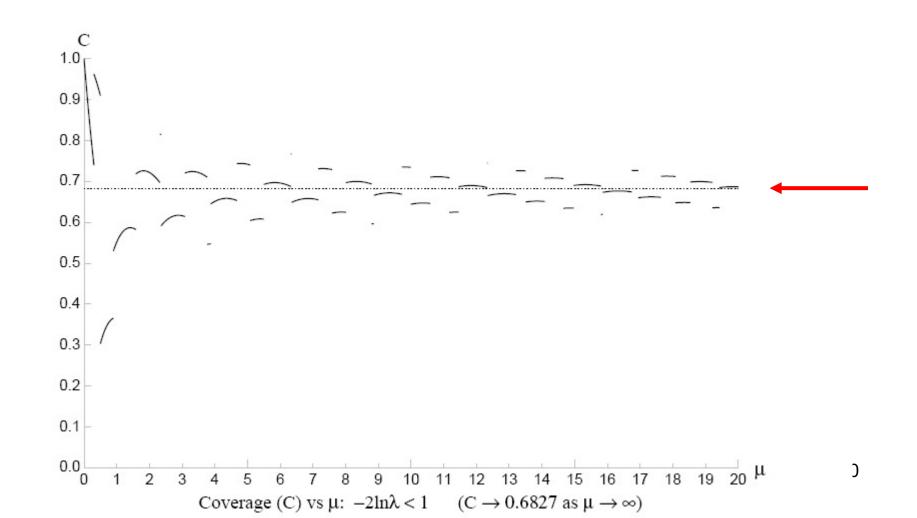
Conservative

Loss of rejection power

Coverage: £ approach (Not Neyman construction)

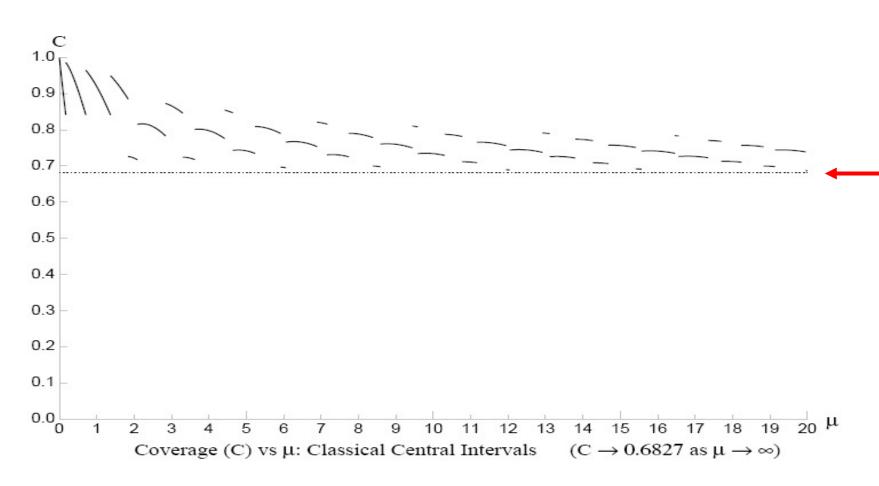
 $P(n,\mu) = e^{-\mu}\mu^n/n!$ (Joel Heinrich CDF note 6438)

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



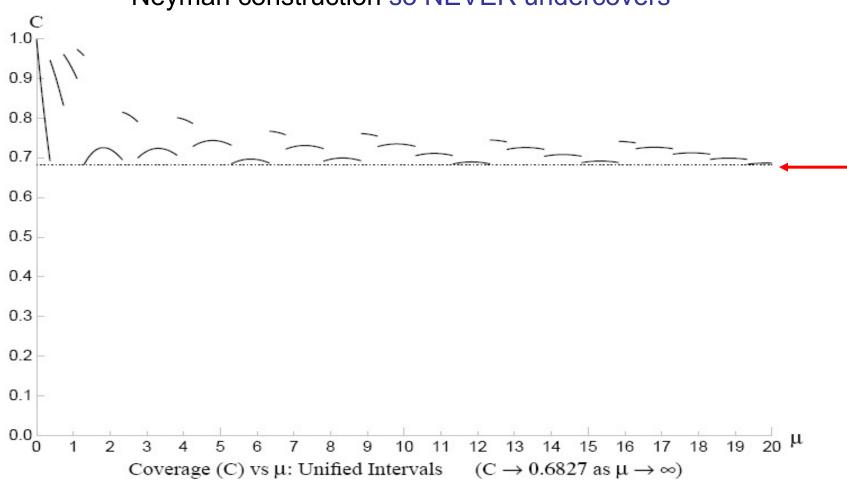
Neyman central intervals, NEVER undercover

(Conservative at both ends)

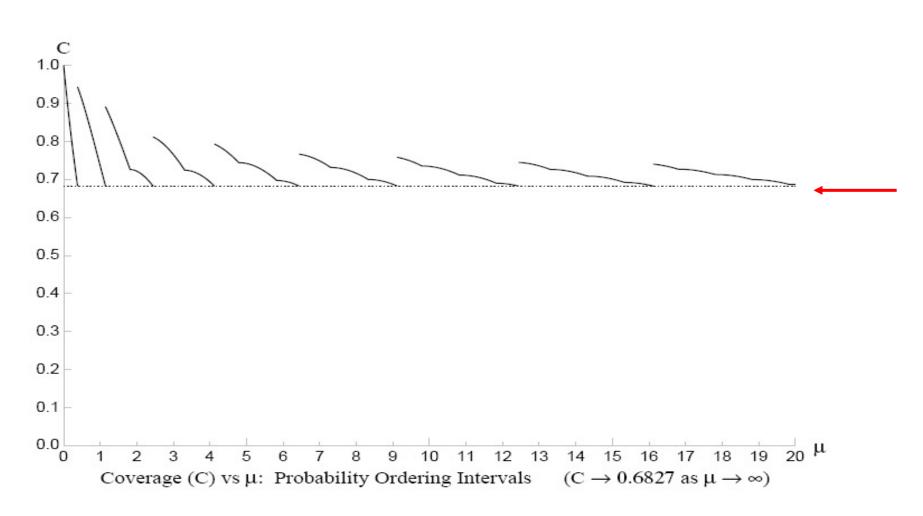


Feldman-Cousins Unified intervals



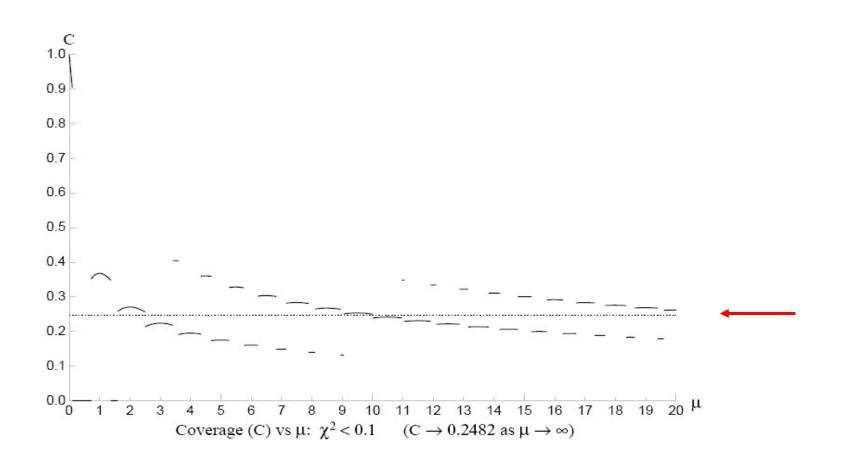


Probability ordering



$$\chi^2 = (n-\mu)^2/\mu$$
 $\Delta \chi^2 = 0.1$ \longrightarrow 24.8% coverage?

NOT Neyman : Coverage = 0% → 100%



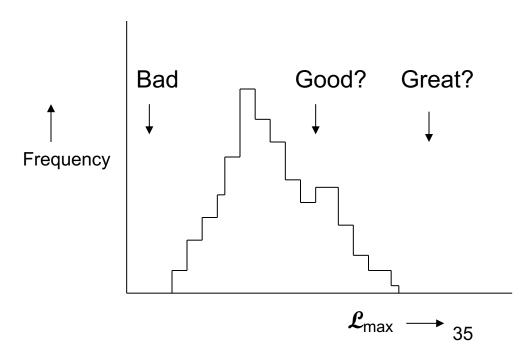
Unbinned \mathcal{L}_{max} and Goodness of Fit?

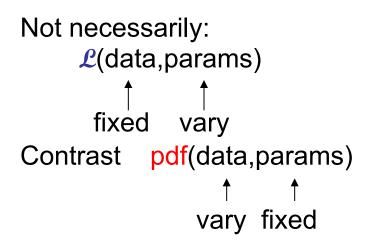
Find params by maximising $\mathcal L$

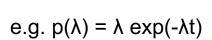
So larger $\mathcal L$ better than smaller $\mathcal L$

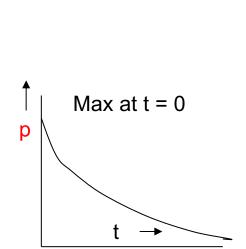
So \mathcal{L}_{max} gives Goodness of Fit??

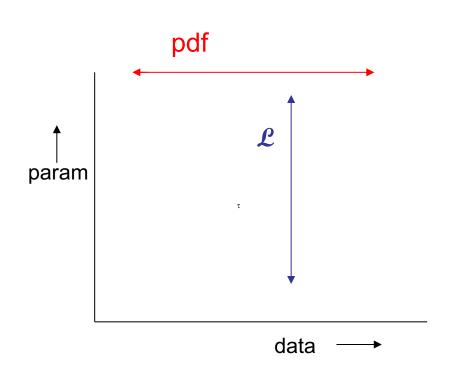
Monte Carlo distribution of unbinned \mathcal{L}_{max}

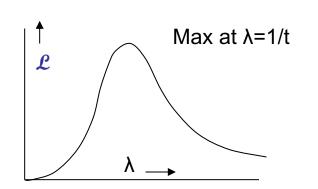












Example 1

Fit exponential to times t₁, t₂,t₃ [Joel Heinrich, CDF 5639]

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

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

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

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

(Average t is a sufficient statistic)

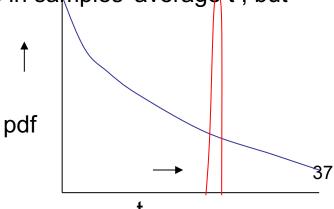
Variation of \mathcal{L}_{max} in Monte Carlo is due to variations in samples' average t, but

NOT TO BETTER OR WORSE FIT



Same average t

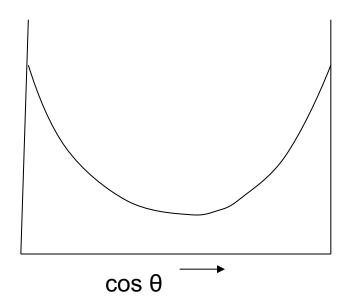
same \mathcal{L}_{max}



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 e.g. all data with $\cos\theta < 0$ and \mathcal{L}_{max} does not know about it.

Example 3

Fit to Gaussian with variable μ , fixed σ

$$p d f = \frac{1}{\sigma \sqrt{2 \pi}} e x p \left\{ -\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right\}$$

$$\ln \mathcal{L}_{\text{max}} = N(-0.5 \ln 2\pi - \ln \sigma) - 0.5 \Sigma (x_i - x_{\text{av}})^2 / \sigma^2$$

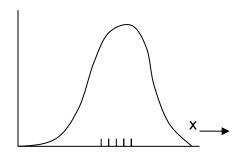
$$\uparrow \qquad \qquad \uparrow$$

$$\text{constant} \qquad \text{~variance}(x)$$

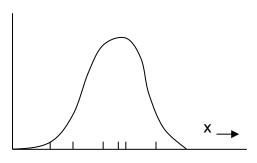
i.e. \mathcal{L}_{max} depends only on variance(x),

which is not relevant for fitting μ ($\mu_{est} = x_{av}$)

Smaller than expected variance(x) results in larger \mathcal{L}_{max}



Worse fit, larger \mathcal{L}_{max}



Better fit, lower \mathcal{L}_{max}

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

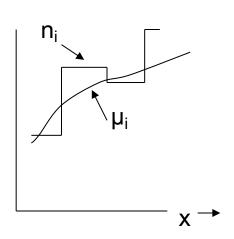
Conclusion:

Let 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 *£*-ratio



$$\mathcal{L} = \prod_{i} p_{ni}(\mu_i)$$

$$\mathcal{L}_{best} = \prod_{i} p_{ni}(\mu_{i,best})$$
$$= \prod_{i} p_{ni}(n_{i})$$

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

$$\overrightarrow{\text{large }\mu_i} \quad \textbf{-0.5}\chi^2$$

 $\overline{\text{large }\mu_i}$ -0.5 χ^2 i.e. Goodness of Fit

 $\mathcal{L}_{\text{best}}$ is independent of parameters of fit, and so same parameter values from \mathcal{L} or \mathcal{L} -ratio

L and pdf

Example 1: Poisson

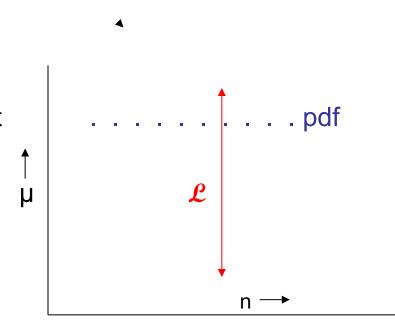
pdf = Probability density function for observing n, given μ

$$P(n;\mu) = e^{-\mu} \mu^{n}/n!$$

From this, construct £ as

$$\mathcal{L}(\mu;n) = e^{-\mu} \mu^n/n!$$

i.e. use same function of μ and n, but for pdf, μ is fixed, but for \mathcal{L} , n is fixed



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

Example 2 Lifetime distribution

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

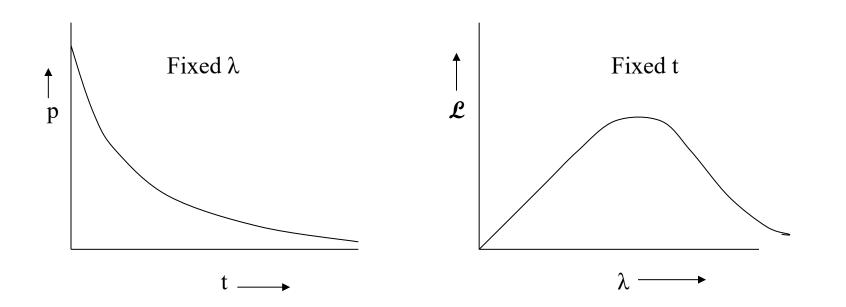
So $\mathcal{L}(\lambda;t) = \lambda e^{-\lambda t}$ (single observed t)

Here both t and λ 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

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

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

N.B. In this case, same functional form for pdf and £

So if you consider just Gaussians, can be confused between pdf and £

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 Likelihood

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

(a') £ 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 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 \mathcal{L}

(However,....)

	pdf(t;λ)	$\mathcal{L}(\lambda;t)$
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

CONCLUSION:

$$\int_{\rho_I}^{\rho_u} L d\rho = \alpha \quad \text{NOT recognised statistical procedure}$$

[Metric dependent:

 τ range agrees with τ_{pred}

 λ range inconsistent with $1/\tau_{pred}$]

BUT

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

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

6) BAYESIAN SMEARING OF X "USE IN I FOR F & 6 P SHEAR IT TO INCORORATE MX SYSTEMATIC UNCERTAINTIES" ENX SCENALIO: UNCERTAINTIES MEMUNED IN SUBSIDIARY EXPT $P(s, \epsilon | n) = P(n | s, \epsilon) T(s, \epsilon)$ P(sIn) = SP(s, e)n) de = $\int Z \pi(s) \pi(e) de$ 11 ds de= $\int Z \pi(s) \pi(s) ds de$ = $\int Z \pi(s) ds ds$ = $\int Z \pi(s) ds$ =

Getting £ wrong: Punzi effect

Giovanni Punzi @ PHYSTAT2003 "Comments on £ fits with variable resolution"

Separate two close signals, when resolution σ varies event by event, and is different for 2 signals

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e.g. 1) Signal 1 1+cos<sup>2</sup>θ
Signal 2 Isotropic
and different parts of detector give different σ
```

2) M (or τ)
Different numbers of tracks \rightarrow different σ_{M} (or σ_{τ})

Events characterised by x_i and σ_i

A events centred on x = 0

B events centred on x = 1

$$\mathcal{L}(f)_{\text{wrong}} = \prod \left[f * G(x_i, 0, \sigma_i) + (1-f) * G(x_i, 1, \sigma_i) \right]$$

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

$$p(S,T) = p(S|T) * p(T)$$

$$p(x_i,\sigma_i|A) = p(x_i|\sigma_i,A) * p(\sigma_i|A)$$

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

So

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

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

but NOT otherwise

Punzi's Monte Carlo for

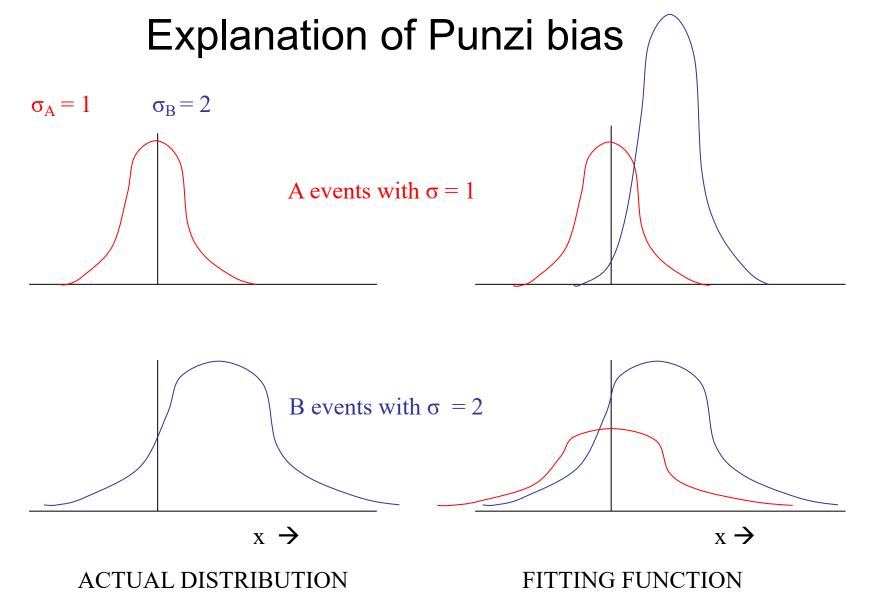
A: $G(x,0,\sigma_A)$

B: $G(x,1,\sigma_B)$

$$f_A = 1/3$$

		$oldsymbol{\mathcal{L}}_{wrong}$		\mathcal{L}_{right}	_	
σ_{A}	σ_{B}	f_A	σ_{f}	f_A σ_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)	0.14	0.335(2) 0.03		
1.0	1 → 2	0.482(9)	0.09	0.333(0) 0		

- 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 σ_f than \mathcal{L}_{wrong}

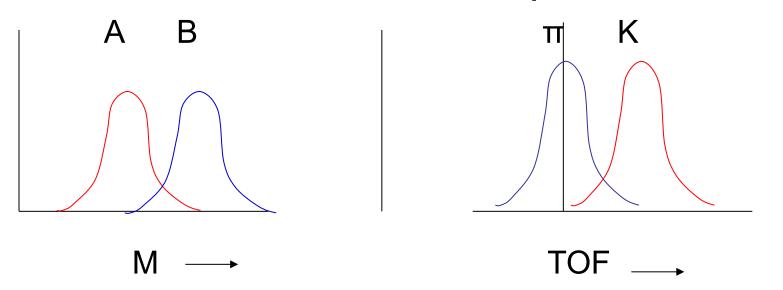


[N_A/N_B variable, but same for A and B events]

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

Another scenario for Punzi problem: PID



Originally:

Positions of peaks = constant

K-peak \rightarrow π -peak at large momentum

$$\sigma_i$$
 variable, $(\sigma_i)_A \neq (\sigma_i)_B$

$$\sigma_i \sim constant, \quad p_K \neq p_{\pi}$$

COMMON FEATURE: Separation/Error ≠ Constant

Where else??

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

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 σ_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

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 £ (Punzi effect)