Marginalising vs Profiling of Nuisance Parameters (Physicist's View)

- In the test statistic
- In simulation to get distribution of test statistic under null/alternative hypotheses

...while maintaining frequentist coverage of the parameter of interest

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Based heavily on my talk at Banff in April 2023,
https://www.birs.ca/workshops/2023/23w5096/files/Bob%20Cousins/cousins_banff_2023.pdf

Define terms, notation

Data vector x is observed, plugged into model to obtain likelihood function $\mathcal{L}(\mu, \beta)$ with
global MLE $\mathcal{L}(\hat{\mu}, \hat{\beta})$, where
μ is parameter of interest (e.g. signal mean) and
β is nuisance parameter (e.g. background mean),

***Profile likelihood function* (of only μ) is $\mathcal{L}(\mu, \hat{\hat{\beta}})$, where, for a given μ, $\hat{\hat{\beta}}$ maximizes $\mathcal{L}$ for that μ. Also written $\sup_{\beta} \mathcal{L}(\mu, \beta)$.**

Common to consider ratio with global MLE as test statistic (PLR)

Integrated/marginalized likelihood function (also of only μ) is $\int \mathcal{L}(\mu, \beta)\, \pi(\beta)\, d\beta$, where $\pi(\beta)$ is a weight function a la Bayesian prior pdf. (More generally, could be $\pi(\beta|\mu)$.)

If one uses either of these as a 1D likelihood function $\mathcal{L}(\mu)$, what are the frequentist properties of intervals constructed for μ ?

Long **Tradition in HEP: Use profile likelihood function and asymptotic Wilks's Theorem to get approximate 1D confidence intervals or (typically) 2D regions.**

Classic FORTRAN program: "Minuit: A System for Function Minimization and Analysis of the Parameter Errors and Correlations" by Fred James and Mats Roos, 1975.

MINUIT calls uncertainties from profile likelihood "MINOS errors".

Name **"Profile likelihood" entered HEP in 2000, with paper by Wolfgang Rolke and Angel Lopez (Fermilab Conf. Limits Wkshp).**

Profile likelihood ratio is the most common test statistic in use today at LHC (in all of HEP?)

See backup slides with some 2003-2005 PhyStat history as Gary Feldman and Kyle Cranmer dissected PLR in Kendall & Stuart, as discussed e.g. in Kyle's https://arxiv.org/pdf/physics/0310108.pdf (Sec. 9).

At some point, a few people started integrating out nuisance parameter(s), typically when Gaussian/normal contribution to likelihood, while treating parameter of interest in frequentist manner.

E.g., (see Backup slides)

Robert Cousins and Virgil Highland, "Incorporating systematic uncertainties into an upper limit" (1992).

For a more enlightened discussion, see our paper on the on/off problem discussed later in this talk,
Cousins, Linnemann, Tucker (2008). "CLT"

Luc Demortier noted that, in these simple cases, what we did was the same math as George Box's prior predictive p-value!

Box calculated a tail probability after obtaining a Bayesian pdf, and we averaged a frequentist tail probability over a Bayesian pdf. Simply reverse order of two integrals; see CLT.

Key paper in 2010, first year of LHC data

Cowan, Cranmer, Gross, and Vitells (CCGV) "Asymptotic formulae for likelihood-based tests of new physics".

Examined profile LR and their preferred variants:

Widely used in HEP, with significant side effect:

Since asymptotic distributions were not known in HEP for other test statistics, the default became profile LR expressions in CCGV, *even for small sample size*, "for consistency".

But…in stats literature, long history of criticism of simple profile LR

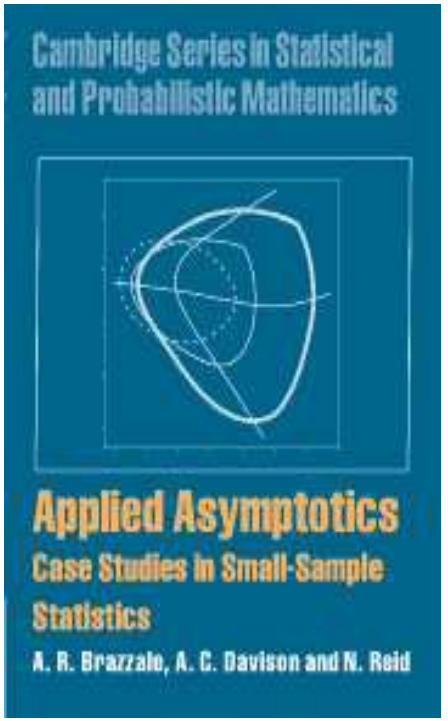
E.g., 2005 PhyStat at Oxford had various reviews of stats literature with higher-order approximations or other improvements: partial likelihood, adjusted likelihood, modified likelihood.

See in particular my talk, Nancy Reid's comments on it, and her workshop summary talk.

Talk by Anthony Davidson at PhyStat-nu 2019, earlier work in Banff challenge after Banff 2006

Talks by statistician Alessandra Brazzale and physicist Igor Volobouev at PhyStat-DM 2019

Virtually none of these developments have been adopted in HEP, as far as I know.



And marginalizing nuisances is rare at LHC (I think)

IMO, three reasons:

1) **The historical precedent of MINUIT MINOS,**
2) **Profiling is natural within context of LR test statistics**
3) **Since CCGV, asymptotic formulas are readily available for profile likelihood but not for marginalization, and are the default in the now-dominant software tools.**

Meanwhile our Bayesian friends have long advocated marginalizing nuisance parameters even if we stick to frequentist treatment of parameter of interest, e.g.,

James O. Berger, Brunero Liseo and Robert L. Wolpert, "Integrated Likelihood Methods for Eliminating Nuisance Parameters", (1999)

From Berger et al rejoinder to comment by Edward Susko:

"Dr. Susko finishes by suggesting that it might be useful to compute both profile and integrated likelihood answers in application, as a type of sensitivity study. It is probably the case that, if the two answers agree, then one can feel relatively assured in the validity of the answer. It is less clear what to think in the case of disagreement, however. If the answers are relatively precise and quite different, we would simply suspect that it is a situation with a 'bad' profile likelihood."

I (BC) agree with Susko's suggestion! More studies are needed in real cases to see if Berger et al are right.

Distribution of the test statistic(s) under hypotheses

Rather than pursuing higher-order corrections to the PLR, the general practice in HEP has been to stick with the PLR test statistic, and:

To use Monte Carlo simulation **(known as "toy MC") to obtain the finite-sample-size distribution(s) of the PLR under the null hypothesis, and under alternative(s) as desired. This is often compared to the relevant asymptotic formula.**

Distribution of the test statistic(s) under hypotheses

So now one has the question: *How should nuisance parameters be treated in the simulation?*

Keep in mind: we want correct frequentist coverage of the parameter of interest when nature is sampling from the unknown *true* values of the nuisance parameters.

***Important constraint* (at least until now): it is generally thought to be impractical to perform M.C. simulation for each of many different values of the nuisance parameters.**
So how to judiciously choose those values used in simulation?

The usual procedure (partially based on a desire to be "fully frequentist"), is to "throw toys" *using the profiled values of the nuisance parameters*, i.e., their ML estimates conditional on whatever value of the parameter(s) of interest are being tested. (Again, see backup slides re Kendall and Stuart.)

At some point, this was identified as the *parametric bootstrap*. (Luc Demortier in PhyStat-LHC 2007 Proceedings, and in email to me in 2011, citing book of Efron and Tibshirani.)

The hope is that the profiled values of the nuisance parameters are a good enough proxy for the unknown true values, even for small sample size.

I would like to see more comparisons of these results with alternatives, particularly those from marginalizing the nuisance parameters with some judiciously chosen priors.

I find it a bit comforting to average over a set of nuisance parameters in the neighborhood of the profiled values. Coverage studies can give guidance on the weight function $\pi(\boldsymbol{\beta})$.

Example

I "cherry-picked" an example that
1) appears often in the statistical literature;
2) is an important prototype in HEP and astronomy; and
3) I happen to be a co-author on studies thereof:

The ratio of Poisson means, which maps onto:
a) the "on/off" problem in astronomy and
b) the "signal band plus sideband" problem in HEP.

For the algebra, see Cousins, Linnemann, Tucker, (2008). "CLT"

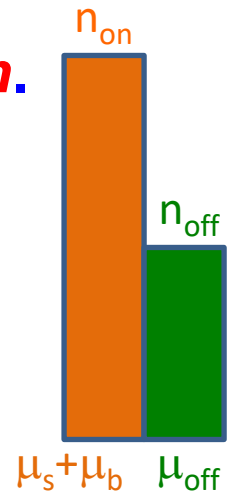
Here I will mostly just give concepts.

Histogram with 2 bins, observed contents n_{on} and n_{off}.

The "on" bin has (potentially) signal and bkg events with unknown Poisson means μ_s and μ_b , total Poisson mean $\mu_s + \mu_b$.

The "off" bin has only bkg with unknown Poisson mean μ_{off} .

Assume ratio of bkg in the two bins, $\tau = \mu_{off} / \mu_b$ is *known*.



Test H_0: $\mu_s = 0$. Rephrase H_0: $\mu_{off} / (\mu_s + \mu_b) = \tau$.
I.e., H_0: ratio of Poisson means of the two bins is τ.
Choice of nuisance param; let it be μ_b .

Std solution: eliminate nuisance by "conditioning":
$n_{tot} = n_{on} + n_{off}$ has no information about ratio;
treat this ancillary statistic as fixed and consider binomial distribution of n_{on} , n_{off} .

Again rephrase H_0: Binomial param ρ is $\mu_b / (\mu_b + \tau\, \mu_b) = 1 / (1+\tau)$.

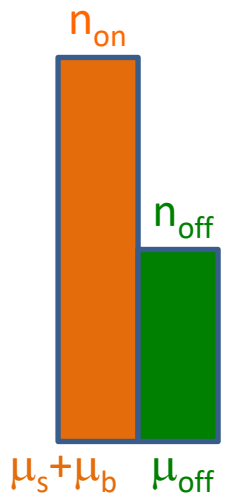
Two ways to write the likelihood function $\mathcal{L}$:

$\mathcal{L}\,(n_{on}\,,\, n_{off}\,;\, \mu_s+\mu_b\,,\, \mu_{off})$

$= \text{Pois}(n_{on}\,;\, \mu_s+\mu_b\,)\ \text{Pois}(n_{off}\,;\, \mu_b)$

$= \text{Pois}(n_{tot}\,;\, \mu_s+\mu_b+\mu_{off})\ \text{Binom}(n_{on}\,;\, n_{tot}\,,\, \rho)$

Where recall H_0: $\mu_s = 0$, equiv to H_0: $\rho = 1 / (1+\tau)$.
So do binomial test of $\rho = 1 / (1+\tau)$, given data n_{on} , n_{tot} .
p-value obtained by inversion of binomial conf intervals.
Convert to Z-value with 1-tailed convention: Z_{Bi}.



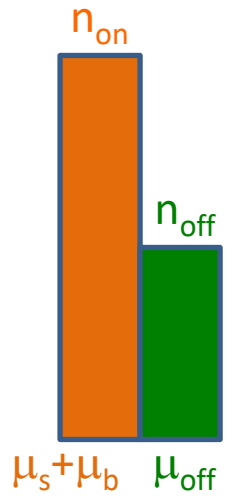
CLT used standard Clopper-Pearson conf intervals.
Very conservative for small n's.
Later paper by Cousins, Hymes, Tucker *preferred Lancaster mid-p confidence intervals.* (Randonness in n_{tot} leads to excellent coverage in ratio of Poisson means.)

Compare other methods to these "exact" intervals.

Marginalization of nuisance μ_b (Bayes-Freq hybrid)

First, consider case when μ_b is known *exactly*.
The p-value (call it p_P) for H_0: $\mu_s = 0$ is Poisson prob of obtaining n_{on} or more events in the "on" bin with true mean μ_b .

Then introduce uncertainty in μ_b in Bayesian-like way, with uniform prior for μ_b (ugh) and likelihood $\mathcal{L}(\mu_b)$ from Poisson probability of observing n_{off} in "off" bin, thus obtaining posterior prob $P(\mu_b|n_{off})$, a Γ function.



Finally, take weighted average of p_P over $P(\mu_b|n_{off})$:

$$P_{\text{B-F hybrid}} = \int p_P \, P(\mu_b|n_{off}) \, d\mu_b.$$ **and map to $Z_{\text{B-F hybrid}}$.**

Jim Linnemann discovered numerically, and then proved, that $Z_{\text{B-F hybrid}} = Z_{\text{Bi}}$ (!) (Called Z_Γ in CLT.)
[See Backup slides for note regarding simulation.]

Parametric Bootstrap treatment of nuisance μ_b

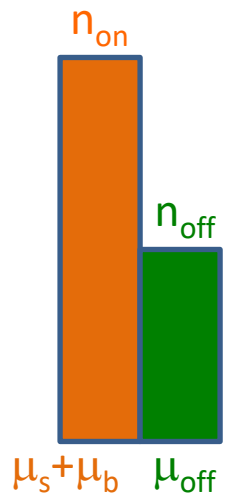
For testing H_0: $\mu_s = 0$, we find the profile likelihood estimate of μ_b. See Li and Ma, cited by CLT, for math.

Conceptually, we can use all the data by noting that $n_{tot} = n_{on} + n_{off}$ is sample from Poisson mean $\mu_b+\mu_{off} = \mu_b(1 + \tau)$.

So profiled MLE of μ_b for $\mu_s=0$ is $(n_{on} + n_{off}) / (1 + \tau)$.

Parametric bootstrap takes this value of μ_b as truth and proceeds to calculate p-value as in p_P above.

Can be done by simulation or direct calculation, leading to Z_{PB}.



Numerical example #1 (skip slide)

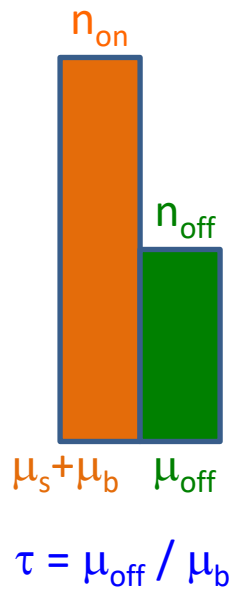
Suppose $\tau = 1$, $n_{on} = 10$, $n_{off} = 2$.

"Exact" $Z_{Bi} = Z_{B\text{-}F\ hybrid}$ (aka Z_Γ) = 2.07

Using Lancaster mid-P binomial: $Z_{mid\text{-}P} = 2.28$

Asymptotic result from Wilks's Thm is $Z_{PL} = 2.41$

Parametric bootstrap:
For $\mu_s = 0$, profiled MLE of $\mu_b = 6$, and so $\mu_{off} = 6$.
So generate toys with $\mu = 6$ in each bin (!) $Z_{PB} = 2.32$



Numerical example #2

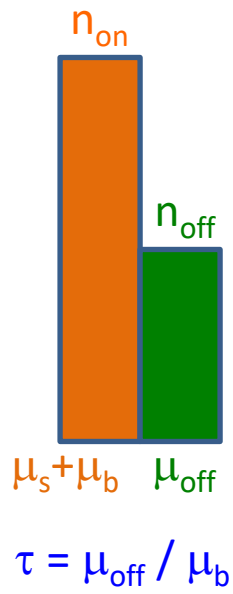
Suppose $\tau = 2$, $n_{on} = 10$, $n_{off} = 2$.

"Exact" $Z_{Bi} = Z_{B\text{-}F\ hybrid}$ (aka Z_Γ) = 3.27

Using Lancaster mid-P binomial: $Z_{mid\text{-}P} = 3.44$

Asymptotic result from Wilks's Thm is $Z_{PL} = 3.58$

Parametric bootstrap:
For $\mu_s = 0$, profiled MLE of $\mu_b = 4$, and so $\mu_{off} = 8$.
So generate toys with $\mu = 4, 8$ in the bins where we observed 10, 2 (!). $Z_{PB} = 3.46$



Superficially, B-F hybrid is "Exact", PB gives larger Z.
But recall: "Exact" overcovers due to discreteness – maybe PB is actually better. Need closer look.

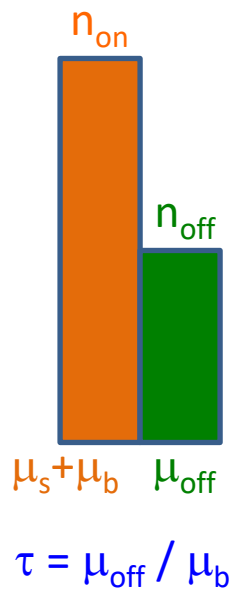
Coverage Studies

Following CLT, we pick a threshold Z_{thresh} (e.g., 3 or 5) and consider a pair of true values of (μ_b , τ).

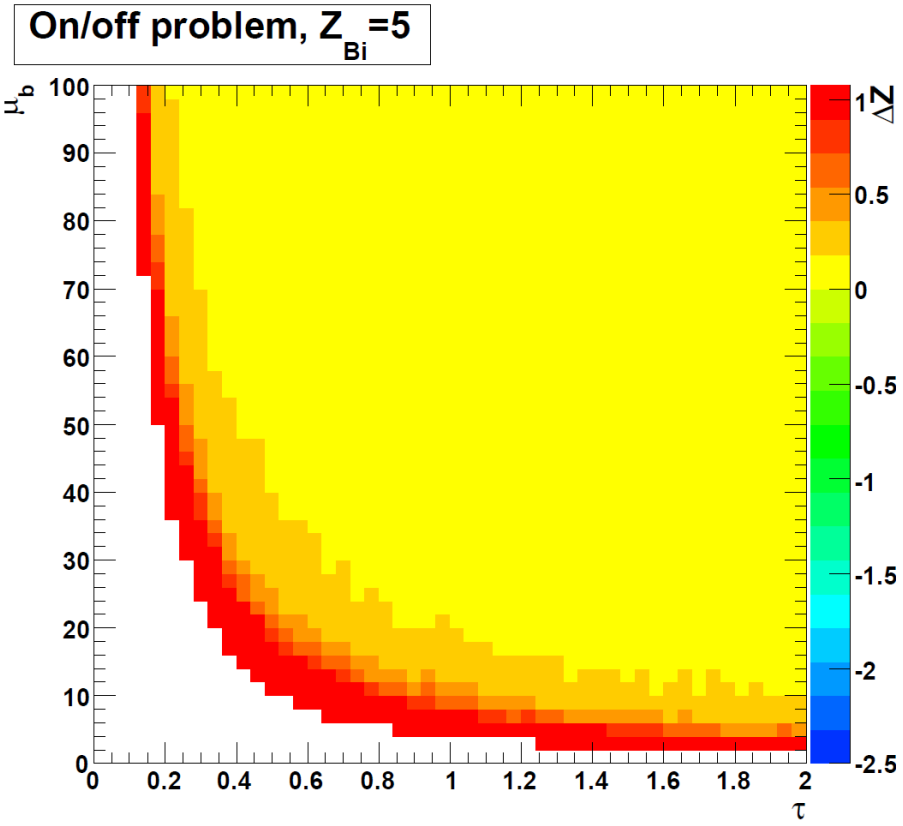
For each pair, we consider all values of (n_{on} , n_{off}), and calculate both the probability of obtaining that data and the claimed Z value for each recipe.

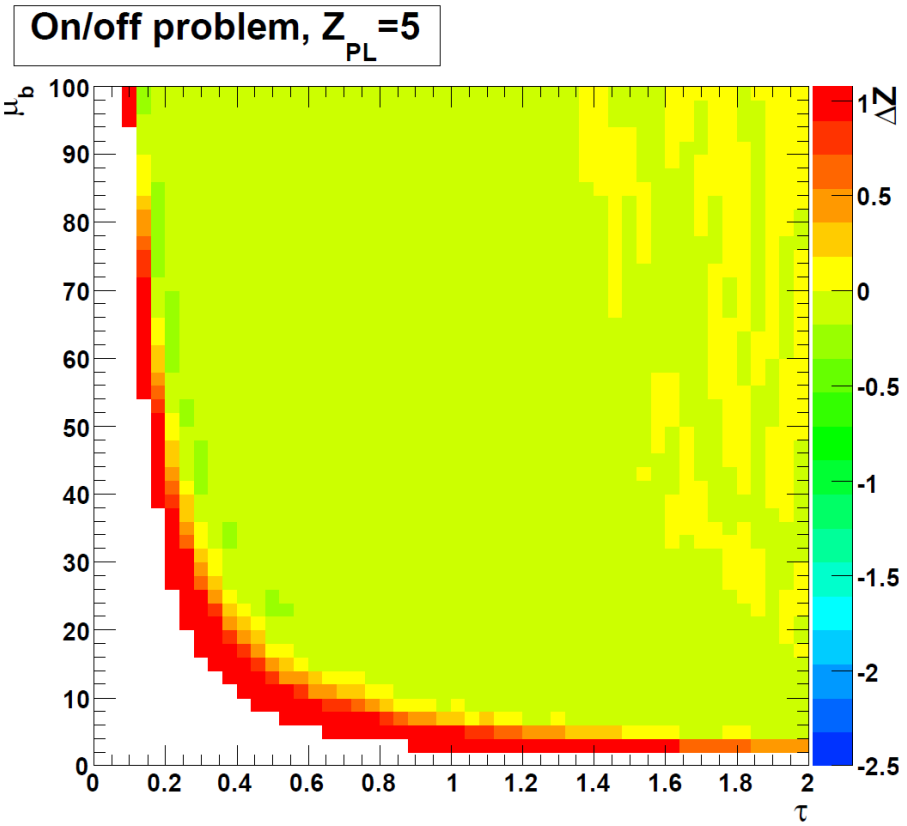
We can then compute the probability that $Z \geq Z_{thresh}$ for each recipe. From this we map to a value Z_{true} that represents the true Z, and compare to Z_{thresh} .

(This could be done by simulation, but we do direct calculation.)



From the CLT (2008) paper





For each fixed value of τ and μ_b , the color indicates $Z_{true} - Z_{claim}$ for the ensemble of expts quoting $Z_{claim} = 5$.

I calculated a couple points using parametric bootstrap Z_{PB} :

For $\tau = 1$ and $\mu_b = 10$, $Z_{claim} = 3$: $Z_{true} = 3.0$ (!)

For $\tau = 1$ and $\mu_b = 20$, $Z_{claim} = 5$: $Z_{true} = 5.0$ (!)

Discussion at Banff BIRS 2023

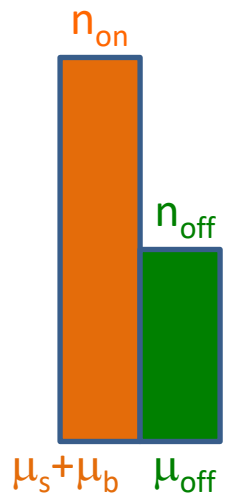
Among the many talks touching on the topic, statistician Anthony Davison's talk was paired with mine, pointing to works including his Banff challenge paper with Sartori, and describing a parametric bootstrap, writing,

"Lee and Young (2005, Statistics and Probability Letters) and DiCiccio and Young (2008, 2010, Biometrika) show that this parametric bootstrap procedure has third-order relative accuracy in linear exponential families, both conditionally and unconditionally, and is closely linked to objective Bayes approaches."

Final remarks

How much is HEP losing by not examining more thoroughly higher-order asymptotic theory?

I cherry-picked my example problem to be one in which I knew that marginalizing the nuisance parameter (with judicious prior) yielded the standard frequentist Z, while doing parametric bootstrap as commonly done at the LHC would give higher Z_{PB}. But in this example, the discrete nature of the problem "saves" the coverage of Z_{PB} !



For *Gaussian* uncertainty on mean μ_b , marginalizing the nuisance parameter can be badly anti-conservative (Kyle Cranmer at Oxford 2005, studied by CLT).

I would urge more exploration of these issues in real HEP analyses!

References (PhyStat at end)

Wolfgang A. Rolke and Angel M. López, Confidence intervals and upper bounds for small signals in the presence of background noise," Nucl. Instrum. Meth.A 458 (2001) 745 e-Print: hep-ph/0005187 [hep-ph]. See also other papers with Lopez et al.

Fred James and Mats Roos (CERN), "Minuit: A System for Function Minimization and Analysis of the Parameter Errors and Correlations", Computer Physics Commun. 10 (1975) 343

Fred James (CERN), "Interpretation of the Shape of the Likelihood Function around Its Minimum", Computer Physics Commun. 20 (1980) 29

Robert D. Cousins and Virgil L. Highland, "Incorporating systematic uncertainties into an upper limit", Nucl. Instr. Meth. A 320 (1992) 331.

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Robert D. Cousins, Kathryn E. Hymes, Jordan Tucker, "Frequentist Evaluation of Intervals Estimated for a Binomial Parameter and for the Ratio of Poisson Means", Nucl. Inst. Meth. A 612 (2010) 388, arXiv:0905.3831

G. Cowan, K. Cranmer, E. Gross, and I. Vitells, "Asymptotic formulae for likelihood-based tests of new physics", Eur. Phys. J. C71 1554 (2011), arXiv:1007.1727. (See also arXiv:1210.6948)

References (cont.)

A. C. Davison and N. Sartori, "The Banff Challenge: Statistical Detection of a Noisy Signal", Stat. Sci. 23 (2008) 354.

James O. Berger, Brunero Liseo, and Robert L. Wolpert, "Integrated Likelihood Methods for Eliminating Nuisance Parameters", Statistical Science 14 (1999) 1.

PhyStat 2005 at Oxford: Talks at https://confs.physics.ox.ac.uk/phystat05/programme.asp, Proceedings at https://confs.physics.ox.ac.uk/phystat05/proceedings/default.htm . See, e.g., Bob Cousins, "Treatment of Nuisance Parameters in High Energy Physics, and Possible Justifications and Improvements in the Statistics Literature, and response by Nancy Reid; also Nancy Reid, "Summary of Some Statistical Issues".

PhyStat-nu 2019 at CERN: https://indico.cern.ch/event/735431/timetable/ , in particular Anthony Davidson, "Almost-perfect Signal Detection".

PhyStat-DM at Stockholm: https://indico.cern.ch/event/769726/timetable/#all.detailed , in particular, Alessandra R. Brazzale, "Likelihood Asymptotics and Beyond," and Igor Volobouev, "Improved Inference for the Signal Significance".

Banff BIRS 2023: https://www.birs.ca/events/2023/5-day-workshops/23w5096/schedule . Multiple relevant talks, most directly the talk by Anthony Davison (paired with my talk): "Marginalise or Profile? A Statisticians' View."

Thanks to all (see note), including my "sponsor", U.S. DOE Office of Science

BACKUP

Approximate Confidence Regions Using $\Delta(-\ln\mathcal{L})$
(included in appendix to MINUIT users guide)

"Interpretation of the Shape of the Likelihood Function around Its Minimum" by Fred James (1980)

It often happens that the solution of a minimum problem is itself straightforward, but the calculation or interpretation of the resulting parameter uncertainties, as determined by the shape of the function at the minimum, is considerably more complicated. The purpose of this note is to clarify the most commonly encountered difficulties in parameter error determination. These difficulties may arise in connection with any fitting program, but will be discussed here with the terminology of the program MINUIT for the convenience of MINUIT users.

The most common causes of misinterpretation may be grouped into three categories:

1. Proper normalization of the user-supplied chi-square or likelihood function, and appropriate ERROR DEF.
2. Non-linearities in the problem formulation, leading to different errors being calculated by different techniques, such as MIGRAD, HESSE and MINOS.
3. Multiparameter error definition and interpretation.

All these topics are discussed in some detail by Eadie et al., which may be consulted for further details.

Table 1
Table of UP for multiparameter confidence regions

Number of parameters	Confidence level (probability contents desired inside hypercontour of "$chi^2 = chi^2$ min + UP")				
	50%	70%	90%	95%	99%
1	0.46	1.07	2.70	3.84	6.63
2	1.39	2.41	4.61	5.99	9.21
3	2.37	3.67	6.25	7.82	11.36
4	3.36	4.88	7.78	9.49	13.28
5	4.35	6.06	9.24	11.07	15.09
6	5.35	7.23	10.65	12.59	16.81
7	6.35	8.38	12.02	14.07	18.49
8	7.34	9.52	13.36	15.51	20 09
9	8.34	10.66	14.68	16.92	21.67
10	9.34	11.78	15.99	18.31	23.21
11	10.34	12.88	17.29	19.68	24.71

If FCN is −log(likelihood) instead of chi-square, all values of UP should be divided by 2.

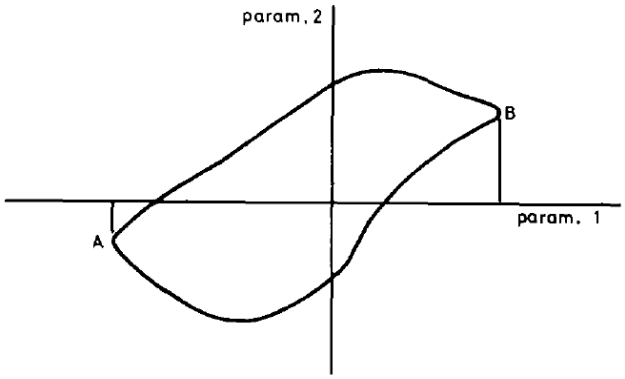

Fig. 1. MINOS errors for parameter 1.

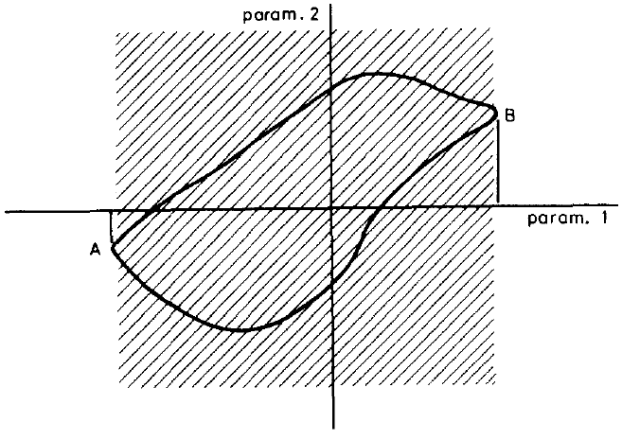

Fig. 2. MINOS error confidence region for parameter 1.

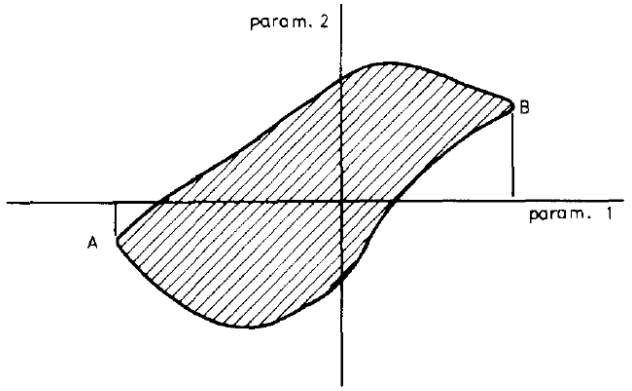

Fig. 4. Optimal confidence region for parameters 1 and 2.

Profile likelihood ratio is most common test statistic in use today at LHC (in all of HEP?)

MINUIT MINOS history, still widely used.

1998 intervals by Feldman and Cousins were recognized as no-nuisance special case of inversion of " exact" PLR test in "Kendall and Stuart".

HEP-invented "modification" called CL_S is ratio of two p-values that are both based on PLR test statistics (with some historical use of marginalization of nuisances).

CHAPTER 22

LIKELIHOOD RATIO TESTS AND TEST EFFICIENCY

The LR statistic

22.1 The ML method discussed in Chapter 18 is a constructive method of obtaining estimators which, under certain conditions, have desirable properties. A method of test construction closely allied to it is the likelihood ratio (LR) method, proposed by Neyman and Pearson (1928). It has played a role in the theory of tests analogous to that of the ML method in the theory of estimation.

As before, we have the LF

$$L(x|\boldsymbol{\theta}) = \prod_{i=1}^{n} f(x_i|\boldsymbol{\theta}),$$

where $\boldsymbol{\theta} = (\boldsymbol{\theta}_r, \boldsymbol{\theta}_s)$ is a vector of $r + s = k$ parameters ($r \geq 1, s \geq 0$) and x may also be a vector. We wish to test the hypothesis

$$H_0 : \boldsymbol{\theta}_r = \boldsymbol{\theta}_{r0}, \tag{22.1}$$

which is composite unless $s = 0$, against

$$H_1 : \boldsymbol{\theta}_r \neq \boldsymbol{\theta}_{r0}.$$

We know that there is generally no UMP test in this situation, but that there may be a UMPU test – cf. **21.31**.

The LR method first requires us to find the ML estimators of $(\boldsymbol{\theta}_r, \boldsymbol{\theta}_s)$, giving the unconditional maximum of the LF

$$L(x|\hat{\boldsymbol{\theta}}_r, \hat{\boldsymbol{\theta}}_s), \tag{22.2}$$

and also to find the ML estimators of $\boldsymbol{\theta}_s$, when H_0 holds,[1] giving the conditional maximum of the LF

$$L(x|\boldsymbol{\theta}_{r0}, \hat{\hat{\boldsymbol{\theta}}}_s). \tag{22.3}$$

$\hat{\hat{\boldsymbol{\theta}}}_s$ in (22.3) has been given a double circumflex to emphasize that it does not in general coincide with $\hat{\boldsymbol{\theta}}_s$ in (22.2). Now consider the likelihood ratio[2]

$$l = \frac{L(x|\boldsymbol{\theta}_{r0}, \hat{\hat{\boldsymbol{\theta}}}_s)}{L(x|\hat{\boldsymbol{\theta}}_r, \hat{\boldsymbol{\theta}}_s)}. \tag{22.4}$$

Since (22.4) is the ratio of a conditional maximum of the LF to its unconditional maximum, we clearly have

$$0 \leq l \leq 1. \tag{22.5}$$

Intuitively, l is a reasonable test statistic for H_0: it is the maximum likelihood under H_0 as a fraction of its largest possible value, and large values of l signify that H_0 is reasonably acceptable. The critical region for the test statistic is therefore

$$l \leq c_\alpha, \tag{22.6}$$

where c_α is determined from the distribution $g(l)$ of l to give a size-α test, that is,

$$\int_0^{c_\alpha} g(l)\,\mathrm{d}l = \alpha. \tag{22.7}$$

Neither maximum value of the LF is affected by a change of parameter from $\boldsymbol{\theta}$ to $\tau(\boldsymbol{\theta})$, the ML estimator of $\tau(\boldsymbol{\theta})$ being $\tau(\hat{\boldsymbol{\theta}})$ – cf. **18.3**. Thus the LR statistic is invariant under reparametrization.

Profile Likelihood Ratio Test in "Kendall & Stuart"

CHAPTER 22

LIKELIHOOD RATIO TESTS AND TEST EFFICIENCY

The LR statistic

22.1 The ML method discussed in Chapter 18 is a constructive method of obtaining estimators which, under certain conditions, have desirable properties. A method of test construction closely allied to it is the likelihood ratio (LR) method, proposed by Neyman and Pearson (1928). It has played a role in the theory of tests analogous to that of the ML method in the theory of estimation.

As before, we have the LF

$$L(x|\boldsymbol{\theta}) = \prod_{i=1}^{n} f(x_i|\boldsymbol{\theta}),$$

where $\boldsymbol{\theta} = (\boldsymbol{\theta}_r, \boldsymbol{\theta}_s)$ is a vector of $r+s=k$ parameters ($r \geq 1, s \geq 0$) and x may also be a vector. We wish to test the hypothesis

$$H_0 : \boldsymbol{\theta}_r = \boldsymbol{\theta}_{r0}, \tag{22.1}$$

which is composite unless $s = 0$, against

$$H_1 : \boldsymbol{\theta}_r \neq \boldsymbol{\theta}_{r0}.$$

We know that there is generally no UMP test in this situation, but that there may be a UMPU test – cf. **21.31**.

The LR method first requires us to find the ML estimators of $(\boldsymbol{\theta}_r, \boldsymbol{\theta}_s)$, giving the unconditional maximum of the LF

$$L(x|\hat{\boldsymbol{\theta}}_r, \hat{\boldsymbol{\theta}}_s), \tag{22.2}$$

and also to find the ML estimators of $\boldsymbol{\theta}_s$, when H_0 holds,[1] giving the conditional maximum of the LF

$$L(x|\boldsymbol{\theta}_{r0}, \hat{\hat{\boldsymbol{\theta}}}_s). \tag{22.3}$$

$\hat{\hat{\boldsymbol{\theta}}}_s$ in (22.3) has been given a double circumflex to emphasize that it does not in general coincide with $\hat{\boldsymbol{\theta}}_s$ in (22.2). Now consider the likelihood ratio[2]

$$l = \frac{L(x|\boldsymbol{\theta}_{r0}, \hat{\hat{\boldsymbol{\theta}}}_s)}{L(x|\hat{\boldsymbol{\theta}}_r, \hat{\boldsymbol{\theta}}_s)}. \tag{22.4}$$

Since (22.4) is the ratio of a conditional maximum of the LF to its unconditional maximum, we clearly have

$$0 \leq l \leq 1. \tag{22.5}$$

Intuitively, l is a reasonable test statistic for H_0: it is the maximum likelihood under H_0 as a fraction of its largest possible value, and large values of l signify that H_0 is reasonably acceptable. The critical region for the test statistic is therefore

$$l \leq c_\alpha, \tag{22.6}$$

where c_α is determined from the distribution $g(l)$ of l to give a size-α test, that is,

$$\int_0^{c_\alpha} g(l)\,dl = \alpha. \tag{22.7}$$

Neither maximum value of the LF is affected by a change of parameter from $\boldsymbol{\theta}$ to $\tau(\boldsymbol{\theta})$, the ML estimator of $\tau(\boldsymbol{\theta})$ being $\tau(\hat{\boldsymbol{\theta}})$ – cf. **18.3**. Thus the LR statistic is invariant under reparametrization.

Define critical region using profile likelihood test statistic.

I recall a long discussion between Gary Feldman and Kyle Cranmer* at a pub at Oxford Phystat in 2005 re how to interpret Eqns. 22.4-22.7.

Are nuisance parameters fixed to PL values, or is the full space of parameters considered when constructing critical region?

I think these are related to the parametric bootstrap and the full method discussed by Larry.

*For historical context in 2003 and 2005, see Kyle's https://arxiv.org/pdf/physics/0310108.pdf (Sec. 9), https://arxiv.org/pdf/physics/0511028.pdf (Sec. 4.3). Also Giovanni Punzi, https://arxiv.org/abs/physics/0511202 .

Robert Cousins and Virgil Highland, "Incorporating systematic uncertainties into an upper limit" (1992).

C-H looked at the case of a physics quantity

$\sigma = \mu_b / L$,

where μ_b = unknown Poisson mean, L is factor called luminosity. One observes a sampled value n from the Poisson distribution.

From n, one obtains an 90% upper confidence limit on μ_b. If L known exactly, scale by 1/L to get upper conf limit on σ.

If instead one has unbiased estimate of L and assumes symmetric pdf for L with known variance, C-H integrate over L, what we now call integrating/marginalizing over the nuisance parameter L.

Our motivation was to ameliorate an effect whereby confidence intervals derived from a discrete observable become shorter when a continuous nuisance parameter is added to the model.

In the initially submitted draft, we did not know that we were grafting a Bayesian pdf onto frequentist Poisson C.L.

(Fred James sorted us out before publication.)

As mentioned in main talk, for a more enlightened discussion, see our paper on the on/off problem discussed later in this talk, Cousins, Linnemann, Tucker (2008). "CLT"

Simulation of marginalization of nuisance μ_b

Sample μ_b from $P(\mu_b|n_{off})$, compute frequentist p_P for each sampled value of μ_b (using same observed n_{on}).

Calculate arithmetic mean of these values of p_P .

Convert to Z_P as desired. (Note that p_P's are averaged, not Z_P's).

Nested Hypothesis Testing Duality

***Given* an ordering:**

Test of $\mu=\mu_0$ vs $\mu\neq\mu_0$ at significance level α
$\leftrightarrow$ Is μ_0 in confidence interval for μ with C.L. = 1- α ?

"There is thus no need to derive optimum properties separately for tests and for intervals; there is a one-to-one correspondence between the problems as in the dictionary in Table 20.1" Stuart99, p. 175. [Table in backup slides] E.g.,

$\alpha \leftrightarrow$ 1 – C.L.

Equal-tailed test $\leftrightarrow$ central confidence intervals

One-tailed tests $\leftrightarrow$ Upper/lower limits

Use of the duality is referred to as "inverting a test" to obtain confidence intervals, and vice versa.

"New" confidence intervals of Feldman & Cousins in 1998 were actually those dual to age-old LR Test in "Kendall and Stuart", minus nuisance parameters.