Real life problems Systematic errors

What are systematic uncertainties
 How to deal with systematic uncertainties

Real-life problems

- Exact calibration of p-values/Z-values possible for counting experiment with background that is *exactly* known.
- Real-life problems are often more difficult
 - Result is (ML) fit to distribution in >=1 dimensions, with model shape uncertainties
 - Background estimate has uncertainty
- *Correct* calculation of significance no longer guaranteed!
 - Q: Is that a problem?
 - A: Yes. If your (naïve) calculation says Z=5, but it is really Z=3, there is a substantial chance your discovery is fake
 - If ATLAS and CMS use different methods one experiment may claim discovery of e.g. Higgs with only half the data of the other because of differences in significance calculation

• Systematic errors

- What are systematic errors
- How to incorporate them in measurement
- Nuisance parameters in limits and intervals

Systematic errors vs statistical errors

• Definitions

```
Statistical error = any error in measurement due to
statistical fluctuations in data
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Systematic errors = **all other errors**

Systematic uncertainty = Systematic error

- But Systematic **error** \neq Systematic **mistake**!
 - Suppose we know our measurement needs to be corrected by a factor of 1.05 ± 0.03
 - Not correcting the data by factor 1.05 introduces a systematic mistake
 - Right thing to do: correct data by factor 1.05 and take uncertainty on factor (0.03) as a systematic error

Classification of systematic errors

- Classification by Pekko Sinerva (PhyStat 2003)
- Good, Bad and Ugly



Source of systematic errors – 'Good' and 'Bad' errors

- 'Good' errors arise from clear causes and can be evaluated
 - Clear cause of error
 - Clear procedure to identify and quantify error
 - Example: Calibration constants, efficiency corrections from simulation
- 'Bad' errors arise from clear causes, but can *not* be evaluated
 - Still clear cause
 - But no unambiguous procedure to quantify uncertainty
 - Example: theory error:
 - Given 2 or more choices of theory model you get 2 or more different answers.
 - What is the error?

Sources of systematic errors – 'Ugly' errors

- 'Ugly' errors arise from sources that have been overlooked
 - Cause unknown \rightarrow error unquantifiable
- 'Ugly' errors are usually found through failed sanity checks
 - Example: measurement of CP violation on a sample of events that is known to have no CP-violation: You find A_{CP} =0.10 ± 0.01
 - Clearly something is wrong What to do?
 - 1) Check your analysis
 - 2) Check your analysis again
 - 3) Phone a friend

. . .

- 4) Ask the audience
- 99) Incorporate as systematic error as last and desperate resort!

What about successful sanity checks?

- Do not incorporate successful checks in your systematic uncertainty
 - Infinite number of successful sanity checks would otherwise lead to infinitely large systematic uncertainty. Clearly not right!
- Define beforehand if a procedure is a sanity check or an evaluation of an uncertainty
 - If outcome of procedure can legitimately be different from zero, it is a systematic uncertainty evaluation
 - If outcome of procedure can only significantly different from zero due to mistake or unknown cause, it is a sanity check

- Two values corresponding to use of two (theory) models A,B
 - What is a good estimate for your systematic uncertainty?
- I) If A and B are *extreme scenarios*, and the truth must always be between A and B
 - Example: fully transverse and fully longitudinal polarization
 - Error is root of variance with uniform distribution with width A-B

$$\sigma = \frac{|A - B|}{\sqrt{12}} \qquad \qquad V(x) = \langle x \rangle^2 - \langle x^2 \rangle = \left(\frac{1}{2}\right)^2 - \int_0^1 x^2 dx = \frac{1}{4} - \frac{1}{3} = \frac{1}{12}$$

- Popular method because sqrt(12) is quite small, but only justified if A,B are truly extremes!
- II) If A and B are typical scenarios
 - Example: JETSET versus HERWIG (different Physics simulation packages)
 - Error is difference divided by sqrt(2)

$$\sigma = \frac{|A - B|}{2} \cdot \sqrt{2} = \frac{|A - B|}{\sqrt{2}}$$

Ν

Factor $\bigvee N_{-1}$

to get unbiased estimate of σ_{parent}

- Two variations of the analysis procedure on the same data
 - Example: fit with two different binnings giving A \pm σ_{A} and B \pm σ_{B}
 - Clearly, results A,B are correlated so $\frac{|A-B|}{\sqrt{\sigma_A^2 + \sigma_B^2}}$ is not a good measure of smallness of error
- Generally difficult to calculate, but can estimate uppper, lower bound on systematic uncertainty

$$\sqrt{\sigma_A^2 - \sigma_0^2} - \sqrt{\sigma_B^2 - \sigma_0^2} \le \sigma_{A-B} \le \sqrt{\sigma_A^2 - \sigma_0^2} + \sqrt{\sigma_B^2 - \sigma_0^2}$$

- Where $\sigma_A > \sigma_B$ and σ_0 is the Minimum Variance Bound. $\sigma_0^2(\hat{a}) = \langle (\hat{a} \langle \hat{a} \rangle)^2 \rangle$
- If the better technique (B) saturates the MVB the range reduces to

$$\sigma_{A-B}^2 = \sigma_A^2 - \sigma_B^2$$

- If MVB is not saturated (e.g. you have low statistics) you will need to use a toy Monte Carlo technique to evaluate σ_{A-B} Wouter Verkerke, UCSB

- Common scenario in HEP analysis: you need to assign systematic uncertainty to shape of distribution obtained from simulated events
 - Measuring data in range [30,90]. Correct for acceptance effect by dividing by efficiency measured from simulated data.
 - Ndata[30,90] = 750

Ntotal = 750 / 0.73 = 1027

- $\text{ eff}_{MC} = 7300/10000 = 0.73$
- What is uncertainty on Ntotal from MC simulation uncertainty?





- Popular but wrong technique: 'Cut variation'
 - Procedure: vary each of your cuts by a little bit. For each change,
 - 1) Measure new yield on data
 - 2) Correct with new MC efficiency.
 - 3) Difference between efficiency corrected results is systematic uncertainty.
 - Example, for a nominal cut in x at 'p' you find N(data)=105, with a MC efficiency ϵ_{MC} =0.835 so that N(corrected)=125.8

	N(data)	ε(MC)	N(corrected)	
p+∆p	110	0.865	127.2	$\sigma_{sys}^{p} = (127.2 - 124.5)/2 = 1.4$
р-∆р	100	0.803	124.5	
				$r = 125.8 \pm 1.4$

 Bad thing to do → error can be dominated by low stats in variation range

- Warning I: Cut variation does not give an precise measure of the systematic uncertainty due data/MC disagreement!
 - Your systematic error is dominated by a potentially large statistical error from the small number of events in data between your two cut alternatives
 - This holds independent of your MC statistics
 - You could see a large statistical fluctuation
 → error overestimated
 - You could see no change due to a statistical fluctuation
 → error underestimated



Wouter Verkerke, UCSB

- Warning II: Cut variation doesn't catch all types of data/MC discrepancies that may affect your analysis
 - Error may be fundamentally underestimated
 - Example of discrepancy missed by cut variation:



Cut variation is a good sanity check,

but not necessarily a good estimator for systematic uncertainty

Systematic errors and correlations

• Pay attention to correlation between systematic errors

$$\sigma_{xy}^{2} = \left(\frac{df}{dx}\right)^{2} \sigma_{x}^{2} + \left(\frac{df}{dy}\right)^{2} \sigma_{y}^{2} + 2\left(\frac{df}{dx}\right)\left(\frac{df}{dy}\right)\rho\sigma_{x}\sigma_{y}$$

- If error uncorrelated, $\rho=0$
 - Add in quadrature
- If error 100% correlated, then $\rho=1$.

- E.g. tracking efficiency uncertainty per track for 6 tracks,

$$\sigma_{3trk} = \sigma_{trk} + \sigma_{trk} + \sigma_{trk} = 3 \cdot \sigma_{trk} \quad (not \ \sqrt{3} \ \cdot \sigma_{trk})$$

- If errors 100% anti-correlated, then ρ =-1
 - This can really happen!
 - Example BF($D^{*0} \rightarrow D^0\pi^0$) =67% and BF($D^{*0} \rightarrow D^0\gamma$) =33%

Combining statistical and systematic uncertainty

- Systematic error and statistical error are independent
 - In 'simple measurements' can be added in quadrature to obtain combined error
 - Nevertheless always quote (also) separately.
 - Also valid procedure if systematic error is not Gaussian:
 Variances can be added regardless of their shape
 - Combined error usually approximately Gaussian anyway (C.L.T)
- You can also incorporate systematic uncertainties directly into a ML of χ^2 fit
 - Advantage: automatic and correct error propagation (including correlations)
 - For ML fit simply multiply your pdf in the parameters with a pdf that describes you systematic uncertainty

Adding uncertainties to a likelihood

- Example: Gaussian signal plus flat background
 - Mean of Gaussian, fraction of signal are parameters
- Case I : Width of Gauss is known exactly

$$F(x;\mu,f,\sigma) = f \cdot G(x,\mu,\sigma) + (1-f) \cdot U(x)$$

$$L(x;\mu,f,\sigma) = -\sum_{D} F(x_{i},\mu,f,\sigma)$$

- Case II: Width of Gaussian is known with 10% uncertainty
 - NB: '10% uncertainty' is ambiguous, choose Gaussian error blow

$$F'(x; \mu, f, \sigma_0, \delta\sigma) = F(x, f, \mu, \sigma) \cdot G(\sigma, \sigma_0, \delta\sigma)$$

 $L(\mu, f, \sigma_0, \delta\sigma) = -\sum_{i} F(x_i, \mu, f, \sigma) - \log(G(\sigma \mid \sigma_0, \delta\sigma))$

Adding uncertainties to a likelihood

• Example 1 – Width known exactly



• Example 2 – Gaussian uncertainty on width



Adding uncertainties to likelihood

 Can in principle also systematic uncertainties of type 'HERWIG simulation' vs 'PYTHIA simulation' directly in likelihood using 'morphing transformation'



- Construct $-\log(L)$ with F_{AB} and let α float in fit
- Optionally, add (Gaussian) constraint term on parameter α

Parameters of interest vs. nuisance parameters

• Typical (likelihood) fit yields many parameters

$$F(x; \mu, f, \sigma) = f \cdot G(x, \mu, \sigma) + (1 - f) \cdot U(x)$$

- Not all are of 'physics interest'
- Terminology to distinguish parameters
 - Parameter(s) of interest \rightarrow Physics we intend to publish (N_{Higgs})
 - Nuisance parameters \rightarrow The others (detector resolution etc...)
- Goal: incorporate uncertainty from nuisance parameters into parameters of interest.
- Each of the three main classes of constructing intervals (Bayesian, likelihood ratio, Neyman confidence intervals) has a way to incorporate the uncertainty on the nuisance parameters in the parameters of interest. But this remains a subject of frontier statistics research.
- Next: introduce methods and their problems

Dealing with nuisance parameters in Bayesian intervals

- Elimination of nuisance parameters in Bayesian interval
 - Construct a multi-D prior pdf P(parameters) for the space spanned by all parameters;
 - Multiply by P(data|parameters) for the data obtained;
 - Integrate over the full subspace of all nuisance parameters;

$$p(s \mid x) = \int \left(L(s, \vec{b}) p(s, \vec{b}) \right) d\vec{b}$$

- You are left with the posterior pdf for the parameter of interest. The math is now reduced to the case of no nuisance parameters.
- Issues
 - The multi-D prior pdf is a problem for both subjective and nonsubjective priors.
 - In HEP there is almost no use of the favored non-subjective priors (reference priors of Bernardo and Berger), so we do not know how well they work for our problems.
 - In case of many nuisance parameters, the high-D numeric integral can be a technical problem (use of Markov Chain Monte Carlo)

Illustration of nuisance parameters in Bayesian intervals

• Example: data with Gaussian model (mean, sigma)



Dealing with nuisance parameters in Frequentist intervals

• (Full) Neyman construction:

- The goal is that the parameter of interest should be covered at the stated confidence for every value of the nuisance parameter
- if there is any value of the nuisance parameter which makes the data consistent with the parameter of interest, that parameter point should be considered:
- eg. don't claim discovery if any background scenario is compatible with data
- Issues
 - Significant over coverage common problem
 - Wilks theorem may not apply due to e.g. 'look elsewhere effects' in nuisance parameters → must rely on toy MC approach, can get very cumbersome



Wilks theorem and nuisance parameters

- Wilks's theorem holds if the true distribution is in the family of functions being considered
 - eg. we have sufficiently flexible models of signal & background to incorporate all systematic effects
 - but we don't believe we simulate everything perfectly
 - ..and when we parametrize our models usually we have further approximated our simulation.
- E.g. if a model has a floating mass, it is clear that there is a degradation in significance due to the lookelsewhere effect (if you look into a wide enough mass range, your always find 'some peak' in the background)
 - Formally, the conditions required for Wilks's theorem do not hold because floating mass parameter makes no sense in a background-only model.

Dealing with nuisance parameters in Likelihood ratio intervals

- Nuisance parameters in LR interval
 - For each value of the parameter of interest, search the full subspace of nuisance parameters for the point at which the likelihood is maximized.
 - Associate that value of the likelihood with that value of the parameter of interest \rightarrow 'Profile likelihood'



Dealing with nuisance parameters in Likelihood ratio intervals



Link between MINOS errors and profile likelihood



Dealing with nuisance parameters in Likelihood ratio intervals

- Issues with Profile Likelihood
 - By using best-fit value of the nuisance parameters corresponding to each value of the parameter of interest, this has a reputation of underestimating the true uncertainties.
 - In Poisson problems, this is partially compensated by effect due to discreteness of n, and profile likelihood (MINUIT MINOS) gives good performance in many problems.
- NB: Computationally Profile Likelihood is quite manageable, even with a large number of nuisance parameters
 - Minimize likelihood w.r.t. 20 parameters quite doable
 - Especially compared to numeric integration over 20 parameters, or constructing confidence belt in 20 dimensions...

Recent comparisons results from PhyStat 2007

A Prototype Problem	BROOKHAVEN NATIONAL LABORATORY			
What is significance Z of an observation $x = 178$ signal like region, if my expected background $\frac{1}{10\%}$ uncertainty?	events in a b =100 with a			
• if you use the ATLAS TDR formula $Z_{5'}=5.5$				
The question seems simple enough, but it is no well-posed	ot actually			
• what do I mean by 10% background uncerta	inty?			
Typically, we consider an auxiliary measuremenestimate background (Type I systematic)	nt y used to			
 eg: a sideband counting experiment where be in sideband is a factor τ bigger than in sign 	ackgrour E	ample Sideband Meas	surement	BROOKHAVEN NATIONAL LABORATORY
$L_P(x, y \mu, b) = Pois(x \mu + b) \cdot Pois(y \mu)$	au b).	aband massurament us	ad š	
Kyle Cranmer (BNL) PhyStat 2007, CERN, June 26, 2007	to the sig	extrapolate / interpolat e background rate in nal-like region	e 20000	$=\frac{\langle y\rangle}{\langle x\rangle}$
	Fo	r now ignore uncertainty trapolation.	/ in 15000	A A A A A A A A A A A A A A A A A A A
			10000	$m_{\gamma\gamma}^{120}$ (GeV)
		$L_P(x,y \mu,b) = Point$	$s(x \mu+b) \cdot Pois(y \tau)$	<i>b</i>).
	Kyle Cra	nmer (BNL) PhyStat 200	7, CERN, June 26, 2007	4

Recent comparisons results from PhyStat 2007

Comparison of Methods for Prototype Problem

In my contribution to PhyStat2005, >130 I considered this problem and 120 compared the coverage for several 110 methods 100

See Linnemann's PhyStat03 paper

Major results:

- Cousins-Highland result (Z_N) badly under-covers (only 4.2σ)!
 - rate of Type I error is 110 times higher than stated!
 - much less luminosity required

Profile Likelihood Ratio (MINUIT/ MINOS) works great out to 5σ!

contours for $\textbf{b}_{true}\text{=}100,$ critical regions for τ = 1 120 No Systematics Z_{5'} 110 Ζ. λ_{G} profile 100 λ_{p} profile ad hoc 90 correct coverage 80 70 60 50 40 60 80 100 120 140 160 180 200

Figure 7. A comparison of the various methods critical boundary $x_{crit}(y)$ (see text). The concentric ovals represent contours of L_G from Eq. 15.

Method	$L_G (Z\sigma)$	$L_P(Z\sigma)$	$x_{crit}(y=100)$
No Syst	3.0	3.1	150
$Z_{5'}$	4.1	4.1	171
Z_N (Sec. 4.1)	4.2	4.2	178
ad hoc	4.6	4.7	188
$Z_{\Gamma} = Z_{Bi}$	4.9	5.0	185
profile λ_P	5.0	5.0	185
profile λ_G	4.7	4.7	${\sim}182$

Kyle Cranmer (BNL)

Hybrid Techniques: Introduction to Pragmatism

- Given the difficulties with all three classes of interval estimation, especially when incorporating nuisance parameters, it is common in HEP to relax foundational rigor and:
 - Treat nuisance parameters in a Bayesian way while treating the parameter of interest in a frequentist way, or
 - Treat nuisance parameters by profile likelihood while treating parameter of interest another way, or
 - Use the Bayesian framework (even without the priors recommended by statisticians), but evaluate the frequentist performance. In effect (as in profile likelihood) one gets approximate coverage while respecting the L.P.

Goal for the LHC a Few Years Ago

- Have in place tools to allow computation of results using a variety of recipes, for problems up to intermediate complexity:
 - Bayesian with analysis of sensitivity to prior
 - Frequentist construction with approximate treatment of nuisance parameters
 - Profile likelihood ratio (Minuit MINOS)
 - Other "favorites" such as LEP's CLS(which is an HEP invention)
- The community can then demand that a result shown with one's preferred method also be shown with the other methods, and sampling properties studied.
- When the methods all agree, we are in asymptopic nirvana.
- When the methods disagree, we learn something!
 - The results are answers to different questions.
 - Bayesian methods can have poor frequentist properties
 - Frequentist methods can badly violate likelihood principle

ATLAS/CMS/ROOT Project: RooStats built on RooFit



- Core developers:
- K. Cranmer (ATLAS)
- Gregory Schott (CMS)
- Wouter Verkerke (RooFit)
- Lorenzo Moneta (ROOT)
- Open project, all welcome to contribute.
- Included in ROOT production releases since v5.22, more soon to come
- Example macros in \$ROOTSYS/tutorials/roostats
- RooFit extensively documented, RooStats manual catching up, code doc in ROOT.

• Create a model - Example

```
Poisson(x | s \cdot r_s + b \cdot r_b) \cdot Gauss(r_s, 1, 0.05) \cdot Gauss(r_b, 1, 0.1)
```

Contents of workspace from above operation

```
RooWorkspace(w) w contents
variables
------
(b, obs, ratioBkgEff, ratioSigEff, s)
p.d.f.s
------
RooProdPdf::PC[ P * sigCon * bkgCon ] = 0.0325554
RooPoisson::P[ x=obs mean=n ] = 0.0325554
RooAddition::n[ s * ratioSigEff + b * ratioBkgEff ] = 150
RooGaussian::sigCon[ x=ratioSigEff mean=1 sigma=0.05 ] = 1
RooGaussian::bkgCon[ x=ratioBkgEff mean=1 sigma=0.1 ] = 1 e, NIKHEF
```

• Confidence intervals calculated with model

-	Profile likelihood	<pre>ProfileLikelihoodCalculator plc; plc.SetPdf(w::PC); plc.SetData(data); // contains [obs=160] plc.SetParameters(w::s); plc.SetTestSize(.1); ConfInterval* lrint = plc.GetInterval(); // that was easy.</pre>
_	Feldman Cousins	<pre>FeldmanCousins fc; fc.SetPdf(w::PC); fc.SetData(data); fc.SetParameters(w::s); fc.UseAdaptiveSampling(true); fc.FluctuateNumDataEntries(false); fc.SetNBins(100); // number of points to test per parameter fc.SetTestSize(.1); ConfInterval* fcint = fc.GetInterval(); // that was easy.</pre>
-	Bayesian (MCMC)	UniformProposal up; MCMCCalculator mc:
		<pre>mc.SetPdf(w::PC); mc.SetData(data); mc.SetParameters(s);</pre>
		<pre>mc.SetProposalFunction(up); mc.SetNumIters(100000); // steps in the chain mc SetTestSize(1): // 90% Cl</pre>
		<pre>mc.SetNumBins(50); // used in posterior histogram mc.SetNumBurnInSteps(40):</pre>
		<pre>ConfInterval* mcmcint = mc.GetInterval();</pre>

• Retrieving and visualizing output

double fcul = fcint->UpperLimit(w::s); double fcll = fcint->LowerLimit(w::s);



- Some notes on example
 - Complete working example (with output visualization) shipped with ROOT distribution (\$ROOTSYS/tutorials/roofit/rs101_limitexample.C)
 - Interval calculators make no assumptions on internal structure of model. Can feed model of arbitrary complexity to same calculator (computational limitations still apply!)



Wouter Verkerke, NIKHEF

'Digital' publishing of results

- A likelihood may be considered the ultimate publication of a measurement
- Interesting to be able to digitally publish actual likelihood rather than
 - Parabolic version (i.e. you publish your measurement and an error)
 - Some parameterized form. Cumbersome in >1 dimension. No standard protocol for exchanging this time of information
- This is trivially possible with RooFit/RooStats
 - Many potential applications, e.g. combining of Higgs channels,



Using persisted p.d.f.s.

• Using both model & p.d.f from file



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 Note that above code is independent of actual p.d.f in file → e.g. full Higgs combination would work with identical code

A toy combination example



Wouter Verkerke, NIKHEF

Work in progress on realistic Higgs limit combination

Combining the inputs

Using the same code as last time, with a few extra lines for the new channels, we arrive at the combined dataset & model

- here the only common parameter is mu, the master signal strength
 - could easily make Higgs mass be the same for all three channels
- the combined model has 27 nuisance parameters





ATLAS Statistics Forum, September 2, 2009



The end – Recommended reading

- Easy
 - R. Barlow, Statistics: A Guide to the Use of Statistical Methods in the Physical Sciences, Wiley, 1989
 - L. Lyons, Statistics for Nuclear and Particle Physics, Cambridge University Press
 - Philip R. Bevington and D.Keith Robinson, Data Reduction and Error Analysis for the Physical Sciences
- Intermediate
 - Glen Cowan, Statistical Data Analysis (Solid foundation for HEP)
 - Frederick James, Statistical Methods in Experimental Physics, World Scientific, 2006. (This is the second edition of the influential 1971 book by Eadie et al., has more advanced theory, many examples)
- Advanced
 - A. Stuart, K. Ord, S. Arnold, Kendall's Advanced Theory of Statistics, Vol. 2A, 6th edition, 1999; and earlier editions of this "Kendall and Stuart" series. (Authoritative on classical frequentist statistics; anyone contemplating a NIM paper on statistics should look in here first!)
- PhyStat conference series:
 - Beginning with Confidence Limits Workshops in 2000, links at http://phystat-lhc.web.cern.ch/phystat-lhc/ and http://www.physics.ox.ac.uk/phystat05/









