

Statistics for the LHC: Quantifying our Scientific Narrative



Kyle Cranmer (NYU)

Introduction

Statistics plays a vital role in science, it is the way that we:

- quantify our knowledge and uncertainty
- communicate results of experiments

Big questions:

- make discoveries, test theories, measure or exclude parameters, etc.
- how do we get the most out of our data
- how do we incorporate uncertainties
- how do we make decisions

Statistics is a very big field, and it is not possible to cover everything in 4 hours. In these talks I will try to:

- explain some fundamental ideas & prove a few things
- enrich what you already know
- expose you to some new ideas

I will try to go slowly, because if you are not following the logic, then it is not very interesting.

Please feel free to ask questions and interrupt at any time

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By physicists, for physicists

G. Cowan, Statistical Data Analysis, Clarendon Press, Oxford, 1998.

R.J.Barlow, A Guide to the Use of Statistical Methods in the Physical Sciences, John Wiley, 1989;

F. James, Statistical Methods in Experimental Physics, 2nd ed., World Scientific, 2006;

• W.T. Eadie et al., North-Holland, 1971 (1st ed., hard to find);

S.Brandt, Statistical and Computational Methods in Data Analysis, Springer, New York, 1998. L.Lyons, Statistics for Nuclear and Particle Physics, CUP, 1986.



My favorite statistics book by a statistician:

Stuart, Ord, Arnold. "Kendall's Advanced Theory of Statistics" Vol. 2A *Classical Inference & the Linear Model*.

Other lectures



Fred James's lectures

http://preprints.cern.ch/cgi-bin/setlink?base=AT&categ=Academic_Training&id=AT00000799

http://www.desy.de/~acatrain/

Glen Cowan's lectures

http://www.pp.rhul.ac.uk/~cowan/stat_cern.html

Louis Lyons

http://indico.cern.ch/conferenceDisplay.py?confld=a063350

Bob Cousins gave a CMS lecture, may give it more publicly

Gary Feldman "Journeys of an Accidental Statistician"

http://www.hepl.harvard.edu/~feldman/Journeys.pdf

The PhyStat conference series at PhyStat.org:





I also gave "Statistics for LHC" academic training lectures in 2009

http://indico.cern.ch/conferenceDisplay.py?confld=48425

Now that we have data, I will put emphasis on realistic problems representative of current analyses 2011

2009

Foundations of Probability

Hypothesis Tests

Confidence Intervals

Generalization for complex problems

Modeling & Scientific Narrative

Hypothesis Tests

Confidence Intervals

Bayesian Methods

Likelihood Methods



Lecture 1



Preliminaries

Probability Density Functions



When dealing with continuous random variables, need to introduce the notion of a **Probability Density Function** (PDF... not parton distribution function)

$$P(x \in [x, x + dx]) = f(x)dx$$

Note, f(x) is NOT a probability

PDFs are always normalized

$$\int_{-\infty}^{\infty} f(x)dx = 1$$



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The Likelihood Function



A Poisson distribution describes a discrete event count *n* for a realvalued mean μ .

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

The likelihood of μ given *n* is the same equation evaluated as a function of μ

- Now it's a continuous function
- But it is not a pdf!

$$L(\mu) = Pois(n|\mu)$$

Common to plot the -2 In L

- helps avoid thinking of it as a PDF
- connection to χ^2 distribution



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

Parametric PDFs



- Many familiar PDFs are considered **parametric**
 - + eg. a Gaussian $G(x|\mu,\sigma)$ is parametrized by (μ,σ)
- defines a family of distributions
- allows one to make inference about parameters
- I will represent PDFs graphically as below (directed acyclic graph)
 - every node is a real-valued function of the nodes below

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Modeling: The Scientific Narrative

Before one can discuss statistical tests, one must have a "**model**" for the data.

- by "model", I mean the full structure of P(data | parameters)
 - holding parameters fixed gives a PDF for data
 - ability to evaluate generate pseudo-data (Toy Monte Carlo)
 - holding data fixed gives a likelihood function for parameters
 - note, likelihood function is not as general as the full model because it doesn't allow you to generate pseudo-data

Both Bayesian and Frequentist methods start with the model

- it's the objective part that everyone can agree on
- it's the place where our physics knowledge, understanding, and intuiting comes in
- building a better model is the best way to improve your statistical procedure

RooFit: A data modeling toolkit



RooFit is a major tool developed at BaBar for data modeling. RooStats provides higher-level statistical tools based on these PDFs.



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The model can be seen as a quantitative summary of the analysis

- If you were asked to justify your modeling, you would tell a story about why you know what you know
 - based on previous results and studies performed along the way
- the quality of the result is largely tied to how convincing this story is and how tightly it is connected to model
- I will describe a few "narrative styles"
 - The "Monte Carlo Simulation" narrative
 - The "Data Driven" narrative
 - The "Effective Modeling" narrative
 - The "Parametrized Response" narrative

Real-life analyses often use a mixture of these

The Monte Carlo Simulation narrative



Let's start with "the Monte Carlo simulation narrative", which is probably the most familiar



Cross-sections and event rates



From the many, many collision events, we impose some criteria to select *n* candidate signal events. We hypothesize that it is composed of some number of signal and background events. Pois(n|s+b)

The number of events that we expect from a given interaction process is given as a product of

- L : a time-integrated luminosity (units 1/cm²) that serves as a measure of the amount of data that we have collected or the number of trials we have had to produce signal events
- σ : "cross-section" (units cm²) a quantity that can be calculated from theory
- ε : fraction of signal events selected by selection criteria



The language of the Standard Model is Quantum Field Theory **Phase space** Ω defines initial measure, sampled via Monte Carlo

$$P = \frac{|\langle f|f \rangle|^{i}}{\langle f|f \rangle \langle i|i \rangle}$$
$$P \to L\sigma$$
$$d\sigma \to |\mathcal{M}|^{2} d\Omega$$

 $|\langle f|_{j}\rangle|^{2}$



The language of the Standard Model is Quantum Field Theory **Phase space** Ω defines initial measure, sampled via Monte Carlo





The language of the Standard Model is Quantum Field Theory **Phase space** Ω defines initial measure, sampled via Monte Carlo $P = \frac{|\langle f|i\rangle|^2}{\langle f|f\rangle\langle i|i\rangle}$ $P \to L\sigma$ $d\sigma \to |\mathcal{M}|^2 d\Omega$ Relative beam sizes around IP1 (Atlas) in collision $\frac{1}{4}\mathbf{W}_{\mu\nu}\cdot\mathbf{W}^{\mu\nu}-\frac{1}{4}B_{\mu\nu}B^{\mu\nu}-\frac{1}{4}G^{a}_{\mu\nu}G^{\mu\nu}_{a}$ $\mathcal{L}_{SM} =$ kinetic energies and self-interactions of the gauge bosons + $\bar{L}\gamma^{\mu}(i\partial_{\mu}-\frac{1}{2}g\tau\cdot\mathbf{W}_{\mu}-\frac{1}{2}g'YB_{\mu})L + \bar{R}\gamma^{\mu}(i\partial_{\mu}-\frac{1}{2}g'YB_{\mu})R$ kinetic energies and electroweak interactions of fermions $\frac{1}{2}\left|\left(i\partial_{\mu}-\frac{1}{2}g\tau\cdot\mathbf{W}_{\mu}-\frac{1}{2}g'YB_{\mu}\right)\phi\right|^{2}-V(\phi)\right|$ W, Z W^{\pm}, Z, γ , and Higgs masses and couplings $g''(\bar{q}\gamma^{\mu}T_aq)G^a_{\mu} + (G_1L\phi R + G_2\bar{R}\phi_cL + h.c.)$ fermion masses and couplings to Higgs interactions between quarks and gluons

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a) Perturbation theory used to systematically approximate the theory.
b) splitting functions, Sudokov form factors, and hadronization models
c) all sampled via accept/reject Monte Carlo P(particles | partons)



- hard scattering
- a dit atre (6. \$2) ⊂ raita carata
- partonic decays, e.g. $t \rightarrow bW$



a) Perturbation theory used to systematically approximate the theory.
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- hard scattering
- (QED) initial/final state radiation
- partonic decays, e.g. $t \rightarrow bW$
- parton shower evolution
- nonperturbative gluon splitting
- colour singlets
- colourless clusters
- cluster fission
- cluster \rightarrow hadrons
- hadronic decays

Next, the interaction of outgoing particles with the detector is simulated. Detailed simulations of particle interactions with matter. Accept/reject style Monte Carlo integration of very complicated function P(detector readout | initial particles)



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In addition to the rate of interactions, our theories predict the distributions of angles, energies, masses, etc. of particles produced

- we form functions of these called **discriminating variables** *m*,
- and use Monte Carlo techniques to estimate f(m)

In addition to the hypothesized signal process, there are known background processes.

- thus, the distribution of f(m) is a mixture model
- the full model is a marked Poisson process



Example model



Here is an example prediction from search for $H \rightarrow ZZ$ and $H \rightarrow WW$

sometimes multivariate techniques are used



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Parametric vs. Non-Parametric PDFs



No parametric form, need to construct **non-parametric** PDFs From Monte Carlo samples, one has empirical PDF





Classic example of a **non-parametric** PDF is the histogram





Classic example of a non-parametric PDF is the histogram but they depend on bin width and starting position





Classic example of a **non-parametric** PDF is the histogram

"Average Shifted Histogram" minimizes effect of binning


Kernel Estimation



Kernel estimation is the generalization of Average Shifted Histograms



"the data is the model"

Adaptive Kernel estimation puts wider kernels in regions of low probability

Used at LEP for describing pdfs from Monte Carlo (KEYS)

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Kernel Estimation has a nice generalizations to higher dimensions

• practical limit is about 5-d due to curse of dimensionality

Max Baak has coded Ndim KEYS pdf described **In** Comput.Phys.Commun. **136** (2001) 2-d projection of in RooFit. slide. These pdfs have been RooNDKeys pdf used as the basis for a automatically models (fine) multivariate correlations discrimination between technique called "PDE"

$$D(\vec{x}) = \frac{f_s(\vec{x})}{f_s(\vec{x}) + f_b(\vec{x})}$$

Correlations

- pdf from previous
- observables ...



Max Baak

Incorporating Systematic Effects



Of course, the simulation has many adjustable parameters and imperfections that lead to systematic uncertainties.

 one can re-run simulation with different settings and produce variational histograms about the nominal prediction



Explicit parametrization



Important to distinguish between the **source** of the systematic uncertainty (eg. jet energy scale) and its **effect**.

- The same 5% jet energy scale uncertainty will have different effect on different signal and background processes
 - not necessarily with any obvious functional form

Usually possible to decompose to independent "uncorrelated" sources

Imagine a table that **explicitly quantifies** the effect of each source of systematic.

Entries are either normalization factors or variational histograms

	sig	bkg 1	bkg 2	•••
syst 1				
syst 2				
•••				

Histogram Interpolation

Several interpolation algorithms exist: eg. Alex Read's "horizontal" histogram interpolation algorithm (RooIntegralMorph in RooFit)

• take several PDFs, construct interpolated PDF with additional nuisance parameter α

A.L. Read | Nuclear Instruments and Methods in Physics Research A 425 (1999) 357-360

interpolation bin-by-bin. Alternative "horizontal" interpolation algorithm b

Simple "vertical"

Alternative "horizontal" interpolation algorithm by Max Baak called "RooMomentMorph" in RooFit (faster and numerically more stable)





Incorporating systematics

Let's consider a simplified problem that has been studied quite a bit to gain some insight into our more realistic and difficult problems

- number counting with background uncertainty
 - in our main measurement we observe n_{on} with s+b expected

$$\operatorname{Pois}(n_{\mathrm{on}}|s+b)$$

- and the background has some uncertainty
 - but what is "background uncertainty"? Where did it come from?
 - maybe we would say background is known to 10% or that it has some pdf $\pi(b)$
 - then we often do a smearing of the background:

$$P(n_{\rm on}|s) = \int db \operatorname{Pois}(n_{\rm on}|s+b) \,\pi(b),$$

- Where does $\pi(b)$ come from?
 - did you realize that this is a Bayesian procedure that depends on some prior assumption about what b is?



Figure 10: Flow chart describing the four data samples used in the $H \rightarrow WW^{(*)} \rightarrow \ell \nu \ell \nu$ analysis. S.R and C.R. stand for signal and control regions, respectively.

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The "on/off" problem



Now let's say that the background was estimated from some control region or sideband measurement.

- We can treat these two measurements simultaneously:
 - main measurement: observe *n*on with *s*+*b* expected
 - sideband measurement: observe $n_{\textit{off}}$ with au b expected

$$\underbrace{P(n_{\rm on}, n_{\rm off}|s, b)}_{P(n_{\rm on}, n_{\rm off}|s, b)} = \underbrace{\operatorname{Pois}(n_{\rm on}|s+b)}_{Pois} \underbrace{\operatorname{Pois}(n_{\rm off}|\tau b)}_{Pois}$$

joint model main measurement sideband

- In this approach "background uncertainty" is a statistical error
- justification and accounting of background uncertainty is much more clear

How does this relate to the smearing approach?

$$P(n_{\rm on}|s) = \int db \operatorname{Pois}(n_{\rm on}|s+b) \,\pi(b),$$

• while $\pi(b)$ is based on data, it still depends on a prior $\eta(b)$ $\pi(b) = P(b|n_{\text{off}}) = \frac{P(n_{\text{off}}|b)\eta(b)}{\int db P(n_{\text{off}}|b)\eta(b)}.$



Often the extrapolation parameter has uncertainty

- Introduce a new measurement to constrain it as in the ABCD method
- what if..., what if ..., what if..., what if ..., what if..., what if ...





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Classification of Systematic Uncertainties

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Taken from Pekka Sinervo's PhyStat 2003 contribution

Type I - "The Good"

- can be constrained by other sideband/auxiliary/ ancillary measurements and can be treated as statistical uncertainties
 - scale with luminosity



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- Type II "The Bad"
 - arise from model assumptions in the measurement or from poorly understood features in data or analysis technique
 - don't necessarily scale with luminosity
 - eg: "shape" systematics



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- Type II "The Bad"
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 - eg: "shape" systematics
- Type III "The Ugly"
 - arise from uncertainties in underlying theoretical paradigm used to make inference using the data
 - a somewhat philosophical issue



Separating the prior from the objective model



Recommendation: where possible, one should express uncertainty on a parameter as a statistical (random) process

- explicitly include terms that represent auxiliary measurements in the likelihood
- **Recommendation:** when using a Bayesian technique, one should explicitly express and separate the prior from the objective part of the probability density function

Example:

- By writing $P(n_{\text{on}}, n_{\text{off}}|s, b) = \text{Pois}(n_{\text{on}}|s+b) \text{Pois}(n_{\text{off}}|\tau b).$
 - the objective statistical model is for the background uncertainty is clear
- One can then explicitly express a prior $\eta(b)$ and obtain:

$$\pi(b) = P(b|n_{\text{off}}) = \frac{P(n_{\text{off}}|b)\eta(b)}{\int db P(n_{\text{off}}|b)\eta(b)}.$$

Constraints on Nuisance Parameters



Many uncertainties have no clear statistical description or it is impractical to provide

Traditionally, we use Gaussians, but for large uncertainties it is clearly a bad choice

quickly falling tail, bad behavior near physical boundary, optimistic p-values, ...

For systematics constrained from control samples and dominated by statistical uncertainty, a Gamma distribution is a more natural choice [PDF is Poisson for the control sample]

Ionger tail, good behavior near boundary, natural choice if auxiliary is based on counting

For "factor of 2" notions of uncertainty log-normal is a good choice

can have a very long tail for large uncertainties

None of them are as good as an actual model for the auxiliary measurement, if available



To consistently switch between frequentist, Bayesian, and hybrid procedures, need to be clear about prior vs. likelihood function

PDF	Prior	Posterior
Gaussian	uniform	Gaussian
Poisson	uniform	Gamma
Log-normal	reference	Log-Normal

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Building the model: HistFactory (RooStats)



Several analyses have used the tool called **hist2workspace** to build the model (PDF)

- command line: hist2workspace myAnalysis.xml
- construct likelihood function below via XML + histograms

$$\mathscr{L}(\mu, \alpha_i) = \prod_{m \in \text{bins}} \text{Pois}(n_m | \mathbf{v}_m) \prod_{i \in \text{Syst}} N(\alpha_i)$$

$$\eta_j(\alpha) = \prod_{i \in \text{Syst}} I(\alpha_i; \eta_{ij}^+, \eta_{ij}^-)$$

$$\sigma_{jm}(\alpha) = \sigma_{jm}^0 \prod_{i \in \text{Syst}} I(\alpha_i; \sigma_{ijm}^+ / \sigma_{jm}^0, \sigma_{ijm}^- / \sigma_{jm}^0)$$

$$\mathbf{v}_m = \mu L \eta_1(\alpha) \ \sigma_{1m}(\alpha) + \sum_{j \in \text{Bkg Samp}} L \eta_j(\alpha) \ \sigma_{jm}(\alpha),$$

$$I(lpha; I^+, I^-) = egin{cases} 1+lpha(I^+-1) & ext{if } lpha > 0 \ 1 & ext{if } lpha = 0 \ 1-lpha(I^--1) & ext{if } lpha < 0 \end{cases}$$

- For each systematic effect, we associated a nuisance parameter α
 - for instance electron efficiency, JES, luminosity, etc.
 - the background rates, signal acceptance, etc. are parametrized in terms of these nuisance parameters
- These systematics are usually known ("constrained") within $\pm 1\sigma$.
 - but here we must be careful about Bayesian vs. frequentist
 - Why is it constrained? Usually b/c we have an auxiliary measurement m and a relationship like:

 $G(m|\alpha,\sigma)$

- Saying that α has a Gaussian distribution is Bayesian.
 - has form "Probability of parameter"
- The frequentist way is to say that that m fluctuates about α

While *m* is a measured quantity (or "observable"), there is only one measurement of *m* per experiment. Call it a "**Global observable**"

An example ModelConfig from HistFactory



The RooStats tools, use the RooFit PDF interface, but the tools need some additional meta information. The **ModelConfig** class encapsulates this meta information

 The PDF itself, the observables, the "global observables", the parameter of interest, and the nuisance parameters. Also the prior for Bayesian methods.

root [7] modelConfig->Print() === Using the following for ModelConfig === **Observables**: RooArgSet:: = (obs_h2e2nu_200)

Parameters of Interest: RooArgSet:: = (SigXsecOverSM)

Nuisance Parameters: RooArgSet:: =

(Lumi,alpha_SysBtagEff,alpha_SysElecScale,alpha_SysElecSmear,alpha_SysJetScale,alpha_SysJetSmear,alpha_SysM ETHadScale,alpha_SysMETHadSmear,alpha_SysMuonScale,alpha_SysMuonSmear,alpha_dieleceff,alpha_mjet2enorm,alpha_signorm,alpha_topnorm,alpha_wnorm,alpha_wwnorm,alpha_wznorm,alpha_znorm,alpha_zznorm)

Global Observables: RooArgSet:: =

(nominalLumi,nom_alpha_dieleceff,nom_alpha_signorm,nom_SysMuonScale,nom_SysMETHadSmear,nom_SysElecSme ar,nom_SysMuonSmear,nom_SysJetSmear,nom_SysBtagEff,nom_SysJetScale,nom_SysMETHadScale,nom_SysElecSc ale,nom_alpha_topnorm,nom_alpha_wwnorm,nom_alpha_wznorm,nom_alpha_zznorm,nom_alpha_wnorm,nom_alpha_z norm,nom_alpha_mjet2enorm)

PDF: RooProdPdf::model_h2e2nu_200[lumiConstraint * alpha_dieleceffConstraint * alpha_signormConstraint * alpha_SysMuonScaleConstraint * alpha_SysMETHadSmearConstraint * alpha_SysElecSmearConstraint * alpha_SysMuonSmearConstraint * alpha_SysJetSmearConstraint * alpha_SysBtagEffConstraint * alpha_SysJetScaleConstraint * alpha_SysMETHadScaleConstraint * alpha_SysElecScaleConstraint * alpha_topnormConstraint * alpha_wnormConstraint * alpha_zznormConstraint * alpha_wnormConstraint * alpha_wnormConstraint * alpha_mjet2enormConstraint * h2e2nu_200_model] = 0

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CMS Higgs example

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The CMS input:

- cleanly tabulated effect on each background due to each source of systematic
- systematics broken down into uncorrelated subsets
- used lognormal distributions for all systematics, Poissons for observations

Started with a txt input, defined a mathematical representation, and then prepared the RooStats workspace

Date: June 22, 2010 Description: HWW>212v, Ojets, cut-and-count for 3 channels: m mH 160 Higgs mass hypothesis comE 7.0 center of mass energy lumi 1 luminosity in fb-1	nu, ee, emu; made-up numbers for a ATLAS+CMS combination exercise	$\left(\left(\sum_{i=0,1} \tilde{n}_{ij} \cdot \kappa_{ijk}^{\theta_k} \right)^{N_i} \right) = \left(\sum_{i=0,1} \tilde{n}_{ij} \cdot \kappa_{ijk}^{\theta_k} \right)^{N_i} = \left(\sum_{i=0,1} \tilde{n}_{ij} \cdot \kappa_{ijk}^{\theta_k}$
imax 3 number of channels jmax 6 number of backgrounds kmax 37 number of nuisance parameters		$ \left(\underbrace{L_{b+rs}}_{i} \right) = \prod_{i} \left \frac{(j=0,1,\dots,j)}{N_{i}!} \cdot \exp\left(-\sum_{j=0,1,\dots,j} \tilde{n}_{ij} \cdot \kappa_{ijk}^{\theta_{k}}\right) \right \cdot \prod_{k} f(\theta_{k}) $
Observation 15 7 13		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 2 2 2 2 3 3 3 3 3 3 Zj tX WW WZ ZZ H Wj Zj tX WW WZ Z 2 3 4 5 6 0 1 2 3 4 5	
rate 10.5 0.01 0.05 0.94 3.39 0.01 0.01 5.39 0.01	05 0.46 1.50 0.05 0.04 10.0 0.01 0.05 1.37 1.88 0.01 0.0	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	00 1.00 1	
3 observables and 37 nuisance paramet	ers	
$n = \mu L \epsilon \sigma_{SM}$		
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ATLAS Higgs Example

The ATLAS input:

- Poisson terms 3 signal regions and 6 control regions
- Initially uncertainties in extrapolation coefficients treated with one Gaussians and it wasn't possible to identify individual systematics effects
 - thus, unable to identify any correlated systematic (eg. theory uncertainty)
- Now individual uncertainties are explicitly parameterized





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The Effective Model



It is common to describe a distribution with some parametric function

- "fit background to a polynomial", exponential, ...
- While this is convenient and the fit may be good, the narrative is weak



The Effective Model narrative



However, sometimes the effective model comes from a convincing narrative

- convolution of resolution with known distribution
- · for example, the "invariant mass" of some final state particles



The parametrized response narrative



The Matrix-Element technique is conceptually similar to the simulation narrative, but the detector response is parametrized.

 Doesn't require building parametrized PDF by interpolating between nonparametric templates.



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Example likelihoods from CDF Z'

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Fast Simulation



Fast simulations based on parametrized detector response are very useful and can often be tuned to perform quite well in a specific analysis context

· For example: tools like PGS, Delphis, ATLFAST, ...

But these tools still use accept/reject Monte Carlo.

 Would be much more useful if the parmaetrized detector response could be used as a transfer function in Matrix-Element approach

Same sign di-lepton + jets + MET search



Narrative styles



The Monte Carlo Simulation narrative (MC narrative)

- each stage is an accept/reject Monte Carlo based on P(out|in) of some microscopic process like parton shower, decay, scattering
- PDFs built from non-parametric estimator like histograms or kernel estimation
 - need to supplement with interpolation procedures to incorporate systematics
 - smearing approach fundamentally Bayesian
- pros: most detailed understanding of micro-physics
- cons: computationally demanding, loose analytic scaling properties, relies on accuracy of simulation
- new ideas: improved interpolation, Radford Neal's machine learning, "design of experiments"

The Data-driven narrative

- independent data sample that either acts as a proxy for some process or can be transformed to do so
- pros: nature includes "all orders", uses real detector
- cons: extrapolation from control region to signal region requires assumptions, introduces systematic effects. Appropriate transformation may depend on many variables, which becomes impractical



Narrative styles

Effective modeling narrative

- parametrized functional form: eg. Gaussian, falling exponential para polynomial fit to distribution, etc.
- pros: fast, has analytic scaling, parametric form may be well justified (eg. phase space, propagation of errors, convolution)
- **cons**: approximate, parametric form may be ad hoc (eg. polynomial from)
- new ideas: using non-parametric statistical methods

Parametrized detector response narrative (eg. kinematic fitting, Matrix-Element method, ~fast simulation)

- pros: fast, maintains analytic scaling, response usually based on good understanding of the detector, possible to incorporate some types of uncertainty in the response analytically, can evaluate P(out|in) for arbitrary out,in.
- cons: approximate, best parametrized detector response is often not available in convenient form
- new ideas: fast simulation is typically parametrized, but we use it in an accept/ reject framework (see Geant5)

Combinations, Rich Modeling, and Publishing

Example of Digital Publishing

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Help

🔀 ROOT Object Browser	File Edit View Onlines Inspect Classes
<u>File View Options</u>	A RooPlot of "x"
🔄 wspace.root 💽 🗈 📴 🔚 📰 📰 🗘 🖒 📀 🕙	S 100 - T
All Folders Contents of "/ROOT Files/wspace.root	
/user/verkerke/roofit/workdir	60 I II
ROOT Files MyWork Space;1	40
wspace.root	
RooFit's Workspace now provides the	
ability to save in a ROOT file the full	9.10 -8 -6 -4 -2 0 2 4 6 8 10 x
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want and the minimal data necessary	8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
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Need this for combinations as n-value	
	2
is not sufficient information for a prope	r 1 - 1

combination.

Kyle Cranmer (NYU)

0

-0.1

-0.08

-0.04

-0.02

04 0.06 0.08 0.1

m

0.02 0.04
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As we saw, constraint terms for nuisance parameters can often be related to auxiliary measurements

- we only considered very simple auxiliary measurements, like number of events in a sideband, but even in that case there are likely to be common systematics
- idea can be generalized to more sophisticated measurements
 - for example, γ-jet or Z-jet balance measurements to constrain the Jet Energy Scale uncertainty
- The point is that combining these models leads to a qualitiative change in how we represent what we know: **rich modeling**

Now the distinction has been blurred between a Higgs combination and a sophisticated modeling of systematics

Examples of Published Likelihoods

RTICLE PHYSICS



The situation 10 years ago...

Origins I: The First "Statistics in HEP" conference

WORKSHOP ON CONFIDENCE LIMITS

CERN, Geneva, Switzerland 17–18 January 2000

CERN 2000-005

Massimo Corradi

Does everybody agree on this statement, to publish likelihoods?

Louis Lyons

Any disagreement? Carried unanimously. That's actually quite an achievement for this Workshop.

...[Fred James wants to be able to calculate coverage, Don Groom wants to able to calculate goodness of fit]...

Cousins

I thought the point of unanimity was that publishing the likelihood function was a *necessary* condition, not a sufficient condition.

But a practical problem remained: *How* to communicate multi-D likelihood?

http://indico.cern.ch/conferenceDisplay.py?confld=100458

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Current scenario

Taken from the GFitter paper

²³This procedure only uses the M_H value under consideration, where Higgs-mass hypothesis and measurement are compared. It thus neglects that in the SM a given signal hypothesis entails background hypotheses for all M_H values other than the one considered. An analysis accounting for this should provide a statistical comparison of a given hypothesis with all available measurements. This however would require to know the correlations among all the measurement points (or better: the full experimental likelihood as a function of the Higgs-mass hypothesis), which are not provided by the experiments to date. The difference to the hypothesis-only test employed here is expected to be small at present, but may become important once an experimental Higgs signal appears, which however has insufficient significance yet

Combining Results: An Example



By using the workspace, it is easy to share results, ideal for combinations.

Example above shows opening an 'atlas' and 'cms' workspace, and performing a combined fit to a common parameter with profile likelihood.

Kyle Cranmer (NYU)



Michelangelo's Likelihood Mandate (MLM):

A general assessment of the status and needs of the tools for setting limits on (or fitting) parameters of BSM models, using the multitude of data from searches at the LHC

Two related communities and ongoing discussions

- Characterization & Simplified Models
- Fitting Model Parameters



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- Fitting Model Parameters

 \rightarrow interpretation



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Potential new tasks

• Input for the Strategy Group

- LPCC and experiments required to produce combined assessment of the 2010-11(-12) findings in Higgs and BSM searches
- TH community, and other expl communities (e.g. LinCol, SuperB, ...), will use this to assess the implications of LHC data for BSM and future exptl projects
- \blacksquare We need to prepare the framework/tools to enable:
 - combination of limits/evidence from ATLAS/CMS(/LHCb)
 - use of the results by the rest of the community (e.g. SUSY-models' fitters)
- This will require coordination with
- ATLAS-CMS statistics forum
- Fitters' groups
- all LHC "search " efforts (Higgs, B decays, exotica of all sorts)

 \rightarrow interpretation



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use of the results by a theorist, in the context of a new model

SUSY Fitting tools

2D 95% CL All measurements

1D 68% CL All measurements

600

2D 95 % contour

400

Usually simplify input from experiments to be a single Gaussian



First interface with SuperBayes

Repeated same analysis as Bridges, KC, Trotta et al (<u>1011.4306</u>) with RooStats likelihood

see consistent results!





Benchmark based on counting



Max Baak's demonstrated interpolation of signal yield and uncertainties in a 3-d mSUGRA scan with a simple number counting analysis



Ultimate Goal

Publish likelihoods along with papers

first goal, the LEP Higgs



Kyle Cranmer (NYU)





CERN Colloquium and Library Science Talk

SPEAKER: Lawrence Lessig (Edmond J. Safra Center for Ethics and Harvard Law School, Cambridge, MA, US)

TITLE: "The architecture of access to scientific knowledge: just how badly we have messed this up"

- DATE: Mon 18/04/2011 16:30
- PLACE: Council Chamber

ABSTRACT

In this talk, Professor Lessig will review the evolution of access to scientific scholarship, and evaluate the success of this system of access against a background norm of universal access. While copyright battles involving artists has gotten most of the public's attention, the real battle should be over access to knowledge, not culture. That battle we are losing.



Kyle Cranmer (NYU)



Lecture 2



Modeling: The Scientific Narrative (continued)

In Monte Carlo Simulation approach, use simulated events to build histograms and construct the "Marked Poisson" model below



Tabulate effect of individual variations of sources of systematic uncertainty

 use some form of interpolation to parametrize *ith* variation in terms of nuisance parameter *α_i*



$$P(\mathbf{m}|\boldsymbol{\alpha}) = \operatorname{Pois}(n|s(\boldsymbol{\alpha}) + b(\boldsymbol{\alpha})) \prod_{j}^{n} \frac{s(\boldsymbol{\alpha})f_{s}(m_{j}|\boldsymbol{\alpha}) + b(\boldsymbol{\alpha})f_{b}(m_{j}|\boldsymbol{\alpha})}{s(\boldsymbol{\alpha}) + b(\boldsymbol{\alpha})}$$

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Something must 'constrain' the α

- the data itself: sidebands; some control region
- constraint term: idealized form of auxiliary measurement or ad hoc 'prior'



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$$\times G(a|\boldsymbol{\alpha}, \sigma)$$

Kyle Cranmer (NYU)

The Data-Driven narrative



In the data-driven approach, backgrounds are estimated by assuming (and testing) some relationship between a control region and signal region

- Ilavor subtraction, same-sign samples, fake matrix, tag-probe,
- **Pros:** Initial sample has "all orders" theory :-) and all the details of the detector **Cons:** assumptions made in the transformation to the signal region can be questioned



Other Examples of data-driven narrative



All-hadronic searches with MHT

Search for high pT jets, high HT and high MHT (= vector sum of jets)

- 3 jets, E_T >50 $|\eta|$ <2.5
- HT > 350 and MHT > 150
- Event cleaning cuts.
- Predict each bkgd separately QCD: rebalance & smear W & ttbar from μ control Z- $\nu\nu$ from γ +jets and Z- $\mu\mu$



 $Z \rightarrow II + jets$ Strength: very clean Weakness: low statistics



W → Iv + jets Strength: larger statistics Weakness: background from SM and SUSY



MET

 γ + jets
Strength: large statistics and clean at high E_T
Weakness: background at low E_T, theoretical errors

CMS SUSY Results, D. Stuart, April 2011, SUSY Recast, UC Davis



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The Effective Model Narrative

It is common to describe a distribution with some parametric function

- "fit background to a polynomial", exponential, ...
- While this is convenient and the fit may be good, the narrative is weak PHYSICAL REVIEW D 79, 112002 (2009)







The Effective Model Narrative



Sometimes the effective model comes from a convincing narrative

- convolution of detector resolution with known distribution
 - + Ex: MissingET resolution propagated through $M_{\tau\tau}$ in collinear approximation
 - + Ex: lepton resolution convoluted with triangular $M_{\rm H}$ distribution



Tools for building effective models



 RooFit's convolution PDFs can aid in building more effective models with a more convincing narrative





Wouter Verkerke, NIKHEF

The parametrized response narrative



The Matrix-Element technique is conceptually similar to the simulation narrative, but the detector response is parametrized.

 Doesn't require building parametrized PDF by interpolating between nonparametric templates.



Kyle Cranmer (NYU)

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Kyle Cranmer (NYU)



-100 T □ 100 V

-200

CDF Run II Preliminary

0.5

Example: CDF Z' $\rightarrow \mu\mu$

"a matrix element based likelihood providing an approximately 20% relative increase in cross section sensitivity at large Z' mass"



79



strategies. No reason we can't propagate uncertainty to next stage.



Kyle Cranmer (NYU)
Fast Simulation



Fast simulations based on parametrized detector response are very useful and can often be tuned to perform quite well in a specific analysis context

· For example: tools like PGS, Delphis, ATLFAST, ...



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Fast Simulation



Fast simulations based on parametrized detector response are very useful and can often be tuned to perform quite well in a specific analysis context

· For example: tools like PGS, Delphis, ATLFAST, ...

But these tools still use accept/reject Monte Carlo.

 Would be much more useful if the parmaetrized detector response could be used as a transfer function in Matrix-Element approach



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Narrative styles



The Monte Carlo Simulation narrative (MC narrative)

- each stage is an accept/reject Monte Carlo based on P(out|in) of some microscopic process like parton shower, decay, scattering
- PDFs built from non-parametric estimator like histograms or kernel estimation
 - need to supplement with interpolation procedures to incorporate systematics
 - smearing approach fundamentally Bayesian
- pros: most detailed understanding of micro-physics
- cons: computationally demanding, loose analytic scaling properties, relies on accuracy of simulation
- new ideas: improved interpolation, Radford Neal's machine learning, "design of experiments"

The Data-driven narrative

- independent data sample that either acts as a proxy for some process or can be transformed to do so
- pros: nature includes "all orders", uses real detector
- cons: extrapolation from control region to signal region requires assumptions, introduces systematic effects. Appropriate transformation may depend on many variables, which becomes impractical



Narrative styles

Effective modeling narrative

- parametrized functional form: eg. Gaussian, falling exponential para polynomial fit to distribution, etc.
- pros: fast, has analytic scaling, parametric form may be well justified (eg. phase space, propagation of errors, convolution)
- **cons**: approximate, parametric form may be ad hoc (eg. polynomial from)
- new ideas: using non-parametric statistical methods

Parametrized detector response narrative (eg. kinematic fitting, Matrix-Element method, ~fast simulation)

- pros: fast, maintains analytic scaling, response usually based on good understanding of the detector, possible to incorporate some types of uncertainty in the response analytically, can evaluate P(out|in) for arbitrary out,in.
- cons: approximate, best parametrized detector response is often not available in convenient form
- new ideas: fast simulation is typically parametrized, but we use it in an accept/ reject framework (see Geant5)



Hypothesis Testing

Hypothesis testing



One of the most common uses of statistics in particle physics is Hypothesis Testing (e.g. for discovery of a new particle)

- assume one has pdf for data under two hypotheses:
 - Null-Hypothesis, H₀: eg. background-only
 - Alternate-Hypothesis H₁: eg. signal-plus-background
- one makes a measurement and then needs to decide whether to reject or accept H₀



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Before we can make much progress with statistics, we need to decide what it is that we want to do.

- first let us define a few terms:
 - Rate of Type I error α
 - Rate of Type II β
 - Power = 1β

			Actual condition	
			Guilty	Not guilty
	Decision	Verdict of 'guilty'	True Positive	False Positive (i.e. guilt reported unfairly) Type I error
		Verdict of 'not guilty'	False Negative (i.e. guilt not detected) Type II error	True Negative

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Treat the two hypotheses asymmetrically

- the Null is special.
 - Fix rate of Type I error, call it "the size of the test"

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Treat the two hypotheses asymmetrically

- the Null is special.
 - Fix rate of Type I error, call it "the size of the test"

Now one can state "a well-defined goal"

Maximize power for a fixed rate of Type I error



- usually 5σ corresponds to $\alpha = 2.87 \cdot 10^{-7}$
 - eg. a very small chance we reject the standard model

In the simple case of number counting it is obvious what region is sensitive to the presence of a new signal





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The Neyman-Pearson Lemma



In 1928-1938 Neyman & Pearson developed a theory in which one must consider competing Hypotheses:

- the Null Hypothesis H_0 (background only)
- the Alternate Hypothesis H_1 (signal-plus-background)

Given some probability that we wrongly reject the Null Hypothesis

 $\alpha = P(x \notin W|H_0)$

(Convention: if data falls in W then we accept H₀)

Find the region W such that we minimize the probability of wrongly accepting the H_0 (when H_1 is true)

 $\beta = P(x \in W | H_1)$



The region W that minimizes the probability of wrongly accepting H_0 is just a contour of the Likelihood Ratio

 $\frac{P(x|H_1)}{P(x|H_0)} > k_{\alpha}$

Any other region of the same size will have less power

The likelihood ratio is an example of a Test Statistic, eg. a real-valued function that summarizes the data in a way relevant to the hypotheses that are being tested



Consider the contour of the likelihood ratio that has size a given size (eg. probability under H₀ is 1- α)

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Now consider a variation on the contour that has the same size



Now consider a variation on the contour that has the same size (eg. same probability under H_0)



 $P(\bigcup |H_1) < P(\bigcup |H_0)k_{\alpha}$

Because the new area is outside the contour of the likelihood ratio, we have an inequality

Kyle Cranmer (NYU)



And for the region we lost, we also have an inequality Together they give...



2 discriminating variables



Often one uses the output of a neural network or multivariate algorithm in place of a true likelihood ratio.

- That's fine, but what do you do with it?
- If you have a fixed cut for all events, this is what you are doing:



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 q_1

Experiments vs. Events

Ideally, you want to cut on the likelihood ratio for your experiment

 equivalent to a sum of log likelihood ratios

Easy to see that includes experiments where one event had a high LR and the other one was relatively small



$$q_{12} = q_1 + q_2$$









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The Test Statistic and its distribution



To get a feel for the different approaches, consider this schematic diagram



The "**test statistic**" is a single number that quantifies the entire experiment, it could just be number of events observed, but often its more sophisticated, like a likelihood ratio. What test statistic do we choose?

And how do we build the **distribution**? Usually "toy Monte Carlo", but what about the uncertainties... what do we do with the nuisance parameters?

Building the distribution of the test statistic



LEP Higgs Working group developed formalism to combine channels and take advantage of discriminating variables in the likelihood ratio.

$$Q = \frac{L(x|H_1)}{L(x|H_0)} = \frac{\prod_{i}^{N_{chan}} Pois(n_i|s_i + b_i) \prod_{j}^{n_i} \frac{s_i f_s(x_{ij}) + b_i f_b(x_{ij})}{s_i + b_i}}{\prod_{i}^{N_{chan}} Pois(n_i|b_i) \prod_{j}^{n_i} f_b(x_{ij})}$$
$$q = \ln Q = -s_{tot} + \sum_{i}^{N_{chan}} \sum_{j}^{n_i} \ln \left(1 + \frac{s_i f_s(x_{ij})}{b_i f_b(x_{ij})}\right)$$



Hu and Nielsen's CLFFT used Fourier Transform and exponentiation trick to transform the log-likelihood ratio distribution for one event to the distribution for an experiment

Cousins-Highland was used for systematic error on background rate.

Getting this to work at the LHC is tricky numerically because we have channels with n_i from 10-10000 events (physics/0312050)

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$$q = \ln Q = -s_{tot} + \sum_{i}^{N_{chan}} \sum_{j}^{n_i} \ln \left(1 + \frac{s_i f_s(x_{ij})}{b_i f_b(x_{ij})}\right)$$

For N events, use Fourier transform to perform N convolutions

$$\rho_{N,i}(q) = \underbrace{\rho_{N,i}(q) \oplus \cdots \oplus \rho_{N,i}(q)}_{N \text{ times}} = \mathcal{F}^{-1} \left\{ \left[\mathcal{F}\left(\rho_{1,i}\right) \right]^N \right\}$$

To include Poisson fluctuations on N for a given luminosity, one can exponentiate

$$\rho_i(q) = \sum_{N=0}^{\infty} P(N; L\sigma_i) \cdot \rho_{N,i}(q) = \mathcal{F}^{-1} \left\{ e^{L\sigma_i \left[\mathcal{F}(\rho_{1,i}(q)) - 1 \right]} \right\}$$

With nuisance parameters: Hybrid Solutions



Goal of Bayesian-frequentist hybrid solutions is to provide a frequentist treatment of the main measurement, while eliminating nuisance parameters (deal with systematics) with an intuitive Bayesian technique.

$$P(n_{\rm on}|s) = \int db \operatorname{Pois}(n_{\rm on}|s+b) \pi(b), \qquad p = \sum_{n=n_{\rm obs}}^{\infty} P(n|s)$$

Tracing back the origin of $\pi(b)$

• clearly state prior $\eta(b)$; identify control samples (sidebands) and use:

$$\pi(b) = P(b|n_{\text{off}}) = \frac{P(n_{\text{off}}|b)\eta(b)}{\int db P(n_{\text{off}}|b)\eta(b)}$$

Note, if we do not want to use the Hybrid Bayesian-Frequentist approach for the nuisance parameters, then we **must consider both** *n*_{on} **and** *n*_{off} **when generating our toy Monte Carlo**

$$P(n_{\rm on}, n_{\rm off}|s, b) = \operatorname{Pois}(n_{\rm on}|s+b) \operatorname{Pois}(n_{\rm off}|\tau b).$$



Coverage as calibration

This prototype problem has been studied extensively.

- instead of arguing about the merits of various methods, just go and check their rate of Type I error (coverage)
- Results indicated large discrepancy in "claimed" coverage and "true" coverage for various methods
- eg. 5 σ is really ~4 σ for some points

Introduce idea of coverage as a calibration of our statistical apparatus



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

$$L_P(x, y | \mu, b) = Pois(x | \mu + b) \cdot Pois(y | \tau b).$$

http://www.physics.ox.ac.uk/phystat05/proceedings/files/Cranmer_LHCStatisticalChallenges.ps

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Recent work by Bob Cousins & Jordan Tucker, [physics/0702156]

$$L_P(x, y|\mu, b) = Pois(x|\mu + b) \cdot Pois(y|\tau b).$$

http://www.physics.ox.ac.uk/phystat05/proceedings/files/Cranmer_LHCStatisticalChallenges.ps

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Define μ to be signal rate in units of SM expectation Define ν to be the shape parameters (nuisance parameters)

In the LEP approach the likelihood ratio is equivalent to: $Q_{LEP} = \frac{L(data|\mu = 1, b, \nu)}{L(data|\mu = 0, b, \nu)}$

• but this variable is sensitive to uncertainty on ν Alternatively, one can define **profile likelihood ratio**

$$\lambda(\mu = 0) = \frac{L(data|\mu = 0, \hat{b}(\mu = 0), \hat{v}(\mu = 0))}{L(data|\hat{\mu}, \hat{b}, \hat{v})},$$

• where $\hat{
u}$ is best fit with μ fixed to 0

• and $\hat{
u}$ is best fit with μ left floating

• conventional ratio is reciprocal in hypo test <-> limit

An example



)5

Essentially, you need to fit your model to the data twice: once with everything floating, and once with signal fixed to 0



Properties of the Profile Likelihood Ratio

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After a close look at the profile likelihood ratio

$$\lambda(\mu=0) = \frac{L(data|\mu=0, \hat{\hat{b}}(\mu=0), \hat{\hat{v}}(\mu=0))}{L(data|\hat{\mu}, \hat{b}, \hat{v})},$$

one can see the function is independent of true values of u

- though its distribution might depend indirectly
- Wilks's theorem states that under certain conditions the distribution of the profile likelihood ratio has an asymptotic form

$$-2\log\lambda(\mu=0)\sim\chi_1^2$$

Thus, we can calculate the p-value for the background-only hypothesis by calculating or equivalently: $-2\log\lambda(\mu=0)$

$$Z = \sqrt{-2\log\lambda(\mu = 0)}$$

Hypothesis Testing



Now on a real PROOF cluster with 30 machines

- real world example throws millions of toys experiments, does full fit on 50 parameters for each toy.
- also supports producing simple shells scripts for use with GRID or batch queues
- Now importance sampling is also implemented,
 - following presentation at Banff with particle physics & statistics experts
 - allows for 1000x speed increase!
 - Still being tested in detail


Experimentalist Justification



So far this looks a bit like magic. How can you claim that you incorporated your systematic just by fitting the best value of your uncertain parameters and making a ratio?

- It won't unless the the parametrization is sufficiently flexible.
- So check by varying the settings of your simulation, and see if the profile likelihood ratio is still distributed as a chi-square



Here it is pretty stable, but it's not perfect (and this is a log plot, so it hides some pretty big discrepancies)

For the distribution to be independent of the nuisance parameters your parametrization must be sufficiently flexible.

Ingredients to Frequentist methods



 $Q_{LEP} = L_{s+b}(\mu = 1)/L_b(\mu = 0)$

RooStats supports several statistical methods used in high energy physics

- Choose a test statistic
 - simple likelihood ratio (LEP)
 - ratio of profiled likelihoods (Tevatron) $Q_{TEV} = L_{s+b}(\mu = 1, \hat{\hat{\nu}})/L_b(\mu = 0, \hat{\hat{\nu}}')$
 - profile likelihood ratio (LHC) $\lambda(\mu) = L_{s+b}(\mu, \hat{\hat{\nu}})/L_{s+b}(\hat{\mu}, \hat{\nu})$
- Define your ensemble (sampling strategy)
 - toy MC randomizing nuisance parameters according to $\pi(\nu)$
 - aka Bayes-frequentist hybrid, prior-predictive, Cousins-Highland
 - toy MC with nuisance parameters fixed (Neyman Construction)
 - assuming asymptotic distribution (Wilks and Wald)



Lecture 3

Confidence Intervals (Limits)



The Neyman-Pearson lemma is **the answer** for simple hypothesis testing

· a hypothesis is **simple** if it has no free parameters and is totally fixed $f(x|H_0)$ vs. $f(x|H_1)$

What about cases when there are free parameters?

• eg. the mass of the Higgs boson $f(x|H_0)$ vs. $f(x|H_1, m_H)$

A test is called **similar** if it has size α for all values of the parameters

A test is called **Uniformly Most Powerful** if it maximizes the power for all values of the parameter

Uniformly Most Powerful tests don't exist in general

Kyle Cranmer (NYU)

Similar Test Examples



- In some cases Uniformly Most Powerful tests do exist:
 - some examples just to clarify the concept:
 - H₀ is simple: a Gaussian with a fixed $\mu = \mu_0, \sigma = \sigma_0$
 - H₁ is composite: a Gaussian with $\mu < \mu_0, \sigma = \sigma_0$
 - consider H₋ and H₋.
 - same size, different power, but both max power



Similar Test Examples



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 - consider H₊ and H₊₊
 - same size, different power, but both max power



Similar Test Examples



Slight variation, a Uniformly Most Powerful test doesn't exit:

- some examples just to clarify the concept:
- H₀ is simple: a Gaussian with a fixed $\mu = \mu_0, \sigma = \sigma_0$
- H₁ is composite: a Gaussian with $\mu = \mu_0, \sigma \neq \sigma_0$
 - Either H+ has good power and H₋ has bad power





When a hypothesis is composite typically there is a pdf that can be parametrized $f(\vec{x}|\theta)$

- ${\scriptstyle \bullet}$ for a fixed θ it defines a pdf for the random variable x
- for a given measurement of x one can consider $f(\vec{x}|\theta)$ as a function of θ called the Likelihood function
- Note, this is not Bayesian, because it still only uses P(data | theory) and
 - the Likelihood function is not a pdf!
- Sometimes θ has many components, generally divided into:
 - parameters of interest: eg. masses, cross-sections, etc.
 - nuisance parameters: eg. parameters that affect the shape but are not of direct interest (eg. energy scale)

A simple example:

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A Poisson distribution describes a discrete event count *n* for a realvalued mean μ .

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

The likelihood of μ given *n* is the same equation evaluated as a function of μ

- Now it's a continuous function
- But it is not a pdf!

$$L(\mu) = Pois(n|\mu)$$

Common to plot the -2 In L

- helps avoid thinking of it as a PDF
- connection to χ^2 distribution





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What is a "Confidence Interval?



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Confidence Interval

What is a "Confidence Interval?

• you see them all the time:





What is a "Confidence Interval?

- you see them all the time:
- Want to say there is a 68% chance that the true value of (m_W, m_t) is in this interval





What is a "Confidence Interval?

you see them all the time:

Want to say there is a 68% chance that the true value of (m_W, m_t) is in this interval

• but that's P(theory|data)!





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- Want to say there is a 68% chance that the true value of (m_W, m_t) is in this interval
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- Correct frequentist statement is that the interval **covers** the true value 68% of the time





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 - remember, the contour is a function of the data, which is random. So it moves around from experiment to experiment





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- but that's P(theory|data)!
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• Bayesian "credible interval" does mean probability parameter is in interval. The procedure is very intuitive:

$$P(\theta \in V) = \int_{V} \pi(\theta | x) = \int_{V} d\theta \frac{f(x | \theta) \pi(\theta)}{\int d\theta f(x | \theta) \pi(\theta)}$$

Neyman Construction example



For each value of θ consider $f(x|\theta)$



Neyman Construction example

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- lacksim we want a test of size lpha
- equivalent to a $100(1-\alpha)\%$ confidence interval on θ
- so we find an **acceptance region** with 1α probability





- No unique choice of an acceptance region
- here's an example of a lower limit





- No unique choice of an acceptance region
- and an example of a central limit





- choice of this region is called an ordering rule
- In Feldman–Cousins approach, ordering rule is the likelihood ratio. Find contour of L.R. that gives size α



Neyman Construction example

Now make acceptance region for every value of θ



Neyman Construction example



This makes a **confidence belt** for θ





This makes a **confidence belt** for θ

the regions of **data** in the confidence belt can be considered as **consistent** with that value of θ





Now we make a measurement x_0

the points θ where the belt intersects x_0 a part of the **confidence interval** in θ for this measurement



Neyman Construction example



For every point θ , if it were true, the data would fall in its acceptance region with probability $1 - \alpha$

If the data fell in that region, the point θ would be in the interval $[\theta_-, \theta_+]$

So the interval $[\theta_{-}, \theta_{+}]$ covers the true value with probability $1 - \alpha$



A Point about the Neyman Construction



This is not Bayesian... it doesn't mean the probability that the true value of θ is in the interval is $1 - \alpha$!





There is a precise dictionary that explains how to move from from hypothesis testing to parameter estimation.

- **Type I error:** probability interval does not cover true value of the parameters (eg. it is now a function of the parameters)
- **Power** is probability interval does not cover a false value of the parameters (eg. it is now a function of the parameters)
 - We don't know the true value, consider each point $heta_0$ as if it were true
- What about null and alternate hypotheses?
 - when testing a point θ_0 it is considered the null
 - all other points considered "alternate"
- So what about the Neyman-Pearson lemma & Likelihood ratio?
 - as mentioned earlier, there are no guarantees like before
 - a common generalization that has good power is:



The Dictionary



There is a formal 1-to-1 mapping between hypothesis tests and confidence intervals:

some refer to the Neyman Construction as an "inverted hypothesis test"

	Property of corresponding
Property of test	confidence interval
Size = α	Confidence coefficient = $1 - \alpha$
Power $=$ probability of rejecting a	Probability of not covering a false
false value of $\theta = 1 - \beta$	value of $\theta = 1 - \beta$
Most powerful	Uniformly most accurate
$\leftarrow \left\{ \begin{array}{c} Unbiased \\ 1-\beta \geq \alpha \end{array} \right\} \longrightarrow$	
Equal-tails test $\alpha_1 = \alpha_2 = \frac{1}{2}\alpha$	Central interval

Table 20.1 Relationships between hypothesis testing and interval estimation

Discovery in pictures



Discovery: test b-only (null: s=0 vs. alt: s>0)

note, one-sided alternative. larger N is "more discrepant"



Sensitivity for discovery in pictures



When one specifies 5σ one specifies a critical value for the data before "rejecting the null".

Leaves open a question of sensitivity, which is quantified as "power" of the test against a specific alternative

- In Frequentist setup, one chooses a "test statistic" to maximize power
 - Neyman-Pearson lemma: likelihood ratio most powerful test for one-sided alternative



Measurements in pictures



Measurement typically denoted $\sigma = X \pm Y$.

- X is usually the "best fit" or maximum likelihood estimate
- ±Y usually means [X-Y, X+Y] is a 68% confidence interval

Intervals are formally "inverted hypothesis tests": (null: $s=s_0$ vs. alt: $s \neq s_0$)

• One hypothesis test for each value of s₀ against a **two-sided** alternative

No "uniformly most powerful test" for a two-sided alternative


Upper limits in pictures

What do you think is meant by "95% upper limit" ?

Is it like the picture below?

• ie. increase s, until the probability to have data "more discrepant" is < 5%



Upper limits in pictures

Upper-limits are trying to exclude large signal rates.

form a 95% "confidence interval" on s of form [0,s95]

Intervals are formally "inverted hypothesis tests": (null: s=s₀ vs. alt: s<s₀)

• One hypothesis test for each value of s₀ against a **one-sided** alternative

Power of test depends on specific values of null so and alternate s'

but "uniformly most powerful" since it is a one-sided alternative



The sensitivity problem



The physicist's worry about limits in general is that if there is a strong downward fluctuation, one might exclude arbitrarily small values of s

 with a procedure that produces proper frequentist 95% confidence intervals, one should expect to exclude the true value of s 5% of the time, no matter how small s is!



Power in the context of limits



Remember, when creating confidence intervals the null is s=s₀

• and power is defined under a specific alternative (eg. s=0)



To address the sensitivity problem, CLs was introduced

- common (misused) nomenclature: CL_s = CL_{s+b}/CL_b
- idea: only exclude if CL_s<5% (if CL_b is small, CL_s gets bigger)

CL_s is known to be "conservative" (over-cover): expected limit covers with 97.5%

• Note: CL_s is NOT a probability



The Power Constraint



An alternative to CLs that protects against setting limits when one has no sensitivity is to explicitly define the sensitivity of the experiment in terms of power.

- A clean separation of size and power. (a new, arbitrary threshold for sensitivity)
- Feldman-Cousins foreshadowed the recommendation sensitivity defined as 50% power against b-only
- David van Dyk presented similar idea at PhyStat2011 [arxiv.org:1006.4334]



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"Power-Constrained" CL_{s+b} limits



Even for s=0, there is a 5% chance of a strong downward fluctuation that would exclude the background-only hypothesis

- we don't want to exclude signals for which we have no sensitivity
- idea: don't quote limit below some threshold defined by an N-σ downward fluctuation of b-only pseudo-experiments (Choose -1σ by convention)



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Coverage Comparison with CLs



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The CLs procedure purposefully over-covers ("conservative")

• and it is not possible for the reader to determine by how much

The power-constrained approach has the specified coverage until the constraint is applied, at which point the coverage is 100%

Imits are not 'aggressive' in the sense that they under-cover



Kyle Cranmer (NYU)

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Discrete Problems

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In discrete problems (eg. number counting analysis with counts described by a Poisson) one sees:

- discontinuities in the coverage (as a function of parameter)
- over-coverage (in some regions)
- Important for experiments with few events. There is a lot of discussion about this, not focusing on it here





Flip-Flopping







The flip-flopping procedure will under-cover

 can be avoided with a 'unified method' or if we always provide both p-value for b-only and 1-sided upper-limit

"As is emphasized in Neal [4], upper and lower one-sided confidence limits should replace confidence intervals, and a full plot of the log-likelihood function is better still." - D. Cox, N. Reid

In practice, we care about coverage on physical parameters (eg. a cross-section, not the number of events). This leads to a subtle semi-philosophical point

 So the relevant 'ensemble' of experiments may be different. With 100x more data one might quickly leave the regions effected by flip-flopping



Feldman & Cousins "Unified Approach" looks like this:

Neyman Construction

- For each $\mu :$ find region R_{μ} with probability $1-\alpha$
- Confidence Interval includes all μ consistent with observation at x_0

Ordering Rule specifies what region

F-C ordering rule is the Likelihood Ratio $R_{\mu} = \left\{ x \mid \frac{L(x|\mu)}{L(x|\mu_{\text{best}})} > k_{\alpha} \right\}$



The F-C ordering rule follows naturally from Neyman-Pearson Lemma

A different way to picture Feldman-Cousins



Most people think of plot on left when thinking of Feldman-Cousins

• bars are regions "ordered by" $R = P(n|\mu)/P(n|\mu_{\text{best}})$, with $\int_{\infty}^{x_2} P(x|\mu)dx = \alpha$.

But this picture doesn't generalize well to many measured quantities.

• Instead, just use R as the test statistic... and R is $\lambda(\mu)$



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Initially, we started with 2 simple hypotheses, and showed the likelihood ratio was most powerful (Neyman-Pearson)



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Then we generalized it to composite hypotheses.





- Initially, we started with 2 simple hypotheses, and showed the likelihood ratio was most powerful (Neyman-Pearson)
- Then we generalized it to composite hypotheses.
- How do we generalize it to include nuisance parameters?



Initially, we started with 2 simple hypotheses, and showed the likelihood ratio was most powerful (Neyman-Pearson)

Then we generalized it to composite hypotheses.

How do we generalize it to include nuisance parameters?

Variable	Meaning
$ heta_r$	physics parameters
$ heta_s$	nuisance parameters
$\hat{ heta}_r, \hat{ heta}_s$	unconditionally maximize $L(x \hat{ heta}_r,\hat{ heta}_s)$
$\hat{\hat{ heta}}_s$	conditionally maximize $L(x heta_{r0},\hat{\hat{ heta}}_s)$



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From Kendal



Initially, we started with 2 simple hypotheses, and showed the likelihood ratio was most powerful (Neyman-Pearson)

Then we generalized it to composite hypotheses.

How do we generalize it to include nuisance parameters?

> 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.

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From Kendal

An example



Essentially, you need to fit your model to the data twice: once with everything floating, and once with signal fixed to 0



Feldman-Cousins with and without constraint



With a physical constraint (μ >0) the confidence band changes, but conceptually the same. Do not get empty intervals.



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Modified test statistic for 1-sided upper limits

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For 1-sided upper-limit one construct a test that is more powerful for all $\mu>0$ (but has no power for $\mu=0$) simply by discarding "upward fluctuations"



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A real life example

Each colored curve is represents a single pseudo-experiment

• the test statistic is changing as μ , the parameter of interest, changes



Recall: Hybrid Solutions

Goal of Bayesian-frequentist hybrid solutions is to provide a frequentist treatment of the main measurement, while eliminating nuisance parameters (deal with systematics) with an intuitive Bayesian technique.

$$P(n_{\rm on}|s) = \int db \operatorname{Pois}(n_{\rm on}|s+b) \pi(b), \qquad p = \sum_{n=n_{obs}}^{\infty} P(n|s)$$

Tracing back the origin of $\pi(b)$

• clearly state prior $\eta(b)$; identify control samples (sidebands) and use:

$$\pi(b) = P(b|n_{\text{off}}) = \frac{P(n_{\text{off}}|b)\eta(b)}{\int db P(n_{\text{off}}|b)\eta(b)}$$

Note, if we do not want to use the Hybrid Bayesian-Frequentist approach for the nuisance parameters, then we **must consider both** *n*_{on} **and** *n*_{off} **when generating our toy Monte Carlo**

$$P(n_{\rm on}, n_{\rm off}|s, b) = \operatorname{Pois}(n_{\rm on}|s+b) \operatorname{Pois}(n_{\rm off}|\tau b).$$

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Conditional vs. Unconditional Ensemble

In the Conditional ensemble the global observables / auxiliary measurements are always the same

- if there are very few events expected, the test statistic takes on discrete values
- discreteness leads to overcoverage in some areas

In the Unconditional ensemble the global observables / auxiliary measurements fluctuate "smearing out" the value of the test statistic.

also more fluctuations in results

More on conditioning tomorrow!



Conditional vs. Unconditional Ensemble

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More on conditioning tomorrow!

Coverage

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Coverage can be different at each point in the parameter space

Example:

G. Punzi - PHYSTAT 05 - Oxford, UK



Poisson(+background), with a systematic uncertainty on efficiency:

 $x \sim Pois(\varepsilon \mu + b) \quad e \sim G(\varepsilon, \sigma)$

e is a measurement of the unknown efficiency ε , with resolution σ ε is the efficiency (a "normalization factor", can be larger than 1).

Neyman Construction with Nuisance parameters



In the strict sense, one wants coverage for μ for all values of the nuisance parameters (here ϵ)

- The "full construction" one n
- Challenge for full Neyman Construction is computational time (scan in 50-D isn't practical) and to avoid significant over-coverage
 - note: projection of nuisance parameters is a union (eg. set theory) not an integration (Bayesian)



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Fermilab Workshop

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The **profile construction** means that one does not need to scan each nuisance parameter (keeps dimensionality constant)

easier computationally

This approximation does not guarantee exact coverage, but

- tests indicate impressive performance
- one can expand about the profile construction to improve coverage, with the limiting case being the full construction



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maximum likelihood estimate)

Construction, based on the profile likelihood
Profile Construction: professional literature



While I have been calling it the "profile construction", it has been called a "hybrid resampling" technique by professional statisticians

 Note: 'hybrid' here has nothing to do with Bayesian-Frequentist Hybrid, but a connection to "boot-strapping"

> Statistica Sinica 19 (2009), 301-314 ON THE UNIFIED METHOD WITH NUISANCE PARAMETERS

Bodhisattva Sen, Matthew Walker and Michael Woodroofe



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Previous ways of addressing spurious exclusion

The problem of excluding parameter values to which one has no sensitivity known for a long time; see e.g.,

Virgil L. Highland, *Estimation of Upper Limits from Experimental Data*, July 1986, Revised February 1987, Temple University Report C00-3539-38.

In the 1990s this was re-examined for the LEP Higgs search by Alex Read and others

T. Junk, Nucl. Instrum. Methods Phys. Res., Sec. A 434, 435 (1999); A.L. Read, J. Phys. G 28, 2693 (2002).

and led to the " CL_s " procedure.