Systematic Uncertainties: Principle and Practice

Outline

1. Introduction to Systematic Uncertainties
2. Taxonomy and Case Studies
3. Issues Around Systematics
4. The Statistics of Systematics
5. Summary

Pekka K. Sinervo,F.R.S.C.
Rosi & Max Varon Visiting Professor
Weizmann Institute of Science
&
Department of Physics
University of Toronto

Introduction

- **Systematic uncertainties play key role in physics measurements**
  - **Few formal definitions exist, much "oral tradition"**
  - **"Know" they are different from statistical uncertainties**

Random Uncertainties

- Arise from stochastic fluctuations
- Uncorrelated with previous measurements
- Well-developed theory
- Examples
  - **measurement resolution**
  - **finite statistics**
  - **random variations in system**

Systematic Uncertainties

- Due to uncertainties in the apparatus or model
- Usually correlated with previous measurements
- Limited theoretical framework
- Examples
  - **calibrations uncertainties**
  - **detector acceptance**
  - **poorly-known theoretical parameters**

Literature Summary

- **Increasing literature on the topic of "systematics"**

  A representative list:

  – R.D.Cousins & V.L. Highland, NIM **A320**, 331 (1992).
  – C. Guinti, Phys. Rev. D **59** (1999), 113009.
  – G. Feldman, "Multiple measurements and parameters in the unified approach," presented at the FNAL workshop on Confidence Limits (Mar 2000).
  – R. J. Barlow, "Systematic Errors, Fact and Fiction," hep-ex/0207026 (Jun 2002), and several other presentations in the Durham conference.
  – G. Zech, "Frequentist and Bayesian Confidence Limits," Eur. Phys. J, **C4:12** (2002).
  – R. J. Barlow, "Asymmetric Systematic Errors," hep-ph/0306138 (June 2003).
  – A. G. Kim et al., "Effects of Systematic Uncertainties on the Determination of Cosmological Parameters," astro-ph/0304509 (April 2003).
  – J. Conrad et al., "Including Systematic Uncertainties in Confidence Interval Construction for Poisson Statistics," Phys. Rev. D **67** (2003), 012002
  – G.C.Hill, "Comment on "Including Systematic Uncertainties in Confidence Interval Construction for Poisson Statistics"," Phys. Rev. D **67** (2003), 118101.
  – G. Punzi, "Including Systematic Uncertainties in Confidence Limits", CDF Note in preparation.

I. Case Study #1: W Boson Cross Section

- **Rate of W boson production**
  - **Count candidates N_s+N_b**
  - **Estimate background N_b & signal efficiency ε**

$$\sigma = (N_c - N_b)/(\varepsilon\, L)$$

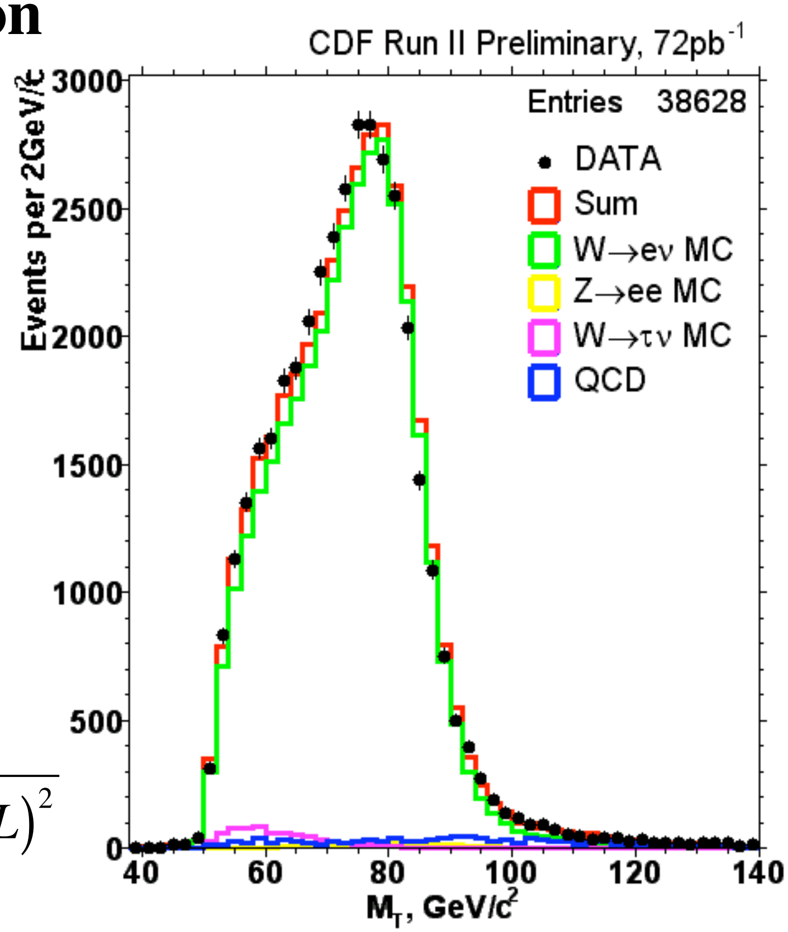
  - **Measurement reported as**

$$\sigma = 2.64 \pm 0.01\,(\text{stat}) \pm 0.18\,(\text{syst})\text{ nb}$$

  - **Uncertainties are**

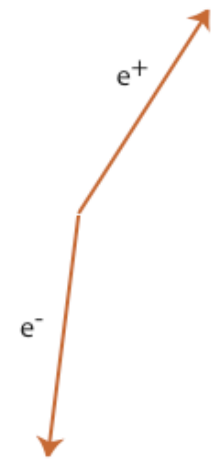
$$\sigma_{stat} \cong \sigma_0^{stat}\sqrt{1/N_c}$$

$$\sigma_{syst} \cong \sigma_0^{syst}\sqrt{(\delta N_b/N_b)^2 + (\delta\varepsilon/\varepsilon)^2 + (\delta L/L)^2}$$



Definitions are Relative

- **Efficiency uncertainty estimated using Z boson decays**
  - **Count up number of Z candidates N_Z^{cand}**
    - Can identify using charged tracks
    - Count up number reconstructed N_Z^{recon}



$$\varepsilon = \frac{N_Z^{recon}}{N_Z^{cand}} \Rightarrow \delta\varepsilon \cong \sqrt{\frac{N_Z^{recon}\left(N_Z^{cand} - N_Z^{recon}\right)}{N_Z^{cand}}}$$

  - **Redefine uncertainties**

$$\sigma_{stat} \cong \sigma_0 \sqrt{1/N_c + \left(\delta\varepsilon/\varepsilon\right)^2}$$

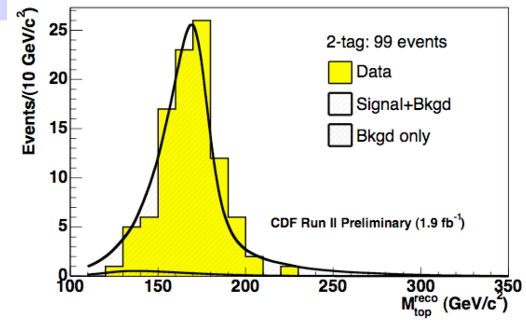
  - $$\sigma_{syst} \cong \sigma_0 \sqrt{\left(\delta N_b / N_b\right)^2 + \left(\delta L / L\right)^2}$$

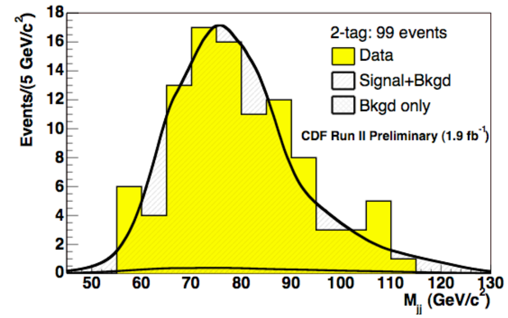
Lessons:
- Some systematic uncertainties are really "random"
- Good to know this
  - Uncorrelated
  - Know how they scale
- May wish to redefine
- Call these
  "CLASS 1" Systematics

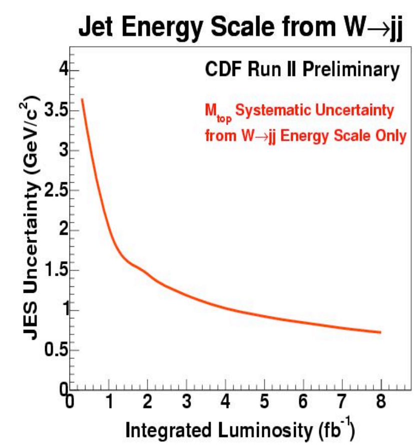
Top Mass Good Example

- **Top mass uncertainty in template analysis**
  - **Statistical uncertainty from shape of reconstructed mass distribution and statistics of sample**
  - **Systematic uncertainty coming from jet energy scale (JES)**
    - Determined by calibration studies, dominated by modelling uncertainties
    - 5% systematic uncertainty
- **Latest techniques determine JES uncertainty from dijet mass peak (W->jj)**
  - **Turn JES uncertainty into a largely statistical one**
  - **Introduce other smaller systematics**

$$M_{top} = 171.8 \pm 1.9\,(\text{stat}+\text{JES}) \pm 1.0\ (\text{syst})\ \text{GeV/c}^2$$
$$= 171.9 \pm 2.1\ \text{GeV/c}^2$$

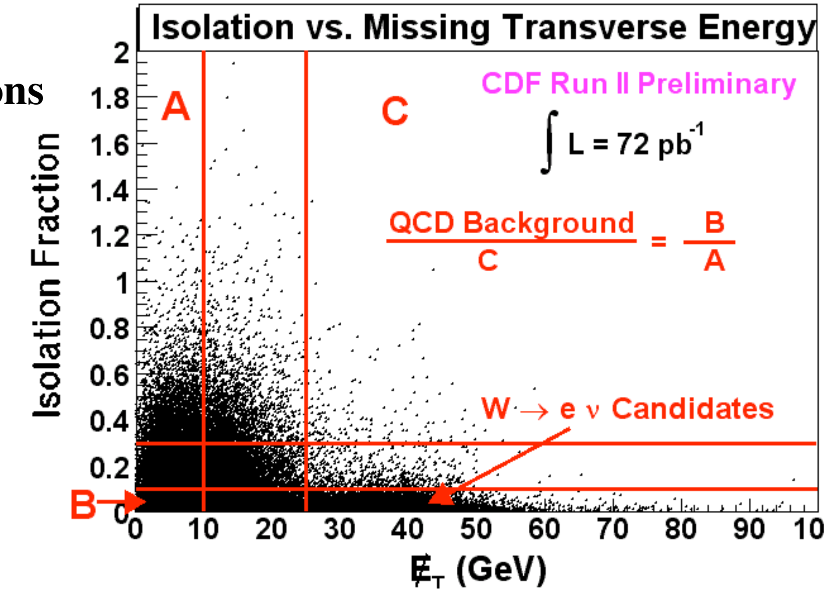






Case Study #2: Background Uncertainty

- **Look at same W cross section analysis**
  - **Estimate of N_b dominated by QCD backgrounds**
    - Candidate event
      - **Have non-isolated leptons**
      - **Less missing energy**
    - Assume that isolation and MET uncorrelated
    - Have to estimate the uncertainty on N_b^{QCD}



  - **No direct measurement has been made to verify the model**
  - **Estimates using Monte Carlo modelling have large uncertainties**

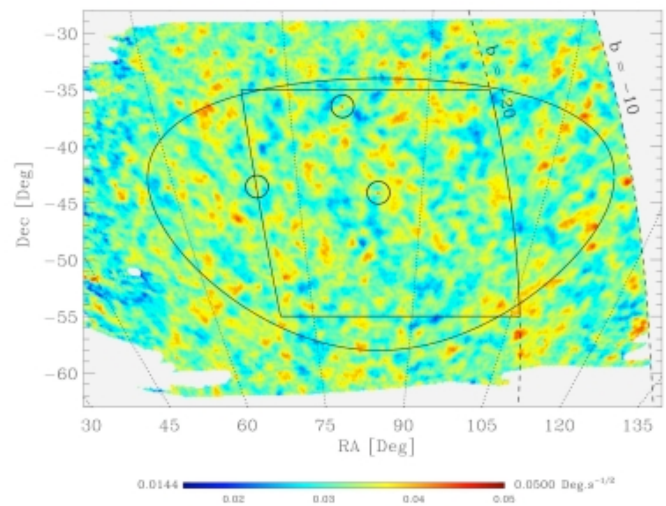
Estimation of Uncertainty

- **Fundamentally different class of uncertainty**
  - **Assumed a model for data interpretation**
  - **Uncertainty in N_b^{QCD} depends on accuracy of model**
  - **Use "informed judgment" to place bounds on one's ignorance**
    - Vary the model assumption to estimate robustness
    - Compare with other methods of estimation
- **Difficult to quantify in consistent manner**
  - **Largest possible variation?**
    - Asymmetric?
  - **Estimate a "1 σ" interval?**
  - **Take** $\sigma \approx \frac{\Delta}{\sqrt{12}}$?

Lessons:
- Some systematic uncertainties reflect ignorance of one's data
- Cannot be constrained by observations
- Call these "CLASS 2" Systematics

Case Study #3: Boomerang CMB Analysis

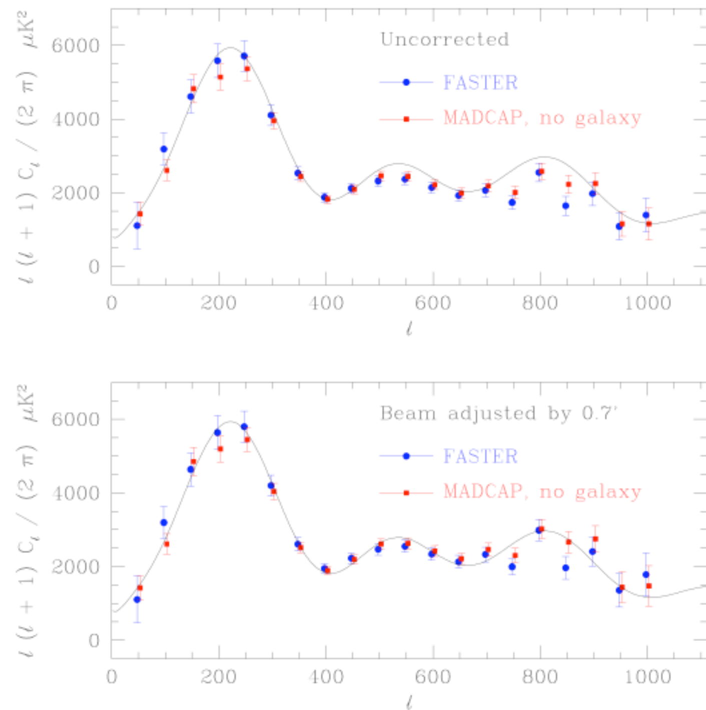
- Boomerang is one of several CMB probes
  - Mapped CMB anisoptropy
  - Data constrain models of the early universe



- Analysis chain:
  - Produce a power spectrum for the CMB spatial anisotropy
    - Remove instrumental effects through a complex signal processing algorithm
  - Interpret data in context of many models with unknown parameters

Incorporation of Model Uncertainties

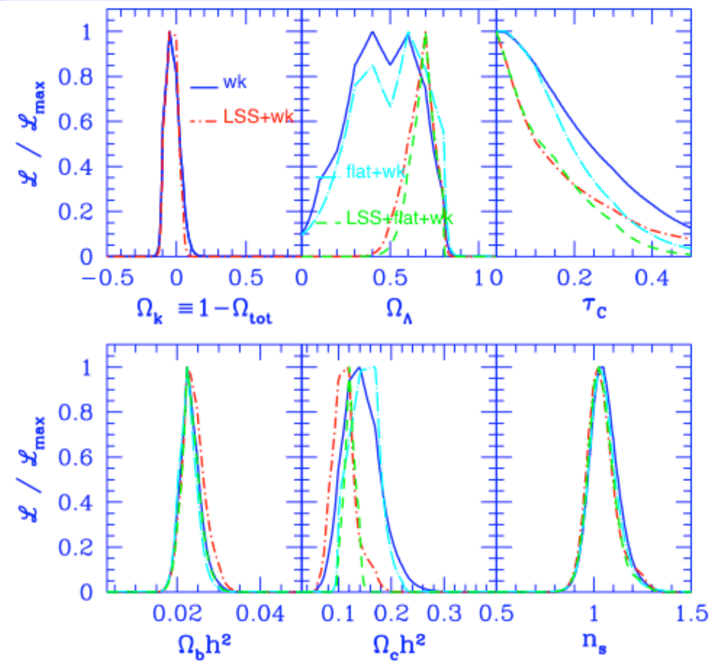
- **Power spectrum extraction includes all instrumental effects**
  - **Effective size of beam**
  - **Variations in data-taking procedures**



- **Use these data to extract 7 cosmological parameters**
  - **Take Bayesian approach**
    - Family of theoretical models defined by 7 parameters
    - Define a 6-D grid (6.4M points), and calculate likelihood function for each

Marginalize Posterior Probabilities

- **Perform a Bayesian "averaging" over a grid of parameter values**
  - **Marginalize w.r.t. the other parameters**
    - NB: instrumental uncertainies included in approximate manner
  - **Chose various priors in the parameters**



- **Comments:**
  - **Purely Bayesian analysis with no frequentist analogue**
  - **Provides path for inclusion of additional data (eg. WMAP)**

Lessons:
- Some systematic uncertainties reflect paradigm uncertainties
- No relevant concept of a frequentist ensemble
- Call these "CLASS 3" Systematics

Proposed Taxonomy for Systematic Uncertainties

- **Three "classes" of systematic uncertainties**
  - **Uncertainties that can be constrained by ancillary measurements**
  - **Uncertainties arising from model assumptions or problems with the data that are poorly understood**
  - **Uncertainties in the underlying models**
- **Estimation of Class 1 uncertainties straightforward**
  - **Class 2 and 3 uncertainties present unique challenges**
  - **In many cases, have nothing to do with statistical uncertainties**
    - Driven by our desire to make inferences from the data using specific models

II. Estimation Techniques

- **No formal guidance on how to define a systematic uncertainty**
  - **Can identify a possible source of uncertainty**
  - **Many different approaches to estimate their magnitude**
    - Determine maximum effect Δ

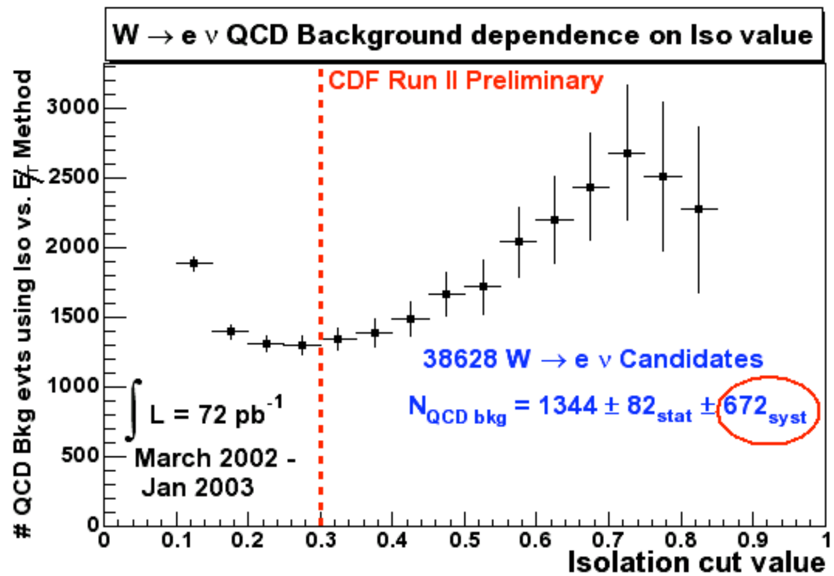
$$\sigma = \frac{\Delta}{2}?$$

$$\sigma = \frac{\Delta}{\sqrt{12}}?$$

- **General rule:**
  - **Maintain consistency with definition of statistical intervals**
  - **Field is pretty glued to 68% confidence intervals**
  - **Recommend attempting to reflect that in magnitudes of systematic uncertainties**
  - **Avoid tendency to be "conservative"**

Estimate of Background Uncertainty in Case Study #2

- **Look at correlation of Isolation and MET**
  - **Background estimate increases as isolation "cut" is raised**
  - **Difficult to measure or accurately model**
    - Background comes primarily from very rare jet events with unusual properties
    - Very model-dependent



- **Assume a systematic uncertainty representing the observed variation**
  - **Authors argue this is a "conservative" choice**

Cross-Checks Vs Systematics

- **R. Barlow makes the point in Durham(PhysStat02)**
  - **A cross-check for robustness is not an invitation to introduce a systematic uncertainty**
    - Most cross-checks confirm that interval or limit is robust,
      - **They are usually not designed to measure a systematic uncertainty**
- **More generally, a systematic uncertainty should**
  - **Be based on a hypothesis or model with clearly stated assumptions**
  - **Be estimated using a well-defined methodology**
  - **Be introduced *a posteriori* only when all else has failed**

III. Statistics of Systematic Uncertainties

- **Goal has been to incorporate systematic uncertainties into measurements in coherent manner**
  - **Increasing awareness of need for consistent practice**
    - Frequentists: interval estimation increasingly sophisticated
      - **Neyman construction, ordering strategies, coverage properties**
    - Bayesians: understanding of priors and use of posteriors
      - **Objective vs subjective approaches, marginalization/conditioning**
  - **Systematic uncertainties threaten to dominate as precision and sensitivity of experiments increase**
- **There are a number of approaches widely used**
  - **Summarize and give a few examples**
  - **Place it in context of traditional statistical concepts**

Formal Statement of the Problem

- **Have a set of observations x_i, $i=1,n$**
  - **Associated probability distribution function (pdf) and likelihood function**

$$\mathrm{p}(x_i \mid \theta) \Rightarrow \mathcal{L}(\theta) = \prod_i \mathrm{p}(x_i \mid \theta)$$

    - Depends on unknown random parameter θ
    - Have some additional uncertainty in pdf
      - **Introduce a second unknown parameter λ**

$$\mathcal{L}(\theta,\lambda) = \prod_i \mathrm{p}(x_i \mid \theta,\lambda)$$

- **In some cases, one can identify statistic y_j that provides information about λ**

$$\mathcal{L}(\theta,\lambda) = \prod_{i,j} \mathrm{p}(x_i, y_j \mid \theta,\lambda)$$

  - **Can treat λ as a "nuisance parameter"**

Bayesian Approach

- **Identify a prior $\pi(\lambda)$ for the "nuisance parameter" λ**
  - **Typically, parametrize as either a Gaussian pdf or a flat distribution within a range ("tophat")**
  - **Can then define Bayesian posterior**

$$\mathcal{L}(\theta,\lambda)\,\pi(\lambda)\,d\theta\,d\lambda$$

  - **Can marginalize over possible values of λ**
    - Use marginalized posterior to set Bayesian credibility intervals, estimate parameters, etc.

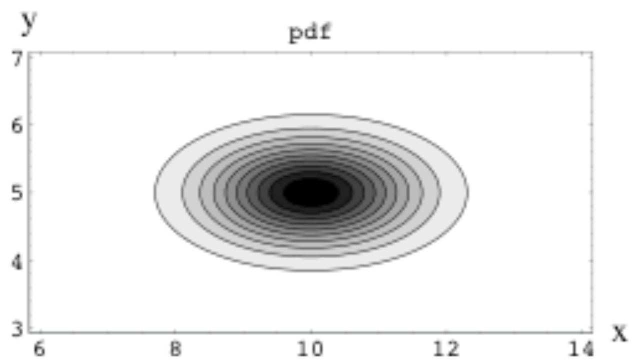
- **Theoretically straightforward ….**
  - **Issues come down to choice of priors for both θ, λ**
    - No widely-adopted single choice
    - Results have to be reported and compared carefully to ensure consistent treatment

Frequentist Approach

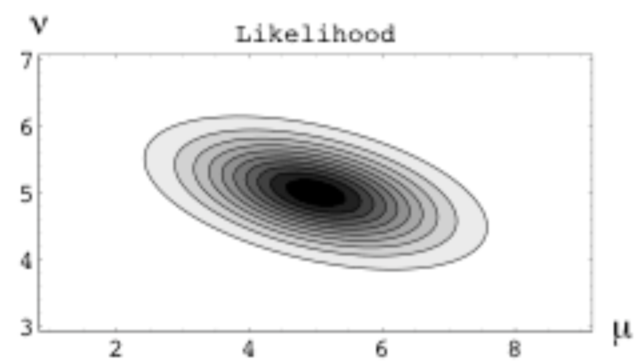
- **Start with a pdf for data** $p(x_i, y_j \mid \theta, \lambda)$
  - **In principle, this would describe frequency distributions of data in multi-dimensional space**
  - **Challenge is take account of nuisance parameter**
  - **Consider a toy model**

$$p(x, y \mid \mu, \nu) = G(x - (\mu + \nu), 1)\, G(y - \nu, s)$$

> Parameter s is Gaussian width for ν



- **Likelihood function (*x=10, y=5*)**
  - **Shows the correlation**
  - **Effect of unknown ν**



Formal Methods to Eliminate Nuisance Parameters

- **Number of formal methods exist to eliminate nuisance parameters**
  - **Of limited applicability given the restrictions**
  - **Our "toy example" is one such case**
    - Replace x with $t=x-y$ and parameter ν with

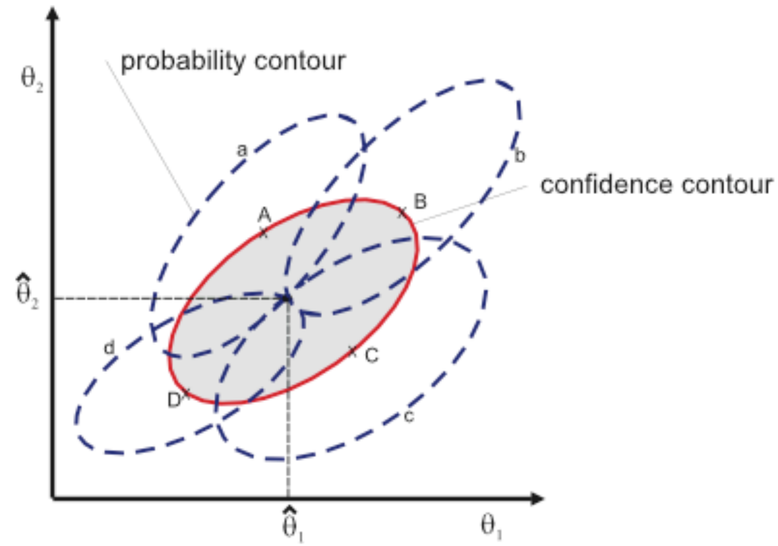
$$\nu' \equiv \nu + \mu s^2 / 1+s^2$$

$$\Rightarrow \mathrm{p}(t,y \mid \mu,\nu') = \mathrm{G}\left(t-\mu, \sqrt{1+s^2}\right)\mathrm{G}\left(y-\nu'+ ts^2 / 1+s^2 ,\ s / \sqrt{1+s^2}\right)$$

    - Factorized pdf and can now integrate over ν'
    - Note that pdf for μ has larger width, as expected
  - **In practice, one often loses information using this technique**

Alternative Techniques for Treating Nuisance Parameters

- **Project Neyman volumes onto parameter of interest**
  - **“Conservative interval”**
  - **Typically over-covers, possibly badly**



From G. Zech

- **Choose best estimate of nuisance parameter**
  - **Known as “profile method”**
  - **Coverage properties require definition of ensemble**
  - **Can possible under-cover when parameters strongly correlated**
    - Feldman-Cousins intervals tend to over-cover slightly (private communication)

Example: Solar Neutrino Global Analysis

- **Many experiments have measured solar neutrino flux**
  - **Gallex, SuperKamiokande, SNO, Homestake, SAGE, etc.**
  - **Standard Solar Model (SSM) describes ν spectrum**
  - **Numerous "global analyses" that synthesize these**
- **Fogli et al. have detailed one such analysis**
  - **81 observables from these experiments**
  - **Characterize systematic uncertainties through 31 parameters**
    - 12 describing SSM spectrum
    - 11 (SK) and 7 (SNO) systematic uncertainties
- **Perform a χ^2 analysis**
  - **Look at χ^2 to set limits on parameters**

Hep-ph/0206162, 18 Jun 2002

Formulation of χ^2

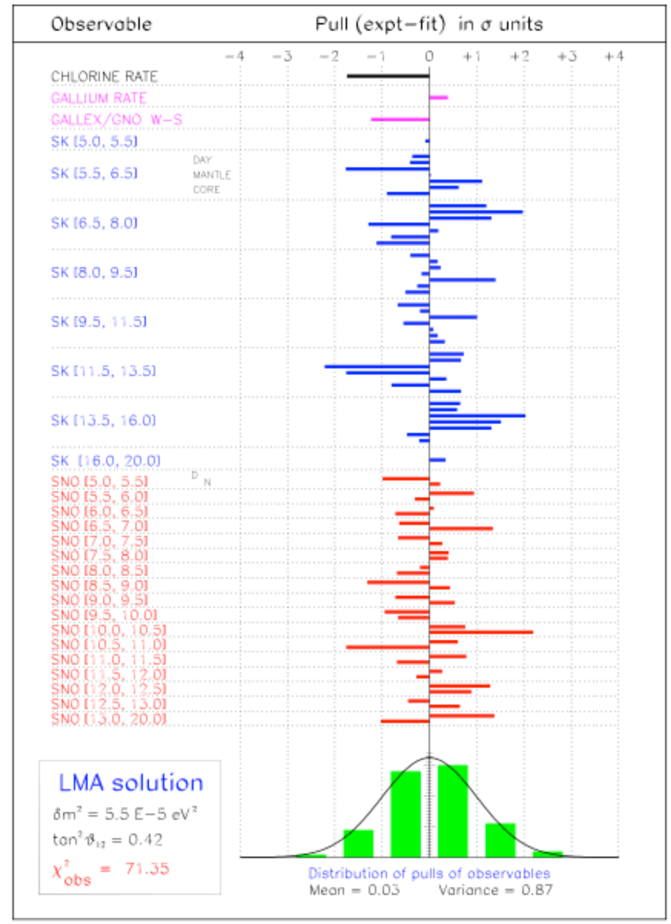
- **In formulating χ^2, linearize effects of the systematic uncertainties on data and theory comparison**

$$\chi^2_{pull} \equiv \min_{\{\xi\}} \left[\sum_{n=1}^{N} \left(\frac{R_n^{\exp t} - R_n^{theor} - \sum (c_n^k \xi_k)}{u_n} \right)^2 + \sum_{k=1}^{K} \xi_k^2 \right]$$

  - Uncertainties u_n for each observable
- **Introduce "random" pull ξ_k for each systematic**
  - Coefficients c_k^n to parameterize effect on *nth* observable
  - Minimize χ^2 with respect to ξ_k
  - Look at contours of equal $\Delta \chi^2$

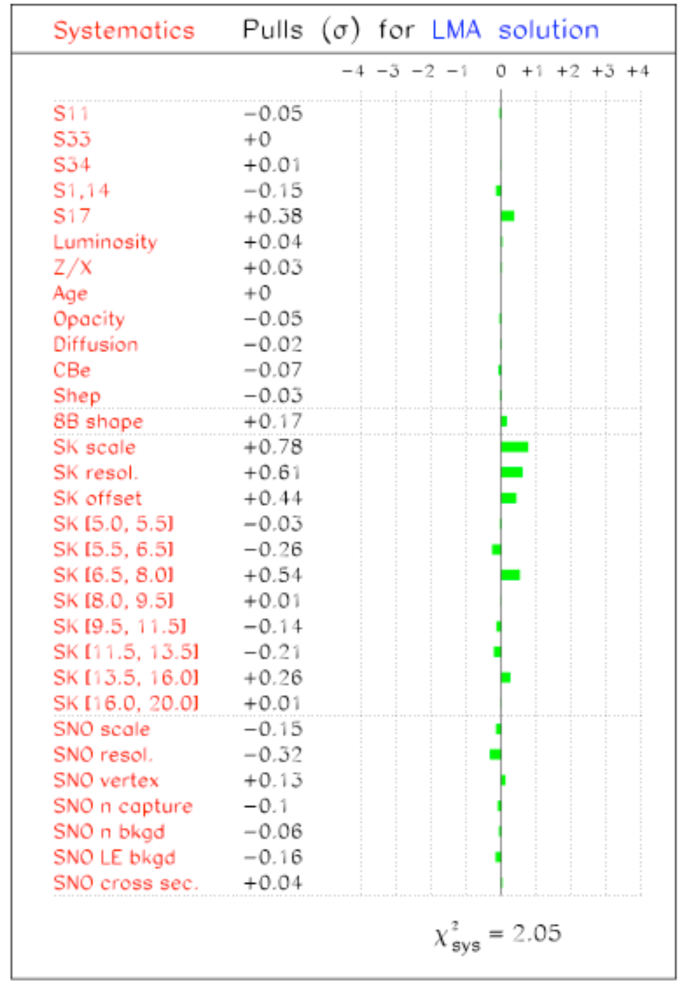
Solar Neutrino Results

- Can look at “pulls” at χ^2 minimum
  - Have reasonable distribution
  - Demonstrates consistency of model with the various measurements
  - Can also separate
    - Agreement with experiments
    - Agreement with systematic uncertainties



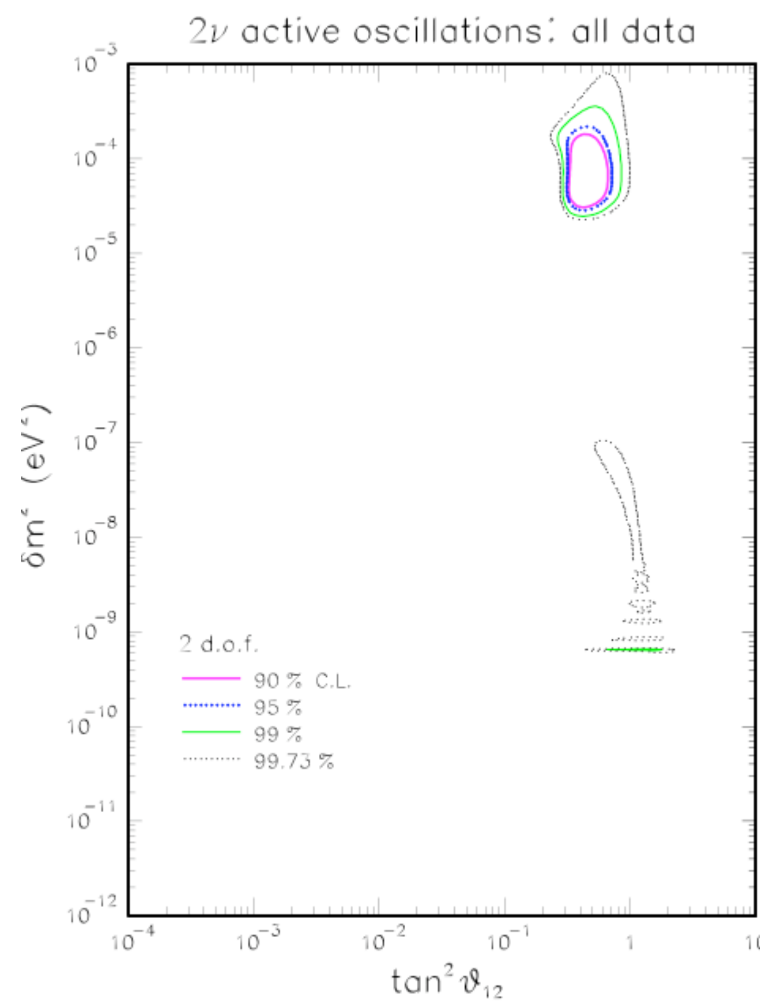
Pull Distributions for Systematics

- **Pull distributions for ξ_k also informative**
  - **Unreasonably small variations**
  - **Estimates are globally too conservative?**
  - **Choice of central values affected by data**
    - Note this is NOT a blind analysis
- **But it gives us some confidence that intervals are realistic**



Typical Solar Neutrino Contours

- Can look at probability contours
  - Assume standard χ^2 form
  - Probably very small probability contours have relatively large uncertainties



Hybrid Techniques

- **A popular technique (Cousins-Highland) does an "averaging" of the pdf**
  - **Assume a pdf for nuisance parameter g(λ)**
  - **"Average" the pdf for data *x***

$$\mathrm{p_{CH}}(x \mid \theta) \equiv \int \mathrm{p}(x \mid \theta, \lambda)\, \mathrm{g}(\lambda)\, d\lambda$$

  - **Argue this approximates an ensemble where**
    - Each measurement uses an apparatus that differs in parameter λ
      - **The pdf g(λ) describes the frequency distribution**
    - Resulting distribution for x reflects variations in λ
- **Intuitively appealing**
  - **But fundamentally a Bayesian approach**
  - **Coverage is not well-defined**

See, for example, J. Conrad et al.

Summary

- **HEP & Astrophysics becoming increasingly "systematic" about systematics**
  - **Recommend classification to facilitate understanding**
    - Creates more consistent framework for definitions
    - Better indicates where to improve experiments
  - **Avoid some of the common analysis mistakes**
    - Make consistent estimation of uncertainties
    - Don't confuse cross-checks with systematic uncertainties
- **Systematics naturally treated in Bayesian framework**
  - **Choice of priors still somewhat challenging**
- **Frequentist treatments are less well-understood**
  - **Challenge to avoid loss of information**
  - **Approximate methods exist, but probably leave the "true frequentist" unsatisfied**