Statistics and Data analysis

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- Why use statistics?
- Have I found something?
- Parameter extraction
- Goodness of fit

What do we want to achieve?

- We aim to make optimal use of the data collected
  - Data are expensive:
    - Use powerful techniques
  - Data processing is also expensive:
    - Mathematical perfection is not the only criterion
  - Systematic errors may well dominate
    - We need to be able to justify our results.

Three Classes of problem

- Hypothesis testing
  - Does this signal exist?
  - Bayes and Frequentist limits
- Parameter extraction
  - What is the mass of the W?
  - Systematic and statistical errors
- Goodness of fit
  - Chi2 test
  - Other tests

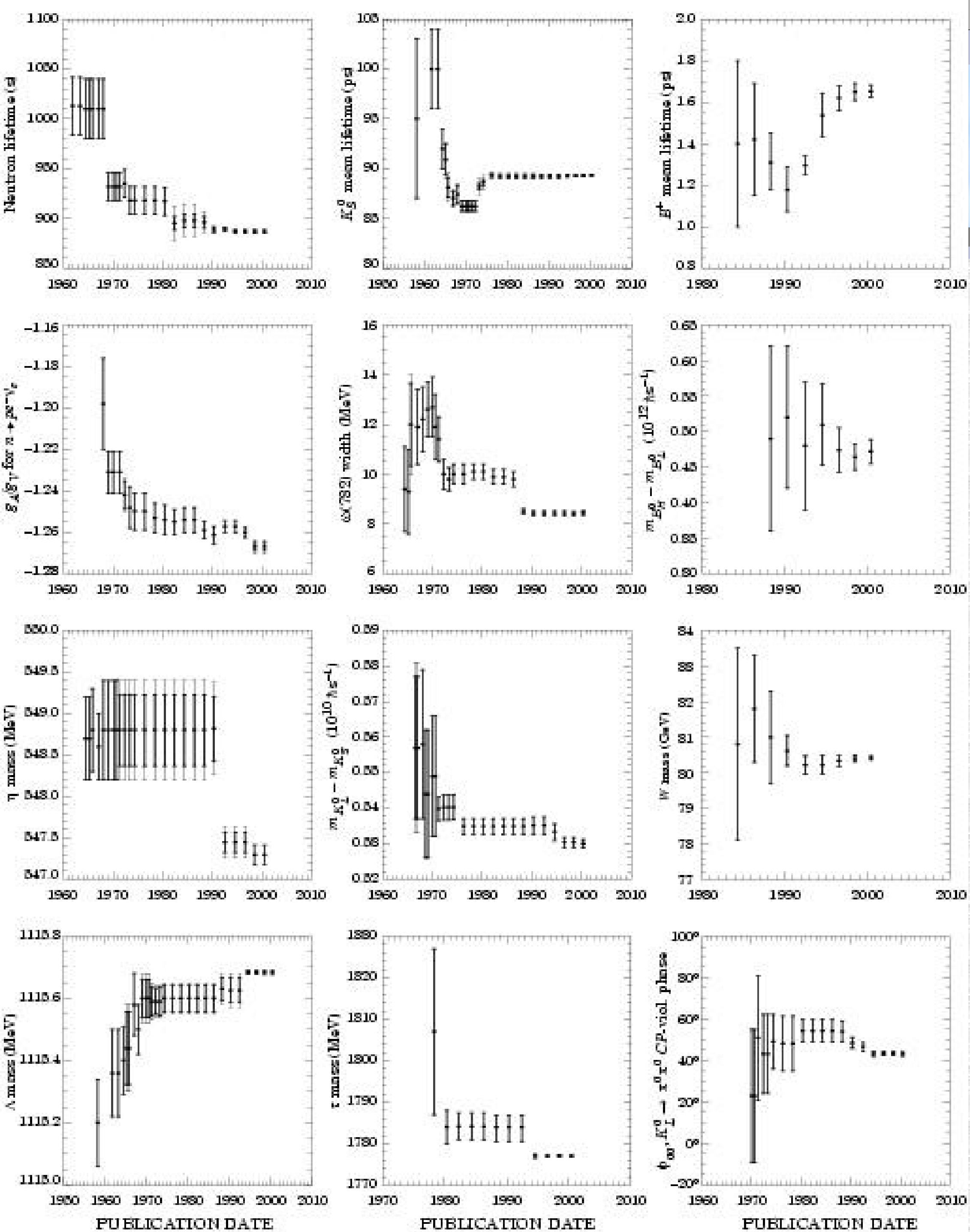


Figure 2: An historical perspective of values of a few particle properties tabulated in this *Review* as a function of date of publication of the *Review*. A full error bar indicates the quoted error; a thick-lined portion indicates the same but without the "scale factor."

History of measurements

Each measurement agrees with preceding one!

Publications which disagree with the standard model/previous estimates are checked more carefully.

If you look you can usually find something

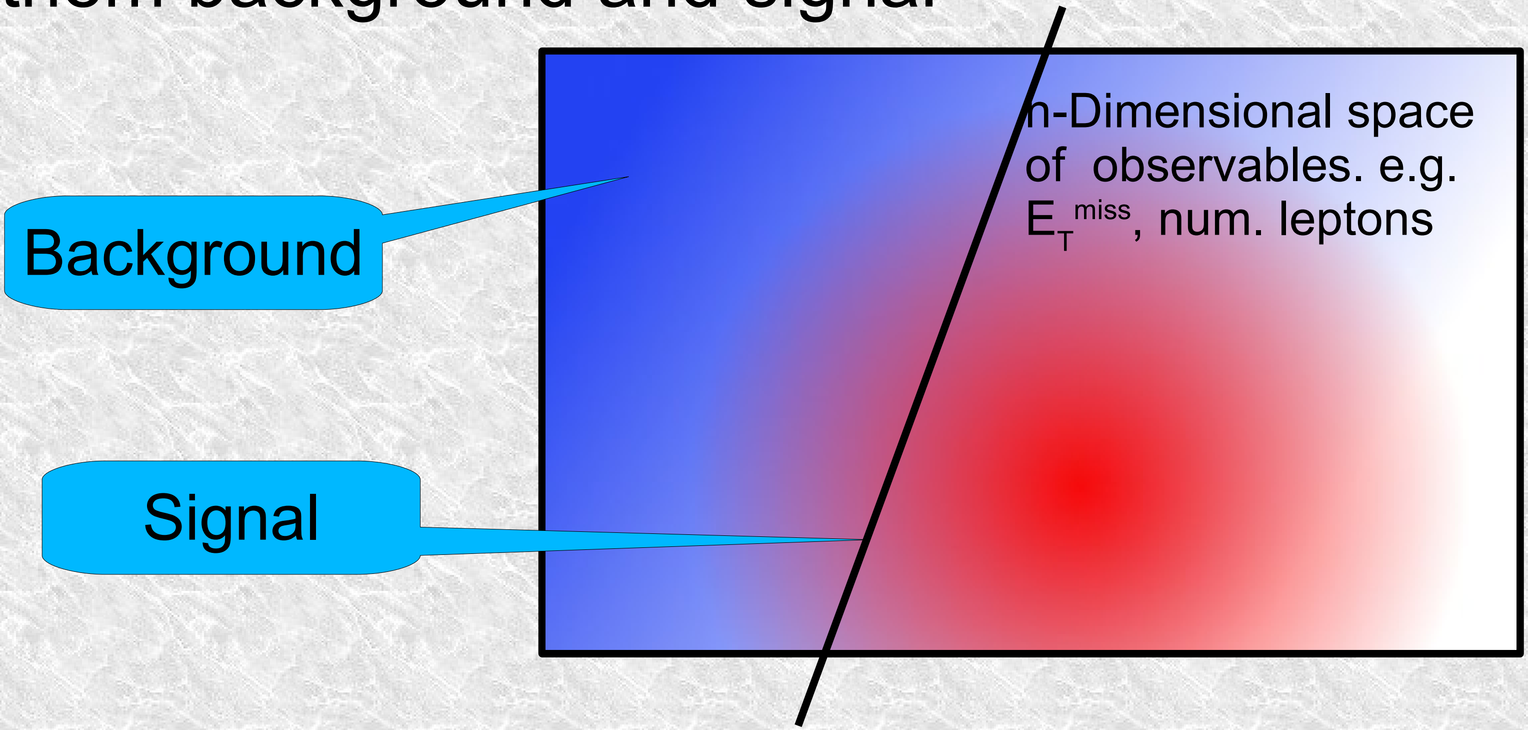
Hence Blind Analysis

Hypothesis Testing

- Have we found a new signal?

Signal Recognition

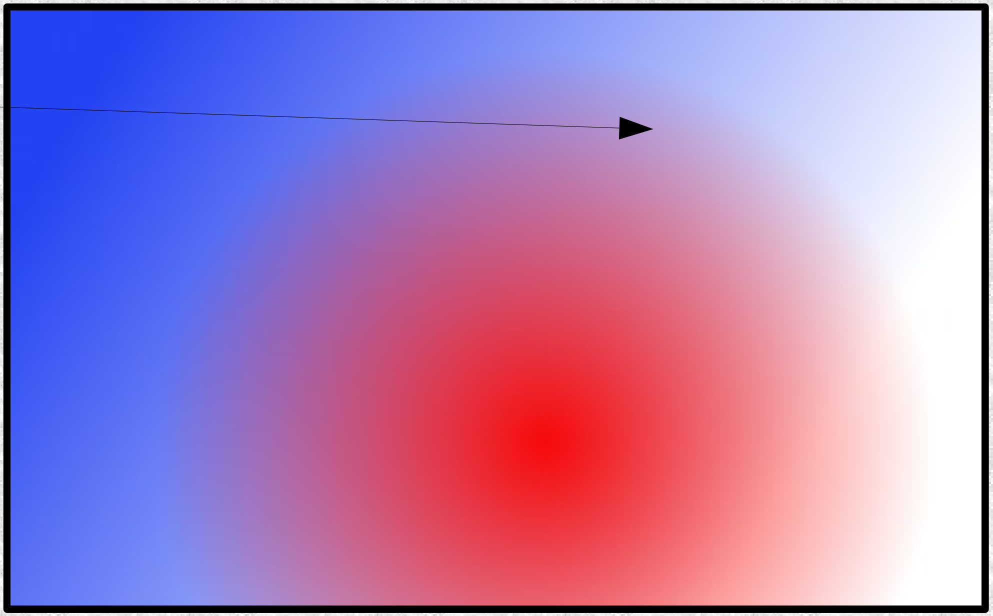
- Consider separating a dataset into 2 classes
  - Call them background and signal



- A simple cut is not optimal

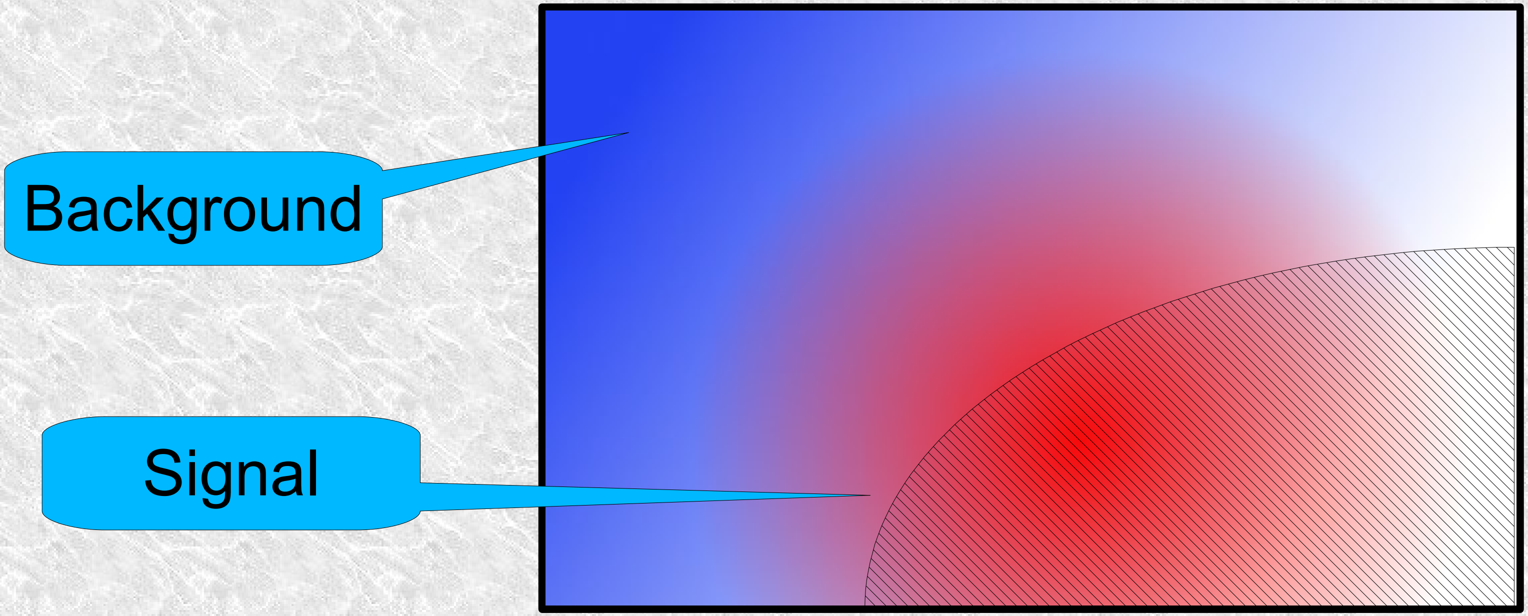
The right answer II

- For an given efficiency, we want to minimize background
- For each event, find ratio of signal and background at that point
- Accept all areas with s/b above some threshold
- Leading to the ***Likelihood Ratio***



The right answer III

- Plot region where events are accepted:



- This is the best possible ***cut***

Is that the best we can do?

- Ordering events by ρ_s/ρ_b and selecting above some threshold gives best possible sample
- But when we ask the question "is there a signal there?" we can extract more information.
- Do a fit to the likelihood-ratios:
  - Use: $\mathcal{L}=1+\rho_s/\rho_b = (\rho_s+\rho_b)/\rho_b$
  - How much more probable if signal also present?
- Take product over all events
  - One event with ρb=0 disproves b
  - 2 events with $\mathcal{L}$=10 same as 1 with $\mathcal{L}$=100
- This product is the most sensitive estimator
  - Neymann-Pearson Lemma

Determination of s, b densities

- We may know matrix elements ("Matrix Element method")
  - Not for e.g. a b-tag
  - But anyway there are detector effects
- Usually taken from simulation

Using MC to calculate density

- Brute force:
  - Divide our n-D space into hypercubes with m divisions of each axis
  - m^n elements, need 100 m^n events for 10% estimate.
  - e.g. 1,000,000,000 for 7 dimensions and 10 bins in each
- This assumed a uniform density – actually need far more
  - The purpose was to separate different distributions

Better likelihood estimation

- Clever binning
  - Starts to lead to tree techniques
- Kernel density estimators
  - Size of kernel grows with dimensions
  - Edges are an issue
- Ignore correlations in variables
  - Very commonly done '**I used likelihood**'
- Assume measured=true, correct later
  - e.g. 'Matrix element' method
  - Bias correction an issue

Alternative approaches

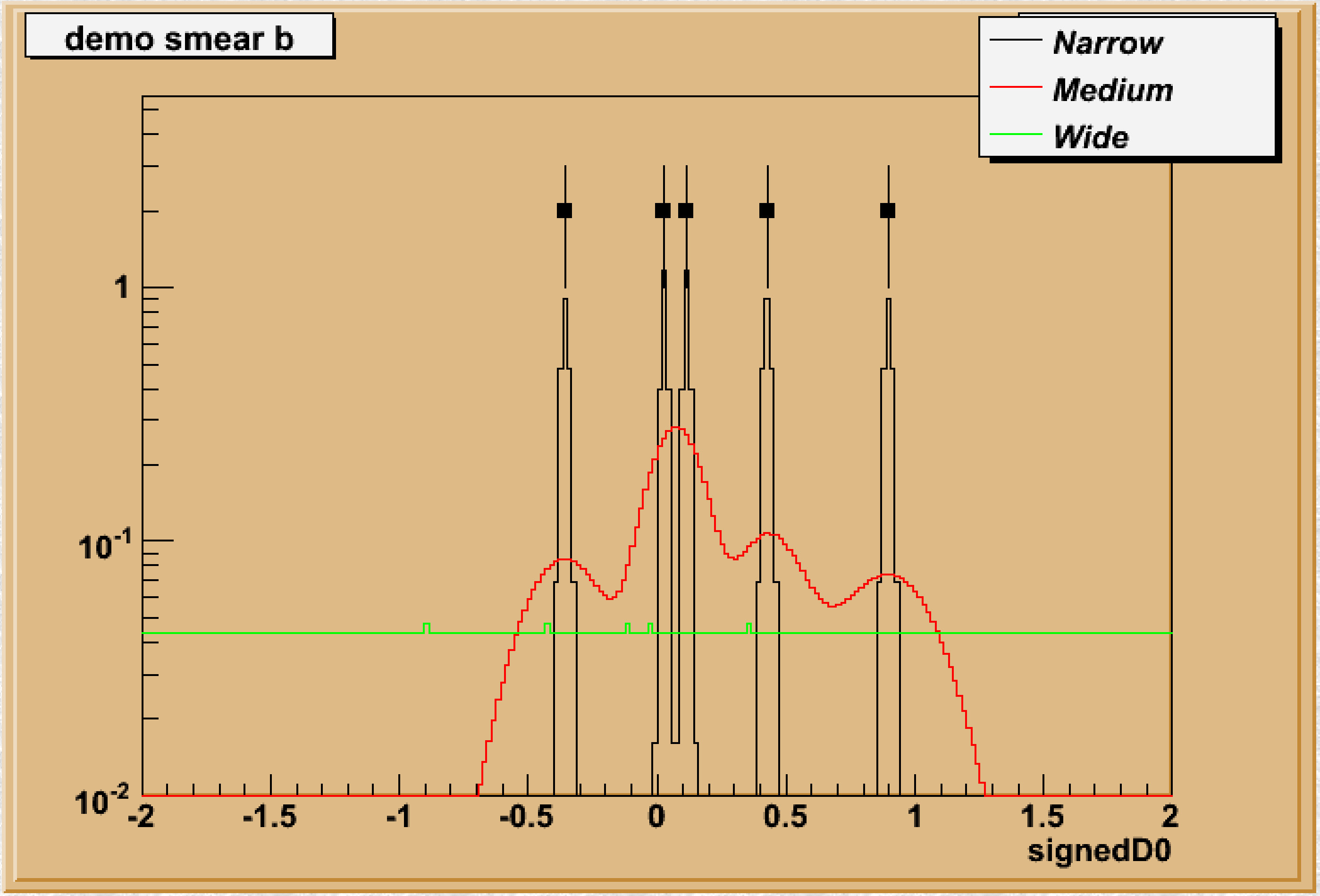
- Neural nets
  - Well known, good for high-dimensions
- Support vector machines
  - Computationally easier than kernel
- Decision trees
  - Boosted or not?

How to calculate densities

Kernel Likelihoods

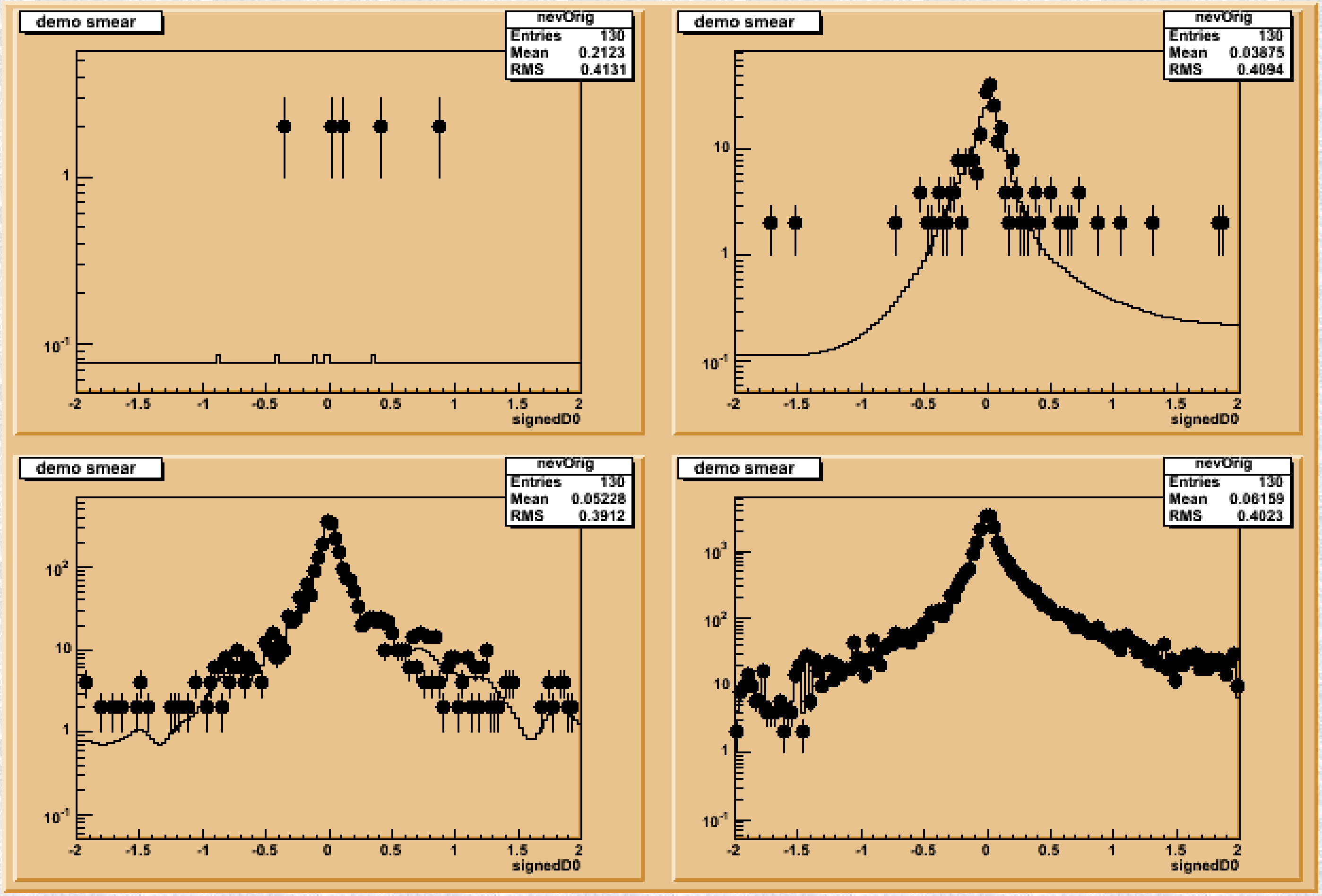
- Directly estimate Probability Density Function of distributions based upon training sample events.
- Some kernel, usually Gaussian, smears the sample
  - increases widths
  - Width of kernel must be optimised
- Fully optimal *if* infinite MC statistics
  - Then we can use narrow kernels

Smearing 5 events, 1D



- The kernel width is crucial
- Problem much worse in higher dimensions

Varying event nos.



- More events always helps

Kernel Likelihoods: nDim

- Metric of kernel, (size, aspect ratio) hard to optimize
  - Watch kernel size dependence on stats.
- Kernel size must grow with dimensions;
  - Lose precision if unnecessary dimensions added
  - Need to choose which variables to use
- Big storage/computational requirements

Taming m^n

Use of an approximately sufficient statistic or likelihood estimate

- No large resolution and acceptance effects:
  Perform fit with uncorrected data and undistorted likelihood function.
- Acceptance losses but small distortions:
  Compute global acceptance by MC and include in the likelihood function.
- Strong resolution effects:
  Perform crude unfolding.

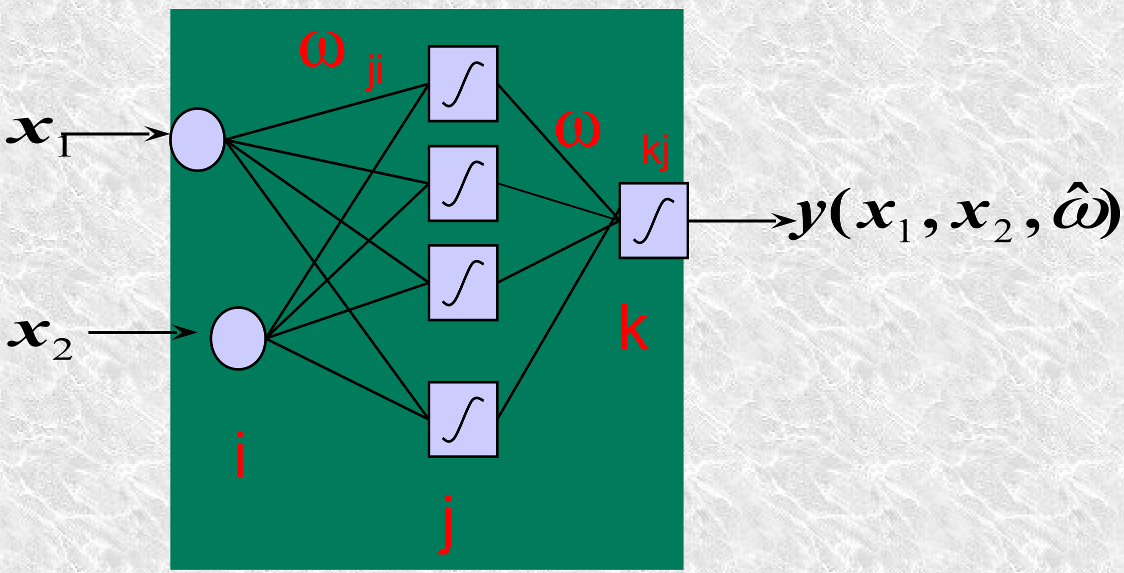
All approximations are corrected by the Monte Carlo simulation.
The loss in precision introduced by the approximations is usually completely negligible.

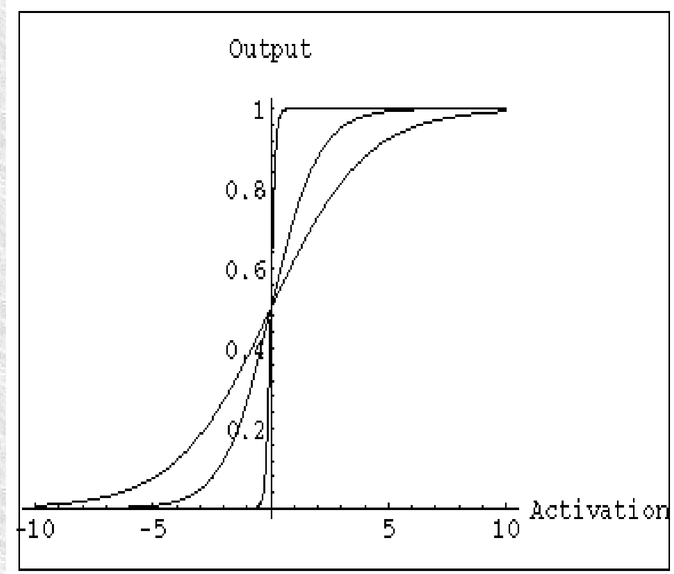
Neural Nets

- Well known in HEP

Multi-Layer Perceptron NN

- A popular and powerful neural network: (in root)





$$F = \sum_j \omega_{kj} \, f\left(\sum_i \omega_{ji} x_i + \theta_j\right) + \theta_k \,; \qquad y = \frac{1}{1 + e^{-F}}$$

Need to find ω 's and θ 's, the free parameters of the model

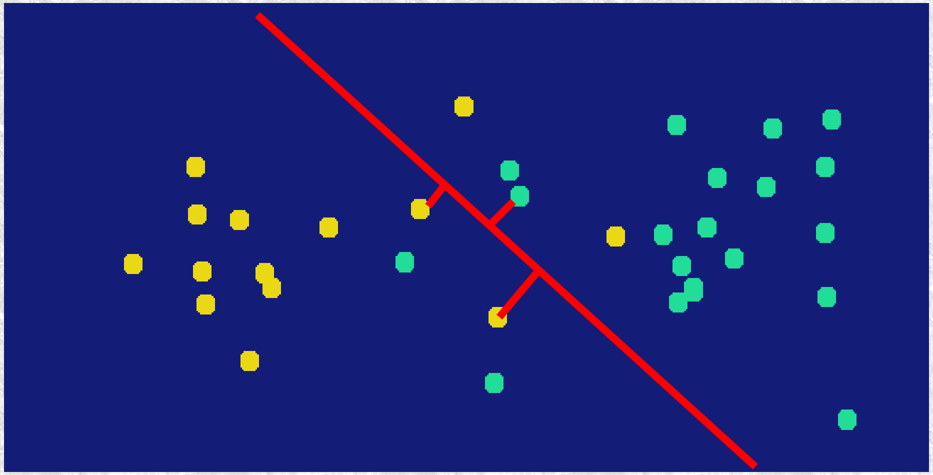
Neural Network Features

- Easy to use – packages exist everywhere
- Performance is good
  - Especially at handling higher dimensionality
  - No need to define a metric
  - But not optimal (we aim to approx. likelihood)
  - And only trained at one point
- Training is an issue
  - Optimization of nodes/layers can be difficult
  - Can over-focus on fluctuations
  - This is a problem for all machine learning
- Often worth a try
  - But it is solving the wrong problem

Support Vector Machines

Vapnik 1996

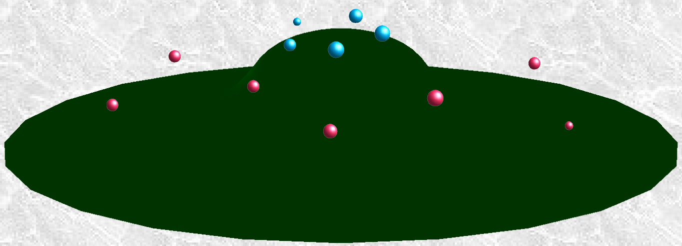
- Simplify storage/computation of separation by storing the 'support vector'



- The straight line is defined by closest points – the support vectors

Straight lines???

- Straight lines are not adequate, in general. Trick is to project from observed space into higher (infinite?) dimensionality space, such that a simple hyperplane defines the surfaces



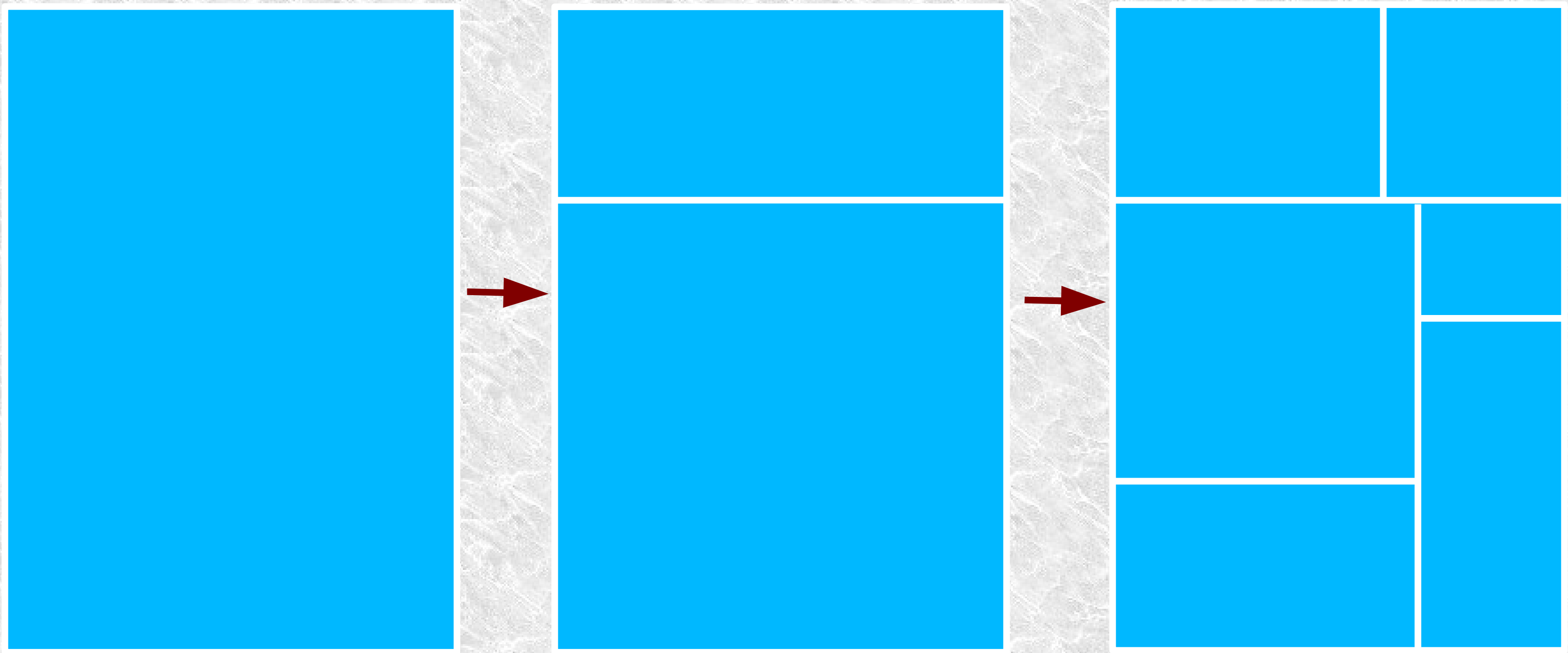
- Projection done implicitly by kernel choice
- Only inner-products are ever evaluated, and these are metric independent, so can be calculated in normal space.
- Never need to explicitly define the higher dimensional space

Support Vector Machines

- Storing just those points lying closest to the line is much easier than storing the entire space
- Defect is that the cut is only well defined near the line
- Computationally much easier then kernel likelihood

Decision Trees

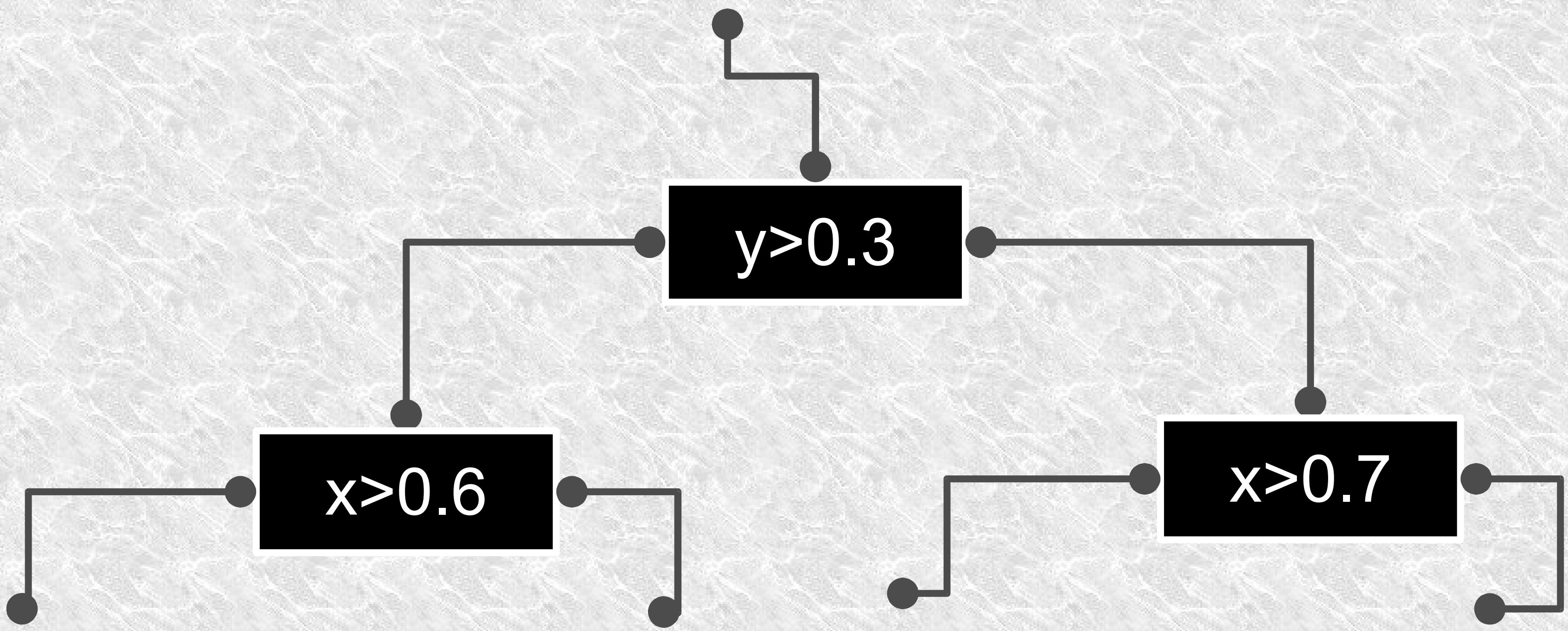
- A standard decision tree divides a problem in a series of steps.



Signal/background evaluated in each box

Decision Trees II

- Very clear: Each decision is binary, and whole tree can be represented as a tree:



This display works for any dimensionality of problem

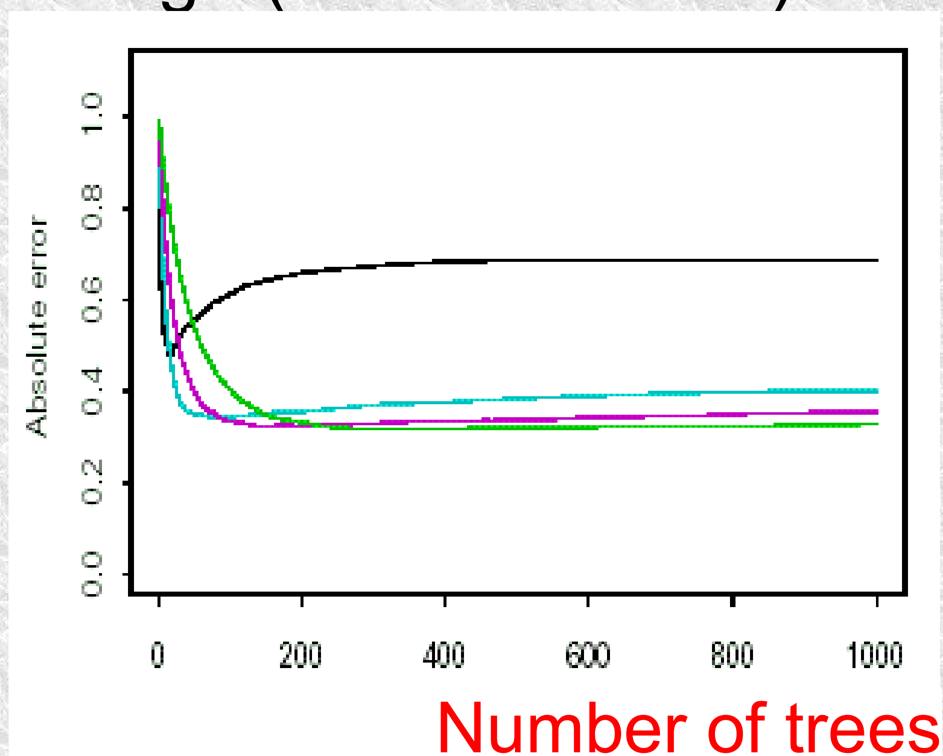
But how much do we value clarity?

Decision Trees III

- Downside is lack of stability
  - First 'cut' affects all later ones, classification can vary widely with a different training set
- Power somewhat below NN/Kernal likelihood for typical HEP problems
- Stopping rule important, affected by sample size.

Boosted Decision Trees

- A first tree is made
- Add more, increasing the weight of the mis-classified events
- Final s/b is average (in some sense) over all trees.



Black, cyan purple and green reflect increasing down-weighting of new trees

Boosted Decision Trees

- Lack of stability removed by averaging
- Computer intensive – but not N^3
- Power very good
- Trees individually small, whole data set is in each – good use of statistics
- Fairly fast.

Breiman: Boosted trees best off the shelf classifier in the world

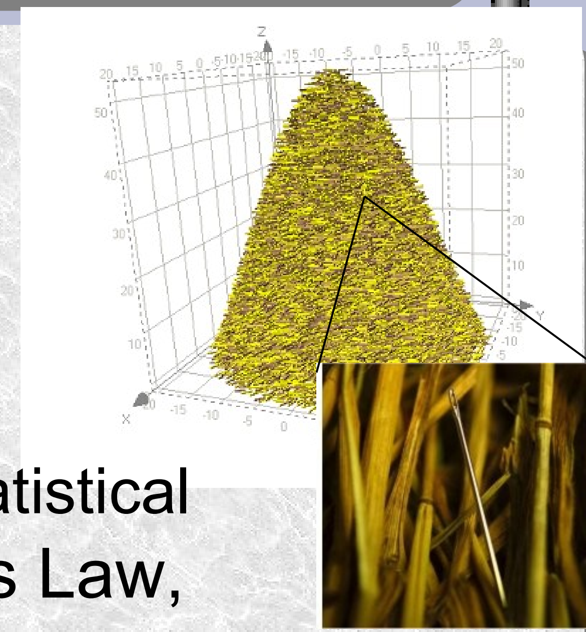
I do not have direct experience here

How to use these?

- Much is available from root
  - TMVA package widely used
  - I have produced 'TNSmooth'
    - Root add-on for kernel likelihood method

Summary of classification:

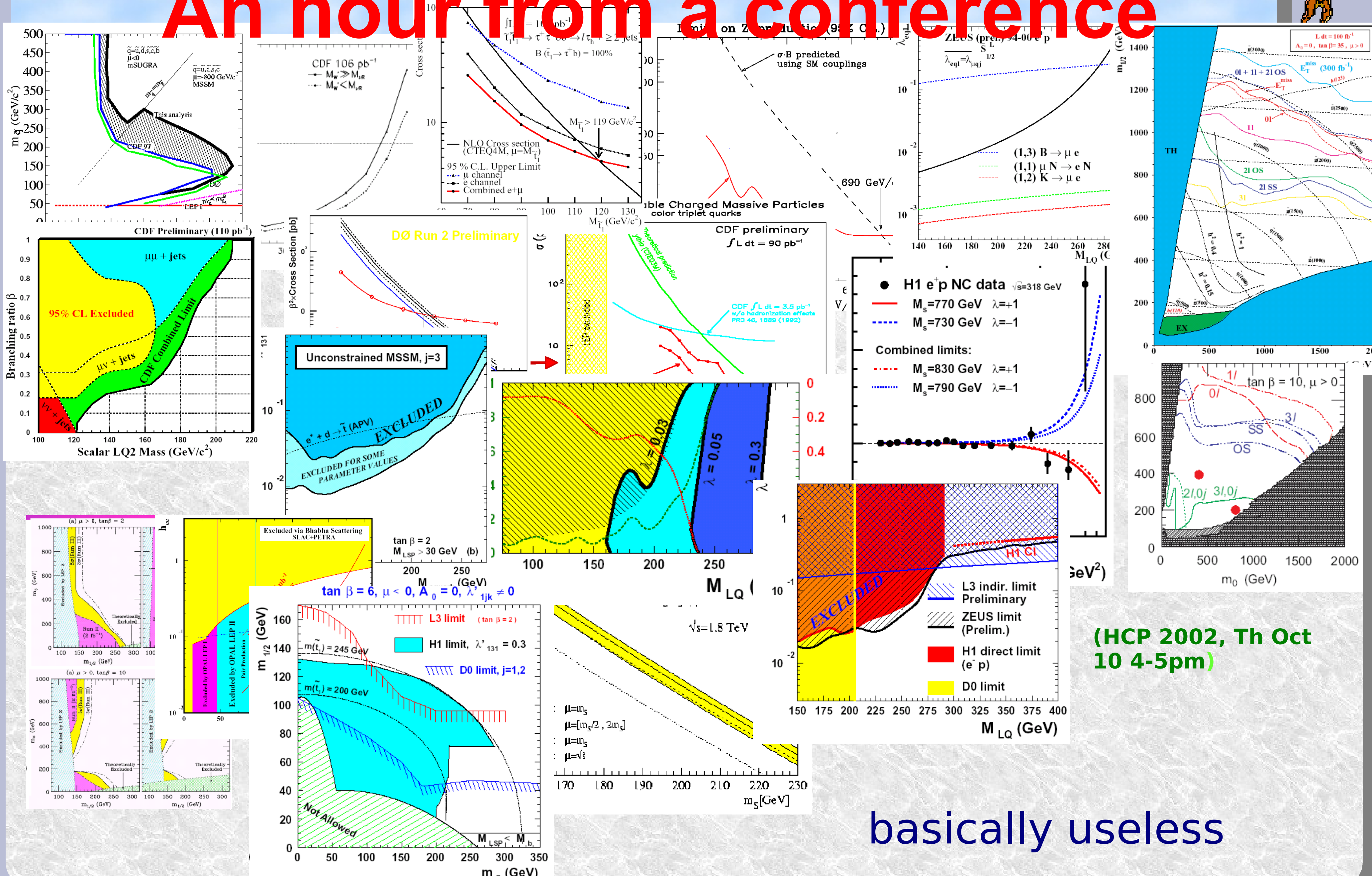
- Looking for
  - Needles in haystacks – the Higgs particle
- Needles are easier than haystacks
- 'Optimal' statistics have poor scaling
  - likelihood techniques: N^3
  - For large data sets main errors are not statistical
- As data and computers grow with Moore's Law, we can only keep up with $N \log N$
- A way out?
  - Discard notion of optimal (data is fuzzy, answers are approximate)
  - Don't assume infinite computational resources or memory
- Requires combination of statistics & computer science



Limits

- Definition of a limit
  - Bayes vs Frequentist
- Errors on limits
- Combining limits
- You need to know: What is being limited?

An hour from a conference



(HCP 2002, Th Oct 10 4-5pm)

basically useless

Bayes and Frequentist Statistics

- Bayes confidence level
  - Probability of theory given data
  - `There is a 5% probability X<0'
  - Right question, but subjective
- Frequentist/Classical P-value
  - Probability of data given theory
  - `If X<0, probability of these (or more extreme) data is 5% or less'
  - Wrong question

Bayes Theorem

- Bayes theorem modifies probabilities in light of data
- But needs an a-priori probability

$$p(a \wedge b) = p(a)\, p(b|_a) = p(b)\, p(a|_b)$$

$$p(b|_a) = \frac{p(b)}{p(a)}\, p(a|_b)$$

Uncontroversial

Requires p(theory)

$$p(theory|_{data}) = \frac{p(theory)}{p(data)}\, p(data|_{theory})$$

- If data plentiful frequentist and Bayesian converge
- Bayesian statistics much easier to use

Frequentist limits

'For this theory, probability of these data is <5%'

- About as useful as:

  'It was raining when I went to the theatre'

- e.g. a Higgs Search, background=3, observed=0
  - S=3: P = 0.2%
  - S=1: P=1.8%
  - S=0: P=5%
- So even a production of 0 Higgses is excluded at 95% CL. (M_H=1000 excluded!)
- Mathematically fine, but not useful

Bayes vs Frequentist Statistics II

- For measurement, almost all results are implicitly Bayesian - but could be justified frequentisticly.

- Limits are much less clear - read the small print
  - Many modifications (e.g. Feldmann & Cousins, RPP 2000) try to give Bayesian properties to classical limits
  - Without such modification, frequentist limits can be meaningless. (e.g. Example on previous page)

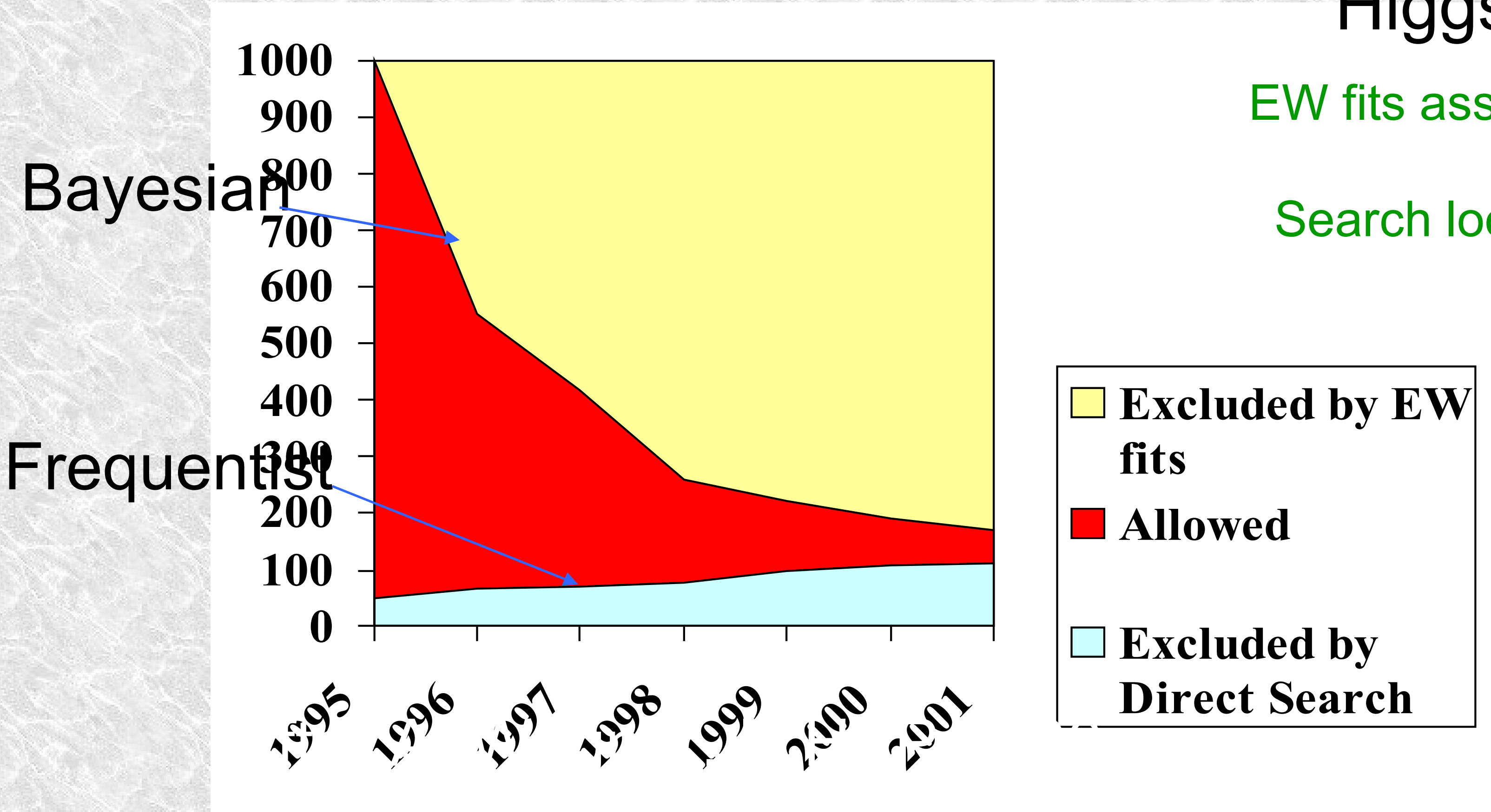
Fundamental problem:

$$P(\text{data}|\text{hypothesis}) \neq P(\text{hypothesis}|\text{data})$$

Error on a limit

- Sometimes people ask: What is the error on this limit?
- *This is the wrong question, it hides two others:*
  - How different would the limit be if
    - the data was a bit different?
    - you quoted 90% or 99% instead of 95%
- It is wrong, because $M_H > 113 \pm 1$ helps no-one. $M_H = 115 \pm 1$ is useful

Mixed up results!



Higgs limits

EW fits assume a Higgs

Search looks for one

To be fair, he had no choice - this is what is provided

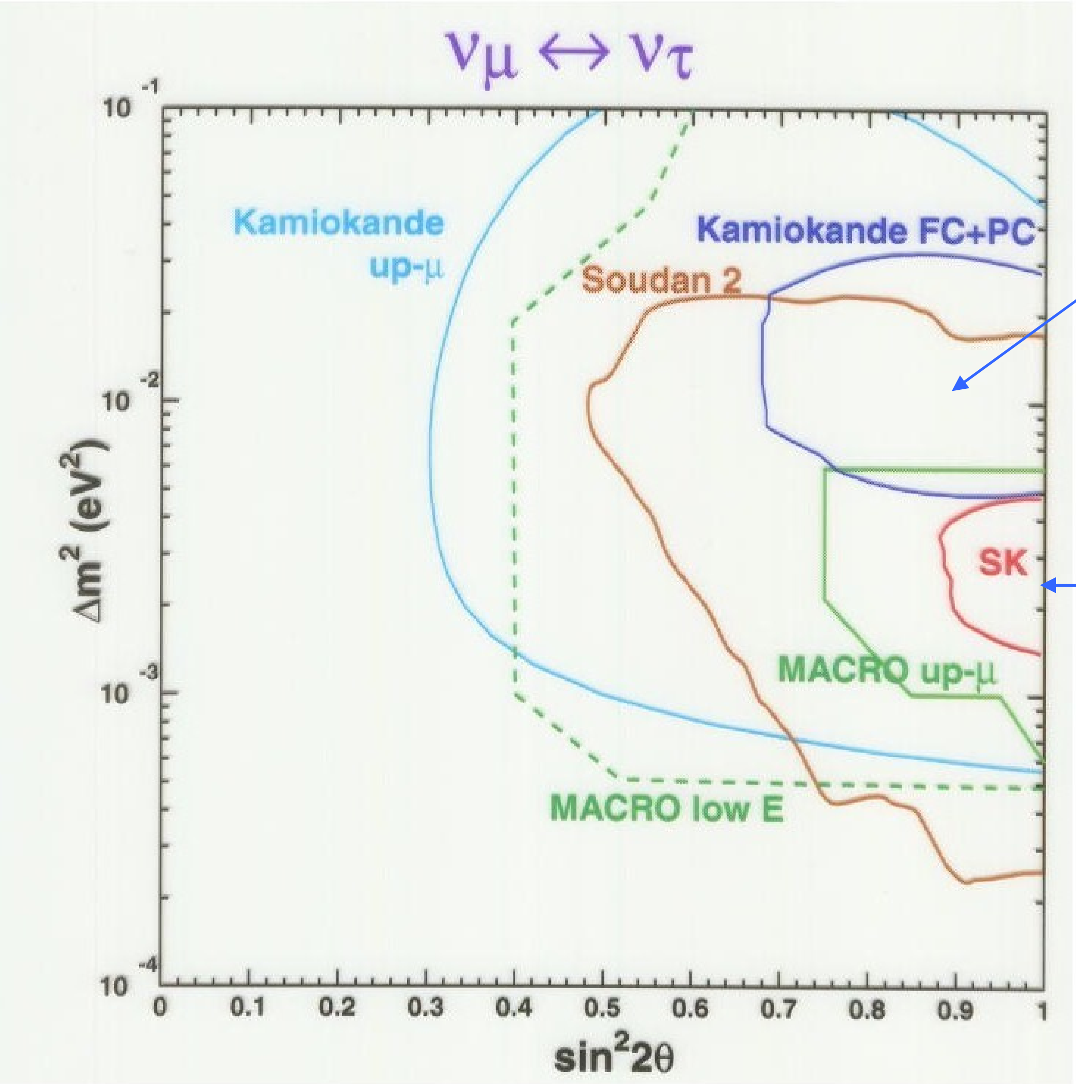
So what does a limit mean?

- Usually, a statement like:

  M_H>113.2GeV/c^2 @ 95%CL

  - Does NOT Mean that there is a 95% probability that M_H>113.2
  - DOES mean that IF MH<113.2 then there was at most a 5% probability we missed it.
- But you should not CARE anyway - it is a *probability*

Combination of limits



Kamiokande 90%

Super-K 90%

Results do not overlap! How can you combine?

Please, don't do it!

Parameter Extraction

Statistics and Systematics

- Data are collected very often in terms of **numbers of events**
- These are converted into cross-sections; rates at which things happen.
- This is true of almost all HEP measurements
- The statistical precision is fairly straightforward to estimate, and will have a Poisson or Binomial form which can often be approximated with a Gaussian (CLT)
- Various systematic effects will also affect the re-sult.

Evaluation of Systematics

- Usually the hardest part of a measure-ment
- Frequently done badly
- Can be under- or over- estimated
  - Sometimes an error source is forgotten
  - Frequently statistics get taken twice

Systematics

- Typical experimental statements:
  - M_W =80.336 ±0.055(stat) ±0.028(sys) ±0.025(FSI) ±0.009(LEP) (DELPHI)
  - M_W = 80.329 ±0.029 (EW group)
- First has statistical and systematic errors
- The second does not. Why?

Systematics in combination

- Take an example: Two measurements of `x'
  - $x_a = 50 \pm 10(stat) \pm 1(sys)$ (expt. a)
  - $x_b = 60 \pm 1(stat) \pm 10(sys)$ (expt. b)
- To combine, use:

$$\frac{x_{tot}}{\sigma^2_{tot}} = \sum_i \frac{x_i}{\sigma^2_i} \qquad \frac{1}{\sigma^2_{tot}} = \sum_i \frac{1}{\sigma^2_i}$$

Correlations?

  - $x_{tot} = 55 \pm 7.11$ (total)
- But either stat. or syst. combined separately is <1!

Errors are completely mixed in combination - must be evaluated on equal footing

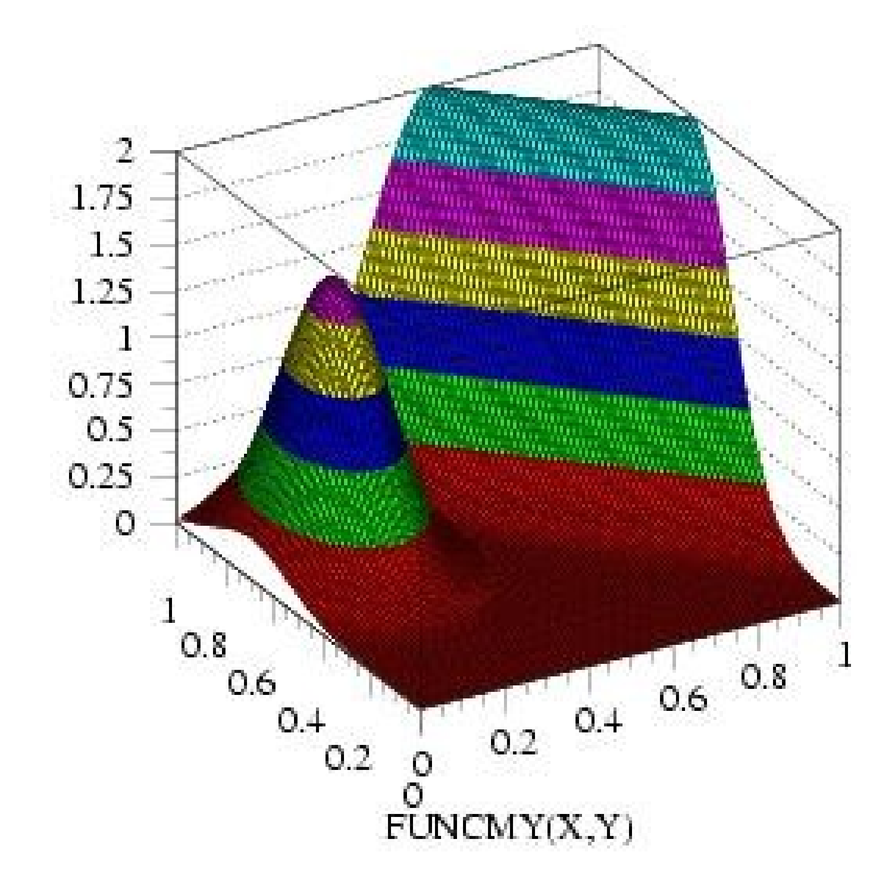
Why is fitting important?

- Experimental data usually used to obtain theoretical parameter values
- There are two distinct questions:
  - What is the best value of X (Parameter optimization)
  - Does the theory explain the data (Goodness of fit)
- The use of is very different

Parameter optimisation

- What value of the free parameters best describes the data?
- `MINUIT' from root/CERNLIB a very common minimization package
- User must specify WHAT is minimized (χ^2, likelihood, etc.)
- MINUIT will (usually) find the optimal parameter set
- Complex functions may have secondary maxima / convergence failure

Example of a hard maximisation



- Subsidiary minimum may confuse algorithm
- Primary maximum has very high parameter correlation
- Likely convergence failure

The right way to fit?

	χ^2	***likelihood***
Binned	Yes	Yes
Unbinned	No	Yes
Works low stats	No	Yes
Unbiased	Sometimes	Yes
Goodness-of-fit	$P(\chi^2)$	Hard

The techniques converge for high statistics

Both can be handled by 'Minuit'

No *right* way

Definition of χ^2

- Compatibility of results with expectation:

$$\chi^2 = \sum_i \frac{(x_i^{obs} - x_i^{pred})^2}{\sigma_x^2}$$

- If counting events in bins then:
- Beware: Is σ $\sqrt{N^{obs}}$ or $\sqrt{N^{pred}}$? - Both are wrong!
- $\sqrt{N^{obs}}$ Biased down if data down... (Mean 5 & 3 = 3.75))
- $\sqrt{N^{pred}}$ Error depends upon theory - biased up (~4.12)

Definition of likelihood

$$L_r = e^{-r} \times \prod_i R_i$$

$$LR = \frac{L_{s+b}}{L_b} = e^{-s} \times \prod_i \frac{S_i + B_i}{B_i}$$

- r: The total rate
- R_i: The density at point i
- s: signal
- b: background

- Likelihood ratio compares two hypotheses.
- Or vary R to maximize L. Maximum likelihood powerful estimator.

$$\log(L_R) = -r + \sum_i \ln R_i$$

← weighted sum of events.

Comparison of definitions

$$\chi^2 = \sum_i \frac{(x_i^{obs} - x_i^{pred})^2}{\sigma_x^2}$$

$$\log(L_R) = -r + \sum_i \ln R_i$$

Take a Gaussian centred on 0, width σ

$$\chi^2 = \sum_i \frac{x_i^2}{\sigma^2}$$

$$\log(L_R) = -r + \sum_i \ln\left(e^{-0.5 x_i^2/\sigma^2}\right)$$

$$\log(L_R) = -r + \sum_i -0.5\frac{x_i^2}{\sigma^2}$$

So: $\delta \chi^2 = -2 * \delta \log(L_R)$ IF GAUSSIAN

Goodness of fit

Averaging two numbers

- Suppose we have two measurements of x:
  10±1 and 11±1
- We know the average:
  10.5±0.7
- But what about
  10±1 and 20±1
- Are we happy with:
  15.0±0.7
- If the errors are Gaussian we should be happy
  - Combining two Gaussians gives a Gaussian
- Or we conclude we have a 'bad fit'

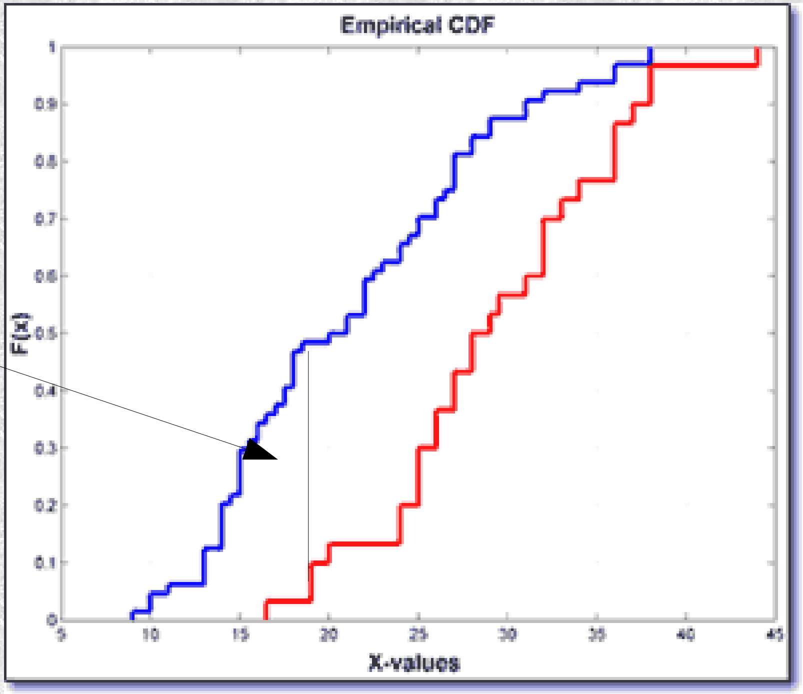
Goodness of fit

Do I believe my fitted results?

- For a χ^2 fit (much the most common) easy
  - Look up Prob(χ^2,NDF) in a table.
  - Good general test
    - often abused, e.g. χ^2/DoF
- For a likelihood fit: hard
  - Can sometimes use simulated trials to find Probability of getting observed result OR \`larger’ one

Kolmogorov-Smirnov Test

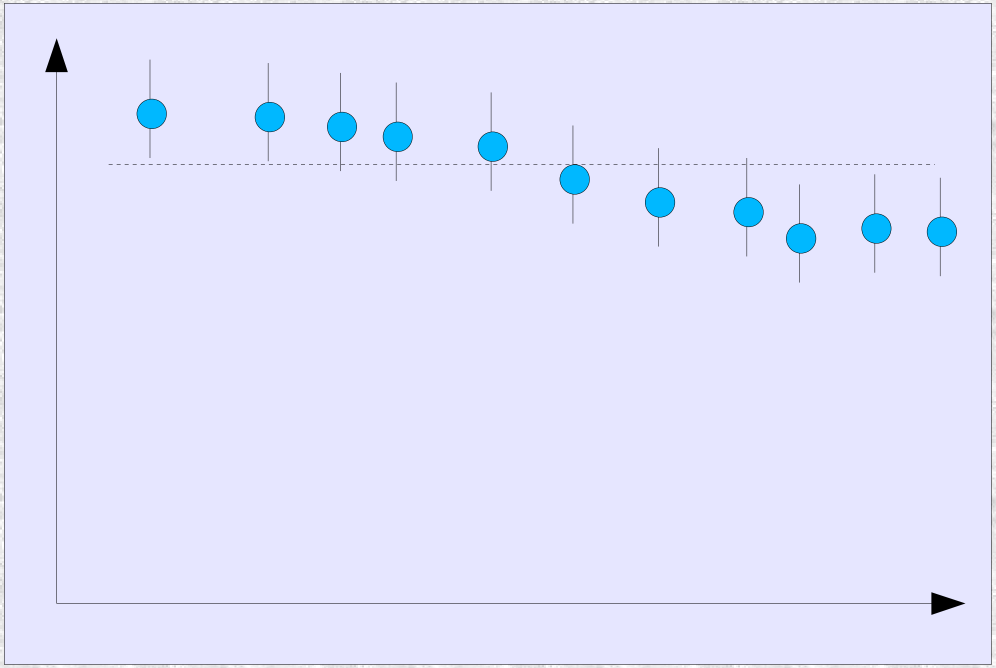
- Are two 1D distributions drawn from a common parent?
- Find integral distribution
- Observe maximum difference between two integrals
- Probability is calculable
- Very bad here!



- K-S very good
  - No allowance for fit
  - Or systematic error

Run test

- Measures 'runs': How often one distribution is above (or below) the other
  - Find length of maximum run
  - Probability of this length is calculable
- This data has good χ^2
- Run test would be poor



Is there a better test than chi^2?

- Yes...and no
- For any given problem, a more sensitive test can be defined
- But you can only define the sensitivity if you know what you are choosing between
- There is no 'most powerful' goodness of fit test.

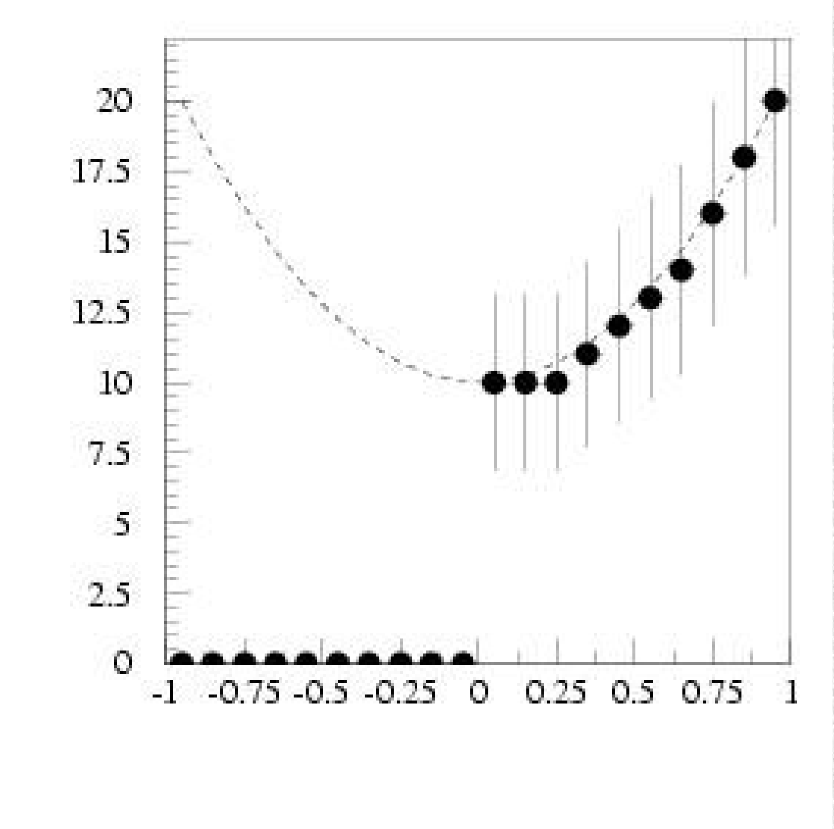
How things can go wrong…

- Example: Fit function

  $y=a + b \cos\theta^2$

- Likelihood fit is not sensitive to sign on θ
- Concludes that dist^n shown is very good fit!

  Nothing is perfect…



Conclusions

- The likelihood ratio underpins everything
  - Use it
- Cost of computing becoming important
  - Optimal methods not *necessarily* optimal
  - But the data is very expensive too.
  - Systematic errors may dominate anyway
- Need to see statistics as a tool
- Please:
  - Ask me if you have statistical questions