Practical Statistics – part I 'Basics Concepts'

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What do we want to know?

- Physics questions we have...
 - Does the (SM) Higgs boson exist?
 - What is its production cross-section?
 - What is its boson mass?

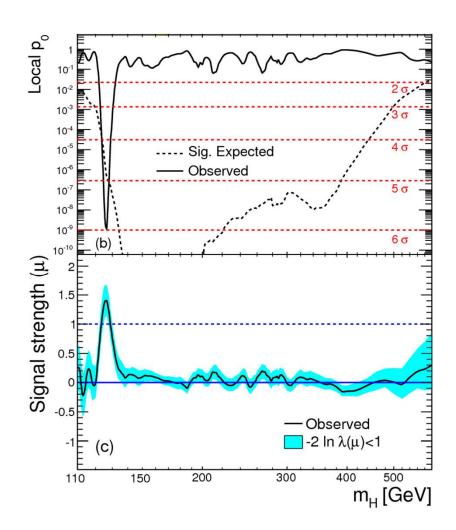


- Statistical tests construct probabilistic statements: p(theo|data), or p(data|theo)
 - Hypothesis testing (discovery)
 - (Confidence) intervals
 Measurements & uncertainties



Result: Decision based on tests

"As a layman I would now say: I think we have it"

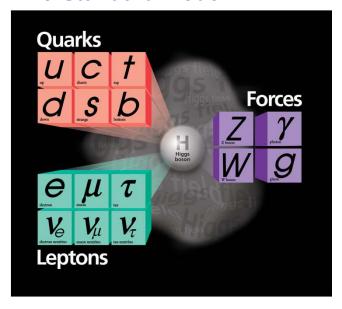




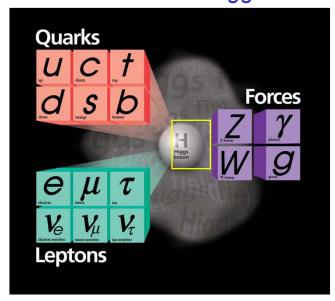
How do we do this?

- All experimental results start with formulation of a (physics) theory
- Examples of HEP physics models being tested

The Standard Model



The SM without a Higgs boson

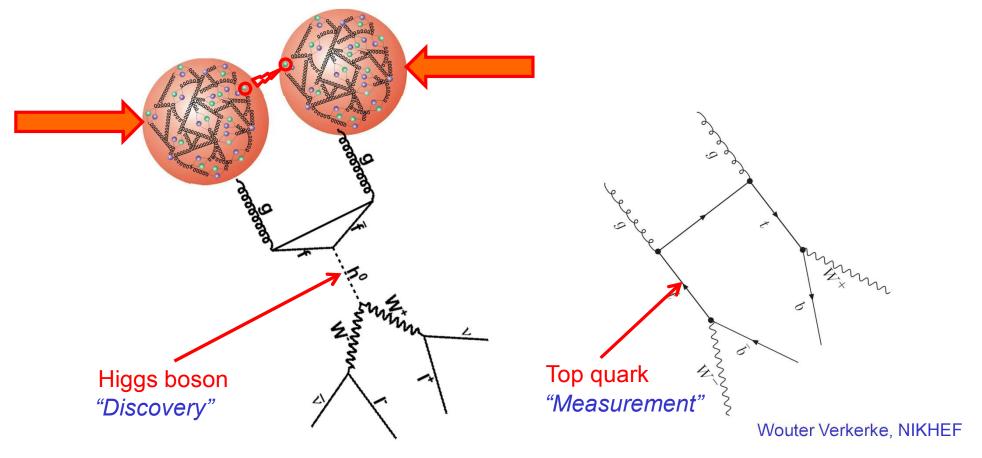


- Next, you design a measurement to be able to test model
 - Via chain of physics simulation, showering MC, detector simulation and analysis software, a physics model is reduced to a statistical model

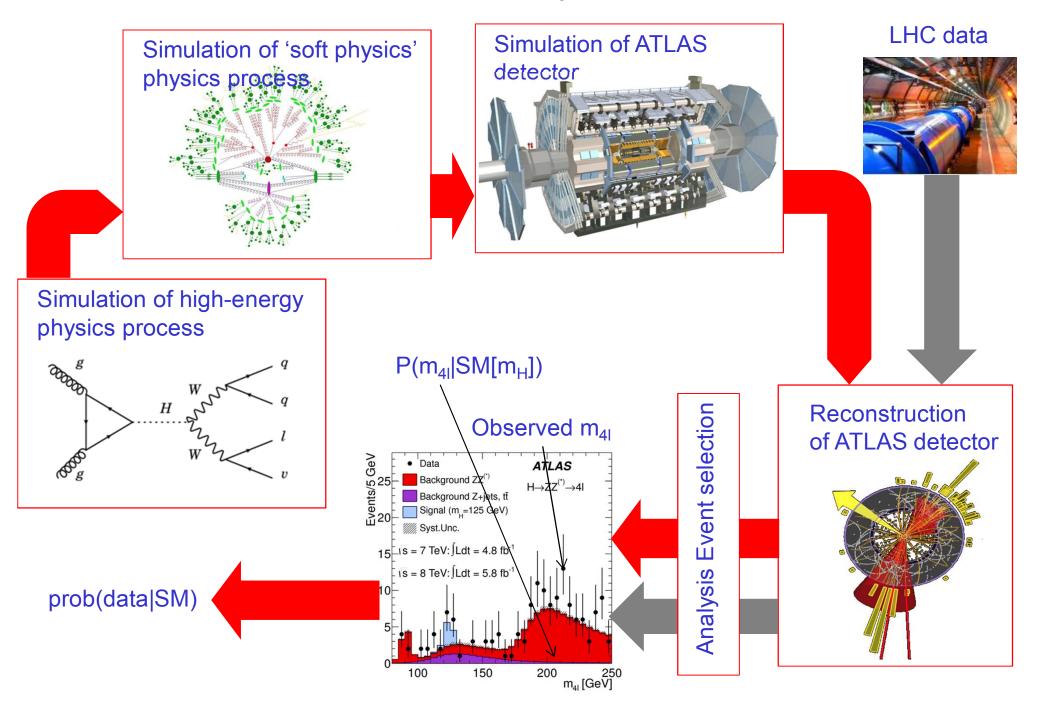
How do we do this?

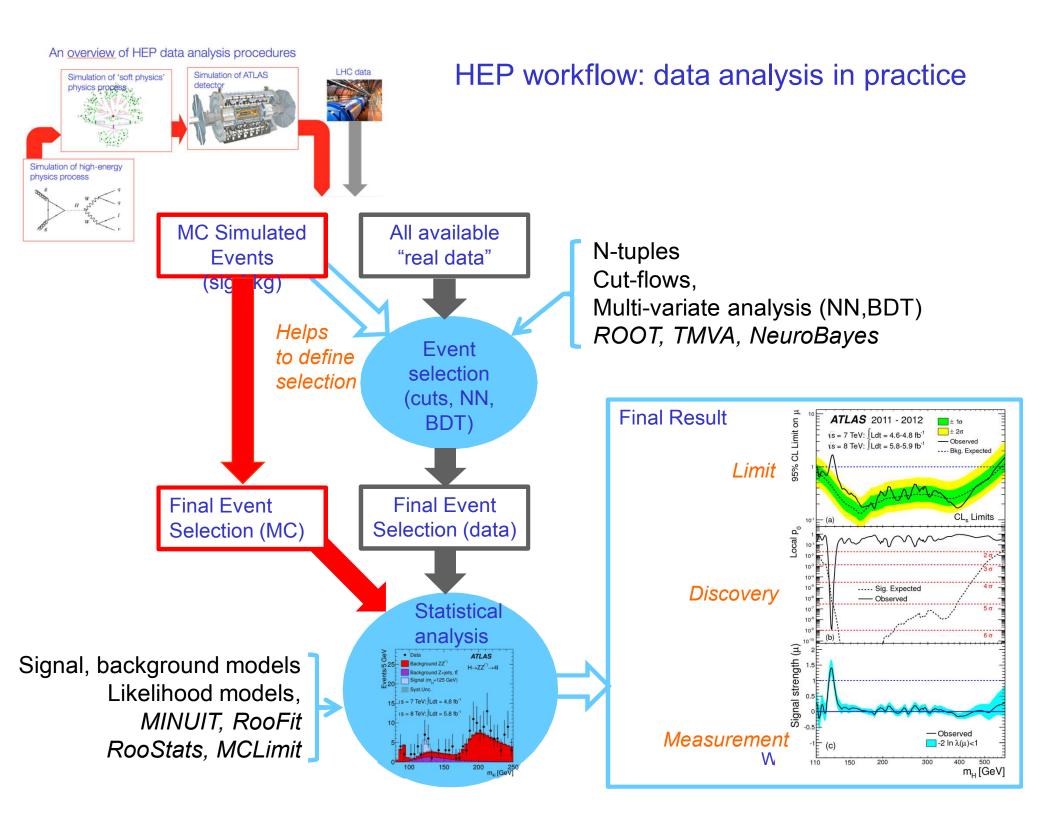


- General infrastructure collider, detector, computing
- Design analysis strategy to
 - observe existence of a particular process,
 - measure property of a produced particle



An overview of HEP data analysis procedures

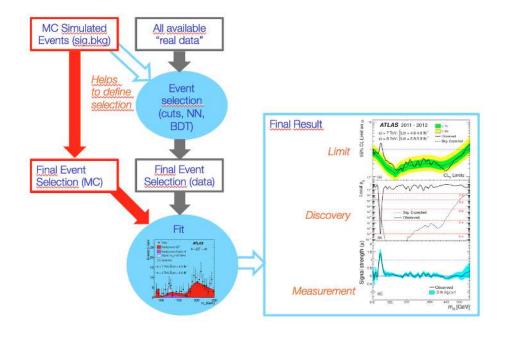




From physics theory to statistical model

 HEP "Data Analysis" is for large part the reduction of a physics theory to a statistical model

Physics Theory: Standard Model with 125 GeV Higgs boson

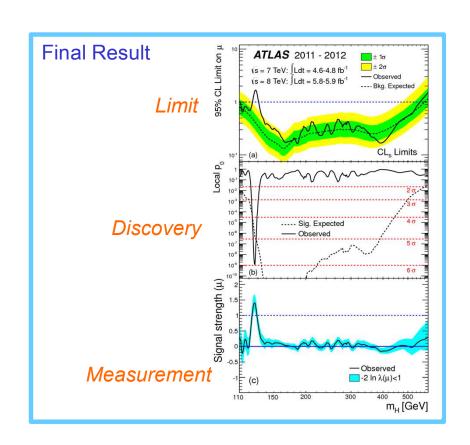


Statistical Model: *Given a measurement x (e.g. an event count)*what is the probability to observe each possible value of x,
under the hypothesis that the physics theory is true.

Once you have a statistical model, all physics knowledge has been abstracted into the model, and further steps in statistical inference are 'procedural' (no physics knowledge is required in principle)

From statistical model to a result

 The next step of the analysis is to confront your model with the data, and summarize the result in a probabilistic statement of some form



'Confidence/Credible Interval'

 σ/σ_{SM} (HIZZ) $|_{mH=150}$ < 0.3 @ 95% C.L.

'p-value'

"Probability to observed this signal or more extreme, under the hypothesis of background-only is 1x109"

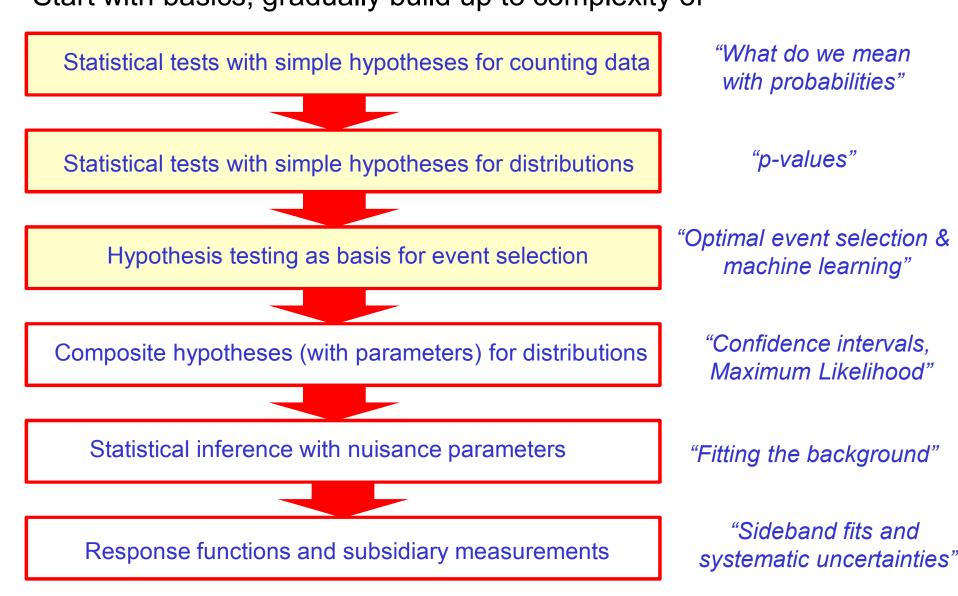
'Measurement with variance estimate' σ/σ_{SM} (HDZZ) $|_{mH=126} = 1.4 \pm 0.3$

 The last step, usually not in a (first) paper, that you, or your collaboration, decides if your theory is valid



Roadmap for this course

Start with basics, gradually build up to complexity of



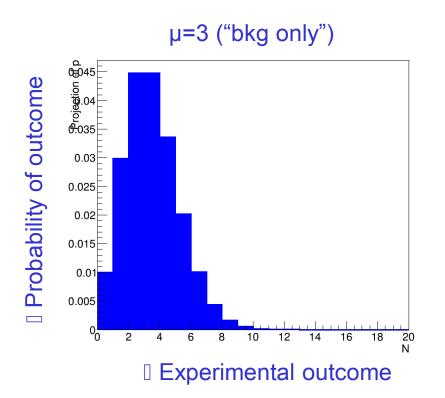
The statistical world

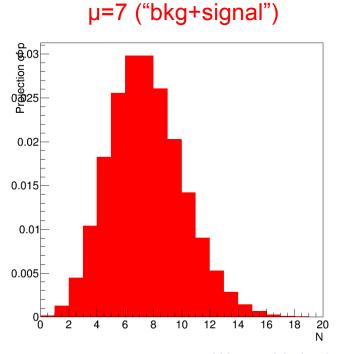
- Central concept in statistics is the 'probability model'
- A probability model assigns a probability to each possible experimental outcome.
- Example: a HEP counting experiment

$$P(N \mid \mu) = \frac{\mu^N e^{-\mu}}{N!}$$

- Count number of 'events' in a fixed time interval

 Poisson distribution
- Given the expected event count, the probability model is fully specified

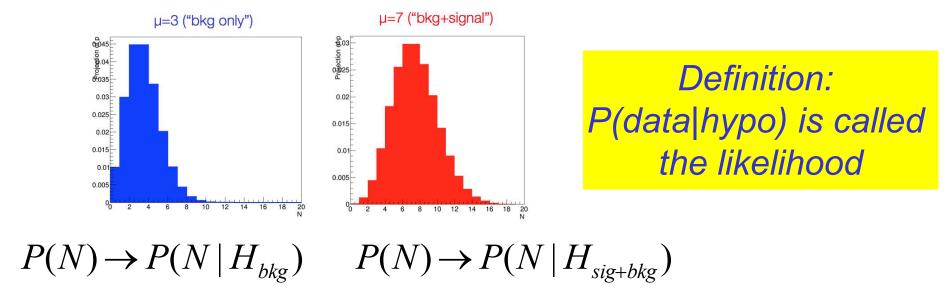




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Probabilities vs conditional probabilities

 Note that probability models strictly give conditional probabilities (with the condition being that the underlying hypothesis is true)



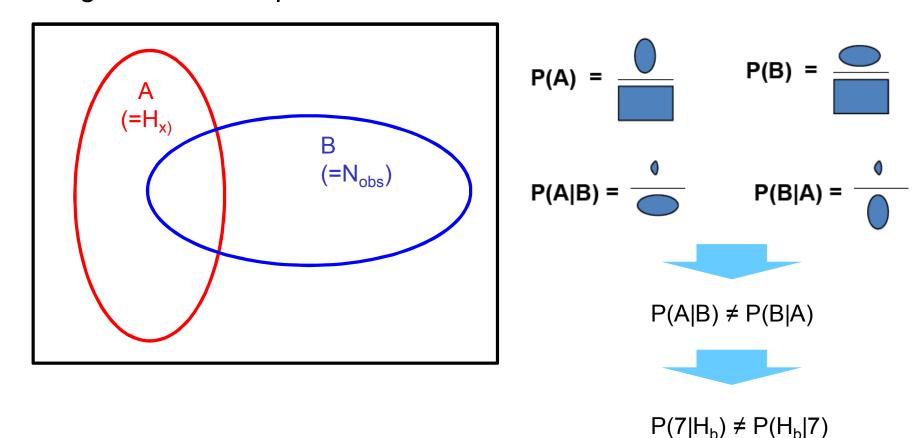
Suppose we measure N=7 then can calculate

$$L(N=7|H_{bkg})=2.2\%$$
 $L(N=7|H_{sig+bkg})=14.9\%$

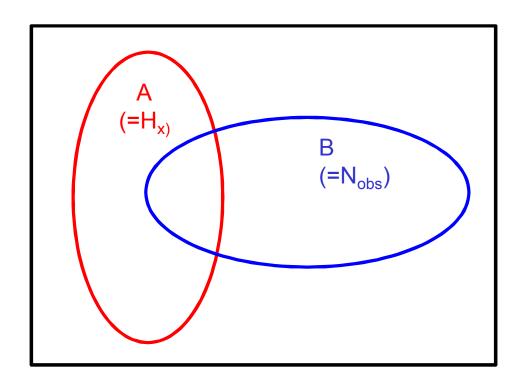
- Data is more likely under sig+bkg hypothesis than bkg-only hypo
- Is this what we want to know? Or do we want to know
 L(H|N=7)?

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- Do you L(7|H_b) and L(7|H_{sb}) provide you enough information to calculate P(H_b|7) and P(H_{sb}|7)
- No!
- Image the 'whole space' and two subsets A and B



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$$P(A) = \frac{0}{|A|} \qquad P(B) = \frac{0}{|A|}$$

$$P(A|B) = \frac{\emptyset}{}$$

$$P(B|A) = \frac{\emptyset}{}$$

$$P(A|B) \neq P(B|A)$$



but you can deduce their relation

$$\Rightarrow$$
 P(B|A) = P(A|B) \times P(B) / P(A)

 This conditionality inversion relation is known as Bayes Theorem

 $P(B|A) = P(A|B) \times P(B)/P(A)$

Essay "Essay Towards Solving a Problem in the Doctrine of Chances" published in Philosophical Transactions of the Royal Society of London in 1764



Thomas Bayes (1702-61)

- And choosing A=data and B=theory
 P(theo|data) = P(data|theo) × P(theo) / P(data)
- Return to original question:

Do you $L(7|H_b)$ and $L(7|H_{sb})$ provide you enough information to calculate $P(H_b|7)$ and $P(H_{sb}|7)$

• No! Need P(A) and P(B) Need P(H_b), P(H_{sb}) and P(P) rerke, NIKHEF

- What is P(data)?
- It is the probability of the data under any hypothesis
 - For Example for two competing hypothesis H_b and H_{sb}

$$P(N) = L(N|H_b)P(H_b) + L(N|H_{sb})P(H_{sb})$$

and generally for N hypotheses

$$P(N) = \sum_{i} P(N|H_i)P(H_i)$$

Bayes theorem reformulated using law of total probability

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P(theo|data) = L(data|theo) \times P(theo)
\Sigma_i L(data|theo-i)P(theo-i)
```

 Return to original question: Do you L(7|H_b) and L(7|H_{sb}) provide you

enough information to calculate $P(H_b|7)$ and $P(H_{sb}|7)$ No! [] Still need $P(H_b)$ and $P(H_{sb})$ Wouter Verkerke, NIKHEF

Prior probabilities

- What is the meaning of P(H_b) and P(H_{sb})?
 - They are the probability assigned to hypothesis H_b prior to the experiment.
- What are the values of P(H_b) and P(H_{sb})?
 - Can be result of an earlier measurement
 - Or more generally (e.g. when there are no prior measurement)
 they quantify a prior degree of belief in the hypothesis
- Example suppose prior belief P(H_{sb})=50% and P(H_b)=50%

$$P(H_{sb}|N=7) = P(N=7|H_{sb}) \times P(H_{sb})$$

$$[P(N=7|H_{sb})P(H_{sb})+P(N=7|H_{b})P(H_{b})]$$

$$= 0.149 \times 0.50 = 87\%$$

$$[0.149 \times 0.5 + 0.022 \times 0.5]$$

Observation N=7 strengthens belief in hypothesis H_{sb}
 (and weakens belief in H_b | 13%)

Interpreting probabilities

We have seen

probabilities assigned observed experimental outcomes (probability to observed 7 events under some hypothesis)

probabilities assigned to hypotheses (prior probability for hypothesis H_{sb} is 50%)

which are conceptually different.

How to interpret probabilities – two schools

Bayesian probability = (subjective) degree of belief P(theo|data)
P(theo|data)

Frequentist probability = fraction of outcomes in P(data|theo) future repeated identical experiments

"If you'd repeat this experiment identically many times, in a fraction P you will observe the same outcome"

Interpreting probabilities

Frequentist:

Constants of nature are fixed – you cannot assign a probability to these. Probability are restricted to observable experimental results

"The Higgs either exists, or it doesn't" – you can't assign a probability to that

Bayesian:

Probabilities can be assigned to constants of nature

Quantify your belief in the existence of the Higgs – can assign a probablity

Example of weather forecast

Bayesian: "The probability it will rain tomorrow is 95%"

Assigns probability to constant of nature ("rain tomorrow")
 P(rain-tomorrow|weather-data) = 95%

Frequentist: "It will rain tomorrow(*)"

(*) 95% of the forecast are correct.

Only states P(weather-data|rain-tomorrow)

Bayesians and Frequentists

A slide from a professional statistician found when Googling...

ACCP 37th Annual Meeting, Philadelphia, PA [2]

Differences Between Bayesians and Non-Bayesians
According to my friend Jeff Gill



Typical Bayesian



Typical Non-Bayesian

Bayesians and Frequentists

Another slide from a particle physicist...

Why isn't everyone a Bayesian?

My suspicion: it is because most people do not understand the frequentist approach. Frequentist statements and Bayesian statements are thought to be about the same logical concept, and the frequentist statement does not require a prior, so ...

A. L. Read, Presentation of search results: the CL_S technique, J. Phys. G: Nucl. Part. Phys. **28** (2002) 2693-2704.

nearly all physicists tend to misinterpret frequentist results as statements about the theory given the data.

Frequentist statements are not statements about the model – only about the data in the context of the model. This is not what we wanted to know ... At least not the ultimate statement.

SOS 12

Formulating evidence for discovery

- Given a scenario with exactly two competing hypotheses
- In the Bayesian school you can cast evidence as an odd-ratio

$$O_{prior} \equiv \frac{P(H_{sb})}{P(H_{b})} = \frac{P(H_{sb})}{1 - P(H_{sb})} \qquad \text{If p(H_{sb})=p(H_{b})} \equiv \text{Odds are 1:1}$$

$$O_{posterior} \equiv \frac{L(x \mid H_{sb})P(H_{sb})}{L(x \mid H_{sb})P(H_{b})} = \frac{L(x \mid H_{sb})}{L(x \mid H_{b})} O_{prior}$$

If $P(data|H_b)=10^{-7}$ P(data|H_{sb})=0.5 K=2.000.000 | Posterior odds are 2.000.000 : 1

Formulating evidence for discovery

- In the frequentist school you restrict yourself to P(data|theory) and there is no concept of 'priors'
 - But given that you consider (exactly) 2 competing hypothesis,
 very low probability for data under Hb lends credence to 'discovery' of Hsb (since Hb is 'ruled out'). Example

P(data|H_b)=
$$10^{-7}$$
 P(data|H_{sb})= 0.5 "H_b ruled out" ["Discovery of H_{sb}"

- Given importance to interpretation of the lower probability, it is customary to quote it in "physics intuitive" form: Gaussian σ .
 - E.g. '5 sigma'
 □ probability of 5 sigma Gaussian fluctuation = 2.87x10⁻⁷
- No formal rules for 'discovery threshold'
 - Discovery also assumed is not too unlikely under Hsb. If not, no discovery, but again no formal rules ("your good physics judgment")
 - NB: In Bayesian case, both likelihoods low reduces Bayes factor K to O(1)

Taking decisions based on your result

- What are you going to do with the results of your measurement?
- Usually basis for a decision
 - Science: declare discovery of Higgs boson (or not), make press release, write new grant proposal
 - Finance: buy stocks or sell
- Suppose you believe P(Higgs|data)=99%.
- Should declare discovery, make a press release?
 A: Cannot be determined from the given information!
- Need in addition: the utility function (or cost function),
 - The cost function specifies the relative costs (to You) of a Type I error (declaring model false when it is true) and a Type II error (not declaring model false when it is false).

Taking decisions based on your result

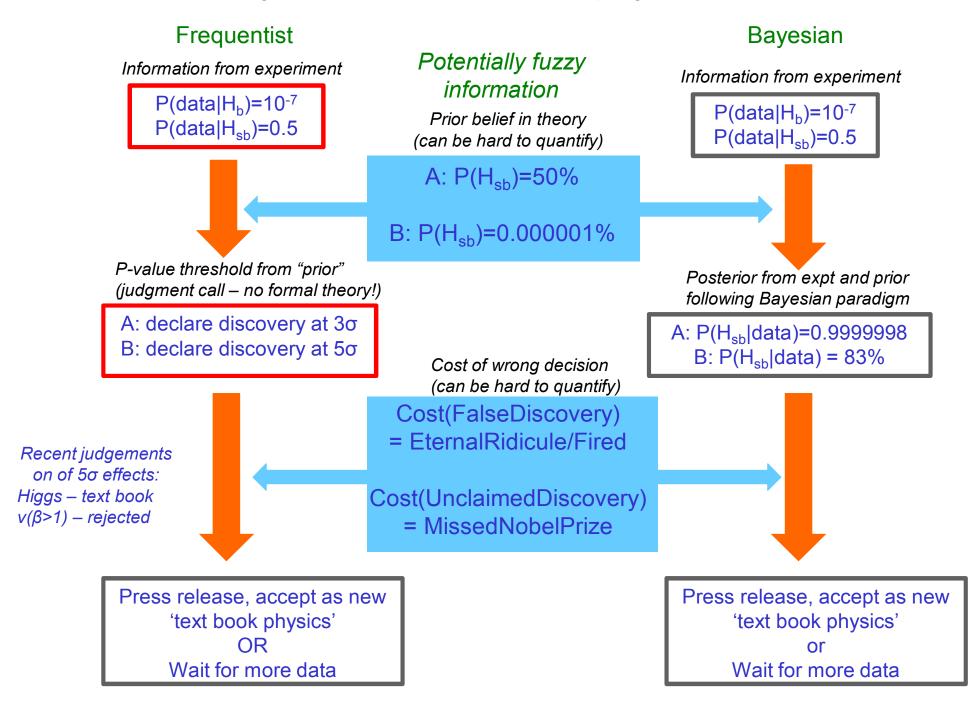
 Thus, your decision, such as where to invest your time or money, requires two subjective inputs:

Your prior probabilities, and

the relative costs to You of outcomes.

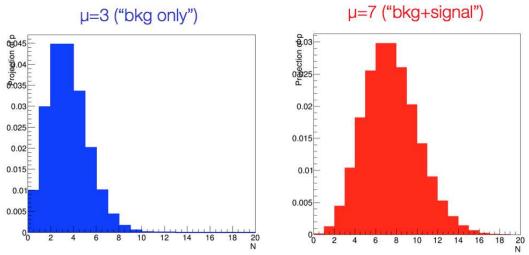
- Statisticians often focus on decision-making; in HEP, the tradition thus far is to communicate experimental results (well) short of formal decision calculations.
- Costs can be difficult to quantify in science.
 - What is the cost of declaring a false discovery?
 - Can be high ("Fleischman and Pons"), but hard to quantify
 - What is the cost of missing a discovery ("Nobel prize to someone else"), but also hard to quantify

How a theory becomes text-book physics



Summary on statistical test with simple hypotheses

- So far we considered simplest possible experiment we can do: counting experiment
- For a set of 2 or more completely specified (i.e. simple) hypotheses

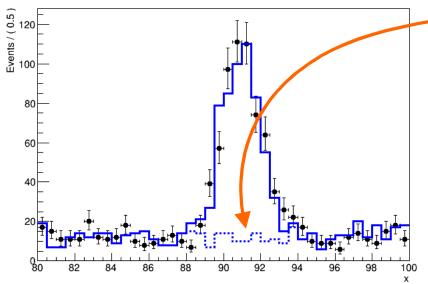


Given probability models P(N|bkg), and P(N|sig)we can calculate P(Nobs|Hx) under both hypothesis

- ☐ With additional information on P(Hi) we can also calculate P(Hx|Nobs)

Practical statistics – (Multivariate) distributions

- Most realistic HEP analysis are not like simple counting expts at all
 - Separation of signal-like and background-like is a complex task that involves study of many observable distributions
- How do we deal with distributions in statistical inference?
 Construct a probability model for the distribution
- Case 1 Signal and background distributions from MC simulation
 - Typically have histograms for signal and background



a counting experiment it of Likelihoods for each bin

$$L(\vec{N} \mid H_b) = \prod_{i} Poisson(N_i \mid \tilde{b}_i)$$

$$L(\vec{N} \mid H_{s+b}) = \prod_{i} Poisson(N_i \mid \tilde{s}_i + \tilde{b}_i)$$

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Working with Likelihood functions for distributions

- How do the statistical inference procedures change for Likelihoods describing distributions?
- Bayesian calculation of P(theo|data) they are exactly the same.
 - Simply substitute counting model with binned distribution model

$$P(H_{s+b} | \vec{N}) = \frac{L(\vec{N} | H_{s+b})P(H_{s+b})}{L(\vec{N} | H_{s+b})P(H_{s+b}) + L(\vec{N} | H_b)P(H_b)}$$

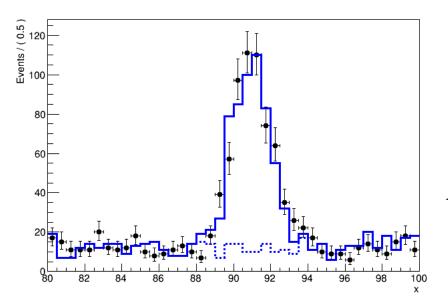


Simply fill in new Likelihood function Calculation otherwise unchanged

$$P(H_{s+b} \mid \vec{N}) = \frac{\prod_{i} Poisson(N_i \mid \tilde{s}_i + \tilde{b}_i)P(H_{s+b})}{\prod_{i} Poisson(N_i \mid \tilde{s}_i + \tilde{b}_i)P(H_{s+b}) + \prod_{i} Poisson(N_i \mid \tilde{b}_i)P(H_b)}$$

Working with Likelihood functions for distributions

 Frequentist calculation of P(data|hypo) also unchanged, but question arises if P(data|hypo) is still relevant?



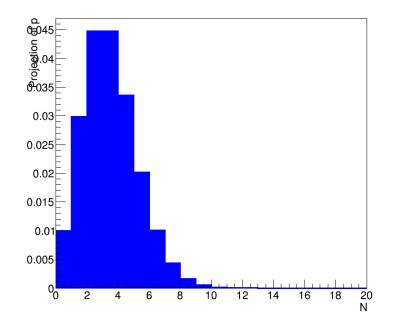
$$L(\vec{N} \mid H_b) = \prod_{i} Poisson(N_i \mid \tilde{b}_i)$$

$$L(\vec{N} \mid H_{s+b}) = \prod_{i} Poisson(N_i \mid \tilde{s}_i + \tilde{b}_i)$$

- L(N|H) is probability to obtain exactly the histogram observed.
- Is that what we want to know? Not really.. We are interested in probability to observe any 'similar' dataset to given dataset, or in practice dataset 'similar or more extreme' that observed data
- Need a way to quantify 'similarity' or 'extremity' of observed data

Working with Likelihood functions for distributions

- Definition: a test statistic T(x) is any function of the data
- We need a test statistic that will classify ('order') all possible observations in terms of 'extremity' (definition to be chosen by physicist)
- NB: For a counting measurement the count itself is already a useful test statistic for such an ordering (i.e. T(x) = x)



Test statistic T(N)=Nobs orders observed events count by estimated signal yield

Low N

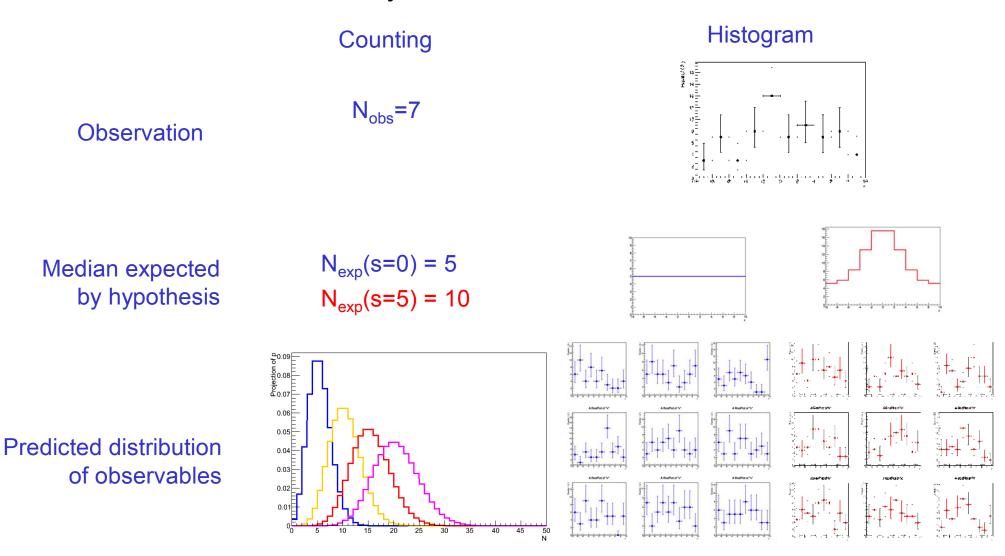
low estimated signal

High N

large estimated signal

Ordering distributions by 'signal-likeness' aka 'extremity'

How to define 'extremity' if observed data is a distribution



Which histogram is more 'extreme'?

The Likelihood Ratio as a test statistic

 Given two hypothesis H_b and H_{s+b} the ratio of likelihoods is a useful test statistic

$$\lambda(\vec{N}) = \frac{L(\vec{N} \mid H_{s+b})}{L(\vec{N} \mid H_b)}$$

- Intuitive picture:
 - If data is likely under H_b,
 L(N|H_b) is large,
 L(N|H_{s+b}) is smaller

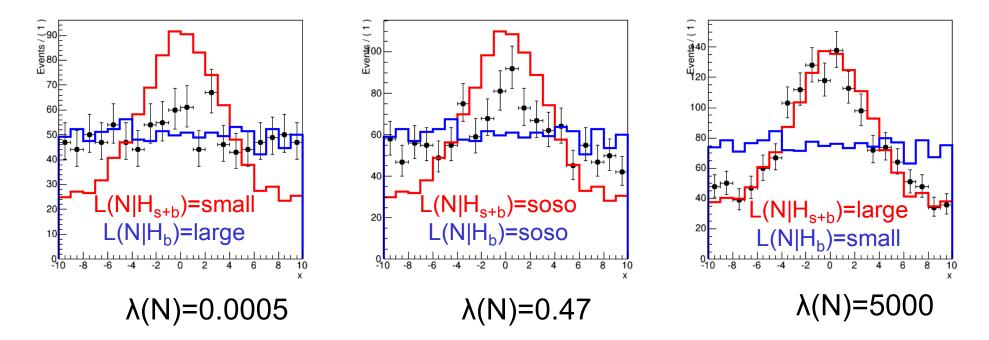
$$\lambda(\vec{N}) = \frac{\text{small}}{\text{large}} = \text{small}$$

□ If data is likely under H_{s+b}
 L(N|H_{s+b}) is large,
 L(N|H_b) is smaller

$$\lambda(\vec{N}) = \frac{\text{large}}{\text{small}} = \text{large}$$

Visualizing the Likelihood Ratio as ordering principle

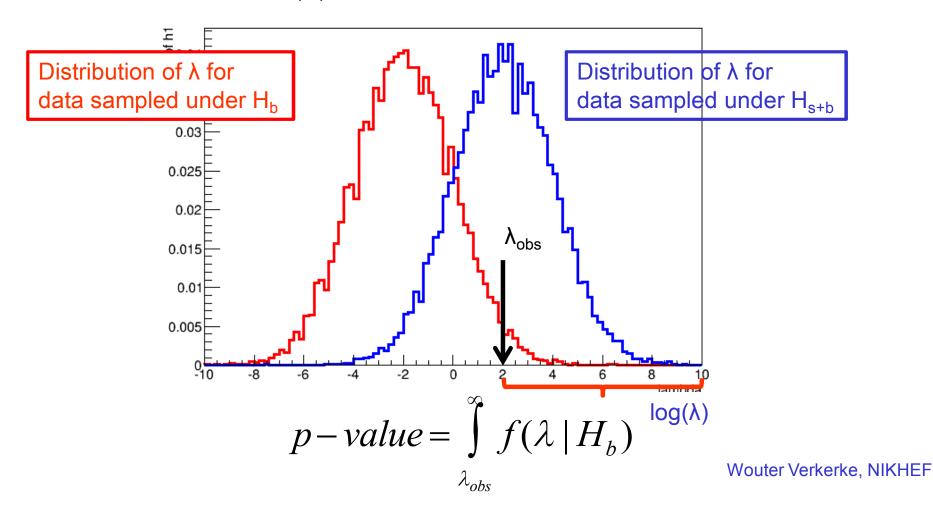
The Likelihood ratio as ordering principle



- Frequentist solution to 'relevance of P(data|theory') is to classify all observed data using a (Likelihood Ratio) test statistic
 - Probability to observe 'similar data or more extreme' then amounts to calculating 'probability to observe test statistic $\lambda(N)$ as large or larger than the observed test statistic $\lambda(N_{obs})$

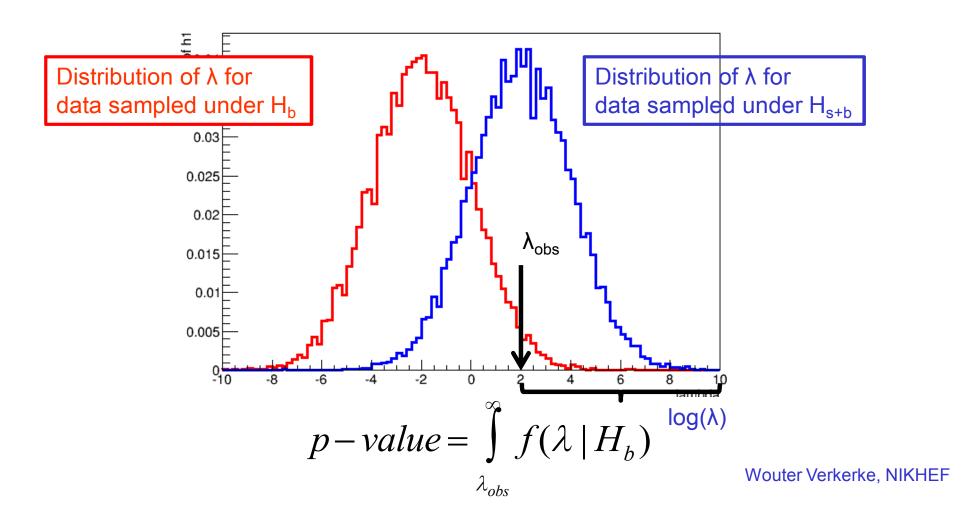
The distribution of the test statistic

- Distribution of a test statistic is generally not known
- Use toy MC approach to approximate distribution
 - Generate many toy datasets N under H_b and H_{s+b} and evaluate λ(N) for each dataset



The distribution of the test statistic

 Definition: p-value: probability to obtain the observed data, or more extreme in future repeated identical experiments (extremity define in the precise sense of the (LR) ordering rule)

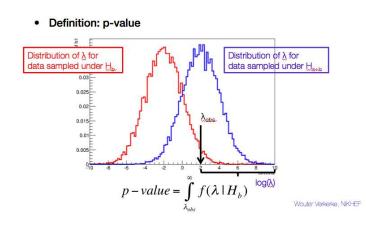


Likelihoods for distributions - summary

- Bayesian inference unchanged
 - simply insert L of distribution to calculate P(H|data)

$$P(H_{s+b} | \vec{N}) = \frac{L(\vec{N} | H_{s+b})P(H_{s+b})}{L(\vec{N} | H_{s+b})P(H_{s+b}) + L(\vec{N} | H_b)P(H_b)}$$

- Frequentist inference procedure modified
 - Pure P(data|hypo) not useful if data is a distribution
 - Order all possible data with a (LR) test statistic in 'extremity'
 - Quote p(data|hypo) as 'p-value' for hypothesis Probability to obtain observed data, or more extreme, is X%



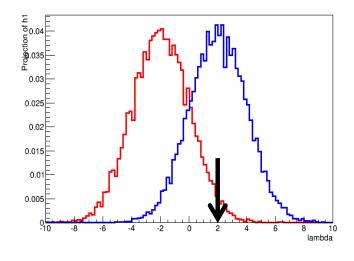
The likelihood principle

- Note that 'ordering procedure' introduced by test statistic also has a profound implication on procedure
- Bayesian inference only uses the Likelihood of the observed data

$$P(H_{s+b} | \vec{N}) = \frac{L(\vec{N} | H_{s+b})P(H_{s+b})}{L(\vec{N} | H_{s+b})P(H_{s+b}) + L(\vec{N} | H_b)P(H_b)}$$

 While the observed Likelihood Ratio also only uses likelihood of observed data.

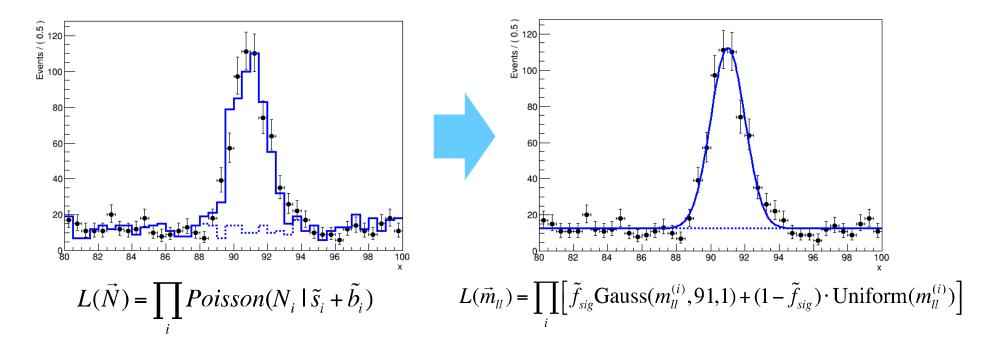
$$\lambda(\vec{N}) = \frac{L(\vec{N} \mid H_{s+b})}{L(\vec{N} \mid H_b)}$$



 Distribution f(λ|N), and thus p-value, also uses likelihood of nonobserved outcomes (in fact Likelihood of every possible outcome is used)

Generalizing to continuous distributions

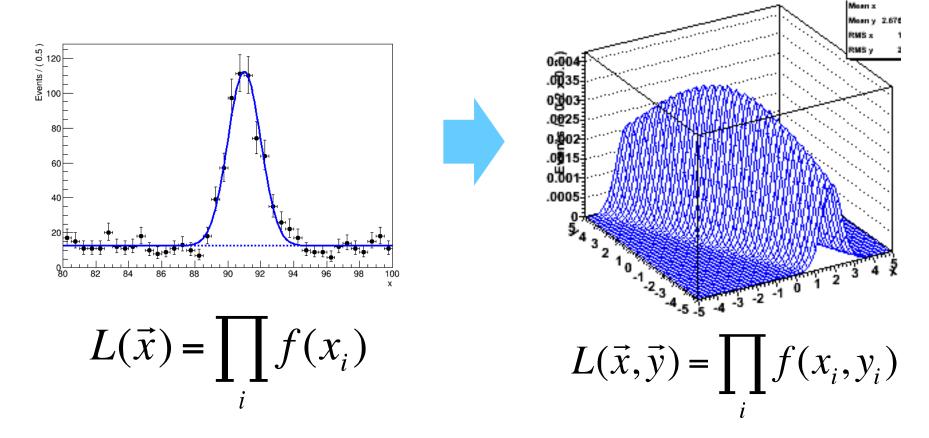
Can generalize likelihood to described continuous distributions



- Probability model becomes a probability density model
 - Integral of probability density model over full space of observable is always 1 (just like sum of bins of a probability model is always 1)
 - Integral of p.d.f. over a range of observable results in a probability
- Probability density models have (in principle) more analyzing power
 - But relies on your ability to formulate an analytical model wouter verkerker NIKHEF

Generalizing to multiple dimensions

Can also generalize likelihood models to distributions in multiple observables



 Neither generalization (binned[continuous, one[multiple observables) has any further consequences for Bayesian or Frequentist inference procedures

The Likelihood Ratio test statistic as tool for event selection

- Note that hypothesis testing with two simple hypotheses for observable distributions, exactly describes 'event selection' problem
- In fact we have already 'solved' the optimal event selection problem! Given two hypothesis H_{s+b} and H_b that predict an complex multivariate distribution of observables, you can always classify all events in terms of 'signal-likeness' (a.k.a 'extremity') with a likelihood ratio

$$\lambda(\vec{x},\vec{y},\vec{z},\ldots) = \frac{L(\vec{x},\vec{y},\vec{z},\ldots|H_{s+b})}{L(\vec{x},\vec{y},\vec{z},\ldots|H_b)}$$

$$p-value = \int_{\lambda_{obs}}^{\infty} f(\lambda|H_b)$$

Distribution of λ for data sampled under H_s .

 $p-value = \int_{\lambda_{obs}}^{\infty} f(\lambda|H_b)$

Wouter Verkerke

 So far we have exploited λ to calculate a frequentist p-value will now explore properties 'cut on λ' as basis of (optimal) event selection

"Likelihood" $L(\mathbf{x}|H_i)$ \mathbf{X}_{obs} MC Simulated All available **Events** "real data" (SIG Kg) Helps **Event** to define selection selection (cuts, NN, BDT) **Final Event Final Event** Selection (data) Selection (MC) Statistical Inference

HEP workflow versus statistical concepts

Note that the Likelihood is key to everything

"Likelihood Ratio"

$$\lambda(\mathbf{x}) \equiv \frac{L(\mathbf{x} | H_{s+b})}{L(\mathbf{x} | H_b)} > \alpha$$

"p-value from Likelihood Ratio test statistic"

$$p_0(\mathbf{x} \mid H_i) = \int_{\lambda_{obs}}^{\infty} f(\lambda \mid H_i)$$

$$P(H_{s+b} | \mathbf{x}) = \frac{L(\mathbf{x} | H_{s+b})P(H_{s+b})}{L(\mathbf{x} | H_{s+b})P(H_{s+b}) + L(\mathbf{x} | H_b)P(H_b)}$$

"Bayesian posterior probability"

Event selection

- The event selection problem:
 - Input: Two classes of events "signal" and "background"
 - Output: Two categories of events "selected" and "rejected"
- Goal: select as many signal events as possible, reject as many background events as possible
- Note that optimization goal as stated is ambiguous.
 - But can choose a well-defined by optimization goal by e.g. fixing desired background acceptance rate, and then choose procedure that has highest signal acceptance.
- Relates to "classical hypothesis testing"
 - Two competing hypothesis (traditionally named 'null' and 'alternate')
 - Here null = background, alternate = signal

Terminology of classical hypothesis testing

- Definition of terms
 - Rate of type-I error = α
 - Rate of type-II error = β
 - Power of test is 1-β

		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

- Treat hypotheses asymmetrically
 - Null hypo is usually special

 Fix rate of type-I error
 - Criminal convictions: Fix rate of unjust convictions
 - Higgs discovery: Fix rate of false discovery
 - Event selection: Fix rate of background that is accepted
- Now can define a well stated goal for optimal testing
 - Maximize the power of test (minimized rate of type-II error) for given α
 - Event selection: Maximize fraction of signal accepted

The Neyman-Pearson lemma

- In 1932-1938 Neyman and Pearson developed a theory in which one must consider competing hypotheses
 - Null hypothesis (H₀) = Background only
 - Alternate hypotheses (H_1) = e.g. Signal + Background

and proved that

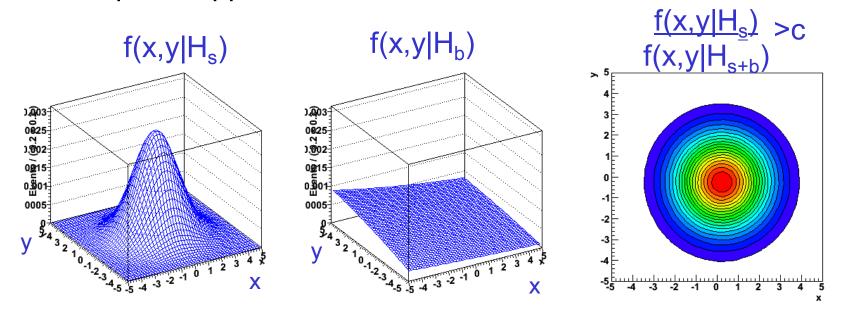
 The region W that minimizes the rate of the type-II error (not reporting true discovery) is a contour of the Likelihood Ratio

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

Any other region of the same size will have less power

The Neyman-Pearson lemma

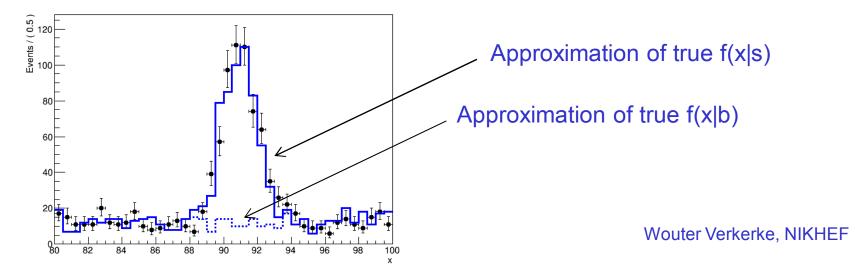
Example of application of NP-lemma with two observables



- Cut-off value c controls type-I error rate ('size' = bkg rate)
 Neyman-Pearson: LR cut gives best possible 'power' = signal eff.
- So why don't we always do this? (instead of training neural networks, boosted decision trees etc)

Why Neyman-Pearson doesn't always help

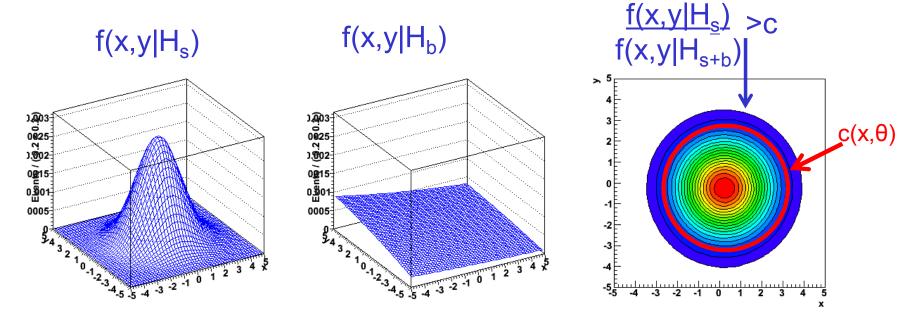
- The problem is that we usually don't have explicit formulae for the $p(f(\vec{x}|s), f(\vec{x}|b)$.
- Instead we may have Monte Carlo samples for signal and background processes
 - Difficult to reconstruct analytical distributions of pdfs from MC samples, especially if number of dimensions is large
- If physics problem has only few observables can still estimate estimate pdfs with histograms or kernel estimation,
 - But in such cases one can also forego event selection and go straight to hypothesis testing / paramater estimation with all events



Hypothesis testing with a large number of observables

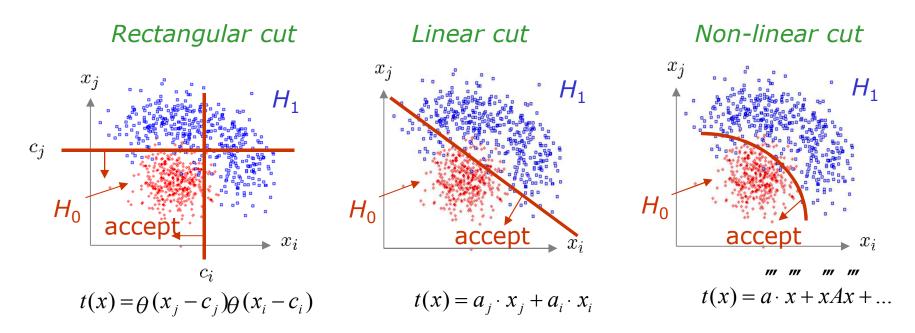
- When number of observables is large follow different strategy
- Instead of aiming at approximating p.d.f.s f(x|s) and f(x|b) aim to approximate decision boundary with an empirical parametric form

$$A_{\alpha}(\vec{x}) = \left[\frac{f(\vec{x} \mid s)}{f(\vec{x} \mid s + b)} > \alpha \right] \implies A_{\alpha}(\vec{x}) = c(\vec{x}, \vec{\theta})$$



Empirical parametric forms of decision boundaries

Can in principle choose any type of Ansatz parametric shape

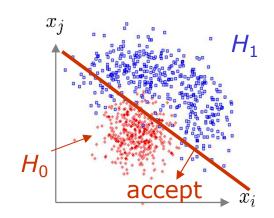


- Goal of Ansatz form is estimate of a 'signal probability' for every event in the observable space x (just like the LR)
- Choice of desired type-I error rate (selected background rate), can be set later by choosing appropriate cut on Ansatz test statistic.

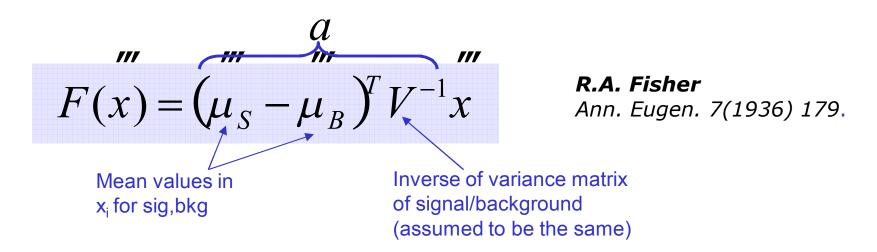
The simplest Ansatz – A linear disciminant

A linear discriminant constructs t(x)
 from a linear combination of the variables x_i

$$t(\vec{x}) = \sum_{i=1}^{N} a_i x_i = \vec{a} \cdot \vec{x}$$

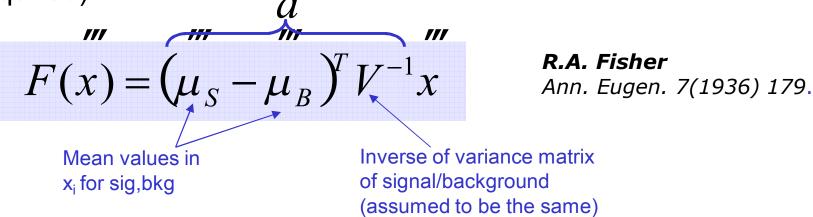


- A cut on t(x) results in a linear decision plane in x-space
- What is optimal choice of direction vector a?
- Solution provided by the Fisher The Fisher discriminant



The simplest Ansatz – A linear disciminant

 Operation advantage of Fisher discrimant is that test statistic parameters can be calculated (no iterative estimation is required)



 Fisher discriminant is optimal test statistic (i.e. maps to Neyman Pearson Likelihood Ratio) for case where both hypotheses are multivariate Gaussian distributions with the same variance, but diffferent means

$$f(x \mid s) = Gauss(\vec{x} - \vec{\mu}_s, V)$$

$$f(x \mid b) = Gauss(\vec{x} - \vec{\mu}_b, V)$$

Multivariate Gaussian distributions with **different means** but **same width** for signal and background

The simplest Ansatz – A linear disciminant

How the Fisher discriminant follows from the LR test statistic

$$-\log\left(\frac{f(x|s)}{f(x|b)}\right) = 0.5\left(\frac{x-\mu_s}{\sigma^2}\right)^2 - 0.5\left(\frac{x-\mu_b}{\sigma^2}\right)^2 + C$$

$$= 0.5\frac{x^2 - 2x\mu_s + \mu_s^2 - x^2 + 2x\mu_b - \mu_b^2}{\sigma^2} + C$$

$$= \frac{x(\mu_s - \mu_b)}{\sigma^2} + C'$$

Generalization for multidimensional Gaussian distributions

$$\log \lambda(x) = \frac{x(\mu_s - \mu_b)}{\sigma^2} + C' \xrightarrow{\sigma^2 \to V} \lambda(x) = \vec{x}(\vec{\mu}_s - \vec{\mu}_b)V^{-1} + C'$$

 Note that since we took -log of λ, F(x) is not signal probability, but we can trivially recover this

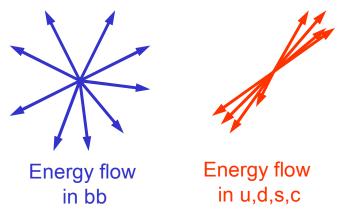
$$P_s(F) = \frac{1}{1 + e^{-F}}$$
 If $\lambda = 1$, x is equally likely under s,b Then F = $-\log(\lambda) = 0$ P = 50% Wouter Verkerke, NIKHEF

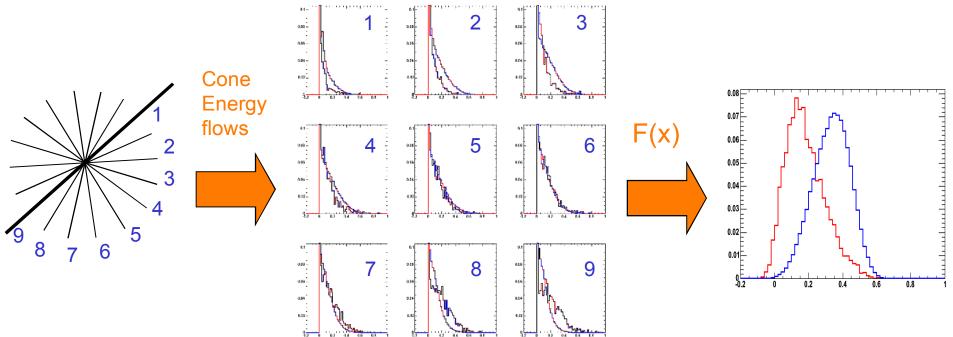
Example of Fisher discriminant use in HEP

- The "CLEO" Fisher discriminant
 - Goal: distinguish between _____
 e+e-

 Y4s

 bb and uu,dd,ss,cc
 - Method: Measure energy flow in 9 concentric cones around direction of B candidate





Non-linear test statistics

- In most real-life HEP applications signal and background are not multi-variate Gaussian distributions with different means
- Will need more complex Ansatz shapes than Fisher discriminant

 x_i

 H_0

- Loose ability analytically calculate parameters of Ansatz model from Likelihood Ratio test statistic (as was done for Fisher)
- Choose an Ansatz shapes with tunable parameters
 - Artificial Neural Networks
 - Decision Trees
 - Support Vector Machines
 - Rule Ensembles

Machine Learning – General Principles

• Given a Ansatz parametric test statistic $T(x|\theta)$, quantify 'risk' due 'loss of performance' due to misclassifications by T as follows

Loss function (~ log of Gaussian Likelihood)

$$R(\theta) = \int \left(T(\vec{x} \mid \theta) - 0\right)^2 f(\vec{x} \mid b) d\vec{x} + \int \left(T(\vec{x} \mid \theta) - 1\right)^2 f(\vec{x} \mid s) d\vec{x}$$
Risk function

Target value of T for background classification

Target value of T for signal classification

• Practical issue: since f(x|s,b) not analytically available, cannot evaluate risk function. Solution \square Substitute risk with 'empirical risk' which substitutes integral with Monte Carlo approximation

$$E(\theta) = \frac{1}{N_b} \sum_{D(x|b)} \left(T(\vec{x}_i \mid \theta) - 0 \right)^2 + \frac{1}{N_s} \sum_{D(x|s)} \left(T(\vec{x}_i \mid \theta) - 1 \right)^2$$
 Empirical Risk function
$$\begin{array}{c} x_i \text{ is a set of points} \\ \text{sampled from f(x|b)} \end{array}$$
 sampled from f(x|s)

Machine Learning – General Principles

- Minimization of empirical risk E(θ) can be performed with numerical methods (many tools are available, e.g. TMVA)
- But approximation of empirical risk w.r.t analytical risk introduces possibility for 'overtraining':

If MC samples for signal and background are small, and number of parameters θ, one can always reduce empirical risk to zero ('perfect selection')

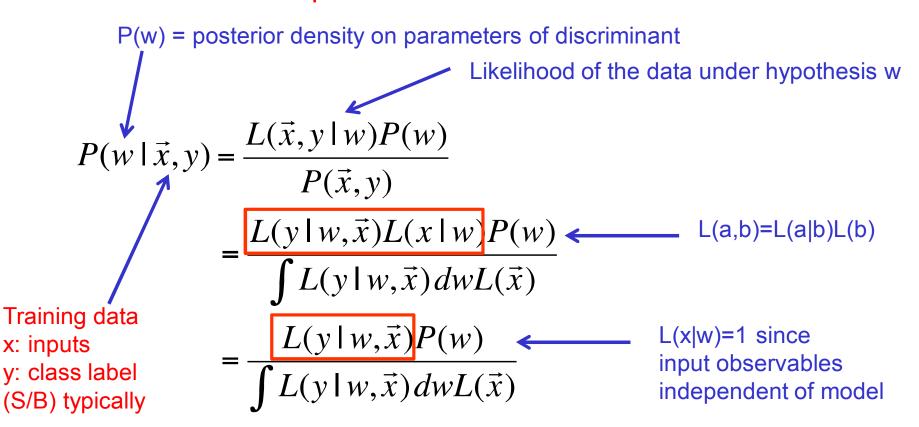
(Conceptually similar to χ^2 fit: if you fit a 10^{th} order polynomial to 10 points – you will always perfectly describe the data. You will however not perfectly describe an independent dataset sampled from the same parent distribution)

- Even if empirical risk is not reduced to zero by training, it may still be smaller than true risk

 Control effect by evaluating empirical risk also on independent validation sample during minimization.
 - If ER on samples start to diverge, stop minimization

Bayesian Learning – General principles

- Can also applied Bayesian methodology to learning process of decision boundaries
- Given a dataset D(x,y) and a Ansatz model with parameters w, aim is to estimate parameters w



Bayesian Learning – General principles

- Inserting a binomial likelihood function to model classification the classification problem
- The parameters w are thus estimated from the Bayesian posteriors densities

$$L(y | x, w) = \prod_{i} T(x_{i}, w)^{y} [1 - T(x_{i}, w)]^{1-y}$$

$$P(w \mid \vec{x}, y) = \frac{L(y \mid w, \vec{x})P(w)}{\int L(y \mid w, \vec{x}) dw L(\vec{x})}$$

- No iterative minimization, but Note that integrals over 'w-space' can usually only be performed numerically and if w contains many parameters, this is computationally challenging
- If class of function T(x,w) is large enough it will contain a function T(x,w*) that represents the true minimum in E(w)
 - I.e. T(x,w*) is the Bayesian equivalent of Frequentist TS that is NP L ratio

- In that case the test statistic is
$$L(y|x,w) = \prod_{i} T(x_i,w)^y [1-T(x_i,w)]^{1-y}$$

$$T(x,w^*) = \int_{i} yL(y|x)dy$$

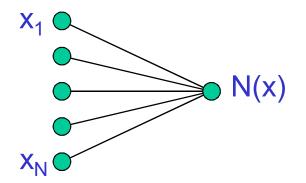
$$= L(y=1|x) = \frac{L(x|y=1)P(y=1)}{L(x|y=0)P(y=0) + L(x|y=1)P(y=1)}$$

Machine/Bayesian learning – Non-linear Ansatz functions

 Artificial Neural Network is one of the most popular non-linear ansatz forms. In it simplest incarnation the classifier function is

$$N(x) = s \left(a_0 + \sum_i a_i x_i\right)$$
 s(t) is the activation function, usually a logistic sigmoid
$$S(t) = \frac{1}{1 + e^{-t}}$$

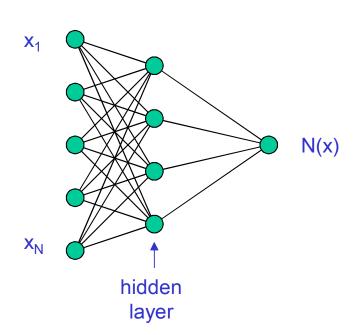
- This formula corresponds to the 'single layer perceptron'
 - Visualization of single layer network topology



Since the activation function s(t) is monotonic, a single layer N(x) is equivalent to the Fisher discriminant F(x)

Neural networks – general structure

 The single layer model and easily be generalized to a multilayer perceptron

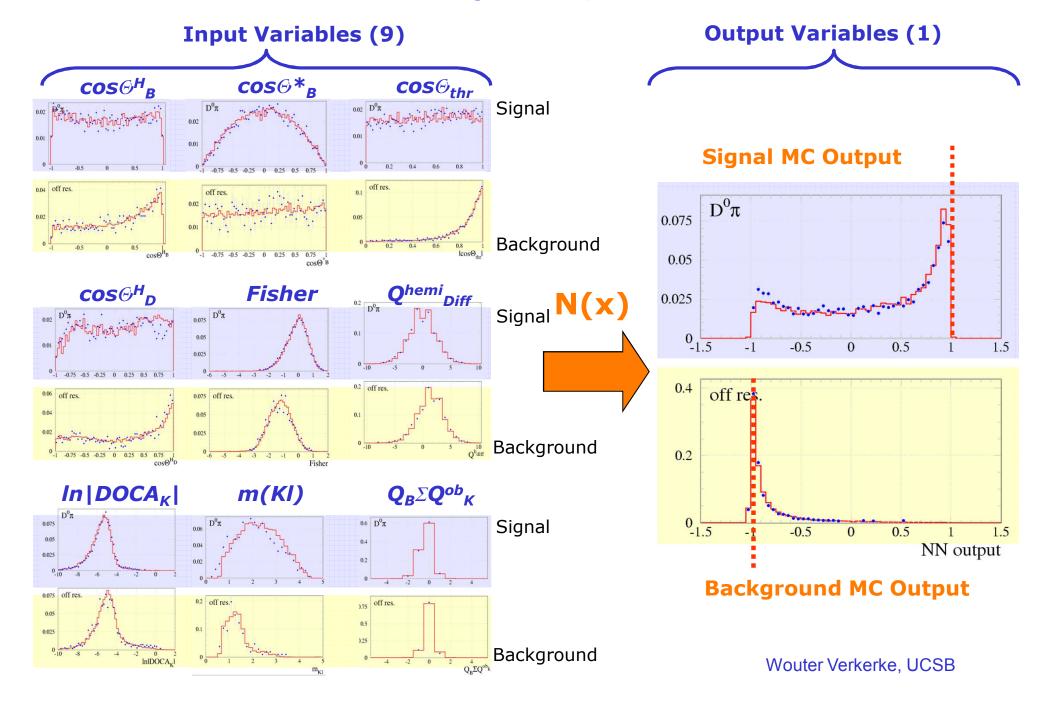


$$N(x) = s(a_0 + \sum_{i=1, m}^{m} a_i h_i(x))$$
with $h_i(x) = s(w_{i0} + \sum_{j=1}^{n} w_{ij} x_j)$

with a_i and w_{ij} weights (connection strengths)

- Easy to generalize to arbitrary number of layers
- Feed-forward net: values of a node depend only on earlier layers (usually only on preceding layer) 'the network architecture'
- More nodes bring N(x) allow it to be closer to optimal (Neyman Pearson / Bayesian posterior) but with much more parameters to be determined

Neural networks – training example



Practical aspects of machine learning

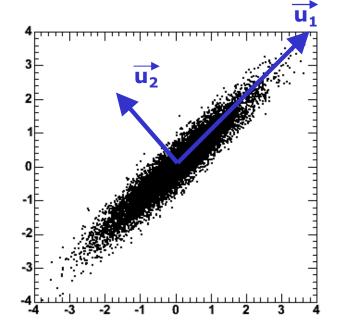
- Choose input variables sensibly
 - Don't include badly understood observables (such as #tracks/evt), variables that are not expected carry useful information
 - Generally: "Garbage in = Garbage out"
- Traditional Machine learning provides no guidance of useful complexity of test statistic (e.g. NN topology, layers)
 - Usually better to start simple and gradually increase complexity and see how that pays off
- Bayesian learning can (in principle) provide guidance on model complexity through Bayesian model selection
 - Bayes factors automatically includes a penalty for including too much model structure.

$$K = \frac{P(D \mid H_1)}{P(D \mid H_2)} = \frac{\int L(D \mid \theta_1, H_1) P(\theta_2 \mid H_1) d\theta_2}{\int L(D \mid \theta_2, H_2) P(\theta_2 \mid H_2) d\theta_2}$$

 But availability of Bayesian model selection depends in practice on the software that you use.

Practical aspects of machine learning

- Don't make the learning problem unnecessarily difficult for the machine
- E.g. remove strong correlation with explicit decorrelation before learning step
 - Can use Principle Component Analysis
 - Or Cholesky decomposition (rotate with square-root of covariance matrix)



- Also: remember that for 2-class problem (sig/bkg) that each have multivariate Gaussian distributions with different means, the optimal discriminant is can be calculated analytically
 - Fisher discriminant is analytical solution. NN solution reduces to single-layer perceptron
- Thus, you can help your machine by transforming your inputs in a form as close as possible to the Gaussian form by transforming your input observables

Gaussianization of input observables

- You can transform any distribution in a Gaussian distribution in two steps
- 1 Probability integral transform

$$y(x) = \int_{-\infty}^{x} f(x'|H)dx'$$

"...seems likely to be one of the most fruitful conceptions introduced into statistical theory in the last few years" -Egon Pearson (1938)

turns any distribution f(x) into a flat distribution in y(x)

• 2 – Inverse error function

$$x^{\text{Gauss}} = \sqrt{2} \cdot \text{erf}^{-1} \left(2x^{\text{flat}} - 1 \right) \qquad \text{erf} \left(x \right) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^{2}} dt$$

turns flat distribution into a Gaussian distribution

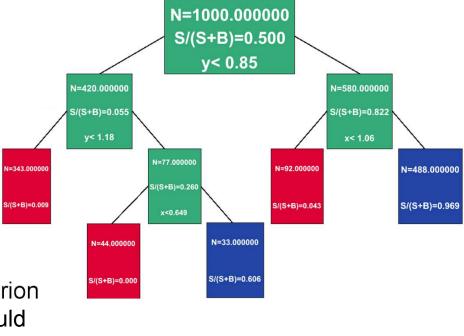
 Note that you can make either signal or background Gaussian, but usually not both

A very different type of Ansatz - Decision Trees

- A Decision Tree encodes sequential rectangular cuts
 - But with a lot of underlying theory on training and optimization
 - Machine-learning technique, widely used in social sciences
 - L. Breiman et al., "Classification and Regression Trees" (1984)

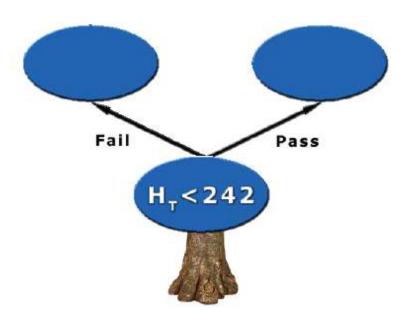
Basic principle

- Extend cut-based selection
- Try not to rule out events failing a particular criterion
- Keep events rejected by one criterion and see whether other criteria could help classify them properly



Building a tree – splitting the data

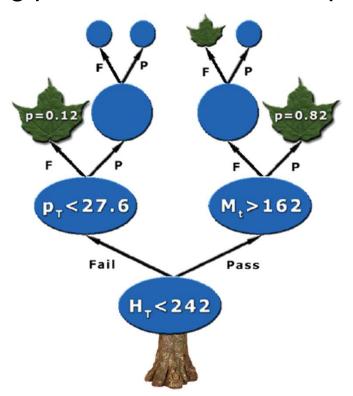
 Essential operation : splitting the data in 2 groups using a single cut, e.g. H_T<242



- Goal: find 'best cut' as quantified through best separation of signal and background (requires some metric to quantify this)
- Procedure:
 - 1) Find cut value with best separation for each observable
 - 2) Apply only cut on observable that results in best separation

Building a tree – recursive splitting

Repeat splitting procedure on sub-samples of previous split



- Output of decision tree:
 - 'signal' or 'background' (0/1) or
 - probability based on expected purity of leaf (s/s+b)

Parameters in the construction of a decision tree

- Normalization of signal and background before training
 - Usually same total weight for signal and background events
- In the selection of splits
 - list of questions (var_i < cut_i) to consider
 - Separation metric (quantifies how good the split is)
- Decision to stop splitting (declare a node terminal)
 - Minimum leaf size (e.g. 100 events)
 - Insufficient improvement from splitting
 - Perfect classification (all events in leaf belong to same class)
- Assignment of terminal node to a class
 - Usually: purity>0.5 = signal, purity<0.5 = background

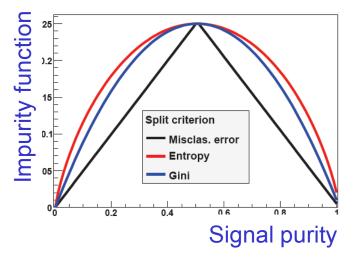
Machine learning with Decision Trees

Instead of 'Empirical Risk' minimize 'Impurity Function' of leaves

Impurity function i(t) quantifies (im)purity of a sample, but is not uniquely

defined

Simplest option: i(t) = misclassification rate



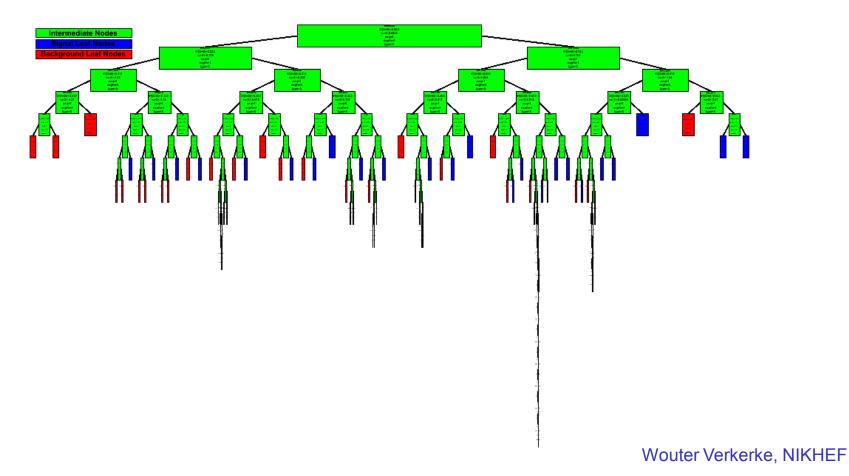
• For a proposed split s on a node t, decrease of impurity is $\Delta i(s,t) = i(t) - p_L \cdot i(t_L) - p_R \cdot i(t_R)$

Impurity Impurity Impurity of sample of 'left' of 'right' before split sample

Take split that results in largest Δi

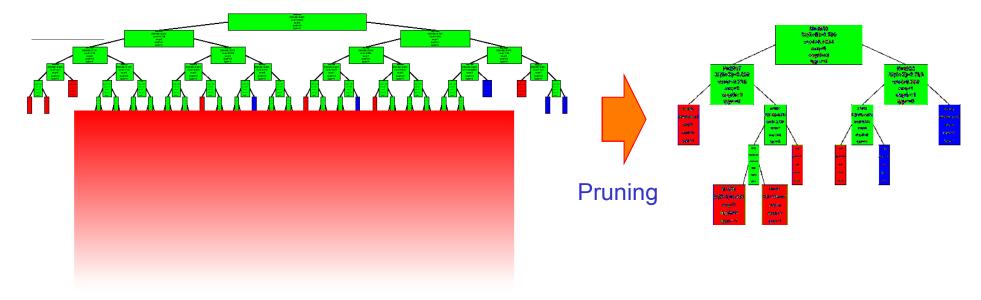
Machine learning with Decision Trees

- Stop splitting when
 - not enough improvement (introduce a cutoff Δi)
 - not enough statistics in sample, or node is pure (signal or background)
- Example decision tree from learning process



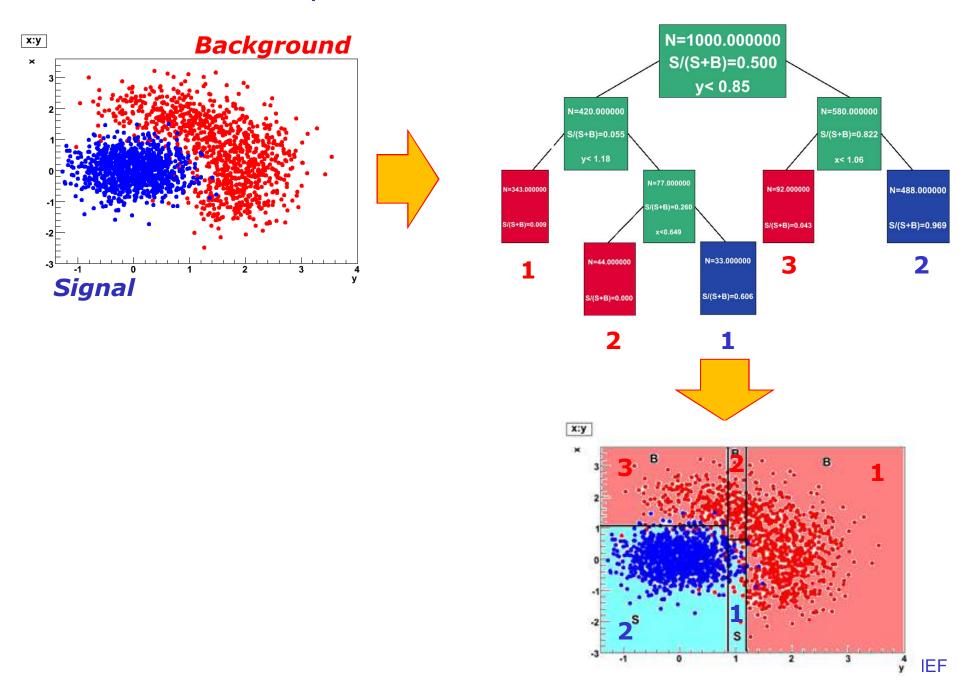
Machine learning with Decision Trees

 Given that analytical pdfs f(x|s) and f(x|b) are usually not available, splitting decisions are based on 'empirical impurity' rather than true 'impurity' | risk of overtraining exists



- Can mitigate effects of overtraining by 'pruning' tree a posteriori
 - Expected error pruning (prune weak splits that are consistent with original leaf within statistical error of training sample)
 - Cost/Complexity pruning (generally strategy to trade tree complexity against performance)

Concrete example of a trained Decision Tree



Boosted Decision trees

- Decision trees largely used with 'boosting strategy'
- Boosting = strategy to combine multiple weaker classifiers into a single strong classifier
- First provable boosting algorithm by Schapire (1990)
 - Train classifier T1 on N events
 - Train T2 on new N-sample,
 half of which misclassified by T1
 - Build T3 on events where T1 and T2 disagree
 - Boosted classifier: MajorityVote(*T1*, *T2*, *T3*)
- Most used: AdaBoost = Adaptive Boosting (Freund & Shapire '96)
 - Learning procedure adjusts to training data to classify it better
 - Many variations on the same theme for actual implementation

AdaBoost

- Schematic view of iterative algorithm
 - Train Decision Tree on (weighted) signal and background training samples
 - Calculate misclassification rate for Tree K (initial tree has k=1)

$$\epsilon_k = \frac{\sum_{i=1}^N w_i^k \times \text{isMisclassified}_k(i)}{\sum_{i=1}^N w_i^k}$$
 "Weighted average of isMisclassified over all training events"

- Calculate weight of tree K in 'forest decision' $lpha_k=eta imes \ln((1-\epsilon_k)/\epsilon_k)$
- Increase weight of misclassified events in Sample(k) to create Sample(k+1)

$$w_i^k \to w_i^{k+1} = w_i^k \times e^{\alpha_k}$$

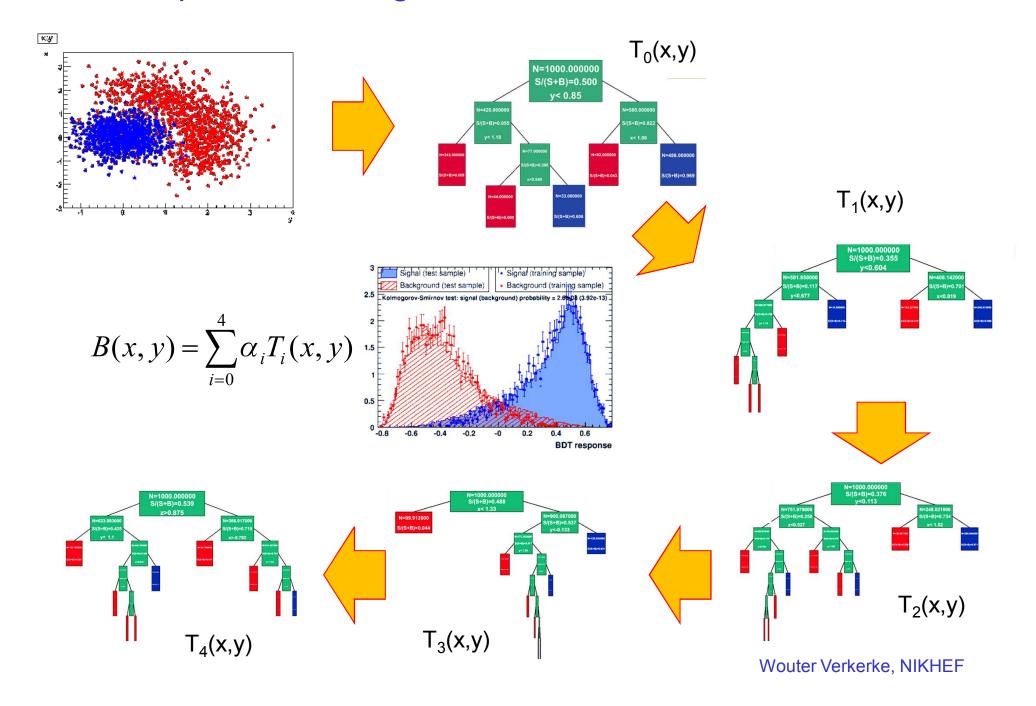
Boosted classifier is result is performance-weighted 'forest'

$$T(i) = \sum_{k=1}^{N_{\text{tree}}} \alpha_k T_k(i)$$
 "Weighted average of Trees by their performance"

AdaBoost by example

- So-so classifier (Error rate = 40%) $\alpha = \ln \frac{1-0.4}{0.4} = 0.4$
 - Misclassified events get their weight multiplied by exp(0.4)=1.5
 - Next tree will have to work a bit harder on these events
- Good classifier (Error rate = 5%) $\alpha = \ln \frac{1-0.05}{0.05} = 2.9$
 - Misclassified events get their weight multiplied by exp(2.9)=19 (!!)
 - Being failed by a good classifier means a big penalty: must be a difficult case
 - Next tree will have to pay much more attention to this event and try to get it right
- Note that boosting usually results in (strong) overtraining
 - Since with misclassification rate will ultimately go to zero

Example of Boosting



"Likelihood" $L(\mathbf{x}|H_i)$ \mathbf{X}_{obs} MC Simulated All available **Events** "real data" (SIG Kg) Helps **Event** to define selection selection (cuts, NN, BDT) **Final Event Final Event** Selection (data) Selection (MC) **Statistical** · Data Inference

HEP workflow versus statistical concepts

"Likelihood Ratio"

$$\lambda(\mathbf{x}) \equiv \frac{L(\mathbf{x} | H_{s+b})}{L(\mathbf{x} | H_b)} > \alpha$$

Or approximation of optimal test statistic with a parametric form from machine learning

Remaining question:
What value of α represents 'optimal cut'?

"Likelihood" $L(\mathbf{x}|H_i)$ \mathbf{X}_{obs} MC Simulated All available **Events** "real data" (SIG Kg) Helps **Event** to define selection selection (cuts, NN, BDT) Final Event **Final Event** Selection (data) Selection (MC) **Statistical** · Data Inference

Choosing the optimal cut on the test statistic

Note that in the limit of an optimal test statistic, and when subsequent using LR hypothesis test, the cut on α has <u>no influence</u> on the statistical inference!

 Purely operational decision (ntuple-sizes etc...)

"Likelihood Ratio"

$$\lambda(\mathbf{x}) \equiv \frac{L(\mathbf{x} | H_{s+b})}{L(\mathbf{x} | H_b)} > \alpha$$

"p-value from Likeliho od Ratio test statistic"

$$p_0(\mathbf{x} \mid H_i) = \int_{\lambda_{obs}}^{\infty} f(\lambda \mid H_i)$$

Choosing the optimal cut on the test statistic

- But reality is usually more complex:
 - Test statistics are usually not optimal,
 - Ingredients to test statistics, i.e. the event selection, are usually not perfectly known (systematic uncertainties)
- In the subsequent statistical test phase we can account for (systematic) uncertainties in signal and background models in a detailed way. In the event selection phase we cannot
- Pragmatically considerations in design of event selection criteria
 - Ability to estimate level of background from the selected data
 - Small sensitivity of signal acceptance to selection criteria used
- Result is that Likelihood Ratio used for event selection and final hypothesis test are different (λ_{selection} ≠ λ_{hypotest})
 □ Cut on λ_{selection} will influence statistical test with λ_{hypotest}
- To be able decide on optimal cut on $\lambda_{\text{selection}}$ you need a figure merit that approximates behavior of statistical test using $\lambda_{\text{hypotest}}$ Wouter Verkerke, NIKHEF

Traditional approximate Figures of Merit

Traditional choices for Figure of Merit

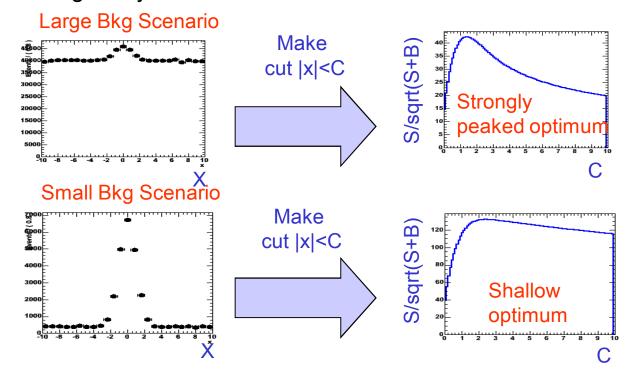
$$F(\alpha) = \frac{S(\alpha)}{\sqrt{B(\alpha)}}$$

$$F(\alpha) = \frac{S(\alpha)}{\sqrt{S(\alpha) + B(\alpha)}}$$
'discovery'
'measurement'

Note that position of optimum depends on

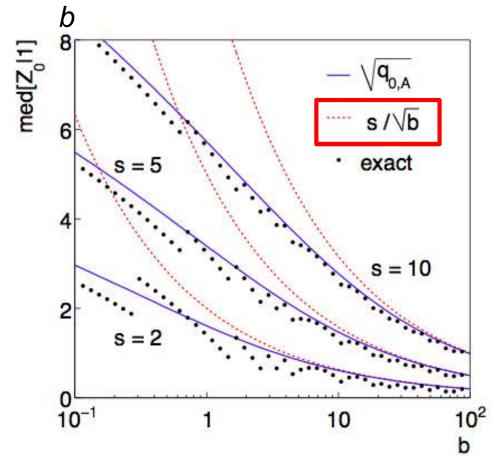
a priori knowledge of signal cross section

 Note: these FOMs quantify best signal significance for a counting experiment with an known level of background, and not e.g. 'strongest upper limit',no accounting for systematic uncertainties



Validity of approximations in Figures of Merit

- Note that approximations made in 'traditional' figure of merit are not always good.
- E.g. for 'discovery FOM' s/ \sqrt{b} illustration of approximation for s=2,5,10 and b in range [0.01-100] shows significant deviations of s/ \sqrt{b} from actual significance at low



Improved discovery F.O.M ("Asimov Z") suggested for situations where s<
b is not true

$$\sqrt{q_{0,\mathrm{A}}} = \sqrt{2\left((s+b)\ln(1+s/b)-s\right)} \; .$$

$$= \frac{s}{\sqrt{b}}\left(1+\mathcal{O}(s/b)\right) \; .$$

Final comments on event selection

- Main issue with event selection is usually, sensitivity of selection criteria to systematic uncertainties
- What you'd like to avoid is your BDT/NN that is trained to get a small statistical uncertainty has a large sensitivity to a systematic uncertainties
- No easy way to incorporate effect of systematic uncertainties in training process
 - Can insert some knowledge of systematic uncertainties included in figure of merit when deciding where to cut in BDT/NN, but proper calculation usually requires much more information that signal and background event counts and is time consuming
- Use your physics intuition...

Roadmap for this course

Tomorrow we with start with hypothesis with parameters

