

Teilchenphysik II - W, Z, Higgs am Collider

Lecture 08: Statistical Analysis

PD Dr. K. Rabbertz, **Dr. Nils Faltermann** | 16. Juni 2023

Statistics and Particle Physics

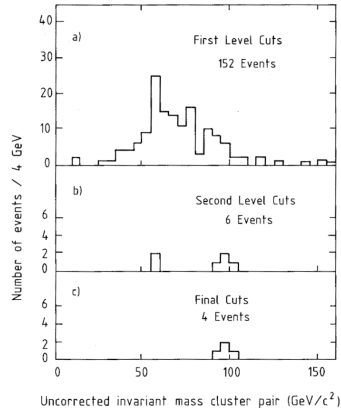
Experiment

- All measurements are derived from **counting experiments**
- **Millions of billions** of particle collision events each year
- Each event **independent** from and (to many extents) identical to all others

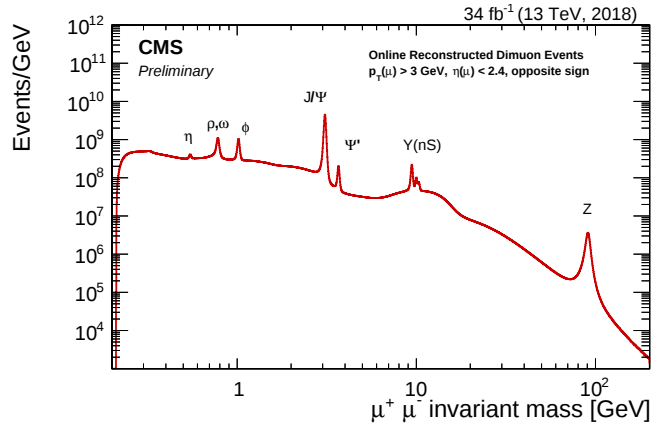
Theory

- Nature intrinsically stochastic
- QM wave functions interpreted as **probability density functions**
- Event-by-event simulation using **Monte Carlo** methods

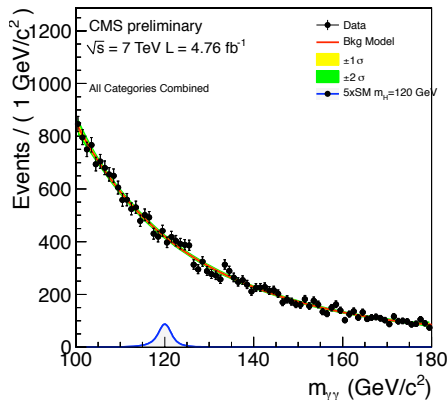
Particle physics experiments perfect application of statistics



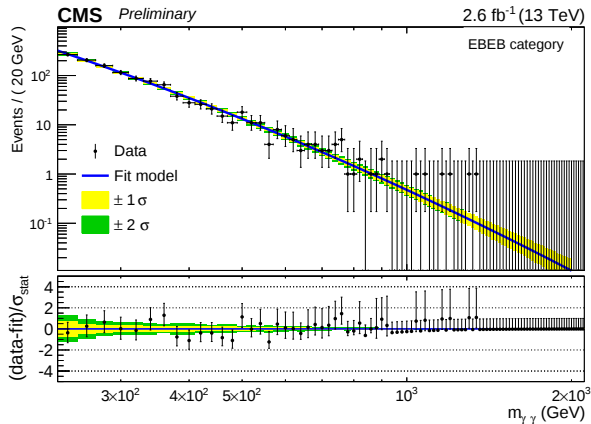
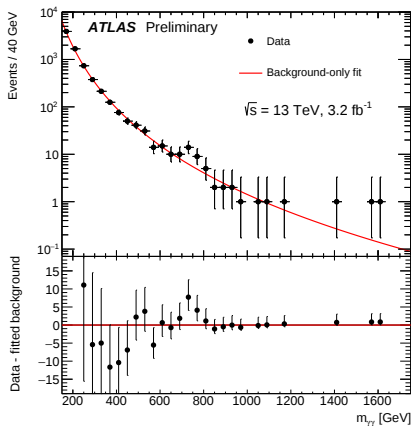
Historically: trust your instincts



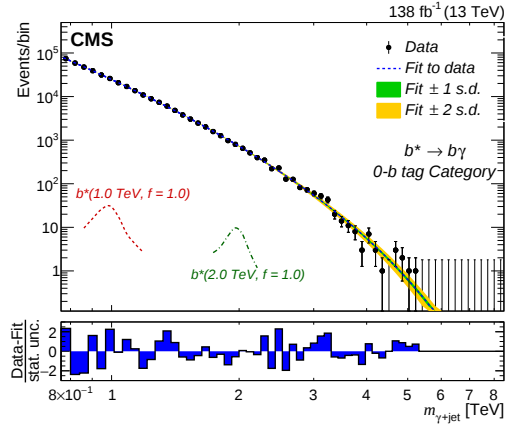
Sometimes unambiguous, clearly there is something!



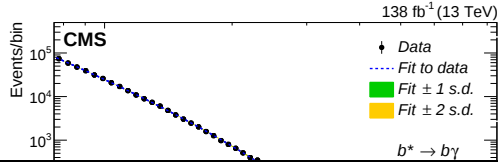
But most of the time not: is there a signal?



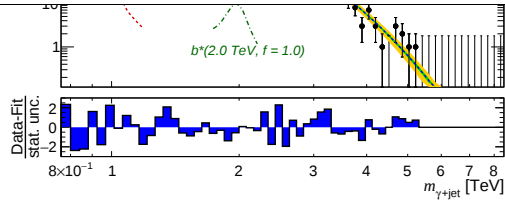
And here at around 750 GeV?
(with more subsequent data: turned out to be nothing)



And what do you do if you don't see anything: just a waste of time?



Particle physics experiments require application of statistical methods

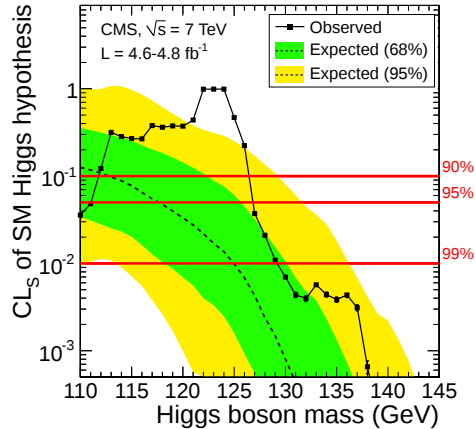


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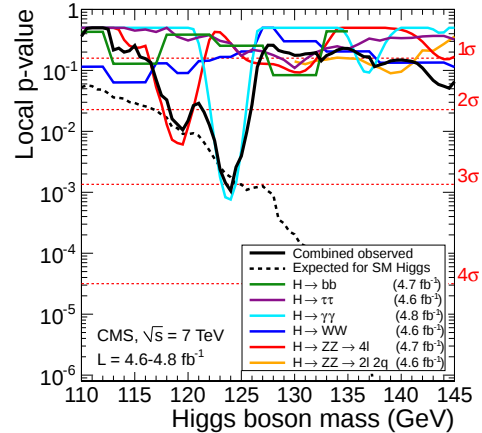
- Statistics is a vast field!
- Here: focus on concepts and techniques needed to **understand experimental particle physics results**
- Questions we will discuss
 - How to interpret the data: are they compatible with my expectation (model)?
 - How do uncertainties enter the game?
 - Can we distinguish between different models?
 - If we don't see any signal, can we still use the data to make statements about the searched-for process?
- Much more details in lecture **Moderne Methoden der Datenanalyse** (summer term)

Outline

- Goal: we want to understand these plots



Phys.Lett. B710 (2012) 26–48

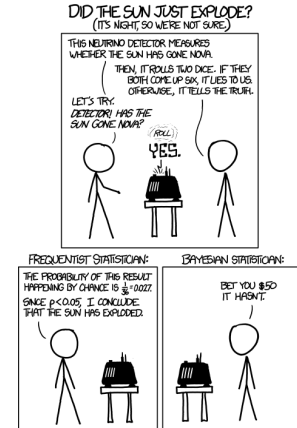


Bayesian and Frequentist Approaches

- Two major approaches in statistical analysis:
 - **Frequentist**: probability purely based on observation, objective
 - **Bayesian**: usage of earlier knowledge (prior), subjective
- Will focus on frequentist approach (but for most concepts Bayesian equivalent, see the literature!)

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<https://xkcd.com/1132/>

Important Probability Density Functions

- Statistical processes underlying the data are assumed to follow a **probability density function (pdf)** $\mathcal{P}$

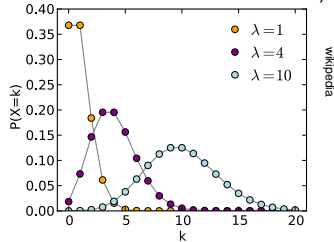
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Poisson:

$$\mathcal{P}(x; \lambda) = \frac{\lambda^x}{x!} e^{-\lambda}$$

e. g. counting experiments
(like cross-section measurements)



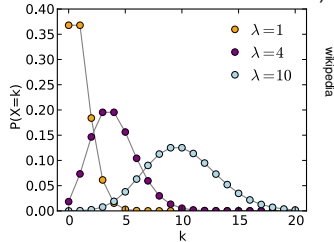
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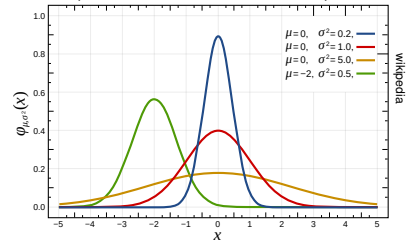
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Gaussian:

$$\mathcal{P}(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2}$$

e. g. parameter estimates
(like mass measurements)



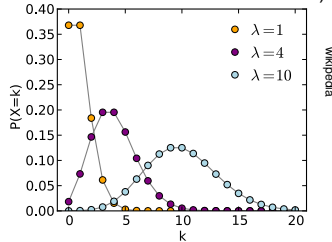
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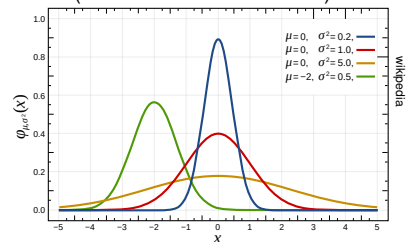
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NB: both are in fact limits of the Binomial distribution for a large number of tries

Likelihood

- The likelihood $\mathcal{L}(n_{\text{obs}}; k) = \prod_i \mathcal{P}(n_{\text{obs},i}; k)$ quantifies

compatibility of the observed data with a given model

- i : independent counting experiments, e. g. bins of a histogram
- $n_{\text{obs}} = \{n_{\text{obs},i}\}$: number of observed events in i , distributed as $\mathcal{P}$
- $k = \{k_j\}$: model parameters in $\mathcal{P}$

→ **function of model parameters and observed data**

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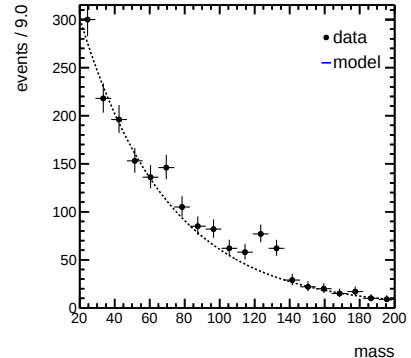
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- Example

- Data: observed events in 20 bins
- Model: known SM process (background)



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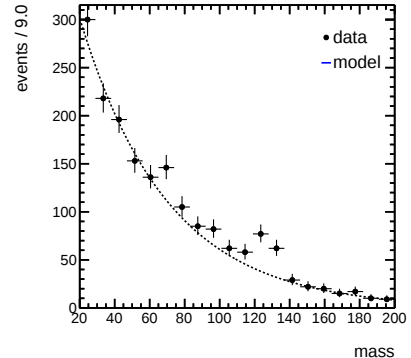
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$$\mathcal{L}(n_{\text{obs}}; b) = \prod_i \text{Poisson}(n_{\text{obs},i}, b)$$



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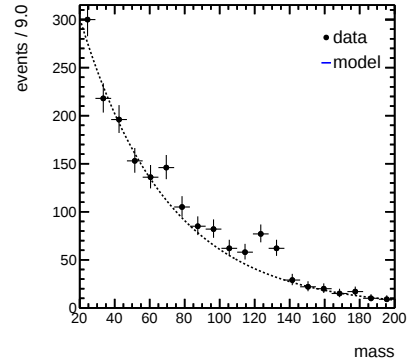
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$$\mathcal{L}(n_{\text{obs}}; b) = \prod_i \frac{(n_{\text{pred},i})^{n_{\text{obs},i}}}{n_{\text{obs},i}!} e^{-n_{\text{pred},i}}$$

$$n_{\text{pred},i}(b) = \underbrace{b \cdot e^{-\alpha x_i}}_{\text{background}}$$



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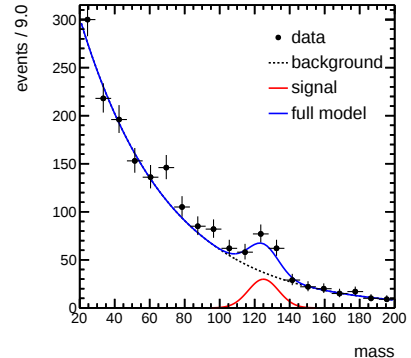
→ function of model parameters and observed data

- Example

- Data: observed events in 20 bins
- Model: known SM process (background) + signal

$$\mathcal{L}(n_{\text{obs}}; b, s) = \prod_i \frac{(n_{\text{pred},i})^{n_{\text{obs},i}}}{n_{\text{obs},i}!} e^{-n_{\text{pred},i}}$$

$$n_{\text{pred},i}(b, s) = \underbrace{b \cdot e^{-\alpha x_i}}_{\text{background}} + \underbrace{s \cdot e^{-(m-x_i)^2}}_{\text{signal}}$$

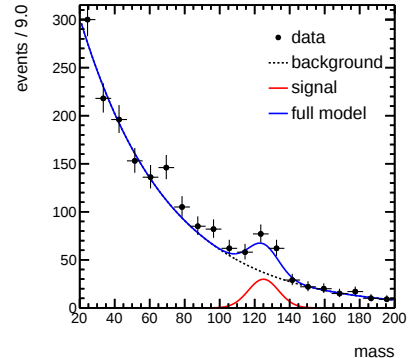


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- **function of model parameters and observed data**
- $\mathcal{L}$ is **not the probability** of a model!
 - Also not the probability of observing the data given the model
- $\mathcal{L}$ is the product of pdfs of the model, used to quantify the compatibility of the data with the model



Parameter Estimation

- Which parameter values of a given model describe best the data?

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Which parameter values lead to the maximum of $\mathcal{L}$?

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- Technically: **minimisation of negative log-likelihood**

$$\text{NLL}(n_{\text{obs}}, k) = -2 \ln \mathcal{L}$$

- Logarithm is monotonic: retains minimum
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- Logarithm is monotonic: retains minimum
- Turns product of pdfs into sum: easier to minimise
- Arbitrarily complex problem, vast amount of techniques and literature
 - e. g. ATLAS+CMS Higgs couplings combination: ≈ 4250 parameters
 - e. g. CMS tracker-alignment problem: $\mathcal{O}(10^6)$ parameters

Maximum-Likelihood Method

- Example: which *signal-strength modifier* μ describes best the data?

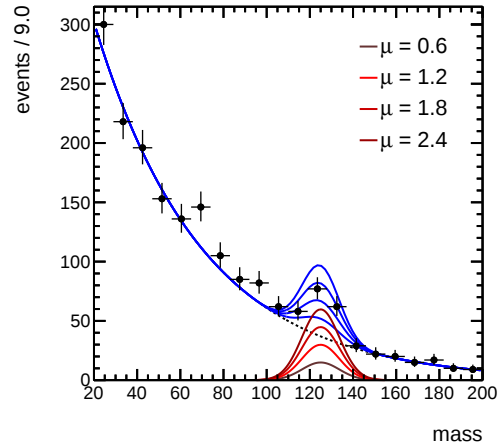
- Common in analyses at the LHC:

$$\mu = (\sigma \cdot \mathcal{B}) / (\sigma_{\text{SM}} \cdot \mathcal{B}_{\text{SM}})$$

$$n_{\text{pred},i}(\mu) = \underbrace{b \cdot e^{-\alpha x_i}}_{\text{background}} + \underbrace{\mu \cdot s_{\text{SM}} \cdot e^{-(m-x_i)^2}}_{\text{signal}}$$

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→ $\hat{\mu}$: maximises $\mathcal{L}(n_{\text{obs}}; \mu)$



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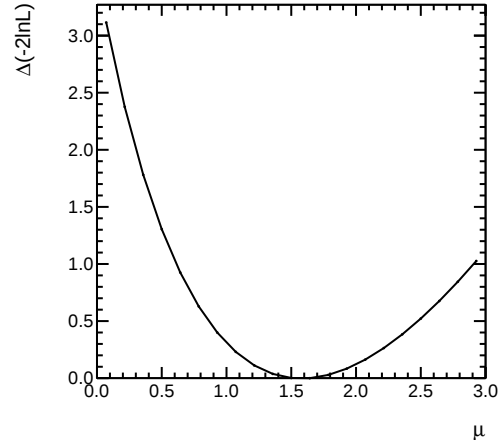
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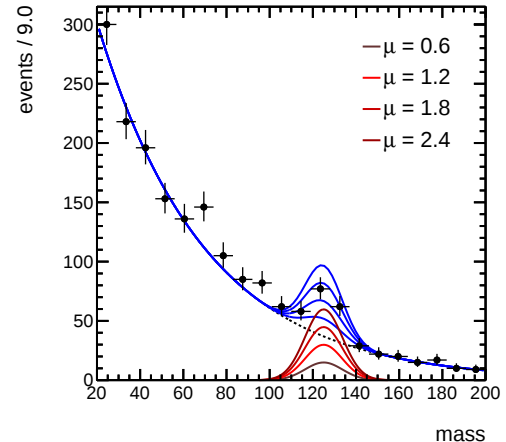
Note: we are usually not interested in the value of $\mathcal{L}$,
only in the difference (Δ) w.r.t. the minimum



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- Important case: **Gaussian distributed measurements**
 - e. g. approximation of Poisson for large number of events (in practice > 10)
- NLL becomes

$$-2 \ln \mathcal{L} = \sum_i \frac{(n_{\text{obs},i} - n_{\text{pred},i})^2}{n_{\text{pred},i}} + \text{const}$$



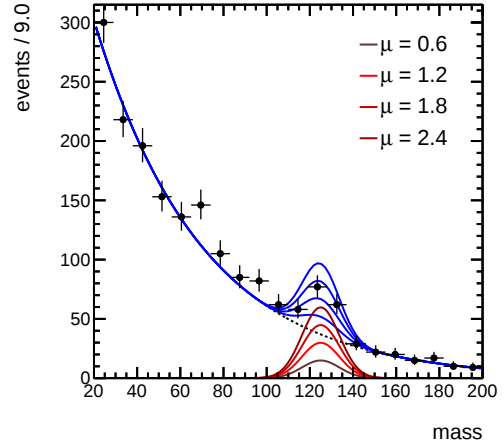
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$$\chi^2 \equiv \sum_i \frac{(n_{\text{obs},i} - n_{\text{pred},i})^2}{n_{\text{pred},i}}$$



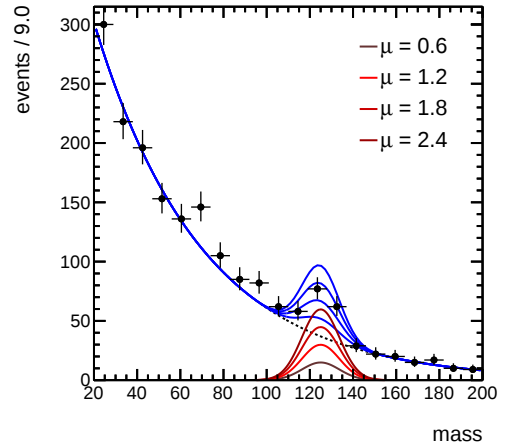
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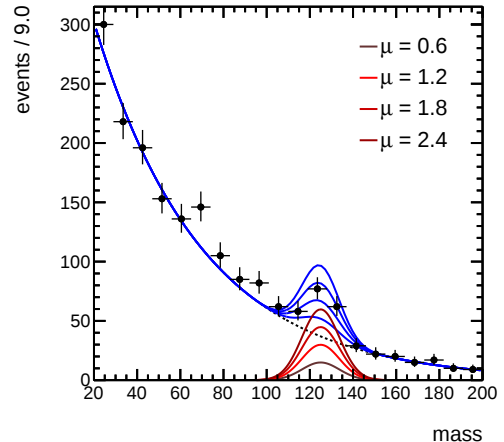
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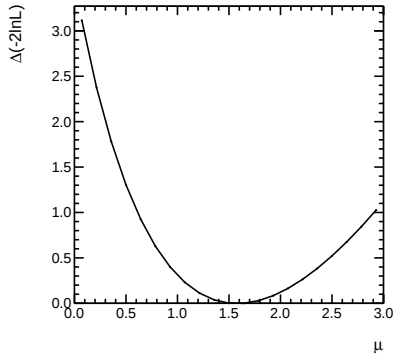
ML estimator is function of the observed data



Maximum-Likelihood Method

- Uncertainty on $\hat{\mu}$ from scan of $\text{NLL} = -2 \ln \mathcal{L}$ around minimum
- **Uncertainty due to fluctuations of data:** “statistical uncertainty”
- For Gaussian pdfs: parabola, standard deviation σ follows from

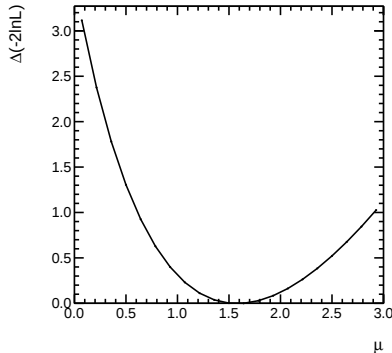
$$\Delta(\text{NLL}) = \text{NLL}(\hat{\mu} \pm r \cdot \sigma) - \text{NLL}(\hat{\mu}) = r$$



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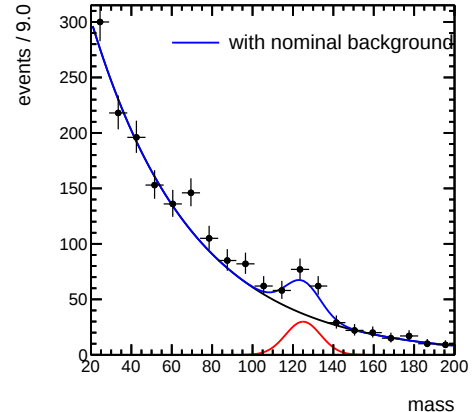
- Other cases can often be approximated by Gaussian case (and true for $n \rightarrow \infty$)
- For strongly asymmetric NLL
 - Often asymmetric intervals quoted
 - Better: variable transformation such that NLL symmetric

Uncertainty vs. Error

- **Uncertainty** reflects degree of precision with which one can deduce a parameter value from the data if one does everything correctly
 - Statistical uncertainties stem from the inherent stochastic nature of the data and finite number of observed events (can not be eliminated, only minimised)
 - Systematic uncertainties stem e. g. from the limited knowledge of the precision of the detector or approximations in theory calculations
 - Uncertainties can (in principle) be quantified
- In contrast, **errors are mistakes**
 - e. g. a loose cable or a wrong method
 - Errors can (and should) be eliminated
- In context of statistical data analysis, we mean uncertainties
 - NB: “Error bars” denote uncertainties!

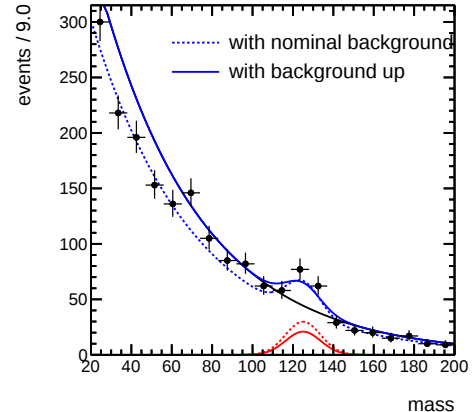
Incorporation of Systematic Uncertainties

- Often, background (and signal) models subject to systematic uncertainties
 - Some (theory or experimental) parameters not exactly known, e. g. cross section or trigger efficiency
- For example, background normalisation b not precisely known but with some uncertainty



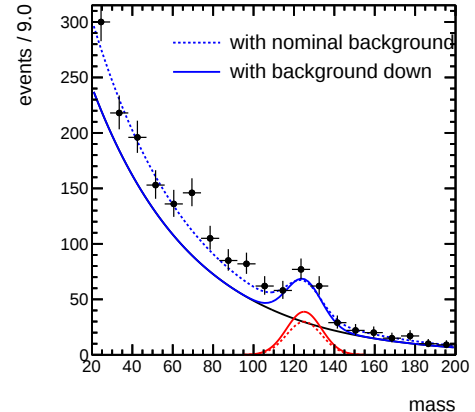
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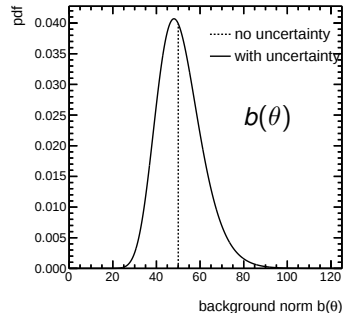
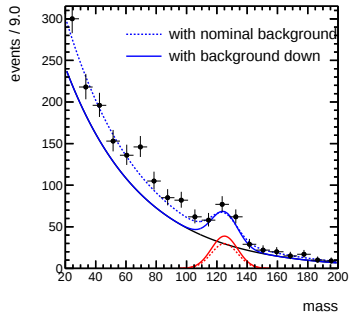


Incorporation of Systematic Uncertainties

- Incorporated into likelihood via **nuisance parameters** θ

$$\mathcal{L}(\mathbf{n}_{\text{obs}}; \mu, \theta) = \prod_i \mathcal{P}(n_{\text{obs}i}; \mu, \theta) \cdot \mathcal{P}_{\tilde{\theta}}(\tilde{\theta}|\theta)$$

- Background normalisation becomes function of θ : $b \rightarrow b(\theta)$

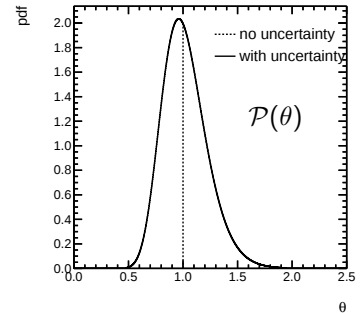
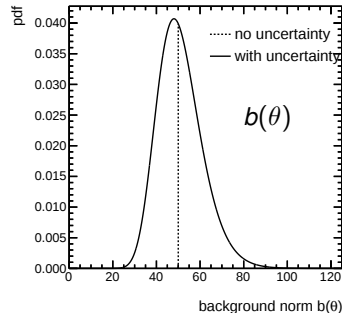
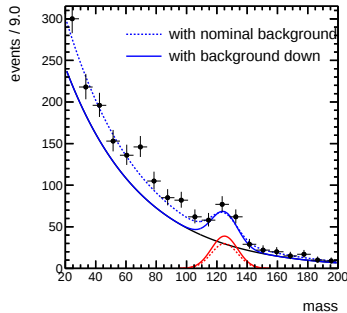


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- Background normalisation becomes function of θ : $b \rightarrow b(\theta)$
 - θ : assumed true value, parameter of the fit
 - $\tilde{\theta}$: best knowledge, e. g. estimate from independent measurement, distributed as $\mathcal{P}_{\tilde{\theta}}(\tilde{\theta}|\theta)$

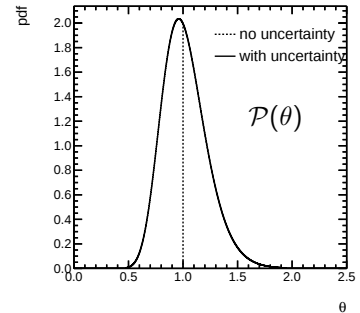
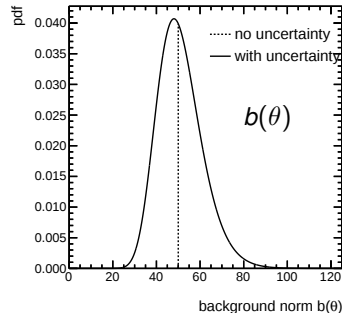
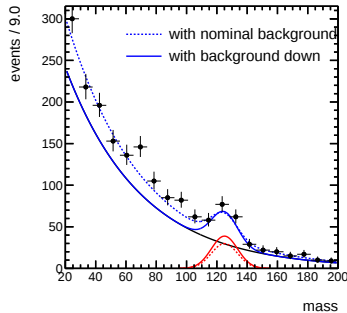


Incorporation of Systematic Uncertainties

- Incorporated into likelihood via **nuisance parameters** θ

$$\mathcal{L}(\mathbf{n}_{\text{obs}}; \mu, \theta) = \prod_i \mathcal{P}(n_{\text{obs}i}; \mu, \theta) \cdot \mathcal{P}_{\tilde{\theta}}(\tilde{\theta}|\theta)$$

- Background normalisation becomes function of θ : $b \rightarrow b(\theta)$
 - ML fit can adjust θ to a value different than $\tilde{\theta}$ to achieve better description of data but at the cost of reducing value of $\mathcal{P}_{\tilde{\theta}}(\tilde{\theta}|\theta)$

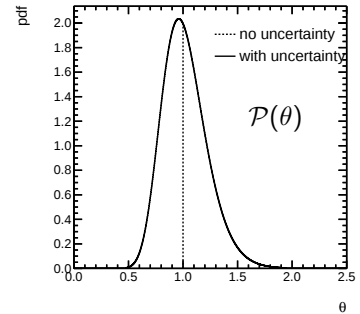
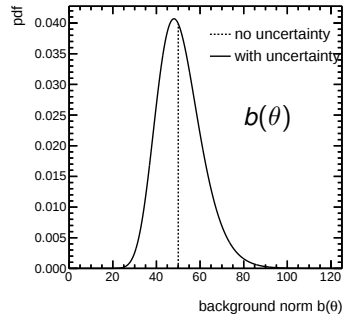
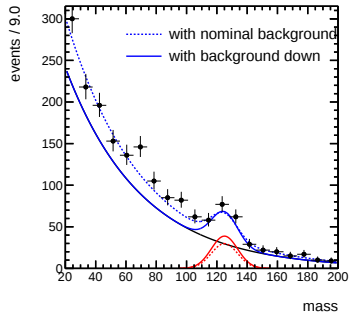


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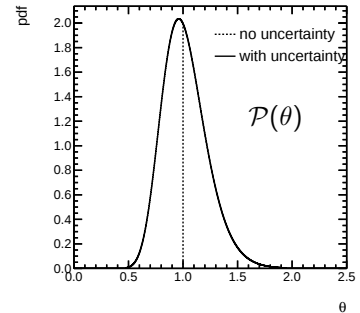
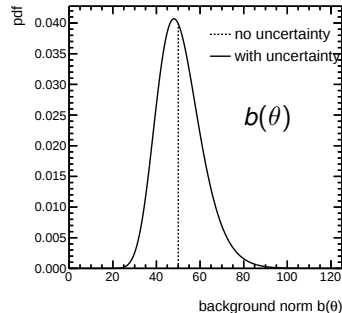
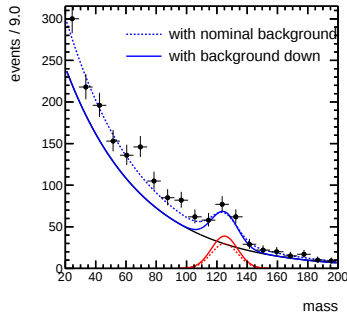
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generally, (anti-)correlated with μ : increased uncertainty on $\hat{\mu} \rightarrow$ smaller sensitivity



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→ can rewrite θ as function of μ

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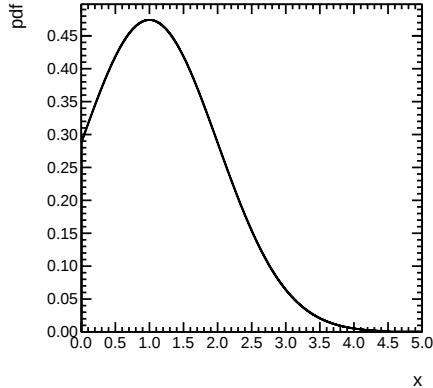
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- $\mathcal{L}_p$ in practice computationally advantageous
 - e. g. need only to consider μ instead of full parameter space (μ, θ) when computing uncertainties

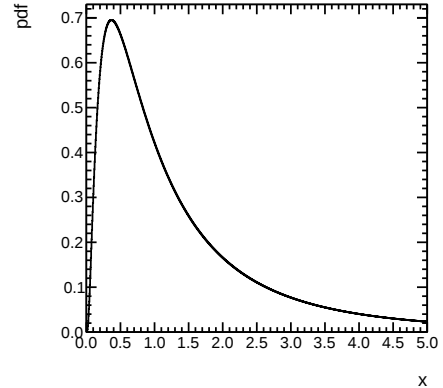
Typical Choices for $\mathcal{P}_\theta(\theta|\tilde{\theta})$

(truncated) Gaussian



$$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

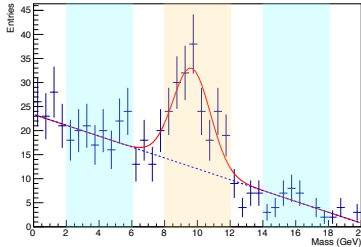
Log-normal



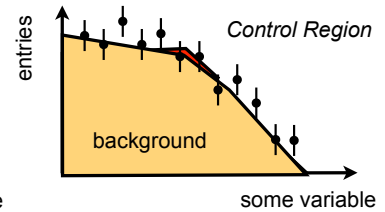
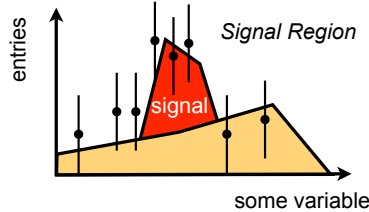
$$\frac{1}{\sqrt{2\pi}\sigma} \frac{1}{x} e^{-\frac{1}{2}\left(\frac{\ln(x)-\mu}{\sigma}\right)^2}$$

Sidebands and Control Regions

sidebands



signal/control region



- Signal-depleted sideband/control region
 - Determine **rate** of background process
 - Determine **shape** of background processes
 - **Constrain uncertainties** on background prediction
- Can be incorporated into likelihood fit via **nuisance parameters**: **simultaneous determination of POI and background parameters**

Confidence Intervals

- Experiment to determine value of some parameter x measures x_{obs}
 - e.g. from maximum likelihood estimate, tag-and-probe measurement
- Want to quote “uncertainty”: interval that reflects statistical precision of measurement
 - Can be estimate of standard deviation from likelihood fit
 - More generally, in particular if non-Gaussian $\mathcal{P}$: **confidence interval**

Confidence Intervals

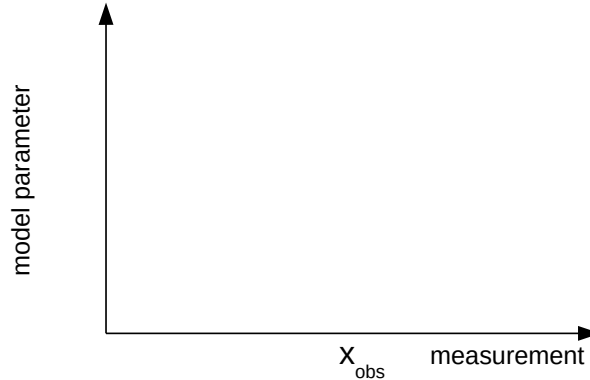
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 - Careful: this is **not** the probability of the true value to lie within the interval
→ there is only one true value either within or not!

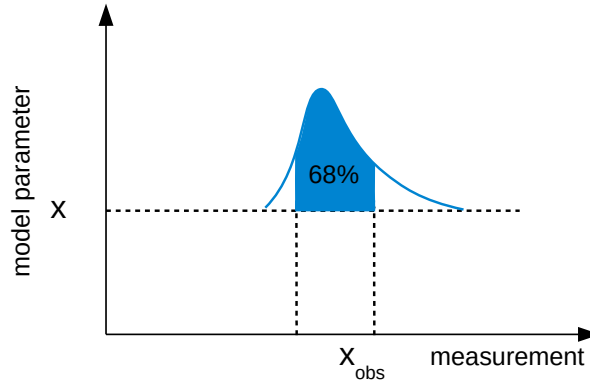
Confidence Intervals

Neyman construction



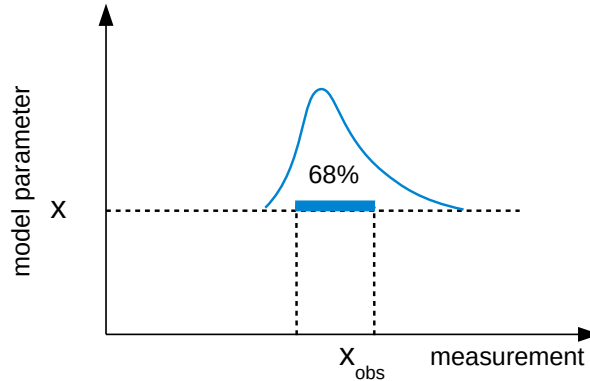
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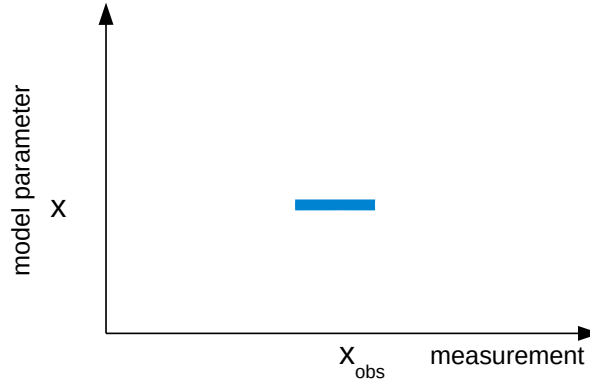
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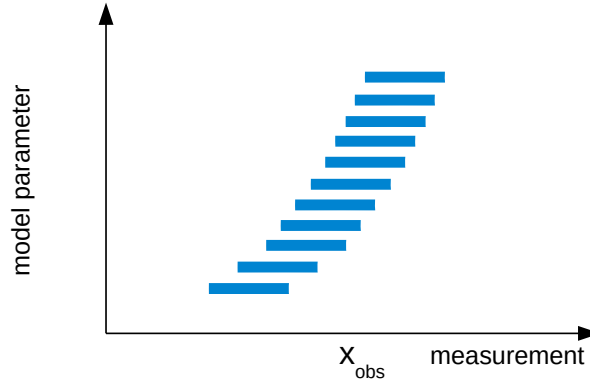
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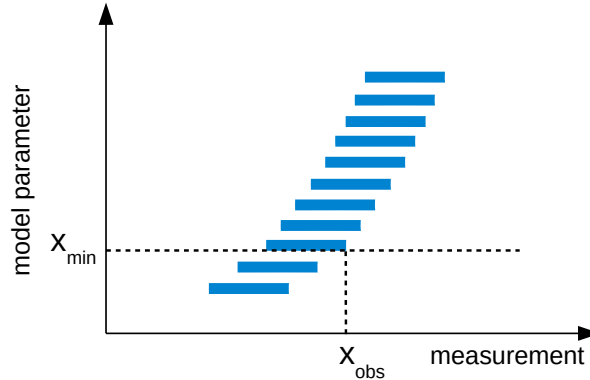
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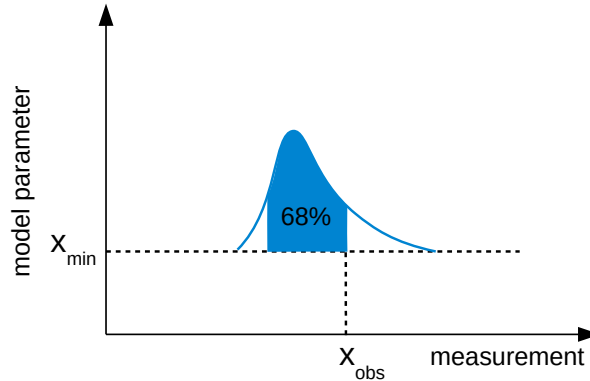
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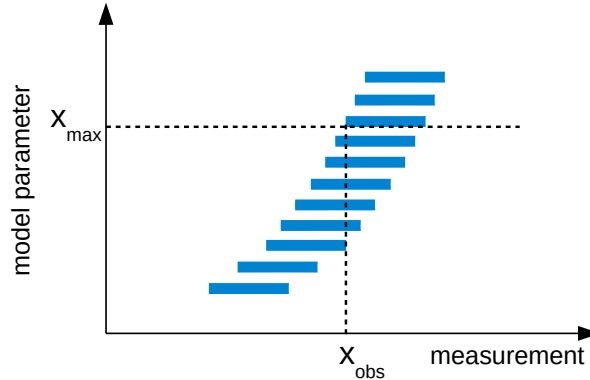
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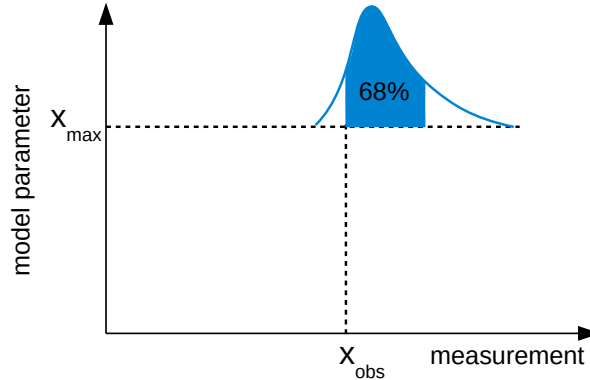
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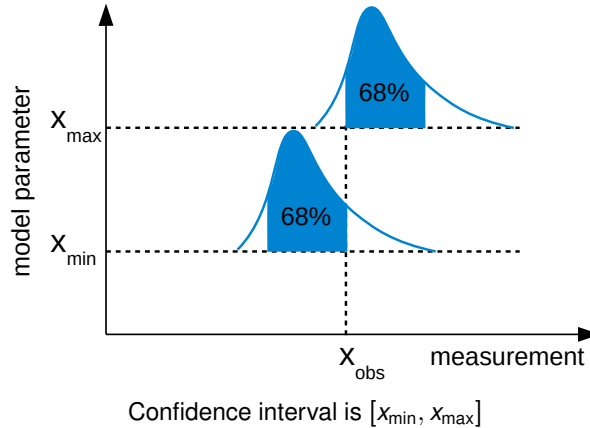
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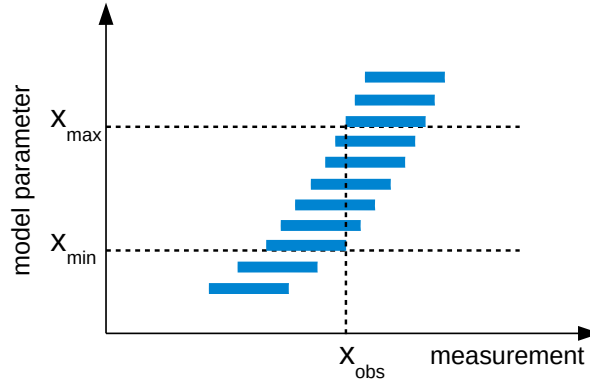
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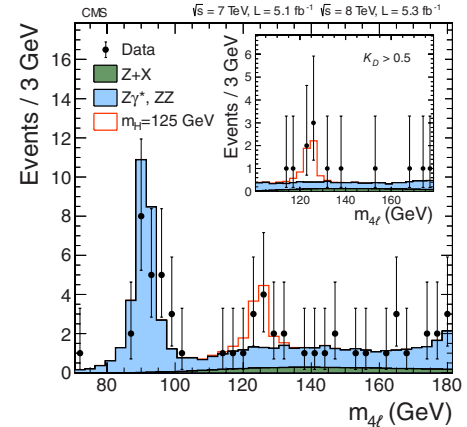
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Confidence interval is $[X_{\text{min}}, X_{\text{max}}]$

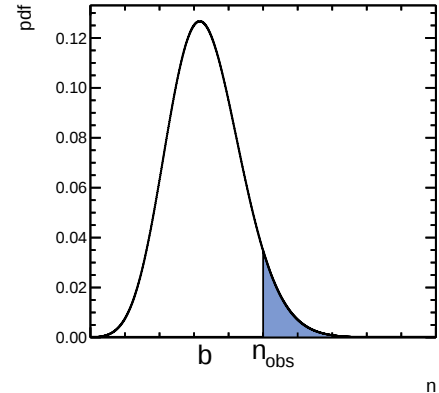
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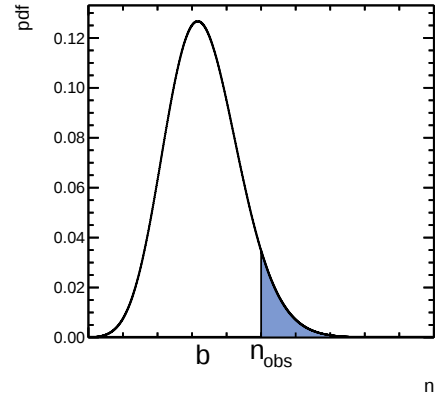


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- “ p value”: **probability of upward fluctuation as large as or larger than observed in data**

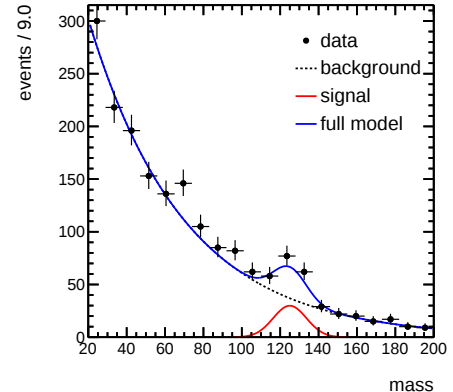
$$p \equiv P(n \geq n_{\text{obs}} | b) = \int_{n_{\text{obs}}}^{\infty} dn \mathcal{P}(n|b)$$

- p value is **not the probability of a hypothesis**
 p quantifies level of (dis-)agreement between model and data:
 → judgement call whether to keep model or reject it



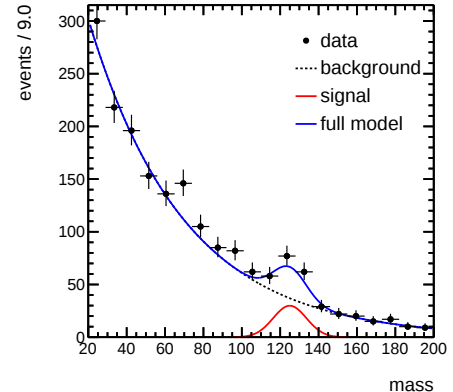
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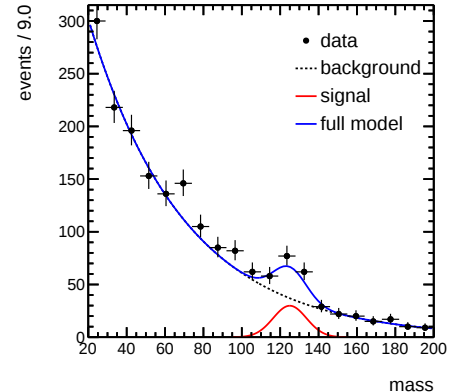
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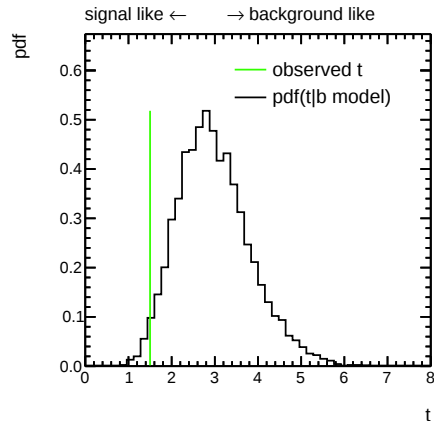


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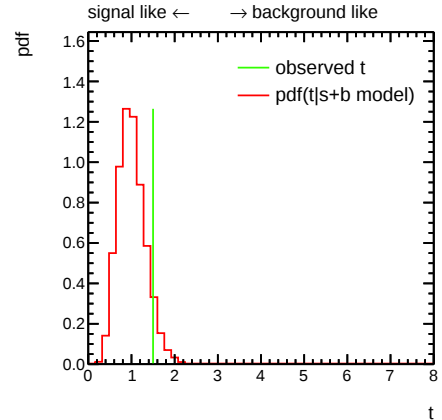


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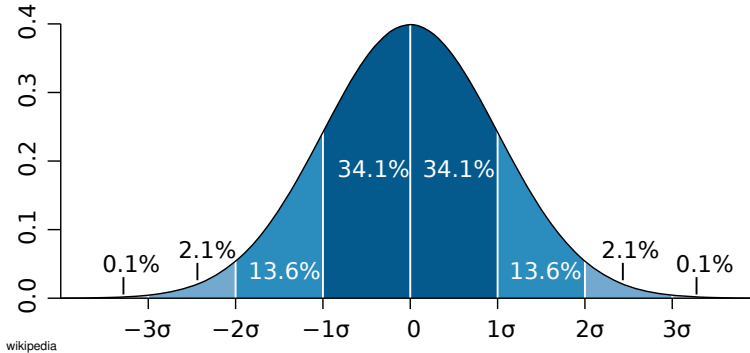


Significance

- Often, p value converted into equivalent **significance Z** :
upward fluctuation from 0 by Z of normal-distributed variable corresponding to same p value
 - Corresponds to Z standard deviations σ of the Gaussian distribution

$$Z = \Phi^{-1}(1 - p)$$

Φ : cumulative (=quantile) function of normal distribution



- Convention** to classify effects by significance:
 - 3σ : *evidence* for a signal
(0.3% chance of background fluctuation)
 - 5σ : *observation* of a signal
(0.00006% chance of background fluctuation)

Distinguishing Hypotheses

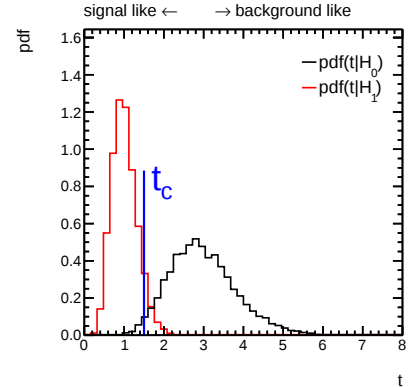
- **Cannot determine whether a hypothesis is true** (frequentist)
- But can **define rules how to reject hypothesis** in favour of an alternative hypothesis
- Can determine **probability of wrong choice**: how often wrong choice is made would the experiment be repeated very often

Distinguishing Hypotheses

- Classification problem: how to interpret outcome of an experiment?
- Want to distinguish between two alternative hypotheses, e. g.
 - H_0 : there are only background events, e. g. no Higgs boson
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 - Define **test statistic** t , e. g. $\mathcal{L}$
 - Construct pdf $\mathcal{P}(t|H_i)$ of t under H_0 and H_1
 - In reality often from simulation
 - How compatible is t_{obs} with H_i ?
- Set a critical value t_c and reject H_0 in favour of H_1 if $t_{\text{obs}} < t_c$



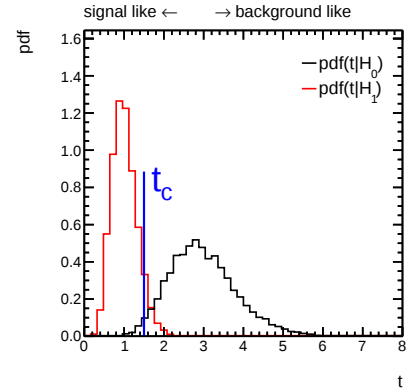
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- Types of errors
 - I: reject H_0 although it is true
 - II: accept H_0 although H_1 is true

$$\begin{aligned} \text{I: } P(t < t_c | H_0) &= \int_{-\infty}^{t_c} dt \mathcal{P}(t | H_0) \equiv \alpha \\ \text{II: } P(t > t_c | H_1) &= \int_{t_c}^{\infty} dt \mathcal{P}(t | H_1) \equiv \beta \end{aligned}$$

α : significance of test

$1 - \beta$: power of test

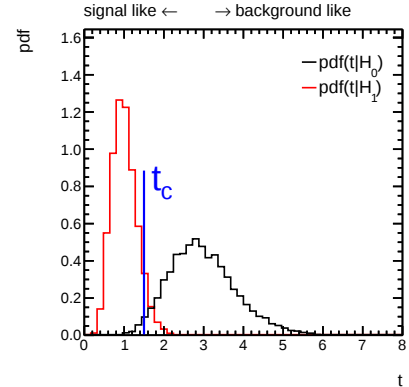


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By choice of t_c (choice of α): association to one or the other hypothesis performed “**at the confidence level α** ”



Difference Between α and p Value?

- In one sense, no difference
 - Both are $\int_x^\infty dx' \mathcal{P}(x')$
- But **conceptually very different**
 - α is computed before one sees the data: predefined property of the test
 - p depends on the data (property of the data) and is a random variable

Neyman-Pearson Lemma

- When performing a test between two hypotheses (models) H_0 and H_1 , the **likelihood ratio test**, which rejects H_0 in favour of H_1 if

$$Q = \frac{\mathcal{L}_{H_1}}{\mathcal{L}_{H_0}} > Q_c \quad \text{with } P(Q > Q_c | H_0) = \alpha$$

is the **most powerful test** at a significance level α (Neyman-Pearson Lemma)

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- For a number of reasons, usually

$$q = -2 \ln Q$$

Test Statistic at the LHC

- Used test statistic in particle-physics experiments evolved with time (LEP → Tevatron → LHC)
 - Different conditions: importance of systematic uncertainties, computational power
- Hypothesis test example
 - H_0 : background-only hypothesis, e. g. SM without Higgs boson
 - H_1 : Higgs boson with fixed mass and signal strength μ (= signal w.r.t. prediction) present in data

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- At the LHC commonly: **profile likelihood ratio test statistic**

$$q_\mu = -2 \ln \frac{\mathcal{L}(n_{\text{obs}}; \mu, \hat{\theta}(\mu))}{\mathcal{L}(n_{\text{obs}}; \hat{\mu}, \hat{\theta})}$$

- Nuisance parameters are profiled in nominator
- Global maximum of $\mathcal{L}$ under (μ, θ) as denominator with $0 \leq \hat{\mu} \leq \mu$
- Allows usage of certain approximations when computing $\mathcal{P}(q_\mu | H_i)$ (“asymptotic formulae” based on Wilks and Wald theorem¹)

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Excluding Parameters

- Assume measurement with a given sensitivity: no signal observed
- How much signal can “hide” in the background fluctuations (+uncertainty)?
- **How large could a signal be at most?**

Excluding Parameters

- No signal observed: **how large could a signal be at most?**
- Formally: test statistic q , depending on signal-strength modifier μ

$$q(\mu) = -2 \ln \frac{\mathcal{L}_{H_1}(\mu)}{\mathcal{L}_{H_0}}$$

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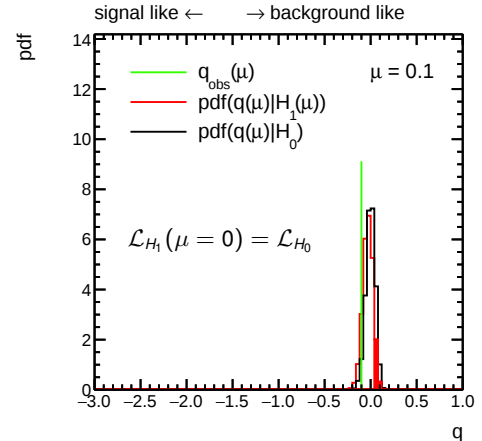
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Excluding Parameters

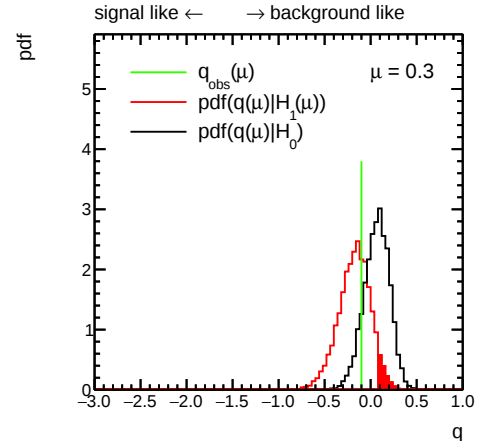
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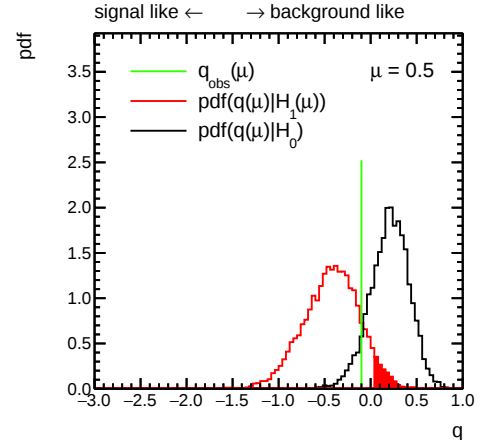
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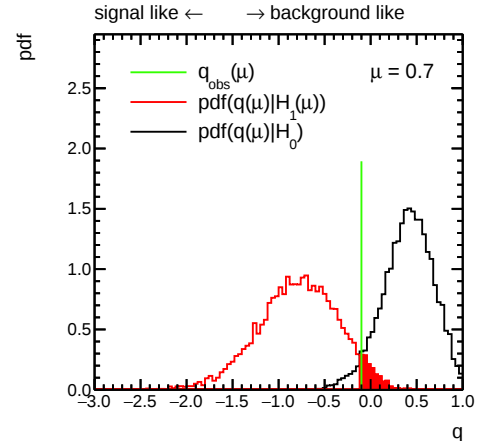
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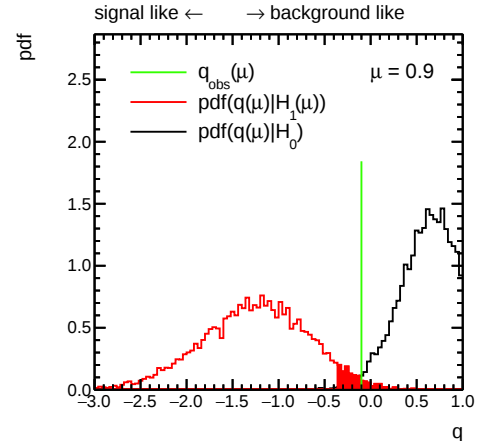
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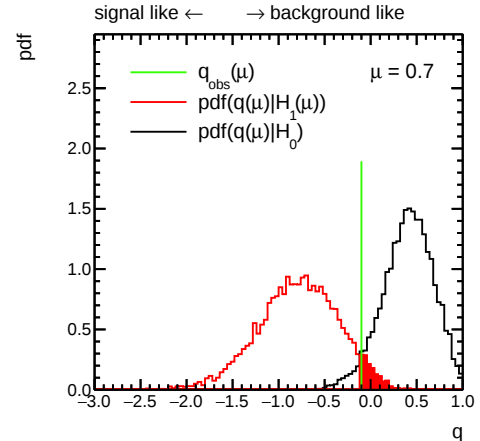
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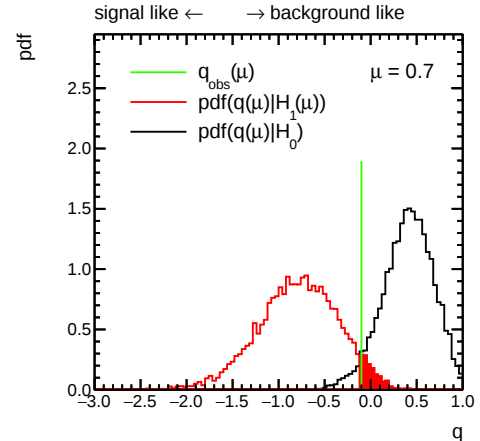
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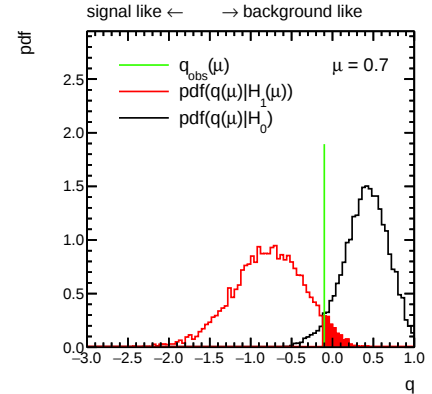
i. e. for $\mu_{1-\alpha}$: $q_{\text{obs}} = q_c$

$\mu_{1-\alpha}$ is called **upper limit** on μ at confidence level
C.L. = $1 - \alpha$
In particle physics usually 95 % C.L. limit



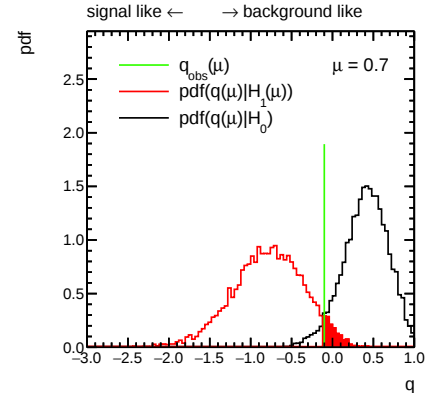
(Observed) Upper Limit: Interpretation

- “Maximal signal that we would still reject”



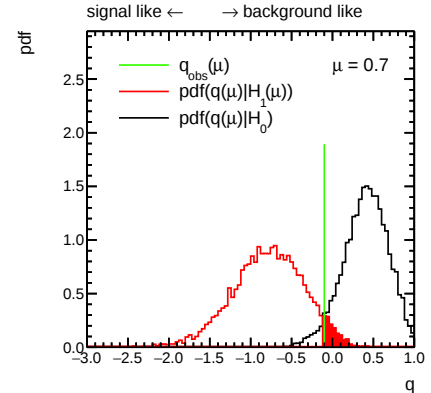
(Observed) Upper Limit: Interpretation

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- 95 % C.L. upper limit on μ : largest value of μ that would still be rejected in a test with significance 5% given the data
 - NB: limit is a **function of the data** (depends on q_{obs})!
- μ for which $\text{CL}_{\text{s+b}} = 0.05$:
$$0.05 = \int_{q_{\text{obs}}}^{\infty} dq \mathcal{P}(q(\mu_{95})|H_1)$$



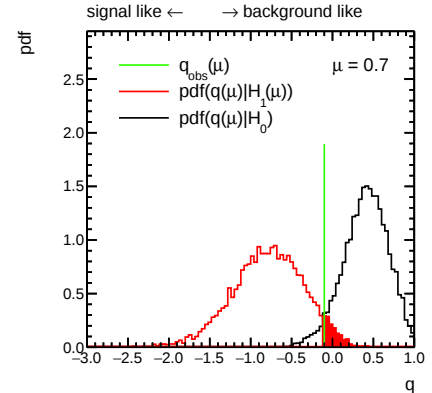
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 - If the experiment is repeated many times, μ_{95} would be larger than μ_{true} in 95 % of the cases



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- Still **5 % chance of wrong exclusion**, i. e. that $\mu_{\text{true}} > \mu_{95}$

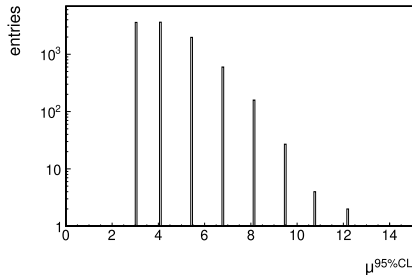


Expected Limit

- Estimate what observed limit would look like in case of no signal

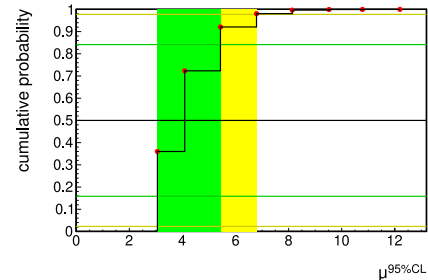
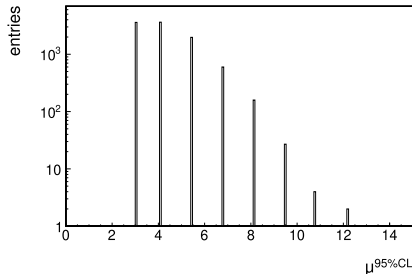
Expected Limit

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- Obtained e. g. from *toy dataset*
 - Sample toy data for q under background-only hypothesis from $\mathcal{P}(q|H_0)$
 - Treat each as observation and compute μ_{95} limit
 - Obtain quantiles from distribution of all μ_{95}



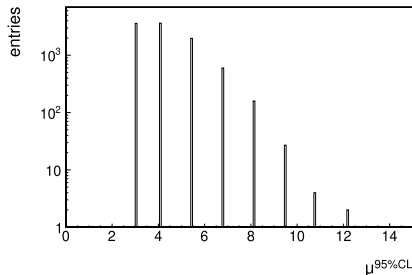
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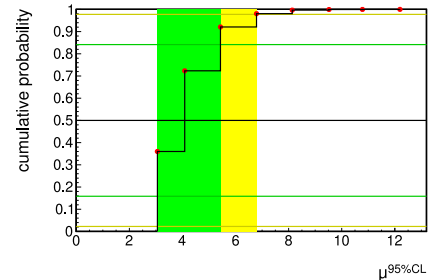


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- **Expected limit = median of μ_{95} distribution**
 - 16 and 84% quantiles: **68% confidence interval**
 - 2.5 and 97.5% quantiles: **95% confidence interval**

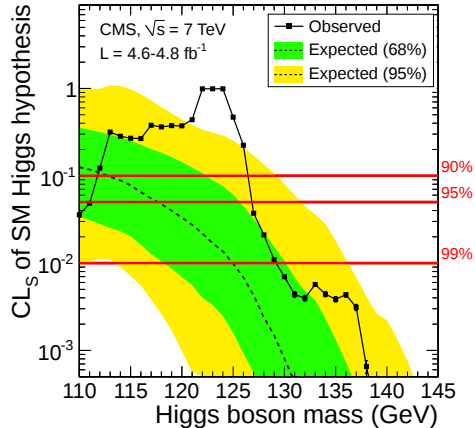


→ “Brazilian band” plots



Before the Higgs-Boson Discovery

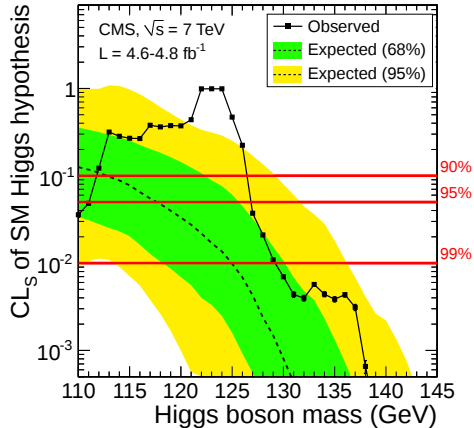
■ Combination of Higgs-boson search results by CMS [Phys.Lett. B710 (2012) 26]



- Tested hypotheses
 - H_0 : no Higgs boson
 - H_1 : SM Higgs boson
- Test statistic q evaluated for SM Higgs boson of different mass ($\mu = 1$ in each case)
- Excluding a SM Higgs boson at 95% CL with masses
 - $m_H > 118$ GeV expected (from toy data under H_0)
 - $m_H > 127$ GeV observed (from real data)

Before the Higgs-Boson Discovery

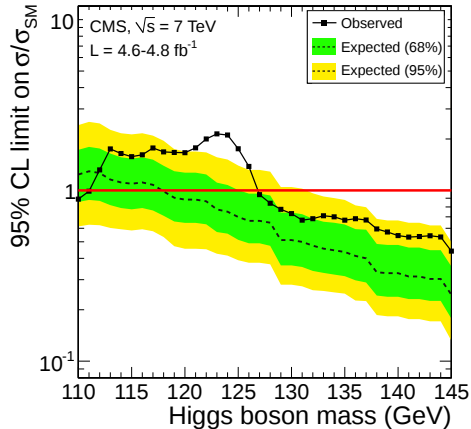
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- Test statistic q evaluated for SM Higgs boson of different mass ($\mu = 1$ in each case)
- Observed exclusion weaker than expected (smaller mass range)
- Around $m_H = 125$ GeV, q_{obs} differs significantly from expectation: **indication that H_0 is wrong!**

Before the Higgs-Boson Discovery

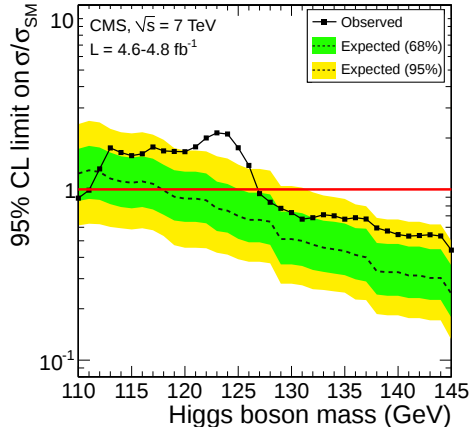
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- Tested hypotheses
 - H_0 : no Higgs boson
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- Test statistic evaluated for a Higgs boson of different mass and variable signal strength
 - Signal strength μ can vary in each case (not SM any more!)
- Exclusion limits on μ for different masses at 95 % C.L.

Before the Higgs-Boson Discovery

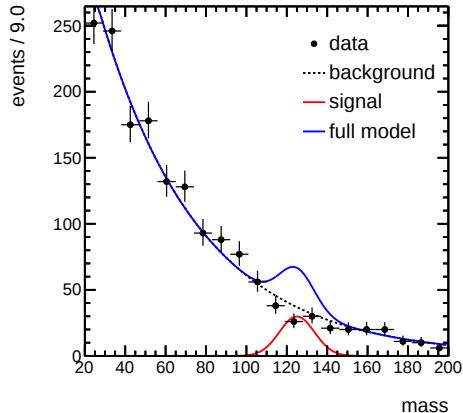
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- Tested hypotheses
 - H_0 : no Higgs boson
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- Test statistic evaluated for a Higgs boson of different mass and variable signal strength
 - Signal strength μ can vary in each case (not SM any more!)
- Striking: observed limit weaker than expected around $m_H = 125$ GeV
- Difference (locally) beyond 2σ : **indication that H_0 is wrong!**

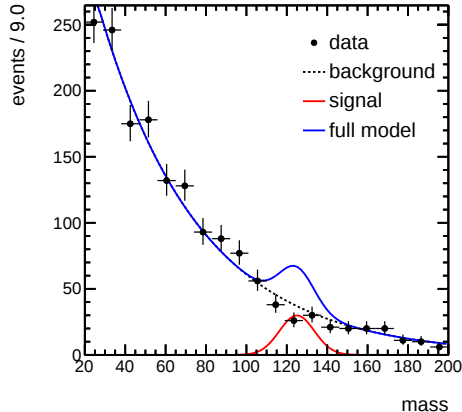
What If the Data Trick Us?

- Suppose **data fluctuates low**, sizably below background expectation
- **CL_{s+b} : artificially strong limit** on signal, i. e. $\mu_{1-\alpha}$ is small



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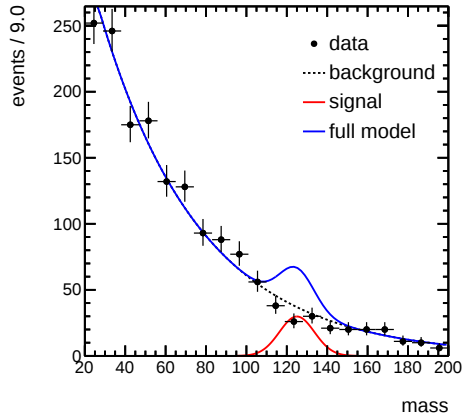
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- In extreme case, $\mu_{1-\alpha} \rightarrow 0$
i. e. exclude signal entirely
- **Not desirable**: just downward fluctuation of the data!
- Often **problem**: **searches in extreme phase-space regions** with few background events

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CL_s method

- Compute both

$$CL_{s+b} = \int_{q_{\text{obs}}}^{\infty} dq \mathcal{P}(q(\mu)|H_1)$$

$$CL_b \equiv \int_{q_{\text{obs}}}^{\infty} dq \mathcal{P}(q(\mu)|H_0)$$

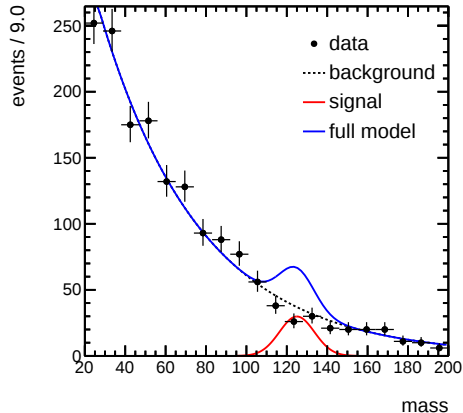
- Define limit as that μ for which

$$CL_s \equiv \frac{CL_{s+b}}{CL_b} = \alpha$$

normalise CL_{s+b} to “background-only p-value”

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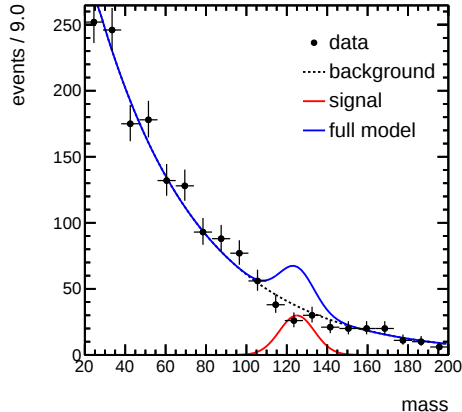
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- In case of extreme under fluctuation: $CL_s \rightarrow 1$
- H_1 not excluded by mistake – but also weaker limit in case of no signal

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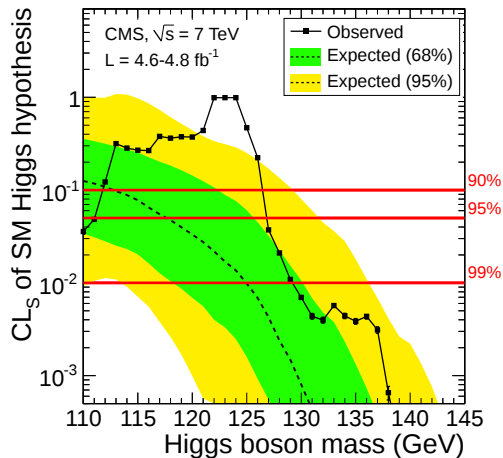
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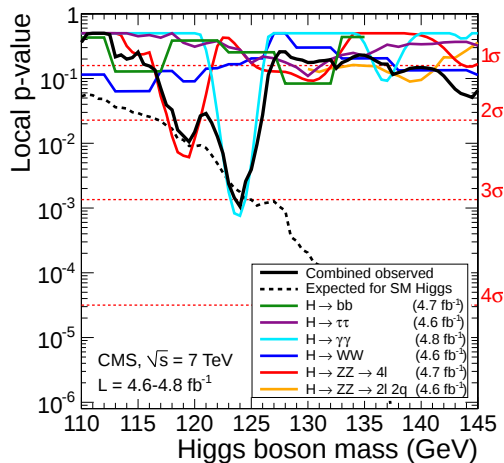
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CL_s protects from fluctuations in the data at cost of lower sensitivity
(procedure used in LHC (Higgs boson) searches)

Et Voilà



Phys.Lett. B710 (2012) 26-48



Summary

- **Statistical analysis crucial tool** in particle physics
- Does not tell probability of a certain model (at least not without further assumptions) but allows
 - quantifying the compatibility of the data with a tested model, e. g. via **p value or significance**
 - determining the parameter values of a given model that describe best the data (estimators), e. g. **via maximum-likelihood fit**
- In practice often **comparison of two alternative hypotheses** H_0 and H_1 , e. g. background-only and signal+background
 - Rules when to reject H_0 in favour of H_1 : allow quantifying type-I/II errors
 - Test statistic combines information of multi-channel data into one single number for application in hypothesis testing
 - **Likelihood ratio is most powerful test statistic**
- Exclusion **limits provide information on model parameter in case no signal found**

Literature

- R. J. Barlow, “Statistics: A Guide to the Use of Statistical Methods in the Physical Sciences”, The Manchester Physics Series **highly recommended**
- G. Cowan, “Statistical Data Analysis”, Oxford Science Publications
- Review “Statistics”, R.L. Workman et al. (Particle Data Group), Prog. Theor. Exp. Phys. 2022, 083C01 (2022) and 2023 update **very good review**
- The ATLAS and CMS Collaborations, “Procedure for the LHC Higgs boson search combination in Summer 2011”, CMS-NOTE-2011-005, ATL-PHYS-PUB-2011-11 **expert document**