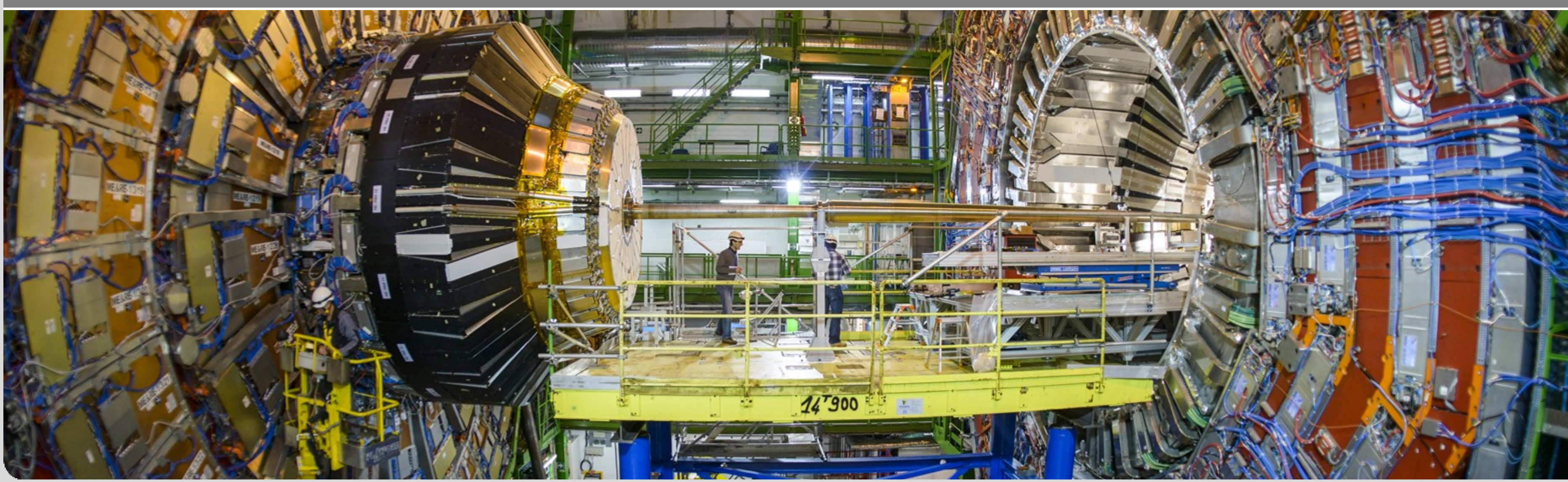
Karlsruhe Institute of Technology

Statistical Methods used for Higgs Boson Searches

Roger Wolf

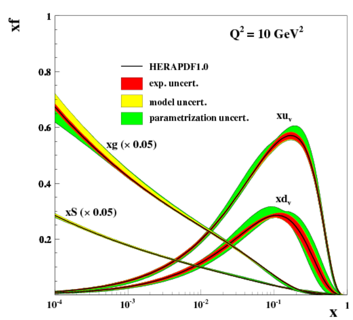
03. June 2014

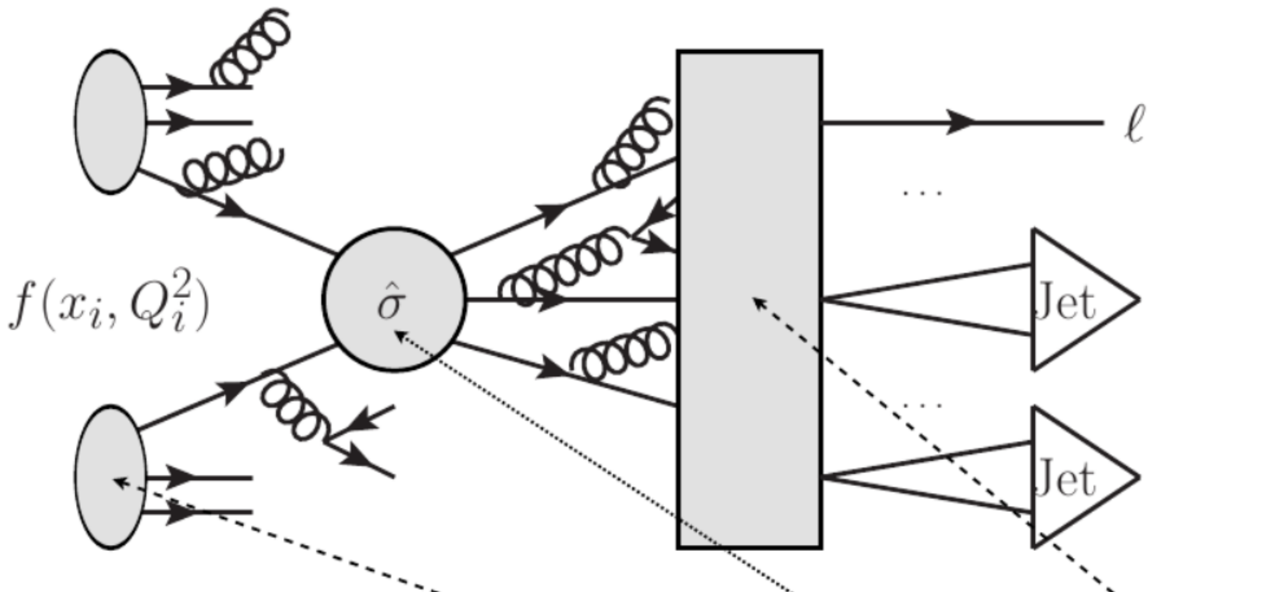
INSTITUTE OF EXPERIMENTAL PARTICLE PHYSICS (IEKP) – PHYSICS FACULTY



Recap from Last Time (Simulation of Processes)

- From “paper & pen” statements to high precision predictions on observable quantities (at the LHC):



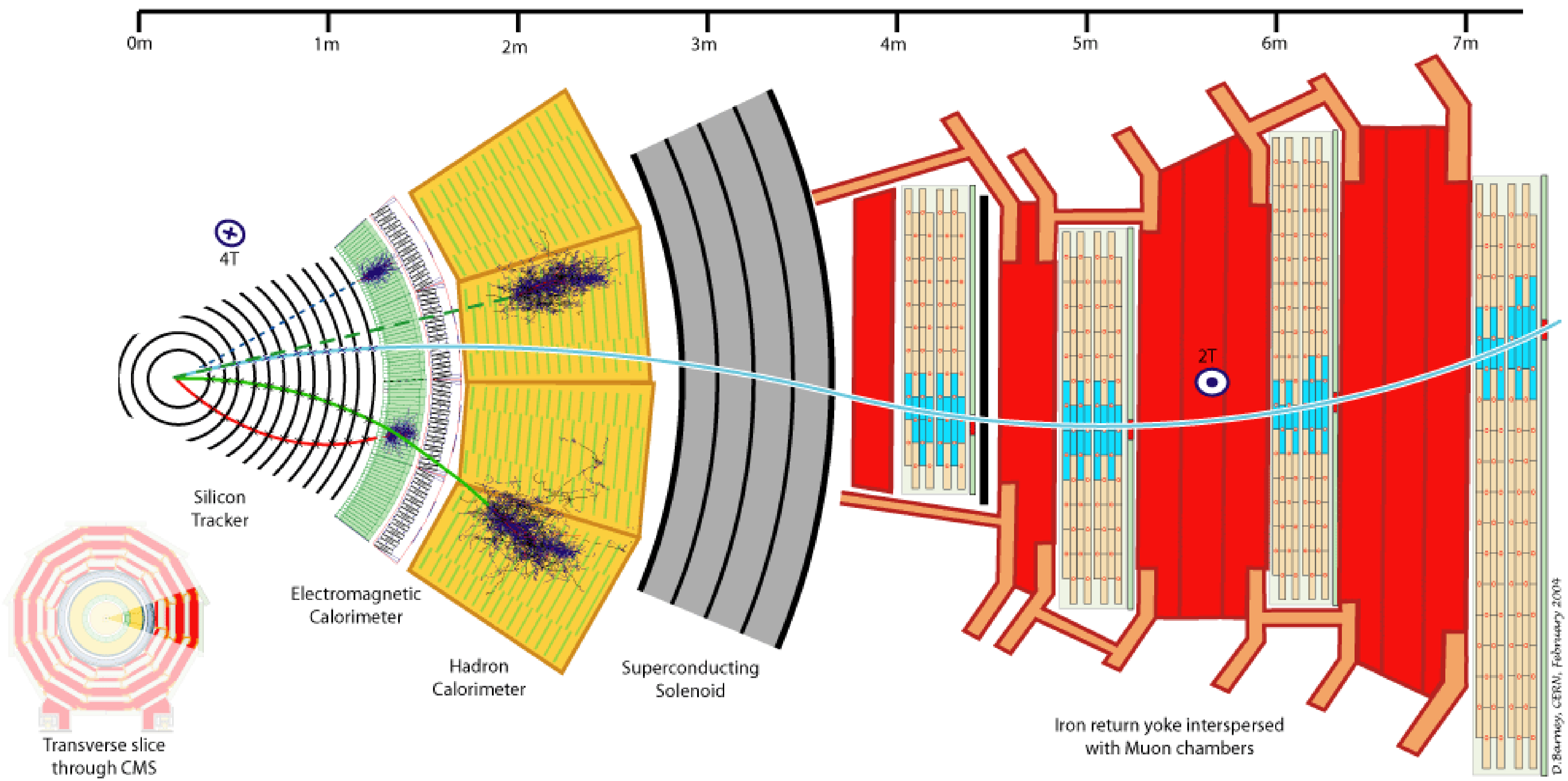


$$\sigma_{QCD} = \sum_{jk} \int \mathrm{d}x_j\, \mathrm{d}x_k\, f_j(x_j, \mu_F^2)\, f_k(x_k, \mu_F^2)\, \hat{\sigma}(x_j x_k s, \mu_F^2, \mu_R^2) \otimes \text{hadronization}$$

- Discussed in lectures 1-3.

Recap from Last Time (Data Analysis)

- Observable → real measurement:



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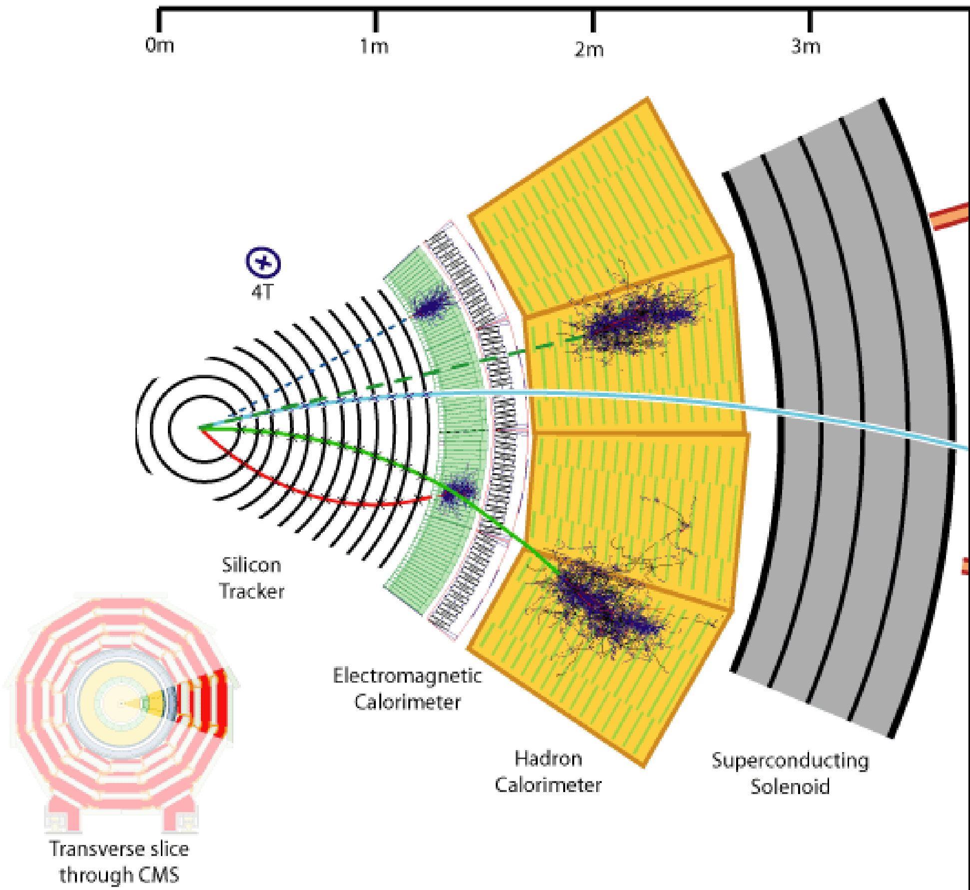
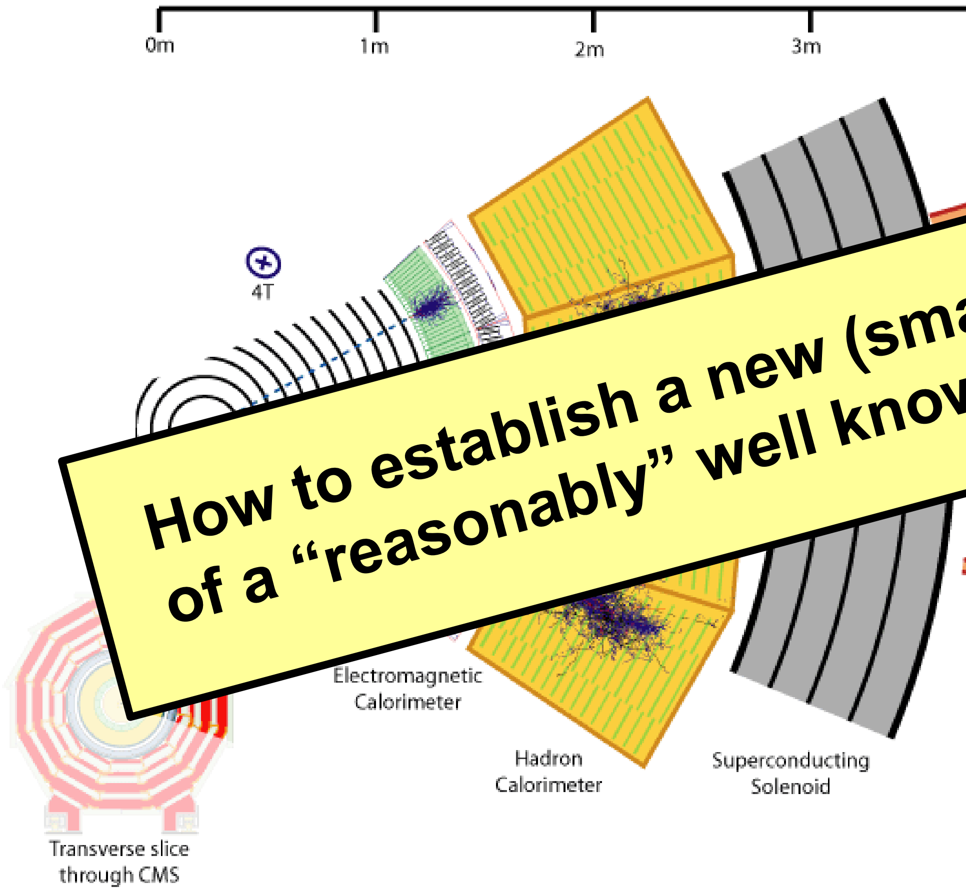


Data preparation techniques:

- Reconstruction of traces in the detector units.
- Alignment of track detectors.
- Calibration of energy response.
- Reconstruction & selection efficiency (“Tag & probe”, “MC Embedding”)
- How well are background processes understood?

• Observable → real measurement:



How to establish a new (small) signal on top of a "reasonably" well known background?

Data preparation tec…niques:

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- …s.
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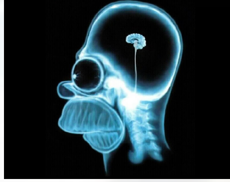
Quiz of the Day



- What is the relation between the Binomial, Gaussian & Poisson distribution?
- What is the relation between a minimal χ^2 fit and a Maximum Likelihood fit?
- How exactly do I calculate a 95% CL limit and how does it relate to classical hypothesis tests?

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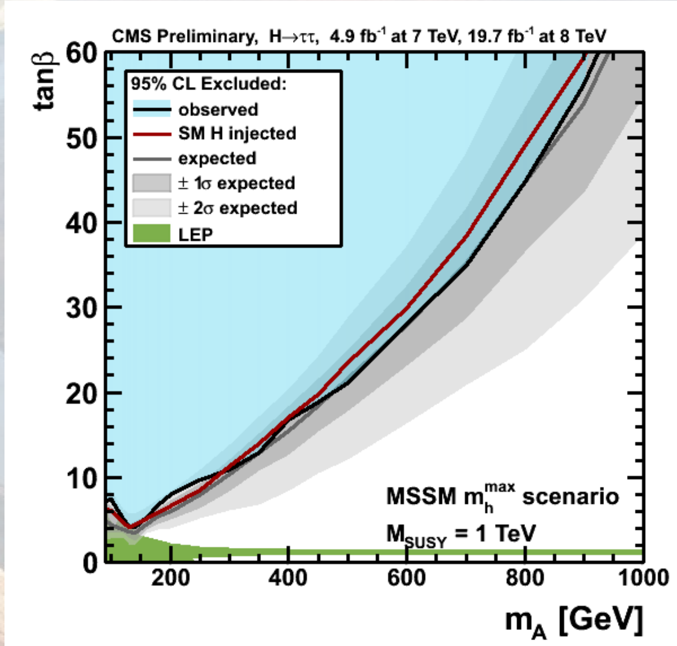

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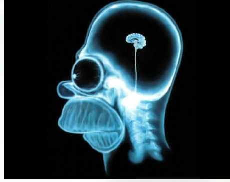

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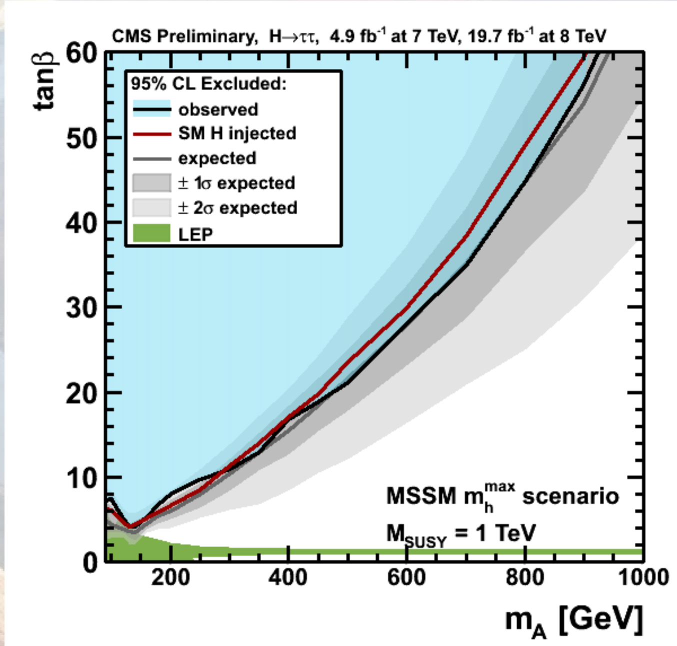

- What does a "3σ evidence" or a "5σ discovery" mean?

Schedule for Today

3

Limits, p-values, significances.

2

Parameter estimates
(=fits).

1

Probability distributions
& Likelihood functions.

Schedule for Today

Walk through statistical methods that will appear in the next lectures:

- You will see all these methods acting in real life during the next lectures.
- To learn about the interiors of these methods check KIT lectures of Modern Data Analysis Techniques.

1 Probability distributions & Likelihood functions.

2 Parameter estimates (=fits).

3 Limits, p-values, significances.

Statistics ↔ Particle Physics

Theory:

- QM wave functions are interpreted as probability density functions.
- The Matrix Element, $\mathcal{S}_{fi}$,gives the probability to find final state f for given initial state i.
- Each of the statistical processes $pdf \rightarrow ME \rightarrow hadronization \rightarrow energy\ loss\ in\ material \rightarrow digitization$ are statistically independent.
- Event by event simulation using Monte Carlo integration methods.

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Experiment:

- All measurements we do are derived from rate measurements.
- We record millions of trillions of particle collisions.
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Experiment:

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- We record millions of trillions of particle collisions.
- Each of these collisions is independent from all the others.

- Particle physics experiments are a perfect application for statistical methods.

Probability Distributions & Likelihood Functions

Characterization of Probability Distributions

- Expectation Value:

$$E[x] = \int_{-\infty}^{\infty} x \cdot pdf(x)\mathrm{d}x = \mu$$

- Variance:

$$V[x] = \int_{-\infty}^{\infty} (x-\mu) \cdot pdf(x)\mathrm{d}x = \sigma^2$$

$$= E[(x-E[x])^2] = E[x^2 - 2xE[x] + E^2[x]] = E[x^2] - E^2[x]$$

- Covariance:

$$cov[x,y] = E[(x-\mu(x)(y-\mu(y))] = \int_{-\infty}^{\infty} x \cdot y \cdot pdf(x,y)\mathrm{d}x = E[xy] - \mu(x)\mu(y)$$

- Correlation coefficient:

$$\rho(x,y) = \frac{cov[x,y]}{\mu(x)\mu(y)}$$

Probability Distributions

	Expectation:	Variance:
$$\mathcal{P}(k,n,p) = \binom{n}{k} p^k \cdot (1-p)^{n-k}$$ (Binomial distribution)	$\mu = np$	$\sigma^2 = np(1-p)$

Probability Distributions

	Expectation:	Variance:
$$\mathcal{P}(k,n,p) = \frac{1}{\sqrt{2\pi np(1-p)}} e^{-\frac{1}{2}\left(\frac{k-np}{np(1-p)}\right)^2}$$ (Gaussian distribution)	$\mu = np$	$\sigma^2 = np(1-p)$
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↑ $n \to \infty$, p fixed

Central limit theorem of de Moivre & Laplace.

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↓ $n \to \infty$, np fixed — Will be shown on next slide.		
$\mathcal{P}(k,n,p) = \frac{(np)^k}{k!} e^{-np}$ (Poisson distribution)	$\mu = np$	$\sigma^2 = \mu = np$

Probability Distributions

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Binomial → Gaussian: $n \to \infty$, p fixed

Central limit theorem of de Moivre & Laplace.

Binomial → Poisson: $n \to \infty$, np fixed

Will be shown on next slide.

$\sigma^2 = \mu = np$ → motivation for $\sqrt{k}$ uncertainty.

Binomial ↔ Poisson Distribution

$$\mathcal{P}(k,n,p) = \binom{n}{k} p^k \cdot (1-p)^{n-k}$$

$$= \frac{n(n-1)(n-2)\cdot\ldots\cdot(n-k+1)}{k!} \cdot \frac{\mu^k}{n^k} \cdot \frac{\left(1-\frac{\mu}{n}\right)^n}{\left(1-\frac{\mu}{n}\right)^k}$$

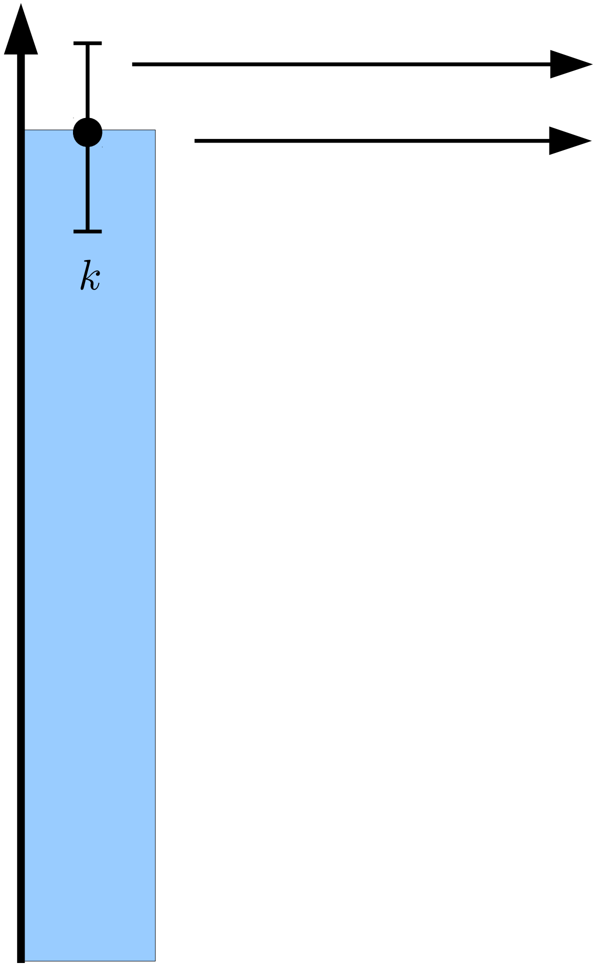
$$= \frac{1\cdot(1-\frac{1}{n})(1-\frac{2}{n})\cdot\ldots\cdot(1-\frac{k-1}{n})}{\left(1-\frac{\mu}{n}\right)^k} \cdot \frac{\mu^k}{k!} \cdot \left(1-\frac{\mu}{n}\right)^n$$

$$= \underbrace{\frac{1}{\left(1-\frac{\mu}{n}\right)} \cdot \frac{(1-\frac{2}{n})}{\left(1-\frac{\mu}{n}\right)} \cdot \frac{(1-\frac{2}{n})}{\left(1-\frac{\mu}{n}\right)} \cdot \ldots \cdot \frac{(1-\frac{k-1}{n})}{\left(1-\frac{\mu}{n}\right)}}_{\to 1} \cdot \frac{\mu^k}{k!} \cdot \underbrace{\left(1-\frac{\mu}{n}\right)^n}_{\to e^{-\mu}}$$

$$= \frac{\mu^k}{k!} e^{-\mu}$$

$$\mu = const, n \to \infty$$

Uncertainties on Counting Experiments



$\sqrt{k}$ uncertainty

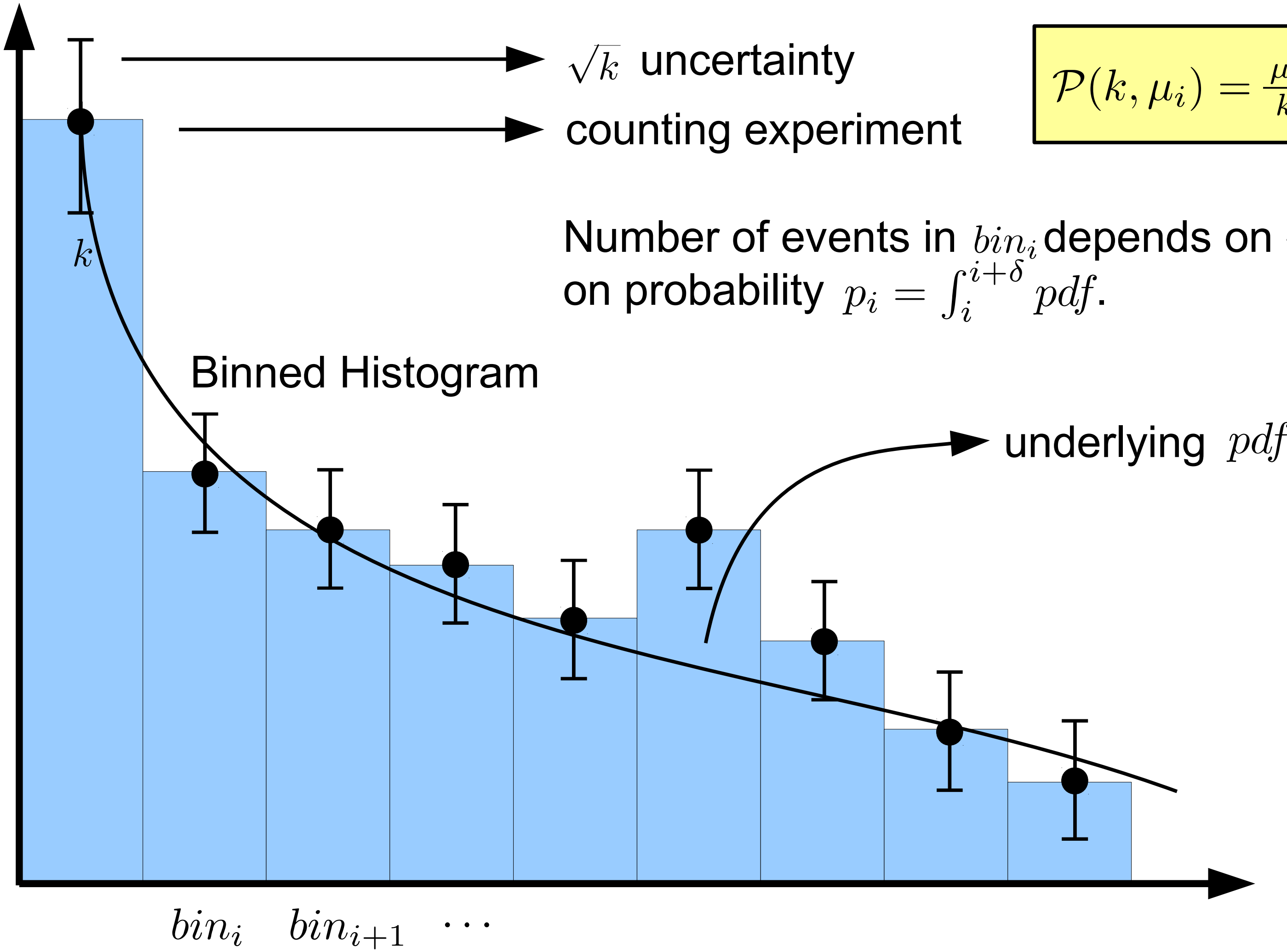
counting experiment

$$\mathcal{P}(k, \mu_i) = \frac{\mu_i^k}{k!} e^{-\mu_i}$$

Uncertainties on Counting Experiments

$$\mathcal{P}(k, \mu_i) = \frac{\mu_i^k}{k!} e^{-\mu_i}$$

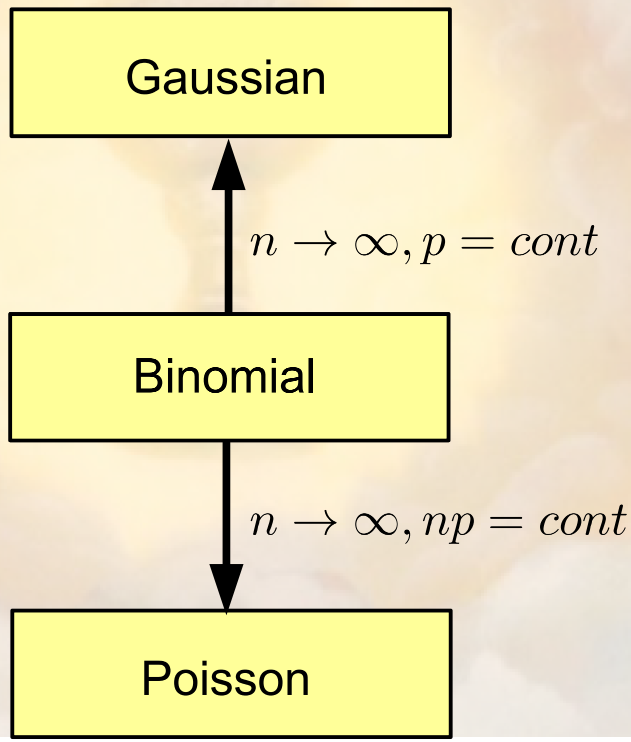
Number of events in bin_i depends on n and on probability $p_i = \int_i^{i+\delta} pdf$.



Relations between Probability Distributions

Central Limit Theorem:

Random variable variable made up of a sum of many single measurements.



Look for something that is very rare very often.

Relations between Probability Distributions

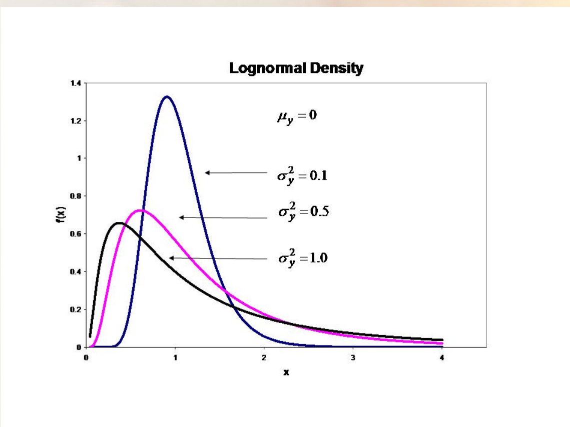
Central Limit Theorem:

Random variable variable made up of a sum of many single measurements.

Log-normal

exp

Random variable variable made up of a product of many single measurements.



Gaussian

$n \to \infty, p = cont$

Binomial

$n \to \infty, np = cont$

Poisson

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Log-normal ←(exp)— **Gaussian** —(log)→ **χ^2 Distribution**

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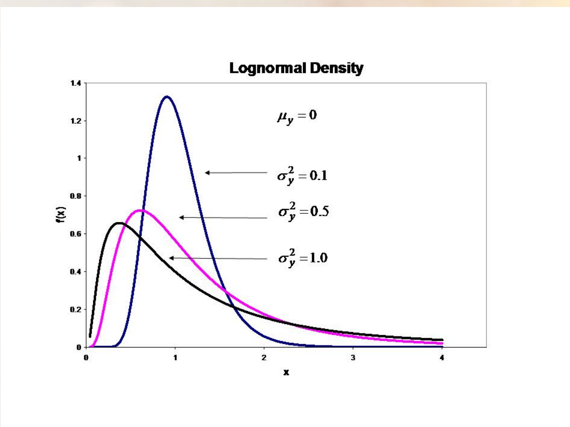
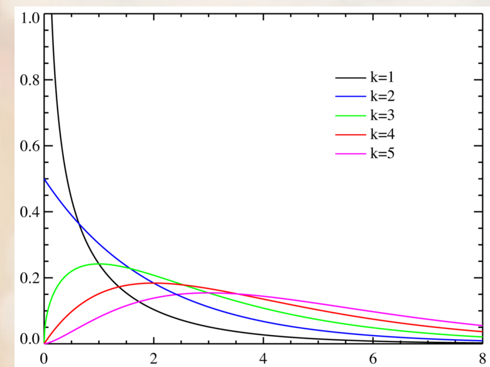


Binomial → **Gaussian**: $n \to \infty, p = cont$

Binomial → **Poisson**: $n \to \infty, np = cont$



What does the parameter k correspond to in the χ^2 distributions?

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Log-normal ← exp ← **Gaussian** → log → **χ^2 Distribution**

Binomial → $n \to \infty, p = cont$ → **Gaussian**

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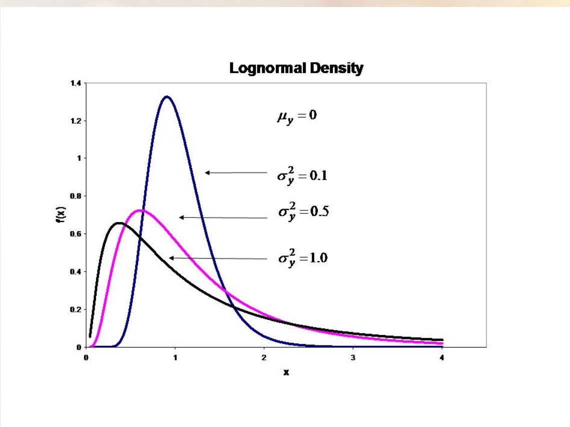

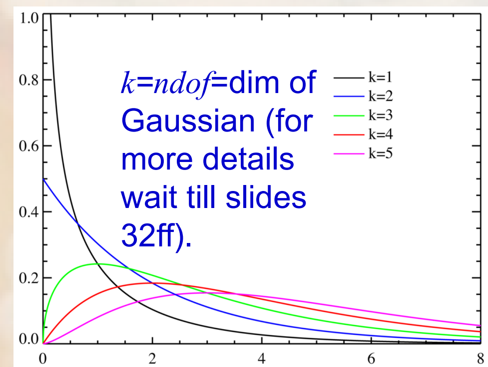

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Likelihood Functions

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- **Problem**: truth is not known!
- Deduce "truth" from measurements (usually in terms of models).
- Likeliness of a model to be true quantified by *likelihood function* $\mathcal{L}(\{k_i\}, \{\kappa_j\})$.

$\{\kappa_j\}$ → model parameters.

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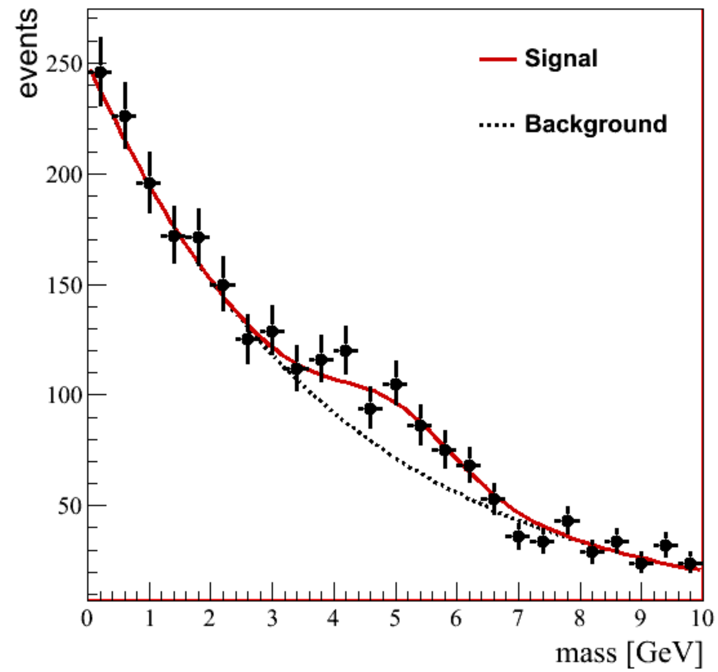
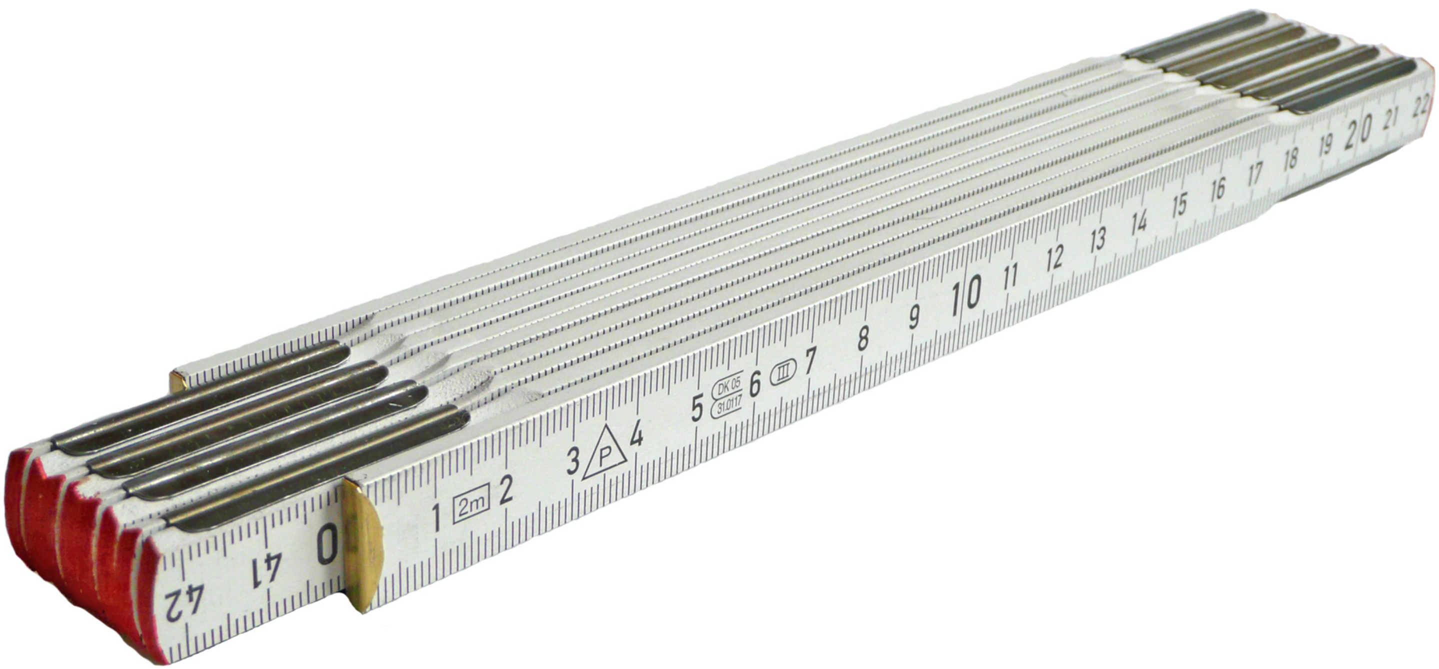


Parameter Estimates



Parameter Estimates

- **Problem**: find most probable parameter(s) κ_j of a given model.
- Usually minimization of negative ln likelihood function (NLL):
  - ln is a monotonic function and very often numerically easier to handle.
  - e.g. products of probability distributions turn into sums.
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$$NLL = -\ln\left(\prod_i e^{-\frac{1}{2}\left(\frac{x_i-\mu_i}{\sigma_i}\right)^2}\right) \propto \sum_i \left(\frac{x_i-\mu_i}{\sigma_i}\right)^2$$

Number of μ_i'i determines dimension of the Gaussian distribution.

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Number of μ_i'i determines dimension of the Gaussian distribution.

- The minimization usually performed:
  - analytically (like in an optimization exercise in school).
  - numerically (usually the more general solution).
  - by scan of the NLL (for sure the most robust method).

Parameter(s) of Interest (POI)

- Each case/problem defines its own *parameter(s) of interest* (POI's):
  - POI could be the mass κ_3.

- Example:
  signal on top of known background in a binned histogram:

$$\mathcal{L}(\{k_i\},\{\kappa_j\}) = \prod_i \underbrace{\mathcal{P}(k_i,\mu_i(\kappa_j))}_{\text{Product of } pdf\text{s for each bin (Poisson).}}$$

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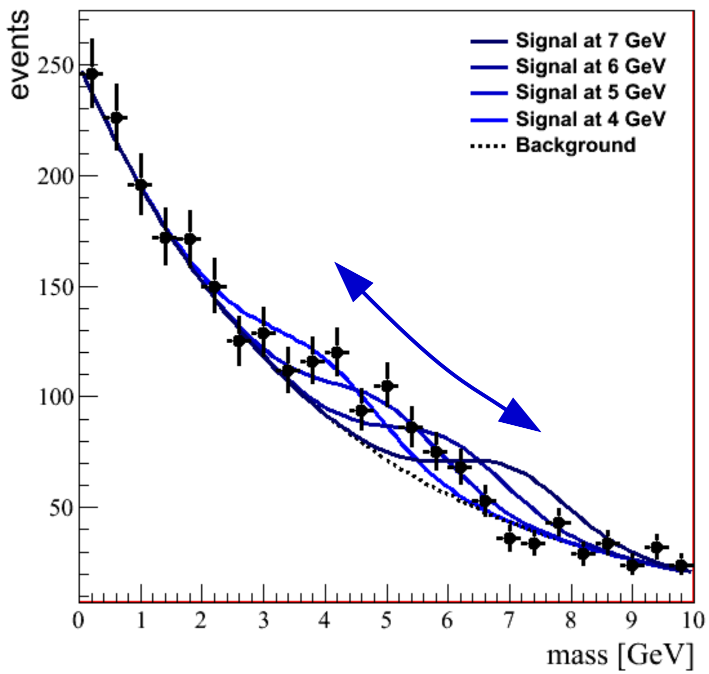

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  - In our case POI usually is the signal strength κ_2 for a fixed value for κ_3.

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Product of *pdf*s for each bin (Poisson).

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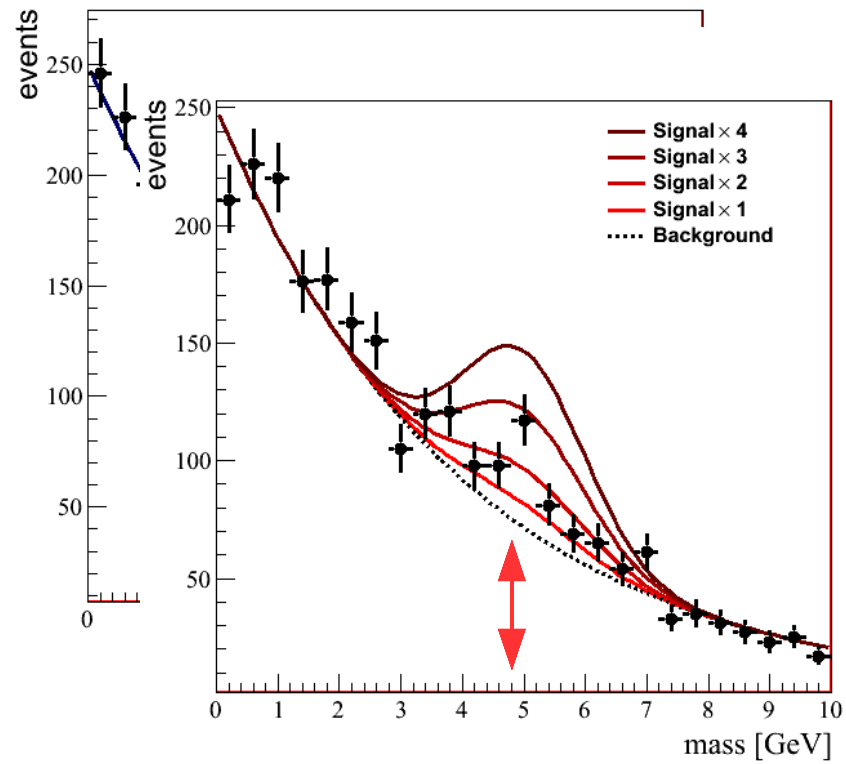

Systematic Uncertainties

- Systematic uncertainties are usually incorporated as *nuisance parameters*:
  - Example: assume background normalization κ_0 is not absolutely known, but with an uncertainty $\sigma(\kappa_0)$:

$$\mu_i(\kappa_j) = \mathcal{P}'(\tilde{\kappa}_0, \kappa_0, \sigma(\kappa_0)) \cdot e^{-\kappa_1 x_i} + \kappa_2 \cdot e^{-(\kappa_3 - x_i)^2}$$

$\tilde{\kappa}_0$: possible values in single measurements; κ_0: expected value; $\sigma(\kappa_0)$: uncertainty

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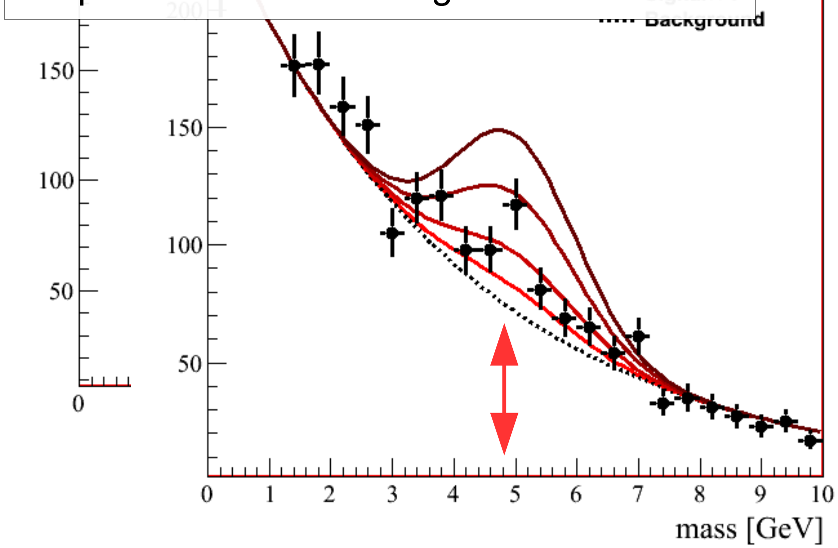


Hypothesis Tests

Hypothesis Separation

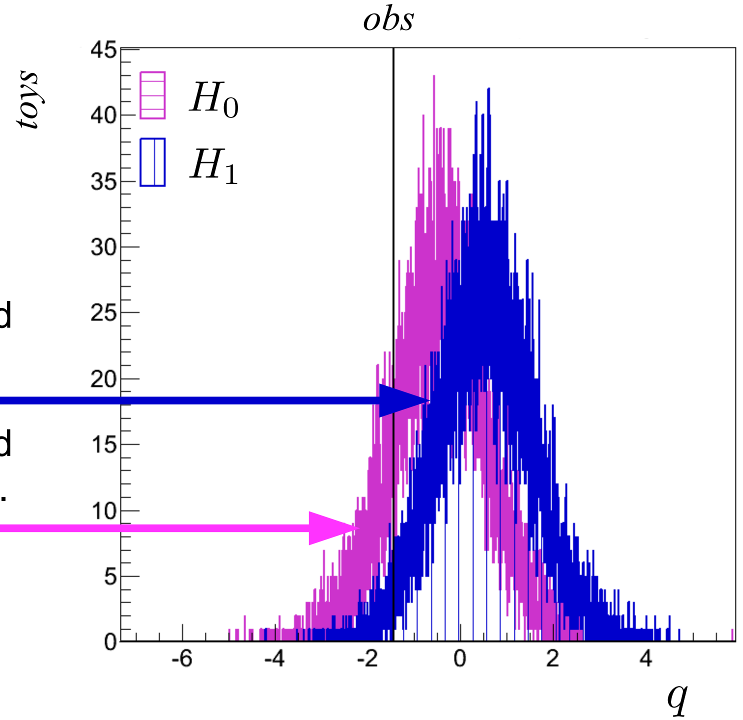
- Start with two alternative hypotheses H_0 & H_1 .
- Define a test statistic $q : \mathbb{R}^n \to \mathbb{R}$ that can distinguish these two hypotheses.
- The test statistic with the best separation power is the likelihood ratio (LR):

$$q = -2\ln\left(\frac{\mathcal{L}(\text{obs})|H_1}{\mathcal{L}(\text{obs})|H_0}\right)$$

- q can be calculated for the observation (obs), for the expectation for H_0 and for the expectation for H_1 :
  - Observed is a single value (outcome of measurement).
  - Expectation is a mean value with uncertainties based on toy measurements.

pdf from toys based on H_1 (usually sig).

pdf from toys based on H_0 (usually BG).



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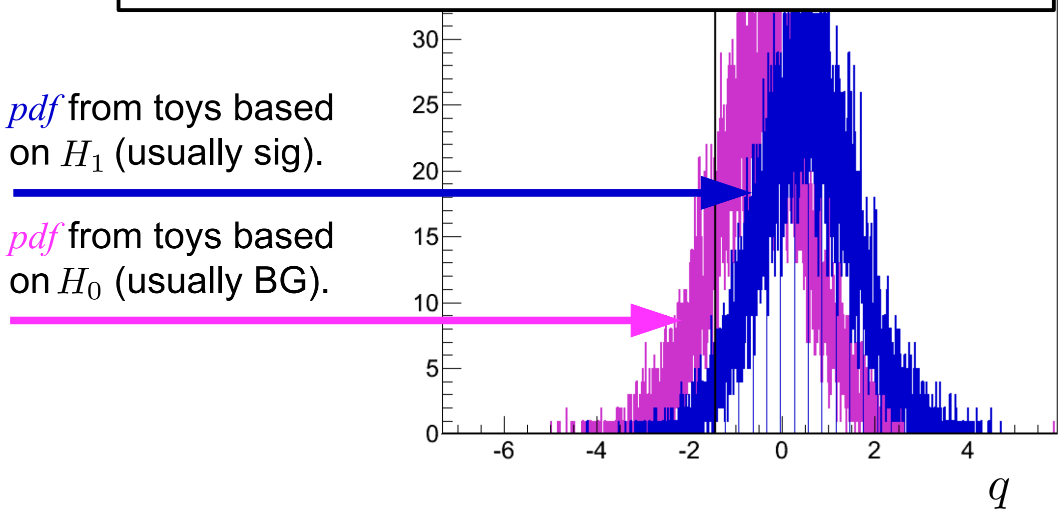
Signal on top of background!

Sorry! No price...



Test Statistics (LEP)

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$$\mathcal{L}(n|\,b(\kappa_j)) = \prod_i \mathcal{P}(n_i|b_i(\kappa_j)) \times \prod_j \mathcal{C}(\kappa_j|\tilde{\kappa}_j)$$

$$\mathcal{L}(n|\,\mu s(\kappa_j) + b(\kappa_j)) = \prod_i \mathcal{P}(n_i|\mu s_i(\kappa_j) + b_i(\kappa_j)) \times \prod_j \mathcal{C}(\kappa_j|\tilde{\kappa}_j)$$

$$q_\mu = -2\ln\left(\frac{\mathcal{L}(\,n|\mu s+b)}{\mathcal{L}(\,n|b)}\right), \quad 0 \leq \mu$$

nuisance parameters $\tilde{\kappa}_j$ integrated out (by throwing toys → MC method) before evaluation of q_μ (→marginalization).

Test Statistics (Tevatron)

- Start with two alternative hypotheses H_0 & H_1 .
- Define a test statistic $q : \mathbb{R}^n \to \mathbb{R}$ that can distinguish these two hypotheses.
- The test statistic with the best separation power is the likelihood ratio (LR):

$$q = -2\ln\left(\frac{\mathcal{L}(\mathrm{obs})|H_1}{\mathcal{L}(\mathrm{obs})|H_0}\right)$$

$$\mathcal{L}(n|\,b(\kappa_j)) = \prod_i \mathcal{P}(n_i|b_i(\kappa_j)) \times \prod_j \mathcal{C}(\kappa_j|\tilde{\kappa}_j)$$

$$\mathcal{L}(n|\,\mu s(\kappa_j) + b(\kappa_j)) = \prod_i \mathcal{P}(n_i|\mu s_i(\kappa_j) + b_i(\kappa_j)) \times \prod_j \mathcal{C}(\kappa_j|\tilde{\kappa}_j)$$

$$q_\mu = -2\ln\left(\frac{\mathcal{L}(\,n|\mu s(\hat{\kappa}_\mu)+b(\hat{\kappa}_\mu))}{\mathcal{L}(\,n|b(\hat{\kappa}_{\mu=0}))}\right), \quad 0 \leq \mu$$

nominator maximized for given μ before marginalization. Denominator for $\mu = 0$. Better estimates on nuisance parameters. Reduces uncertainties on nuisance parameters.

Test Statistics (LHC)

- Start with two alternative hypotheses H_0 & H_1.
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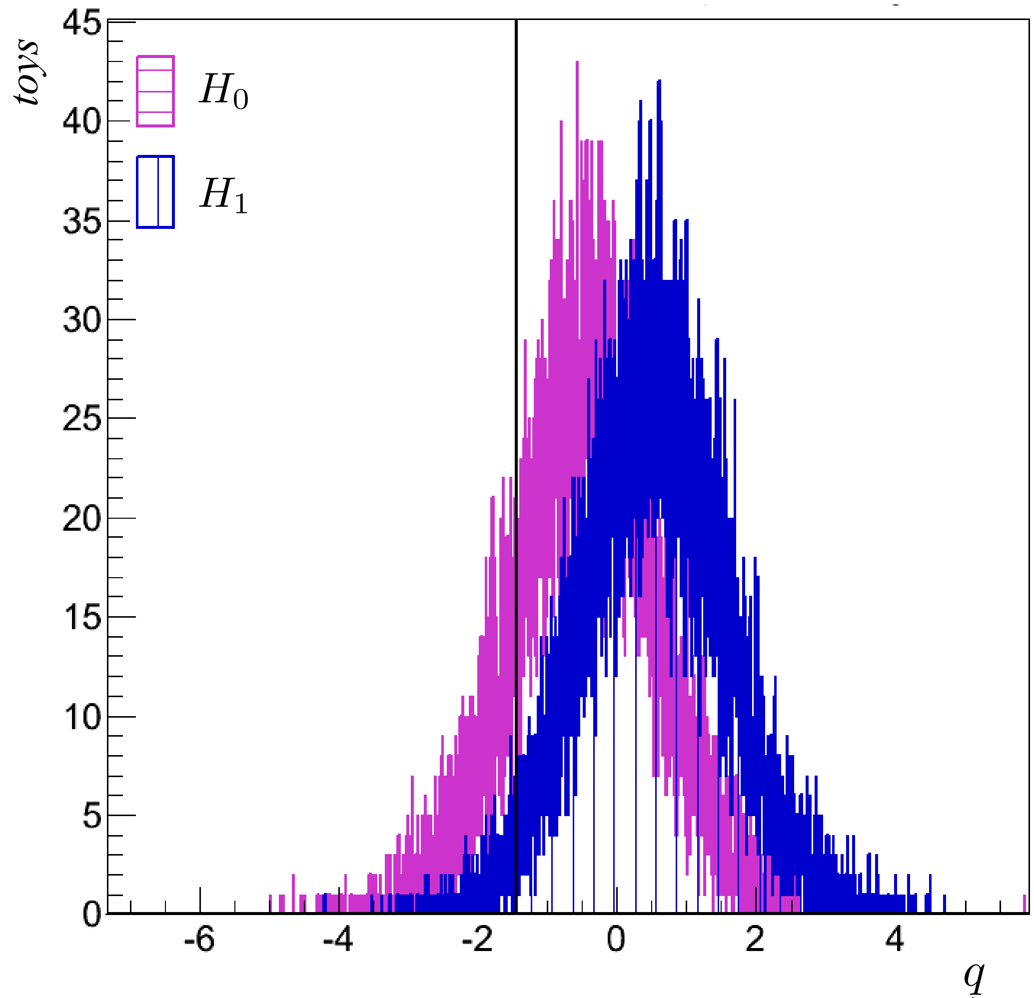
nominator maximized for given μ before marginalization. For the denominator a global maximum is searched for at $\hat{\mu}$. In addition allows use of asymptotic formulas (→ no need for toys).

Classical Hypothesis Testing

- Classical hypothesis test interested in probability to observe q_{obs} given that H_0 or H_1 is true:

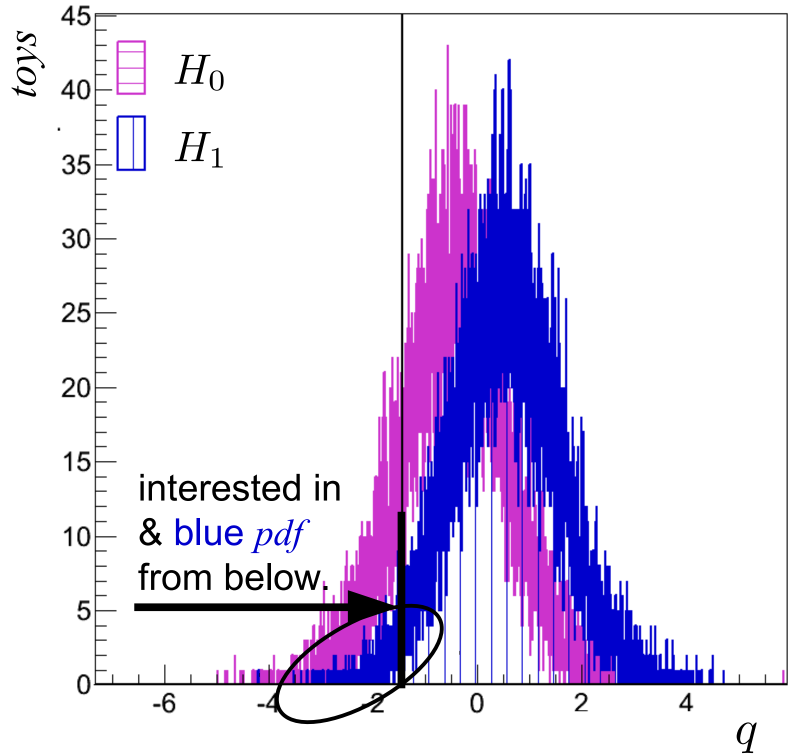
$q \leq q_{\mathrm{obs}}\|_{H_1}$	$q \geq q_{\mathrm{obs}}\|_{H_1}$
$q \leq q_{\mathrm{obs}}\|_{H_0}$	$q \geq q_{\mathrm{obs}}\|_{H_0}$
q_{obs} defines upper bound	q_{obs} defines lower bound

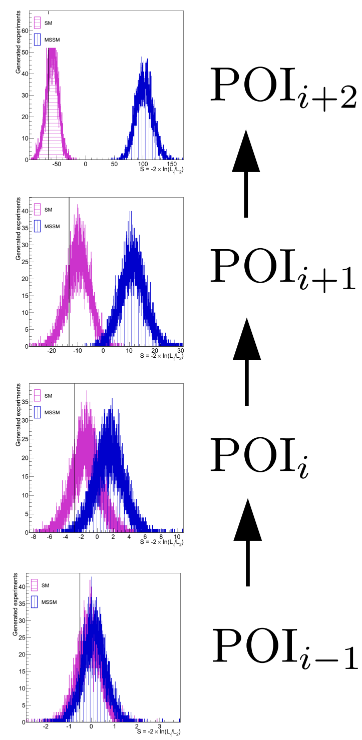
- We are usually interested in "upper limits", which corresp. to "lower bounds" (→ how often signal ≤ observed deviation?).



95% CL Upper Limits

- Our *pdf*'s usually depend on another parameter, which is the actual *POI* (μ in SM, $\tan\beta$ in MSSM case).
- Traditionally we set 95% CL upper limits on this POI.





- *pdf*'s move apart from each other.
- The more separate the *pdf*'s are the more H_0 & H_1 are distinguishable.
- Find POI_i for which:

  $$\mathcal{I}_{\mathrm{POI}} = \int_{-\infty}^{q_{\mathrm{obs}}} pdf = 0.05$$

  for this POI_i in 95% of all toys $q \geq q_{\mathrm{obs}}$.

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95% CL Upper Limit:

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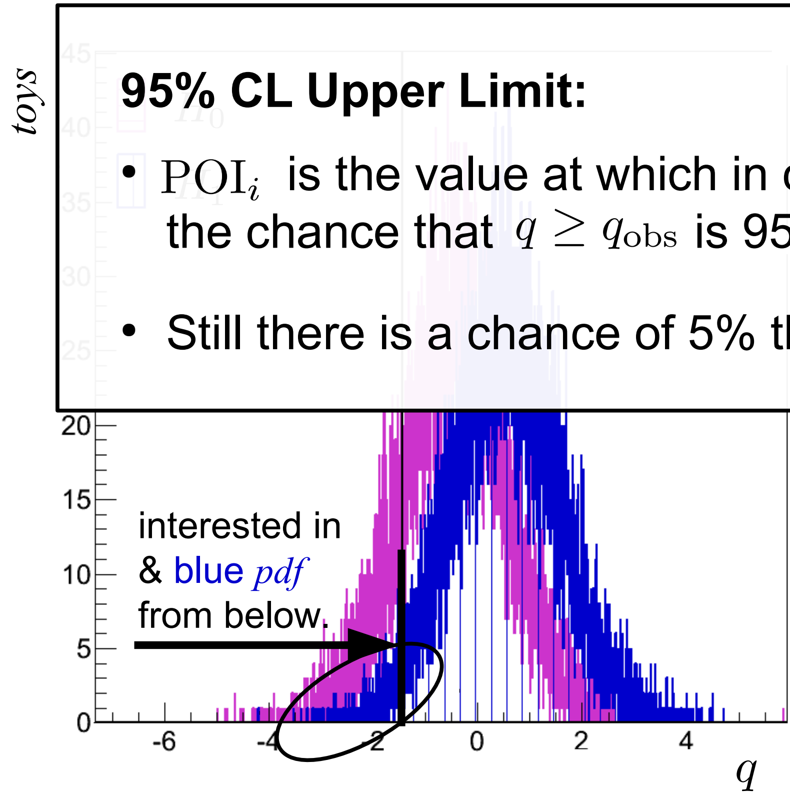
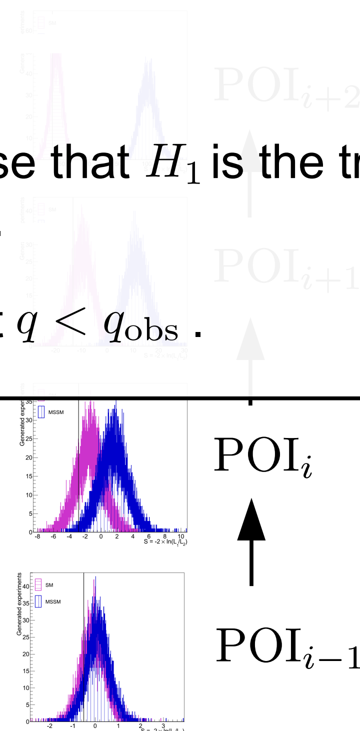
- Still there is a chance of 5% that $q < q_{\mathrm{obs}}$.





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- Assume our POI is μ: does the 90% CL upper limit on μ correspond to a higher or a lower value $\mu_{90\%}$? ⟶ It's lower!

$\mu_{99\%}$ ⟶ 1%

$\mu_{95\%}$

$\mu_{90\%}$ ⟶ 10%

probability of q to be "more background like" than q_{obs}.

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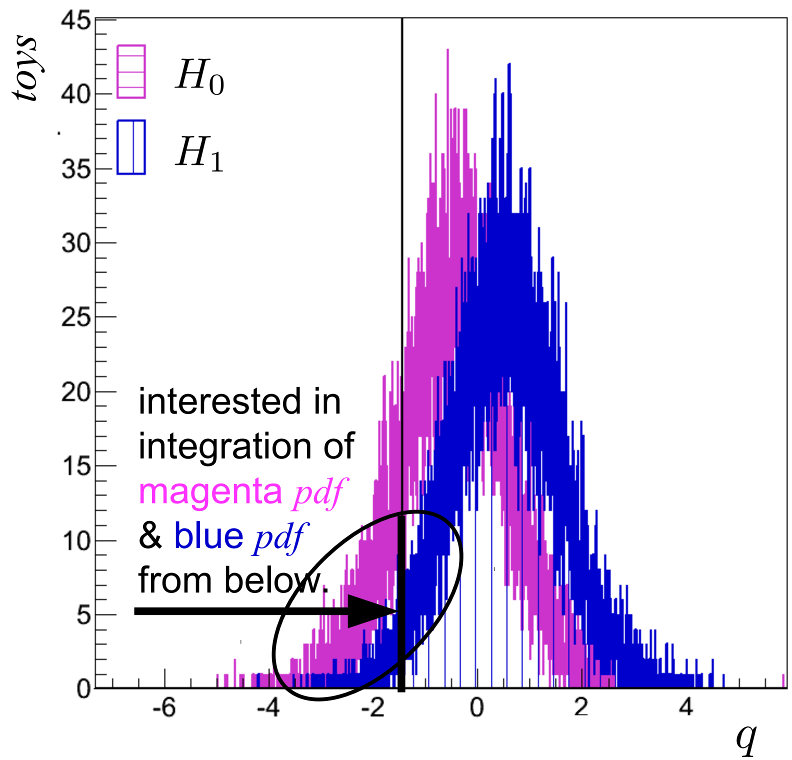
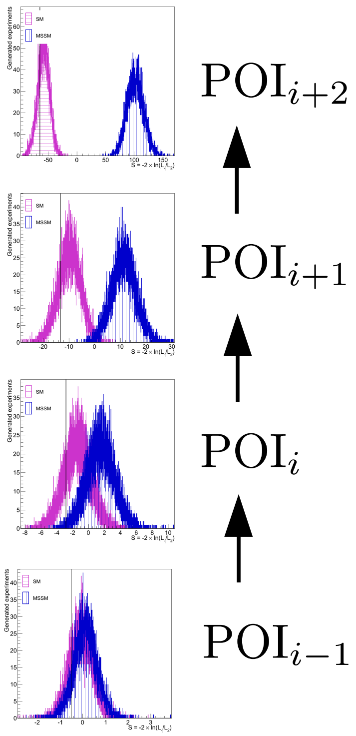
CLs Limits

- In particle physics we set more conservative limits than this, following the *CLs* method:
- Assume H_1 to be signal+background and H_0 to be background only hypothesis.





$$\mathrm{CL(S+B)} = \int_{-\infty}^{q_{\mathrm{obs}}} pdf_{H_1}$$

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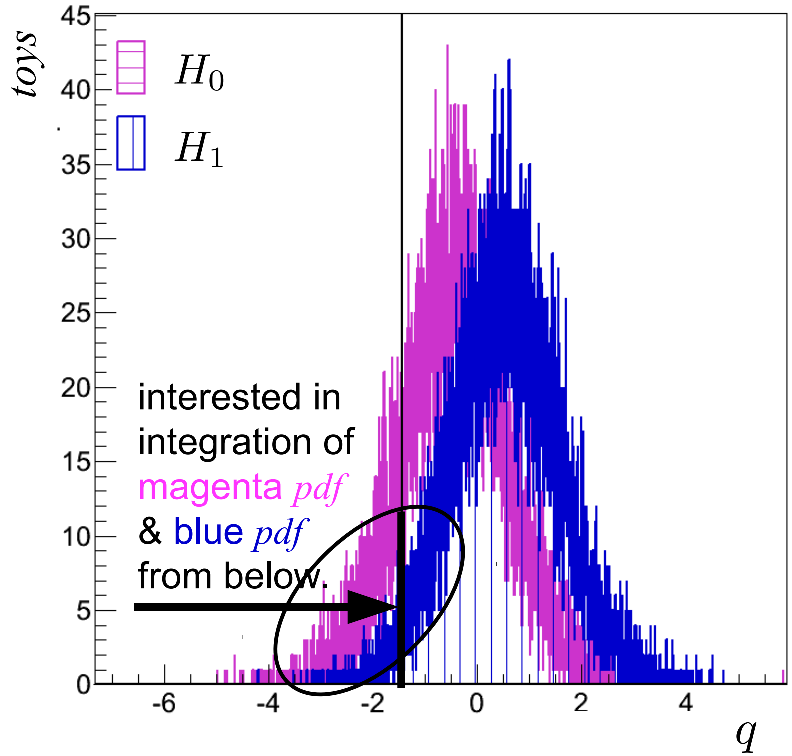

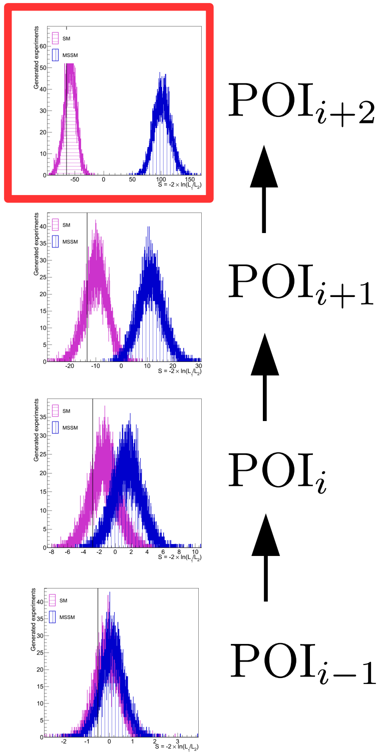

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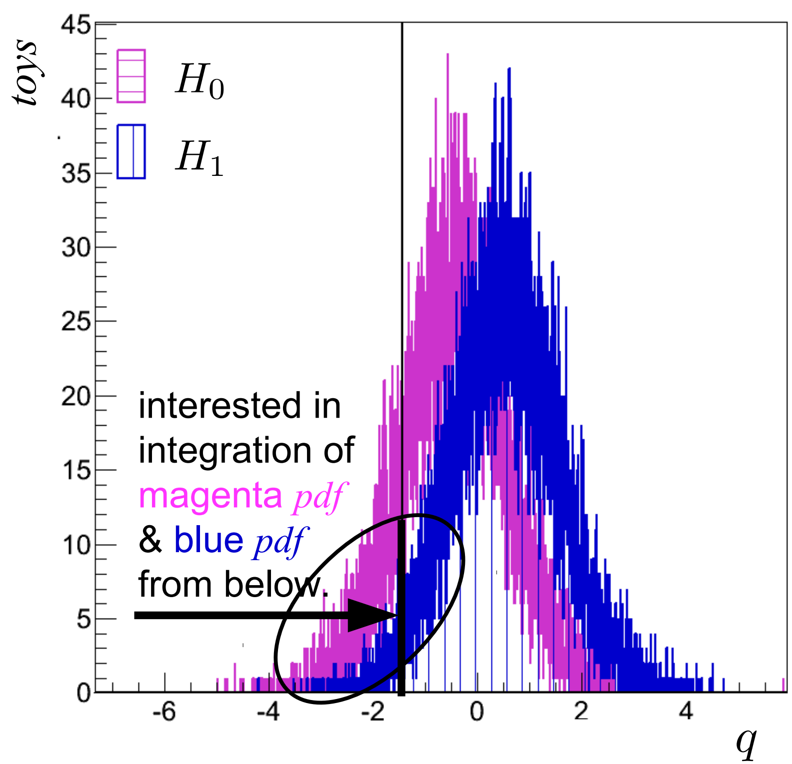

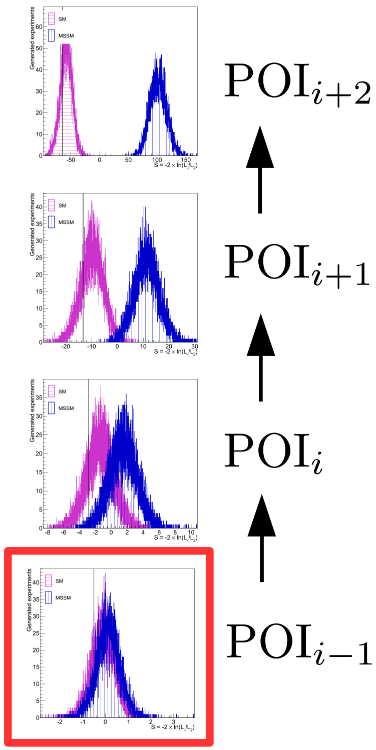

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- If H_0 & H_1 are clearly distinguishable $\mathrm{CL_S} \rightarrow \mathrm{CL(S+B)}$.
- If they cannot be distinguished $\mathrm{CL_S} > \mathrm{CL(S+B)}$.

CLs Limits (more schematic)

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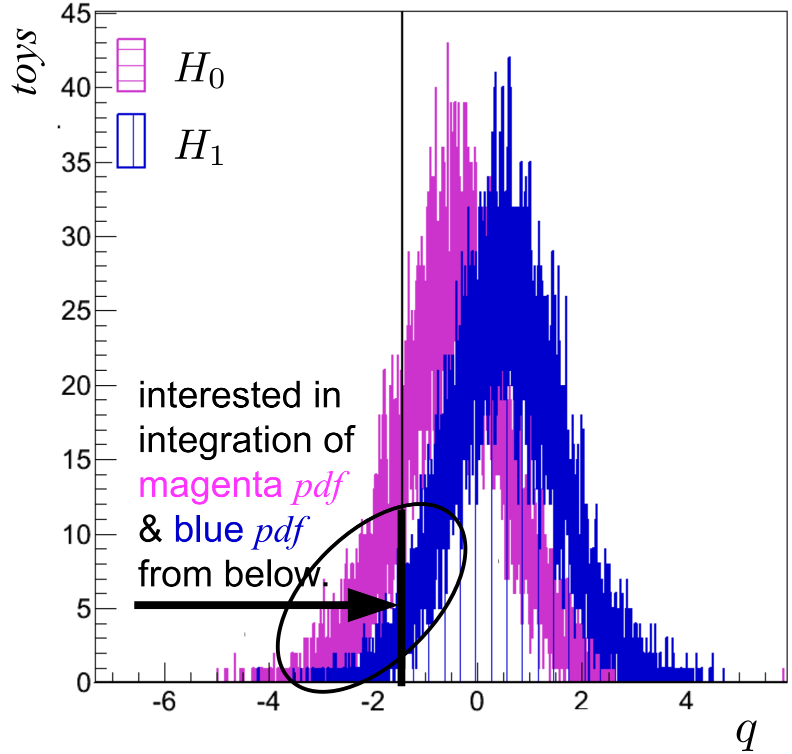
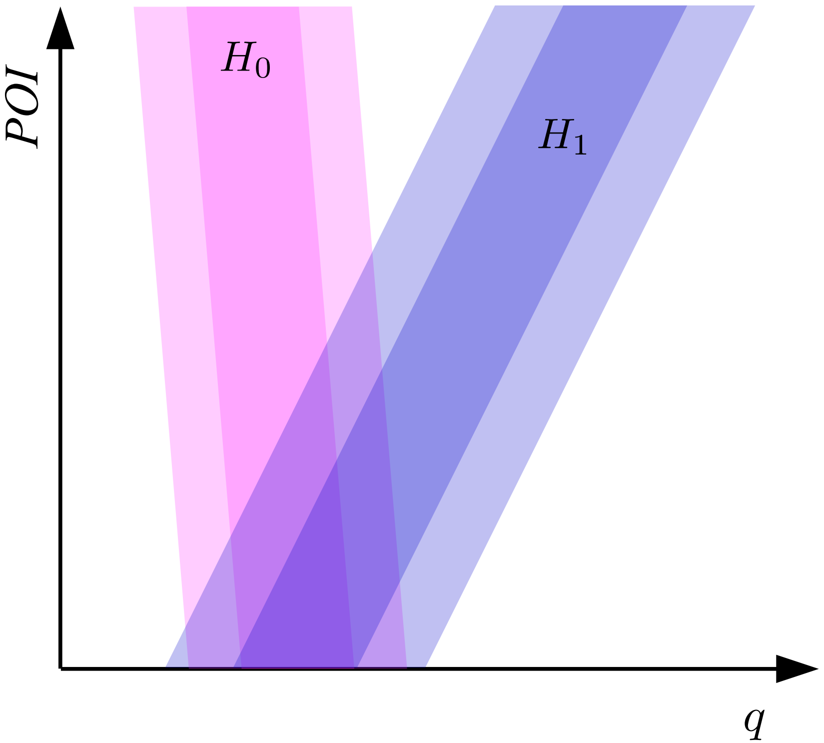
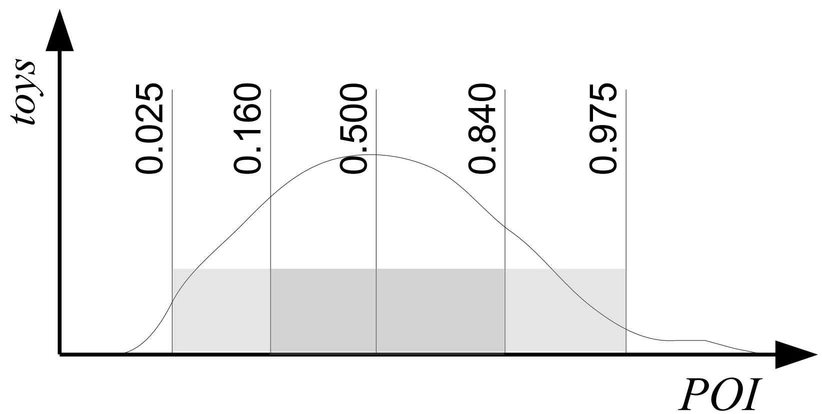
- Assume H_1 to be signal+background and H_0 to be background only hypothesis.

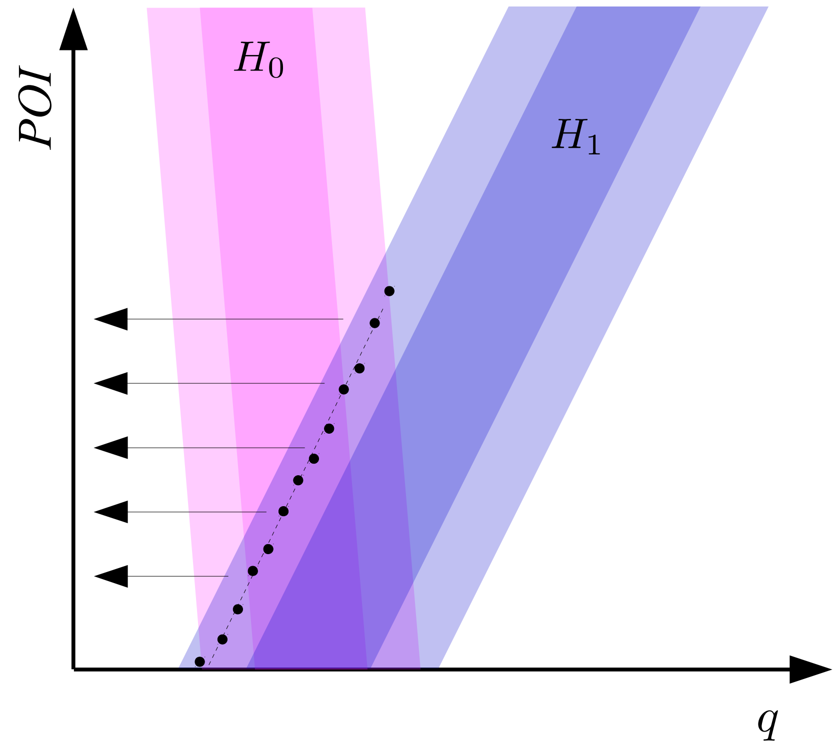




Expected Limit (canonical approach)

- To obtain the expected limit mimic calculation of observed, but base it on toy experiments.
- Make use of the fact that the *pdf*'s do not depend on toys (i.e. schematic plot on the left does not change).
- Throw number of toys under the BG only hypothesis (H_0) determine distribution of 95% CL limits on *POI*.





- Obtain quantiles for expected limit from this distribution.

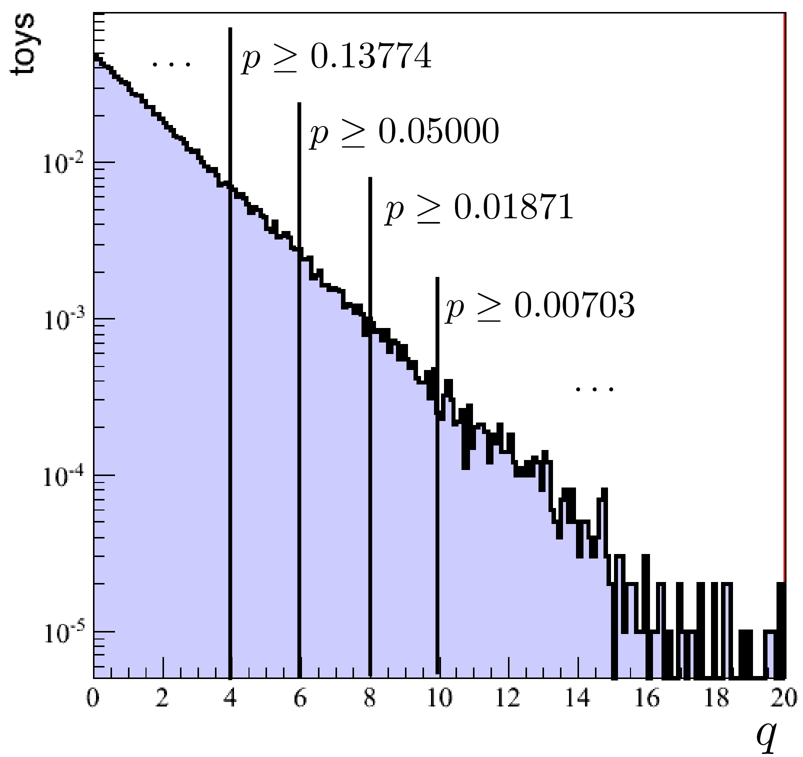
And if the signal shows up...

p-Value

- How do we know whether what we see is not just a background fluctuation?
- The p-value is the probability $\mathcal{P}(q \geq q_{\text{obs}}|H_0)$ to observe values of q larger than q_{obs} under the assumption that the background only hypothesis H_0 is the true hypothesis.
- Think of...

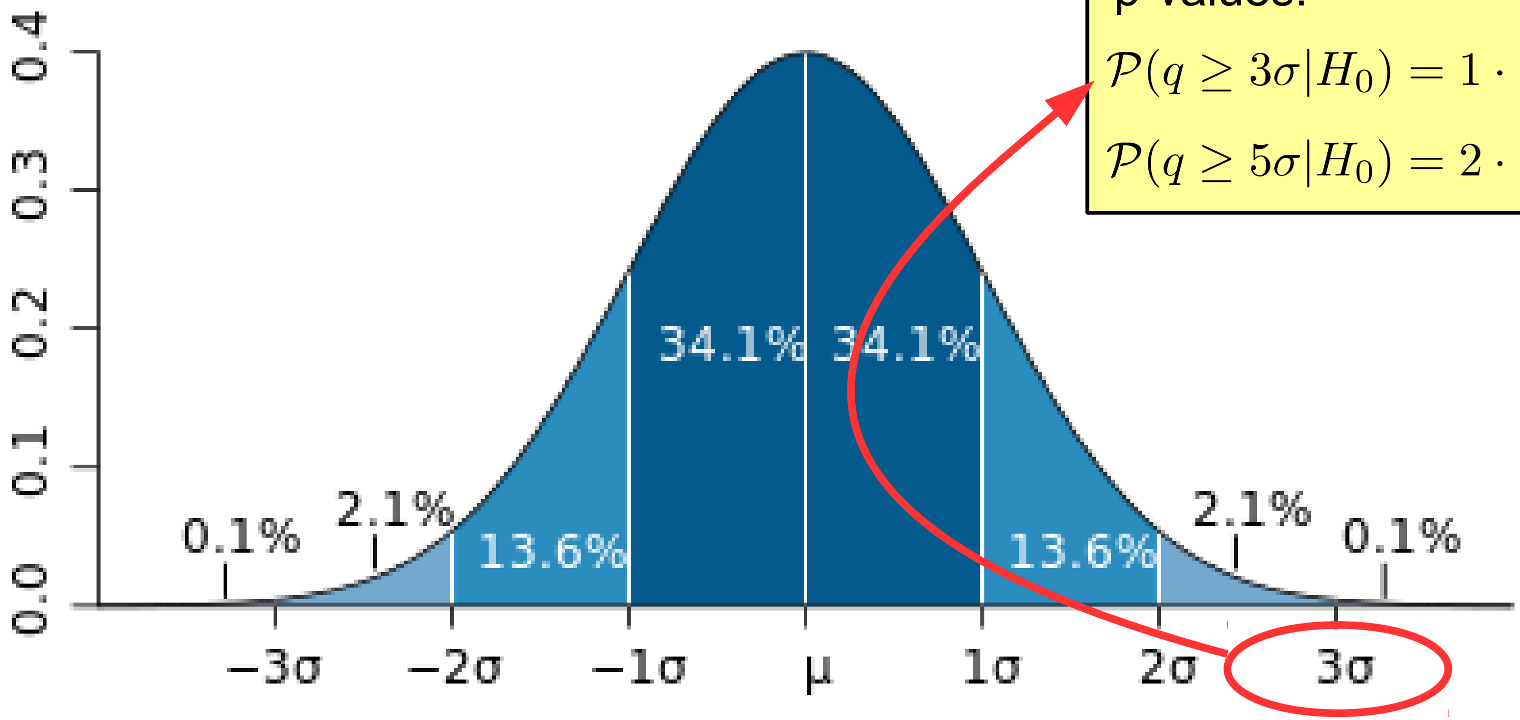
  … the limit as a way to falsify the signal plus background hypothesis (H_1).

  … the p-value as a way to falsify the background only hypothesis (H_0).



Significance

- If the measurement is normal distributed q is distributed according to a χ^2 distribution.
- The χ^2 probability can then be interpreted as a Gaussian confidence interval.



p-values:

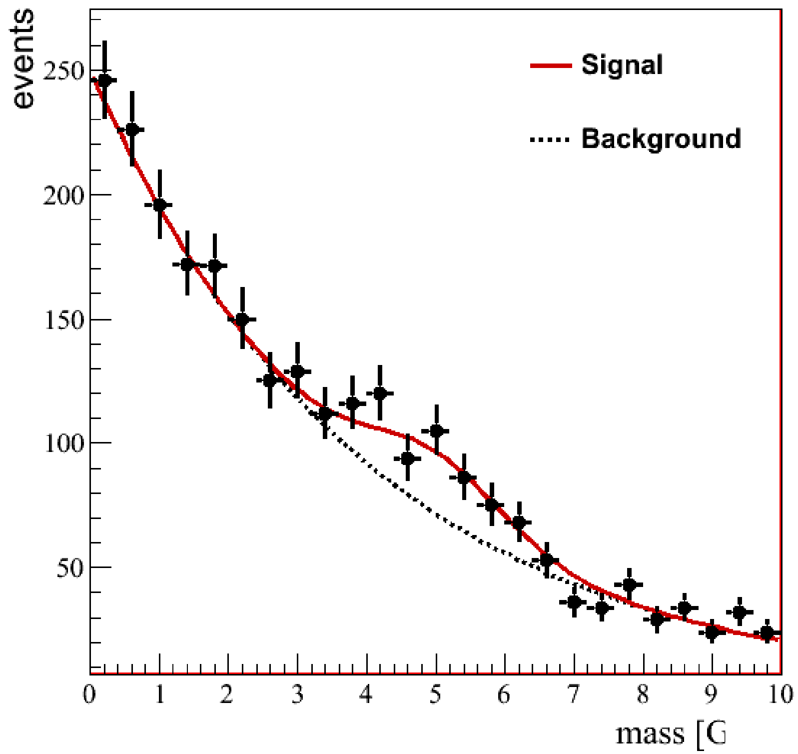
$$\mathcal{P}(q \geq 3\sigma | H_0) = 1 \cdot 10^{-3}$$

$$\mathcal{P}(q \geq 5\sigma | H_0) = 2 \cdot 10^{-5}$$

Significance (in practice)

- If the measurement is normal distributed q is distributed according to a χ^2 distribution.
- The χ^2 probability can then be interpreted as a Gaussian confidence interval.
- Usual approximation in practice is to estimate significances by:

$$\mathcal{S} = \frac{n_{\mathrm{obs}} - n_b}{\sqrt{n_b}}$$



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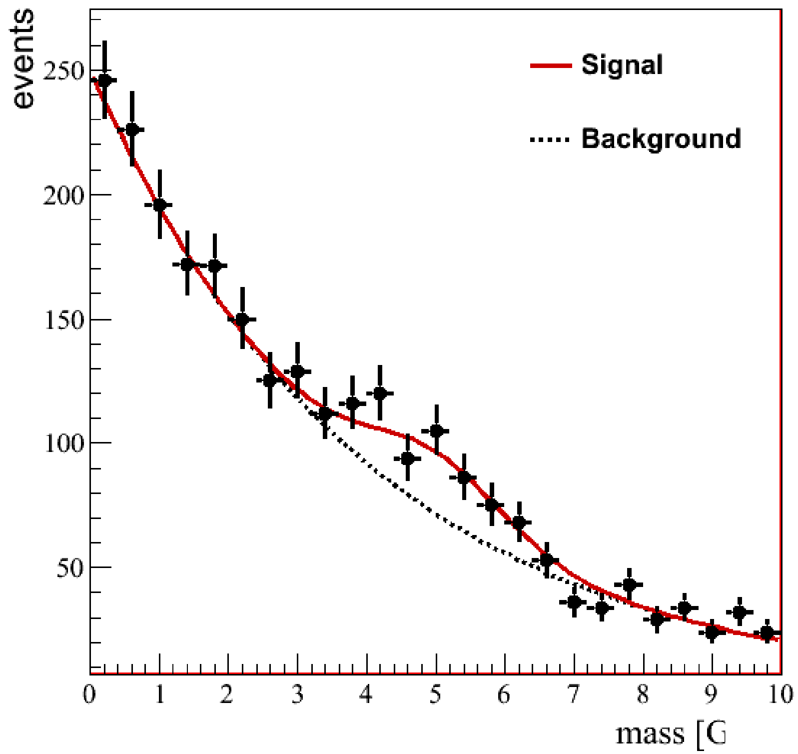

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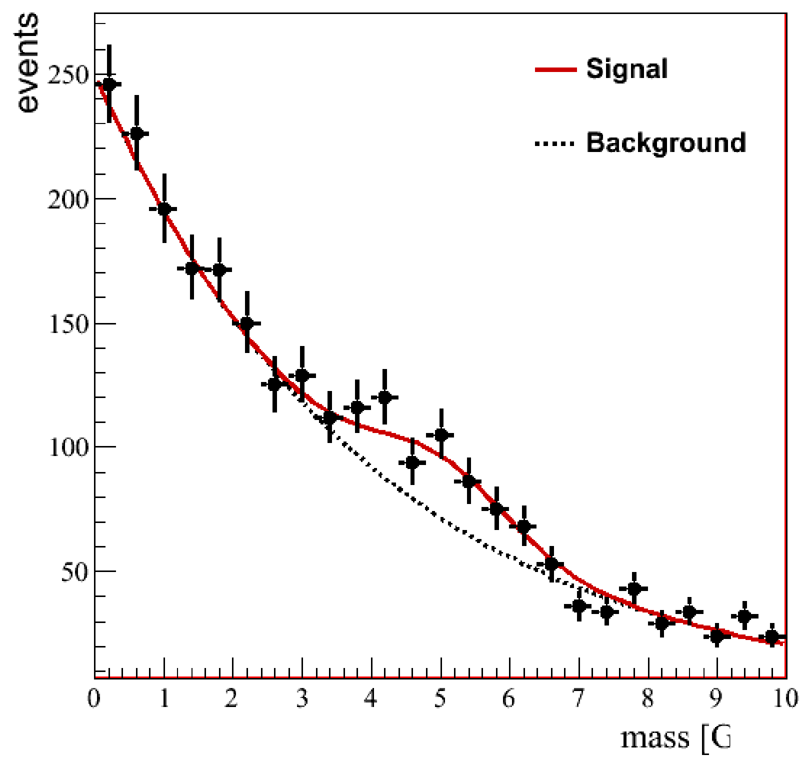
Poisson uncertainty on expected background events.



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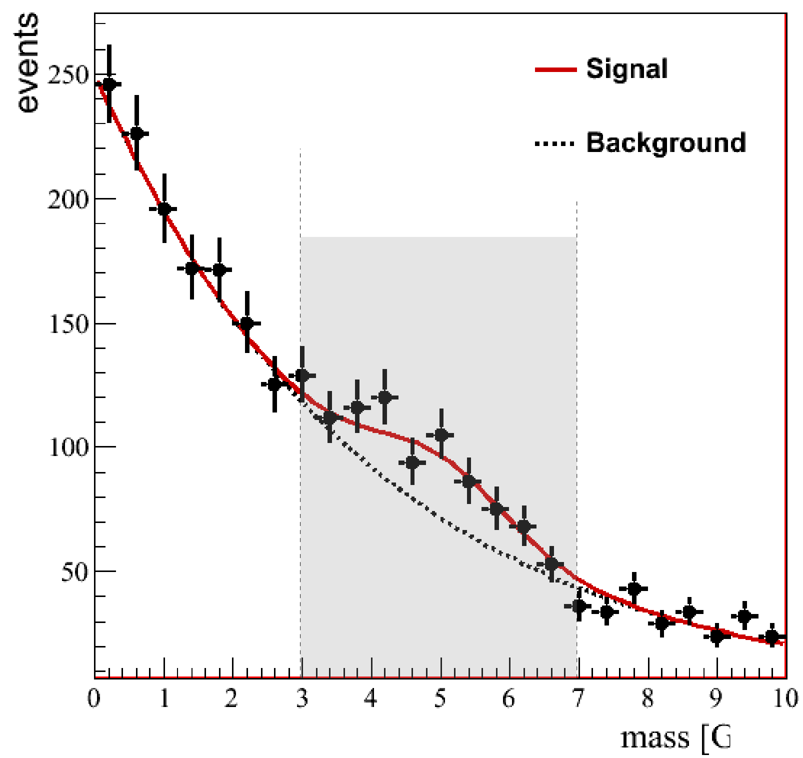

Concluding Remarks

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- Reviewed all statistical tools necessary to search for the Higgs signal ($\rightarrow$ as a small signal above a known background):
  - Probability distributions, likelihood functions, limits, p-values, ...
- Limits are a usual way to 'exclude' the signal hypothesis (H_1).
- p-values are a usual way to 'exclude' the background hypothesis (H_0).
- Under the assumption that the test statistic q is χ^2 distributed p-values can be translated into Gaussian confidence intervals σ.
- In particle physics we call an observation with $\geq 3\sigma$ an evidence.
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- In particle physics we call an observation with $\geq 3\sigma$ an evidence.
- We call an observation with $\geq 5\sigma$ a discovery.
- Once a measurement is established the search is over! Measurements of properties are new and different world!

Sneak Preview for Next Week

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- Review indirect estimates of the Higgs mass and searches for the Higgs boson that have been made before 2012:
- Estimates of m_t and m_H from high precision measurements at the Z-pole mass at LEP.
- Direct searches for the Higgs boson at LEP.
- Direct searches for the Higgs boson at the Tevatron.
- For the remaining lectures we then will turn towards the discovery of the Higgs boson at the LHC.

During the next lectures we will see 1:1 life examples of all methods that have been presented here.

Backup & Homework Solutions