

Course Outline

Previously in this course:

Statistics basics

Describing measurements

Determining the value of a parameter

Today:

Computing statistical results:

Discovery testing

Confidence intervals

Limits

Expected limits

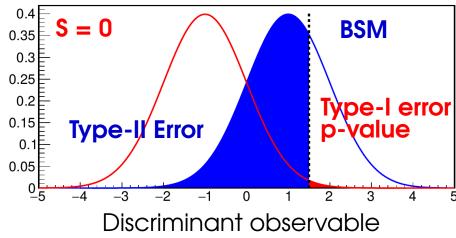
Hypothesis Testing

Hypothesis: assumption on model parameters, say value of S (e.g. H_0 : S=0)

	Data disfavors H ₀ (Discovery claim)		Data favors H (Nothing found	•
H ₀ is false (New physics!)	Discovery!		Type-II error (Missed discovery)	
H ₀ is true (Nothing new)	Type-I error (False discovery)		No new physics, none found	

Lower Type-I errors \Leftrightarrow **Higher Type-II errors** and vice versa: cannot have everything!

→ Goal: test that minimizes Type-II errors for given level of Type-I error.



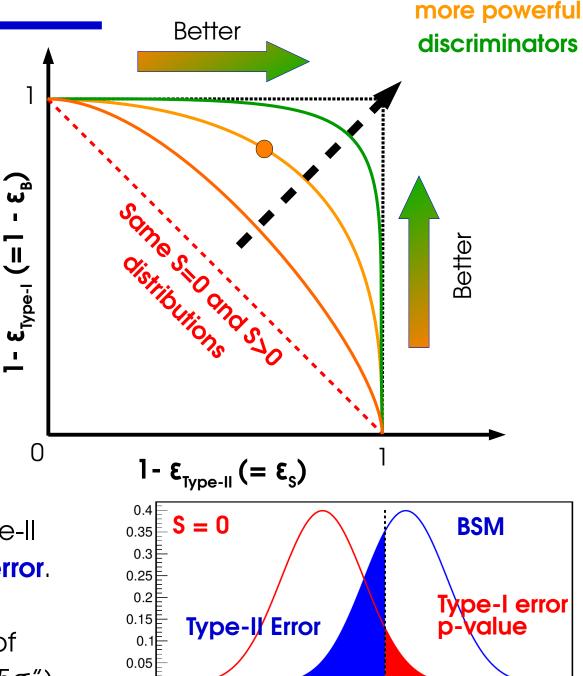
ROC Curves

"Receiver operating characteristic" (ROC) Curve:

- → Plot Type-I vs Type-II rates for different cut values
- \rightarrow All curves monotonically decrease from (0,1) to (1,0)
- → Better discriminators more bent towards (1,1)



→ Usually set predefined level of acceptable Type-I error (e.g. "5σ")



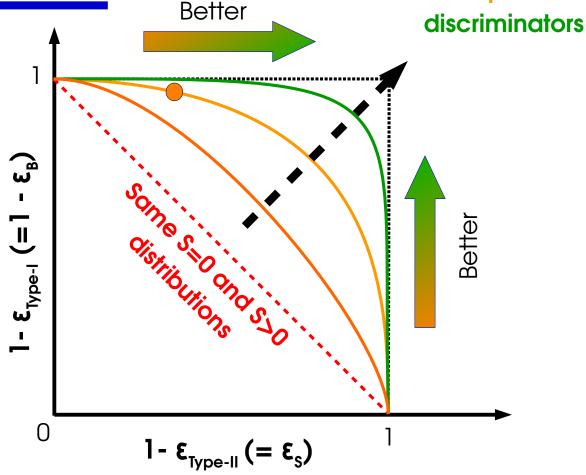
Discriminant observable

Increasingly

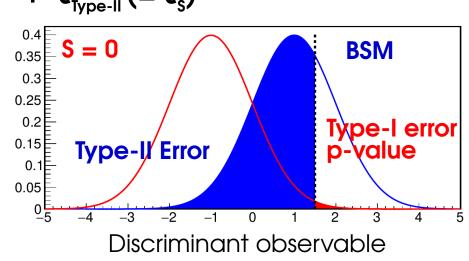
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Increasingly

more powerful

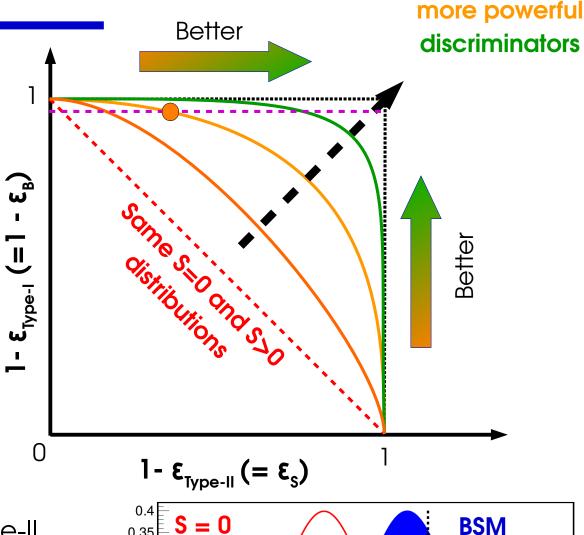
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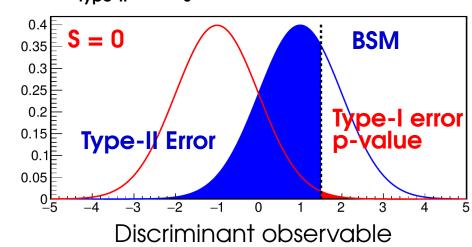
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Increasingly

Hypothesis Testing with Likelihoods

Neyman-Pearson Lemma

When comparing two hypotheses H_0 and H_1 , the optimal discriminator is the **Likelihood ratio** (LR)

$$\frac{L(\mathbf{H}_{1}; data)}{L(\mathbf{H}_{0}; data)}$$

e.g.
$$L(S = 5; data)$$

 $L(S = 0; data)$

Caveat: Strictly true only for *simple* hypotheses (no free parameters)

As for MLE, choose the hypothesis that is more likely **given the data we have**.

- → Minimizes Type-II uncertainties for given level of Type-I uncertainties
- → Always need an **alternate hypothesis** to test against.
- → In the following: all tests based on LR, will focus on p-values (Type-I errors), trusting that Type-II errors are anyway as small as they can be...

Discovery: Test Statistic

Discovery:

H₀: background only (S = 0) against

S=0

- H_{1} : presence of a signal (S > 0)
- \rightarrow For H₁, any S>0 is possible, which to use ? The one preferred by the data, \hat{S} .

⇒ Use Likelihood ratio:
$$\frac{L(S=0)}{L(\hat{S})}$$

→ In fact use the **test statistic**

$$q_0 = -2\log\frac{L(S=0)}{L(\hat{S})}$$

Note: for $\hat{S} < 0$, set $q_0 = 0$ to reject negative signals ("one-sided test statistic")

Discovery p-value

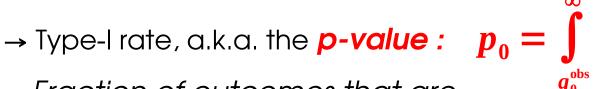
Large values of
$$-2\log\frac{L(S=0)}{L(\hat{S})}$$
 if:

- ⇒ observed Ŝ is far from 0
- \Rightarrow $H_0(S=0)$ distavored compared to $H_1(S\neq 0)$.

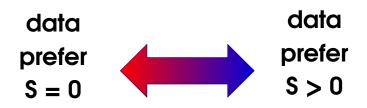
How large q₀ before we can exclude H₀?

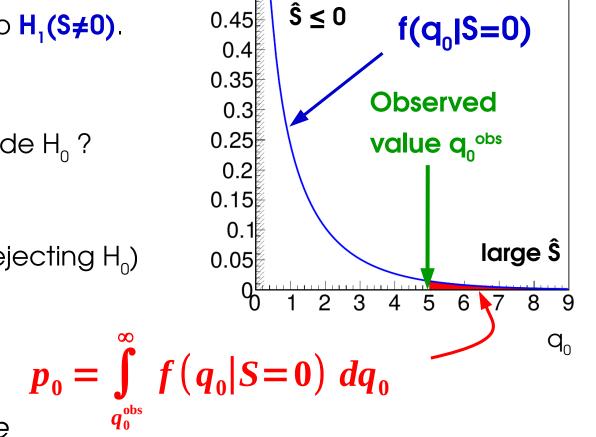
(and claim a discovery!)

→ Need small Type-I rate (falsely rejecting H_n)



= Fraction of outcomes that are





0.5₽

at least as extreme (signal-like) as data, when H_0 is true (no signal).

Asymptotic distribution of q₀

Gaussian regime for \$ (e.g. large n_{evts}, Central-limit theorem):

Wilk's Theorem (*) : for S = 0

q_0 is distributed as χ^2 (n_{par})

$$\Rightarrow$$
 n_{par} = 1 : $\sqrt{q_0}$ is distributed as a Gaussian

→ Can compute p-values from Gaussian quantiles

$$p_0 = 1 - \Phi(\sqrt{q_0})$$

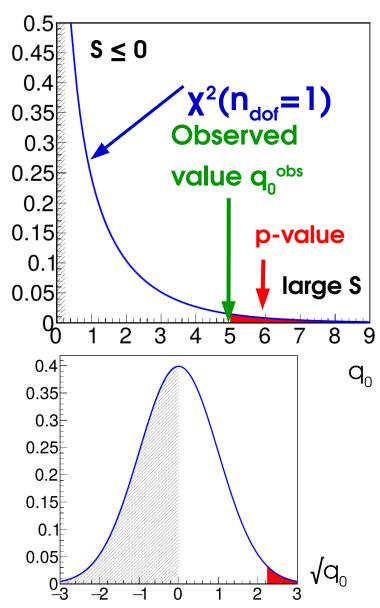
⇒ Even more simply, the significance is:

$$Z = \sqrt{q_0}$$

Typically works well already for for event counts of O(5) and above ⇒ Widely applicable

(*) 1-line "proof": asymptotically L and S are Gaussian, so

$$L(S) = \exp \left[-\frac{1}{2} \left(\frac{S - \hat{S}}{\sigma} \right)^2 \right] \Rightarrow q_0 = \left(\frac{\hat{S}}{\sigma} \right)^2 \Rightarrow \sqrt{q_0} = \frac{\hat{S}}{\sigma} \sim G(0, 1) \Rightarrow q_0 \sim \chi^2(n_{\text{dof}} = 1)$$

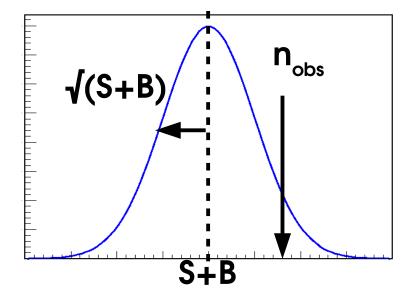


Homework 1: Gaussian Counting

Count number of events n in data

- → assume n large enough so process is Gaussian
- → assume B is known, measure S

Likelihood:
$$L(S; n_{\text{obs}}) = e^{-\frac{1}{2} \left(\frac{n_{\text{obs}} - (S+B)}{\sqrt{S+B}}\right)^2}$$



- \rightarrow Find the best-fit value (MLE) \hat{S} for the signal (can use $\lambda = -2 \log L$ instead of L for simplicity)
- \rightarrow Find the expression of q_0 for $\hat{S} > 0$.
- → Find the expression for the significance

$$Z = \frac{\hat{S}}{\sqrt{B}}$$

Homework 2: Poisson Counting

Same problem but now **not** assuming Gaussian behavior:

$$L(S;n)=e^{-(S+B)}(S+B)^n$$

(Can remove the n! constant since we're only dealing with L ratios)

- \rightarrow As before, compute \hat{S} , and q_0
- \rightarrow Compute Z = $\sqrt{q_0}$, assuming asymptotic behavior

Solution:

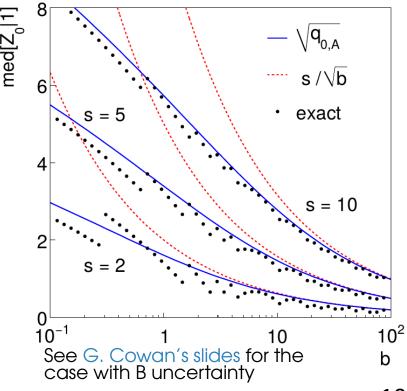
$$Z = \sqrt{2\left[\left(\hat{S} + B\right)\log\left(1 + \frac{\hat{S}}{B}\right) - \hat{S}\right]}$$

Exact result can be obtained using

pseudo-experiments \rightarrow close to $\sqrt{q_0}$ result

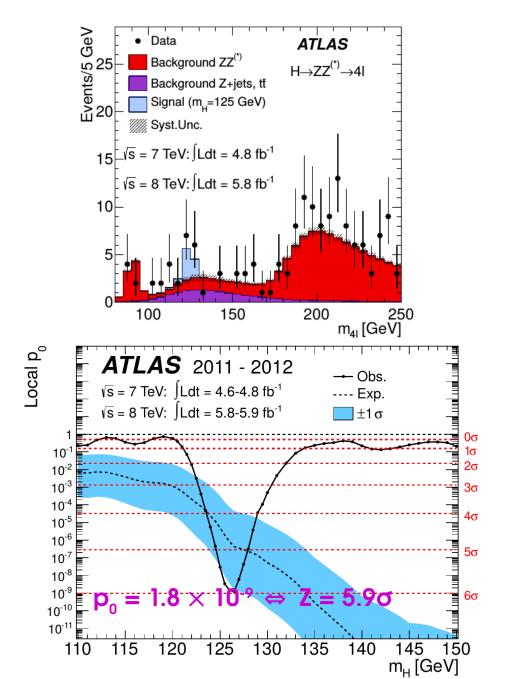
Asymptotic formulas justified by Gaussian regime, but remain valid even for small values of S+B (down to 5 events!)

Eur.Phys.J.C71:1554,2011

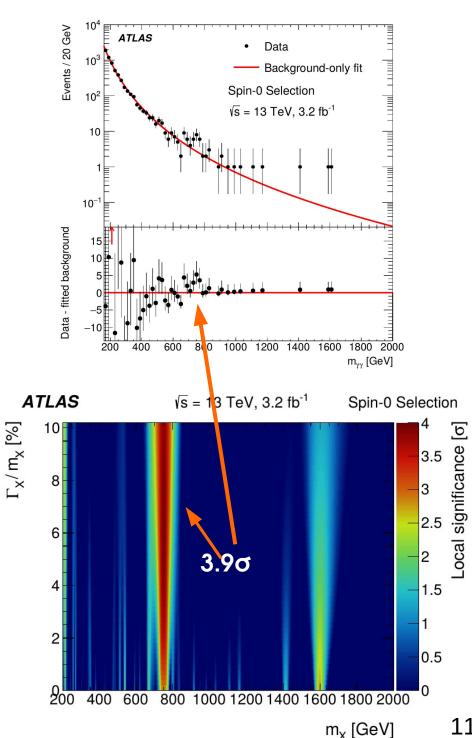


Some Examples

Higgs Discovery: Phys. Lett. B 716 (2012) 1-29



High-mass X→yy Search: JHEP 09 (2016) 1



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Discovery Thresholds

Evidence: $3\sigma \Leftrightarrow p_0 = 0.3\% \Leftrightarrow 1$ chance in 300

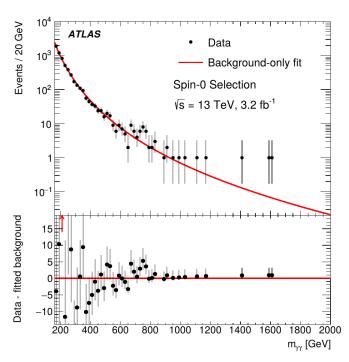
Discovery: $5\sigma \Leftrightarrow p_0 = 3 \cdot 10 - 7 \Leftrightarrow 1 \text{ chance in } 3.5\text{M}$

Why so high thresholds? (from Louis Lyons):

 Look-elsewhere effect: searches typically cover multiple independent regions ⇒ Higher chance to have a fluctuation "somewhere"

 $N_{trials} \sim 1000 : local 5\sigma \Leftrightarrow O(10^{-4})$ more reasonable

 Mismodeled systematics: factor 2 error in syst-dominated analysis ⇒ factor 2 error on Z...



History: 3
 o and 4
 o excesses do occur regularly, for the reasons above

Extraordinary claims require extraordinary evidence!

Takeaways

Given a statistical model P(data; μ), define likelihood $L(\mu) = P(data; \mu)$

To estimate a parameter, use the value $\hat{\mathbf{p}}$ that maximizes $L(\mu) \rightarrow \text{best-fit value}$

To decide between hypotheses H_n and H_{τ} , use the likelihood ratio

$$\frac{L(H_0)}{L(H_1)}$$

To test for **discovery**, use

$$q_0 = -2\log\frac{L(S=0)}{L(\hat{S})} \quad \hat{S} \ge 0$$

For large enough datasets (n >~ 5), $Z = \sqrt{a_n}$

$$Z = \sqrt{q_0}$$

For a Gaussian measurement, $Z = \frac{\hat{S}}{\sqrt{R}}$

$$Z = \frac{\hat{S}}{\sqrt{B}}$$

For a Poisson measurement, $Z = \sqrt{2\left[(\hat{S} + B) \log \left(1 + \frac{\hat{S}}{B} \right) - \hat{S} \right]}$

Outline

Computing statistical results

Discovery Testing

Confidence intervals

Upper limits on signal yields

Expected limits

Confidence Intervals

Last lecture we saw how to estimate (=compute) the value of a parameter

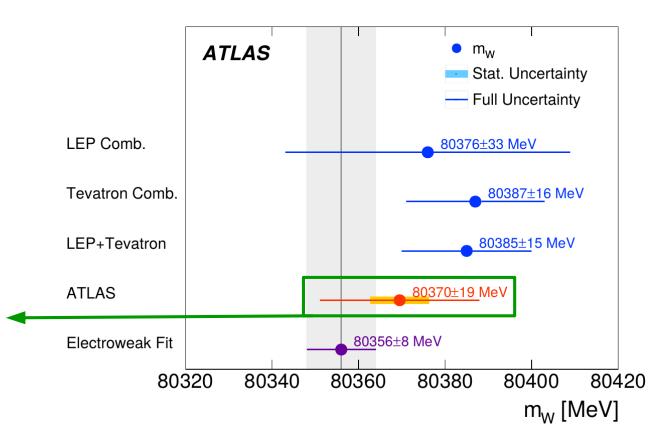
Maximum Likelihood Estimator (MLE) µ:

$$\hat{\mathbf{\mu}} = arg \, max \, L(\mathbf{\mu})$$

However we also need to estimate the associated uncertainty.

What is the meaning of an uncertainty?

We don't know what the true value is, but there is a 68% chance that it is within the orange interval



Gaussian Intervals

If $\hat{\mu} \sim G(\mu^*, \sigma)$, known quantiles :

$$P(\mu^* - \sigma < \hat{\mu} < \mu^* + \sigma) = 68\%$$

This is a probability for $\hat{\mu}$, not μ^* !

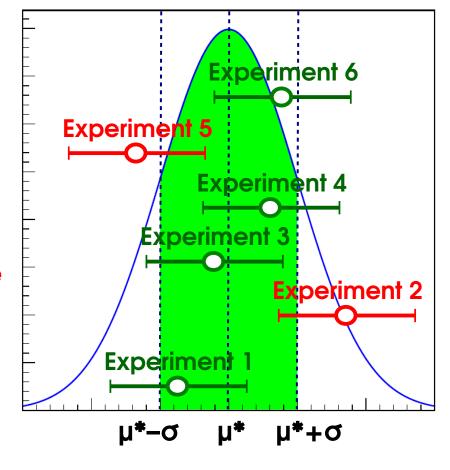
 $\rightarrow \mu^*$ is a fixed number, not a random variable

But we can invert the relation:

$$P(\mu^* - \sigma < \hat{\mu} < \mu^* + \sigma) = 68\%$$

$$\Rightarrow P(|\hat{\mu} - \mu^*| < \sigma) = 68 \%$$

$$\Rightarrow P(\hat{\mu} - \sigma < \mu^* < \hat{\mu} + \sigma) = 68 \%$$



 \rightarrow If we repeat the experiment many times, $[\hat{\mu} - \sigma, \hat{\mu} + \sigma]$ will **contain the true** value 68.3% of the time: $\mu^* = \hat{\mu} \pm \sigma$

This is a statement on the interval $[\hat{\mu} - \sigma, \hat{\mu} + \sigma]$ obtained for each experiment

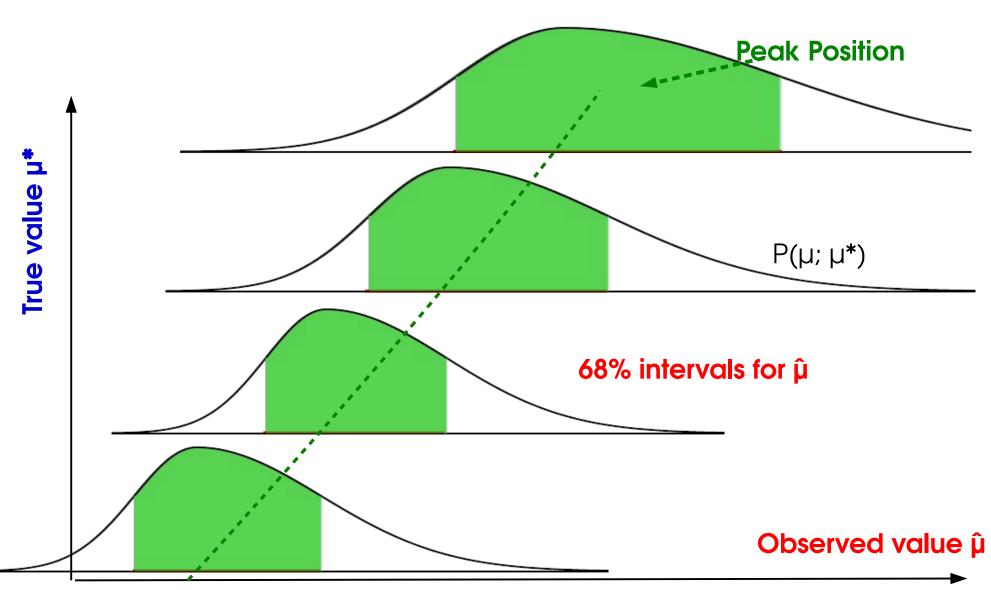
Works in the same way for other interval sizes: $[\hat{\mathbf{p}} - \mathbf{Z}\mathbf{\sigma}, \hat{\mathbf{p}} + \mathbf{Z}\mathbf{\sigma}]$ with

Z	1	1.96	2
CL	68.3%	95%	95.5%

Neyman Construction

General case: Build 10 intervals of observed values for each true value

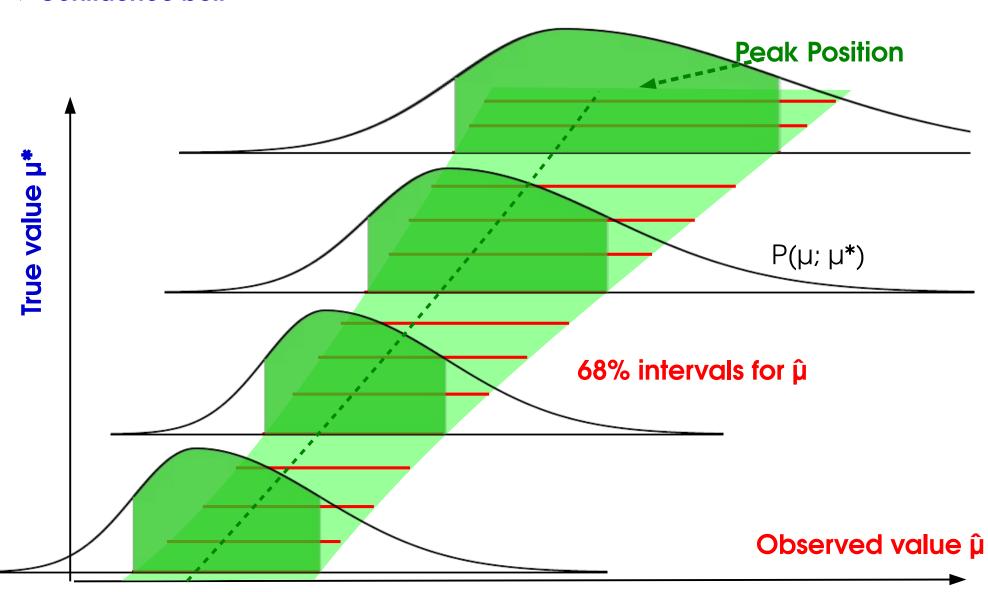
⇒ Confidence belt



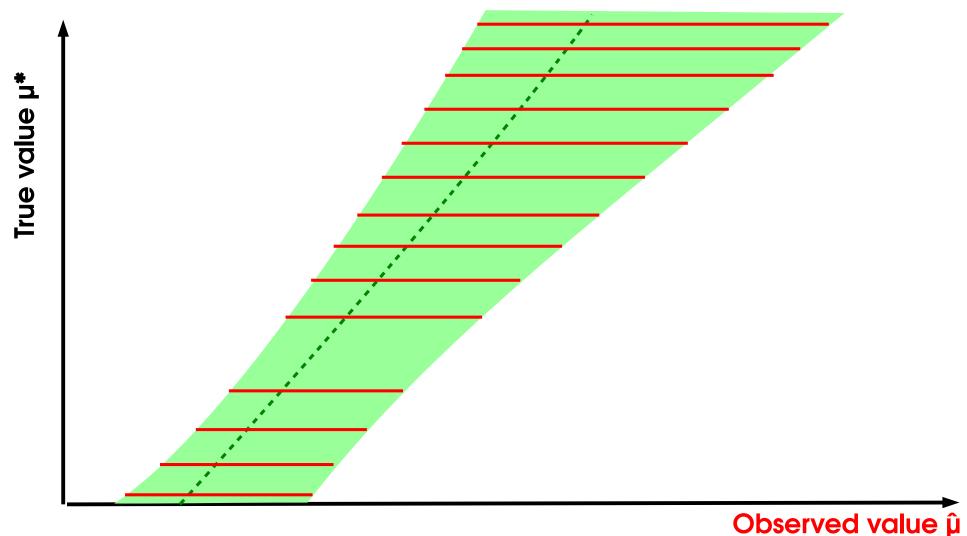
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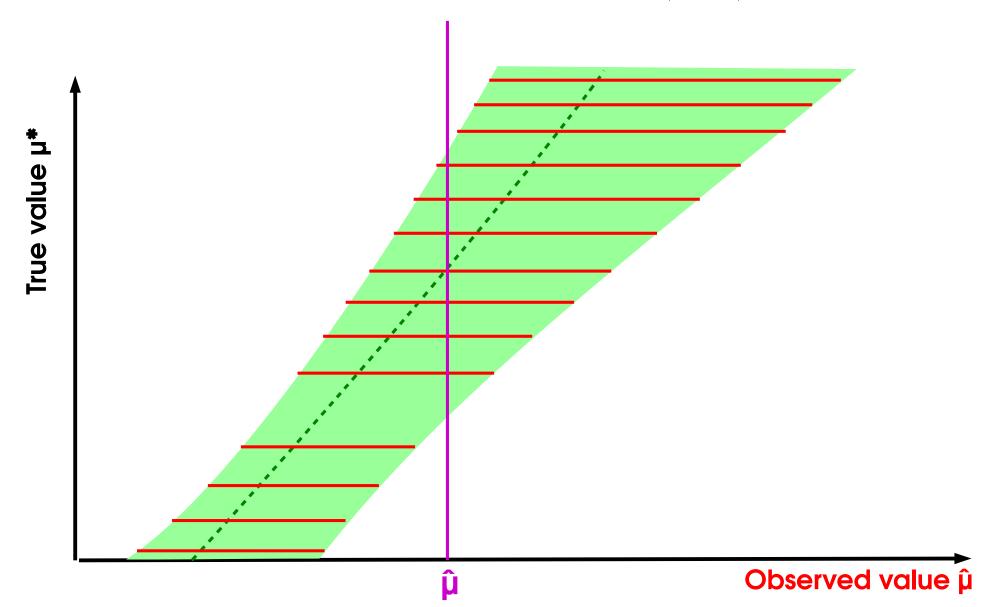
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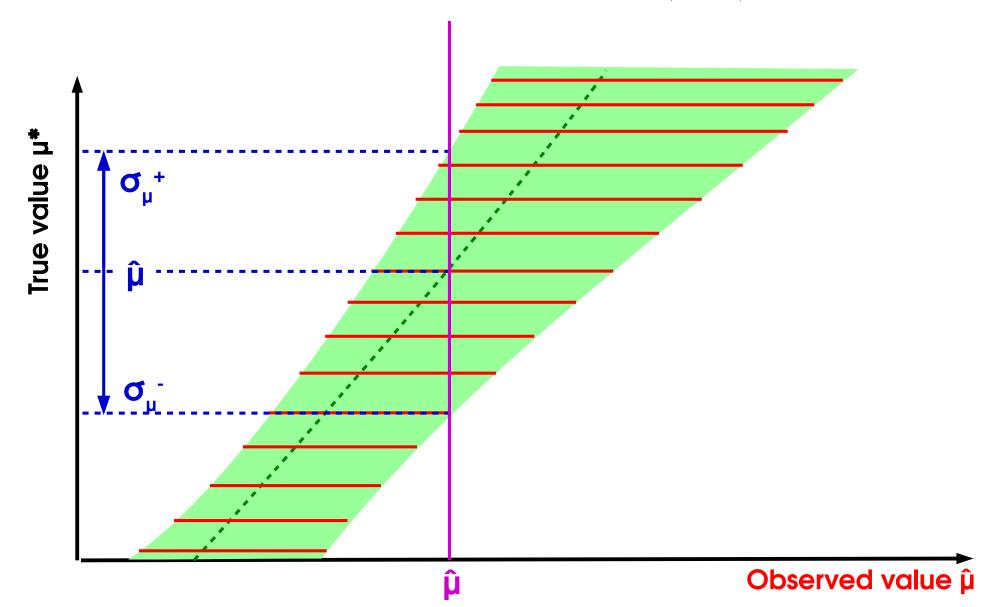
General case: Intersect belt with given $\hat{\mu}$, get $P(\hat{\mu} - \sigma_{\mu} < \mu^* < \hat{\mu} + \sigma_{\mu}) = 68 \%$



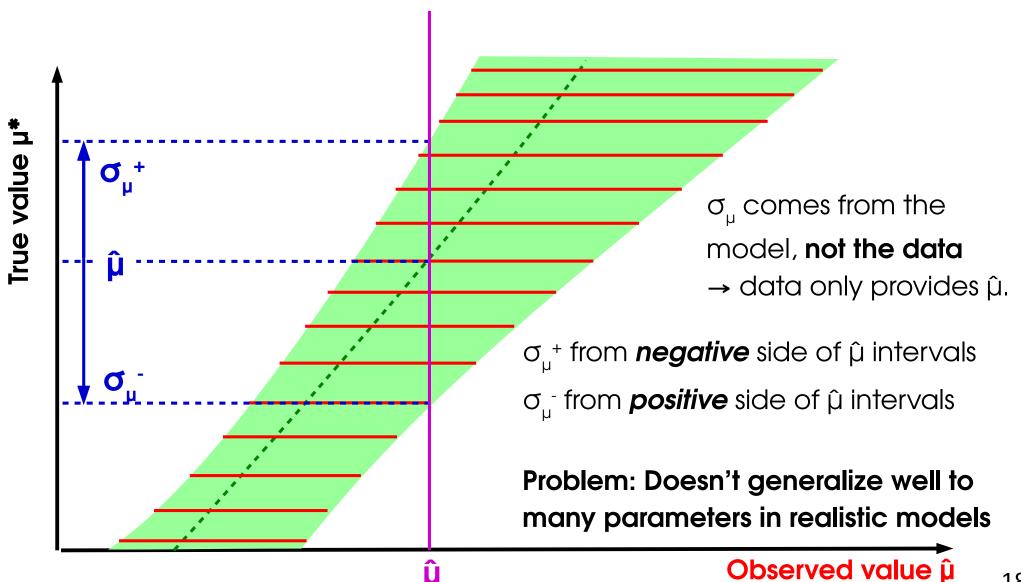
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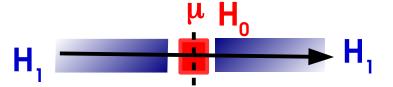
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Likelihood Intervals



Confidence intervals from L:

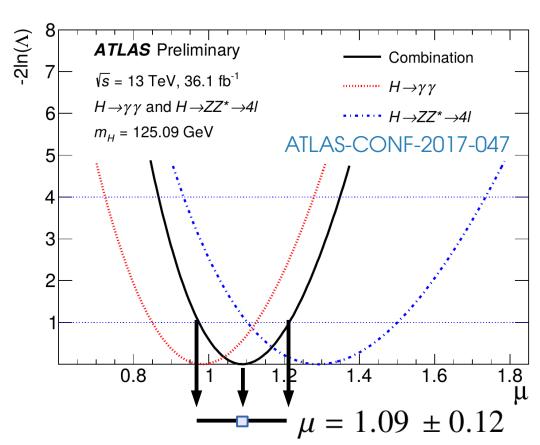
- Test $H(\mu_0)$ against alternative using
- $t_{\mu_0} = -2\log\frac{L(\mu = \mu_0)}{L(\hat{\mu})}$ Two-sided test since true value can be higher or lower than observed

Gaussian L:

- $t_{\mu_0} = \left(\frac{\hat{\mu} \mu_0}{\sigma_{\mu}}\right)^2$: parabolic in μ_0 .
- Minimum occurs at $\mu = \hat{\mu}$
- Crossings with $t_{\parallel} = 1$ give the 1_o interval

General case:

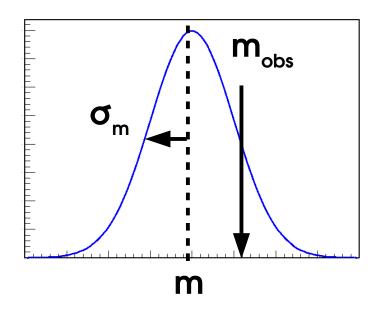
- Generally not a perfect parabola
- Minimum still occurs at $\mu = \hat{\mu}$
- Still define 1σ interval from the $t_{1} = \pm 1$ crossings



Homework 3: Gaussian Case

Consider a parameter m (e.g. Higgs boson mass) whose measurement is Gaussian with known width $\sigma_{m'}$ and we measure m_{obs} :

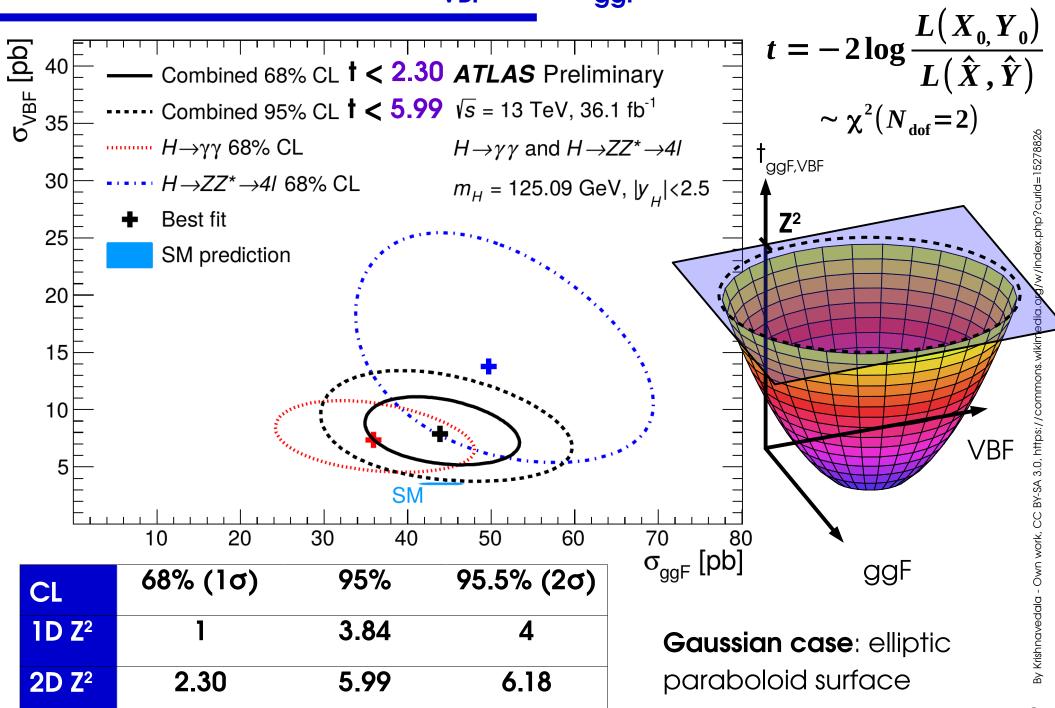
$$L(m; m_{\text{obs}}) = e^{-\frac{1}{2} \left(\frac{m - m_{\text{obs}}}{\sigma_m}\right)^2}$$



- → Compute the best-fit value (MLE) m̂
- → Compute t_m
- \rightarrow Compute the 1- σ (Z=1, ~68% CL) interval on m

Solution: $m = m_{obs} \pm \sigma_m$

- → Not really a surprise the method works as expected on this simple case
- → General method can be applied in the same way to more complex cases



Outline

Computing statistical results

Discovery Testing

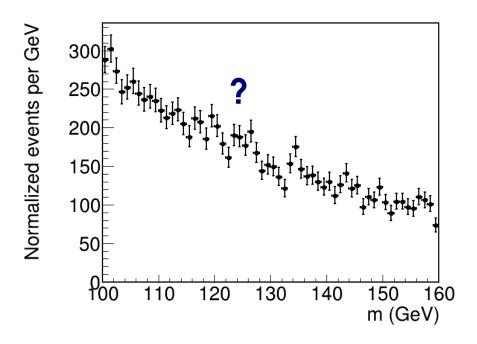
Confidence intervals

Upper limits on signal yields

Expected Limits

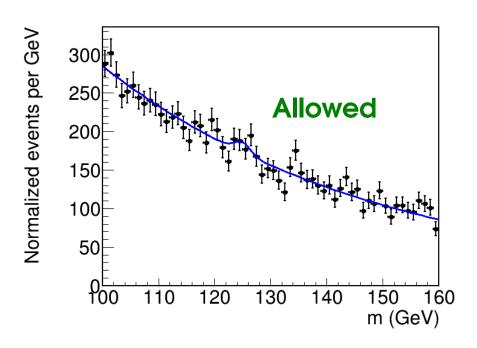
If no signal in data, testing for discovery not very relevant (report 0.2 σ excess?)

- → More interesting to exclude large signals
- → Upper limits on signal yield



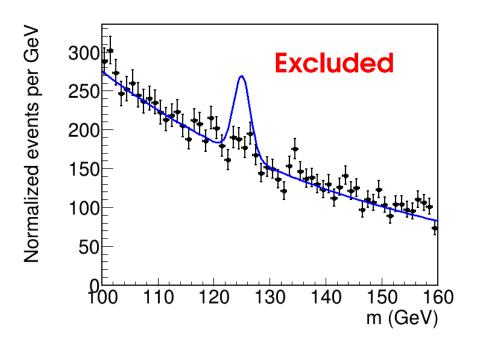
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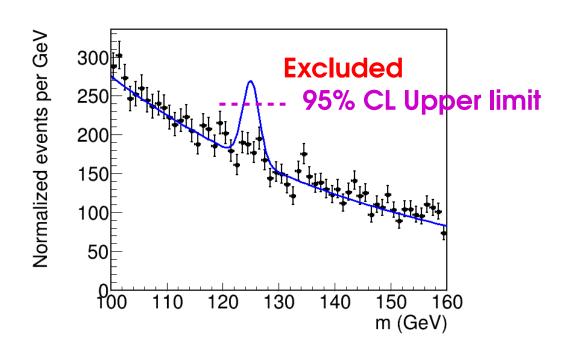
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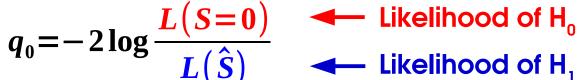
Test Statistic for Limit-Setting

Discovery:

- $H_0 : S = 0$
- $H_1: S > 0$

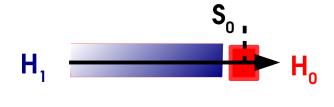


Compare



Limit-setting

- $H_0 : S = S_0$
- H₁: S < S₀

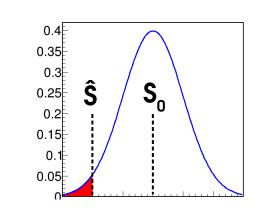


Compare

Same as q_0 :

 \rightarrow large values \Rightarrow good rejection of H₀.

Asymptotic case: p-value $p_{S_a} = 1 - \Phi(\sqrt{q_{S_a}})$



 $(\hat{S} > 0)$

 $(\hat{S} < S_0)$

Inversion: Getting the limit for a given CL

Procedure:

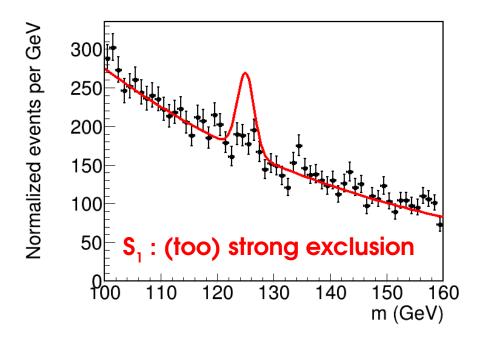
→ Compute q_{S0} for some S_0 , get the exclusion p-value p_{S0} .

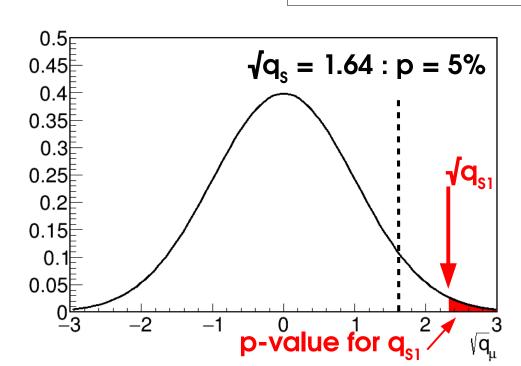
→ Adjust S₀ until 95% CL exclusion ($p_{s0} = 5\%$) is reached Asymptotic case: need $\sqrt{q_{s0}} = 1.64$

Asymptotics

$$\sqrt{q_{S_0}} = \Phi^{-1}(1-p_0)$$

CL	Region	
90%	$\sqrt{q_{_{\rm S}}} > 1.28$	
95%	$\sqrt{q_{s}} > 1.64$	
99%	$\sqrt{q_s} > 2.33$	





Inversion: Getting the limit for a given CL

Procedure:

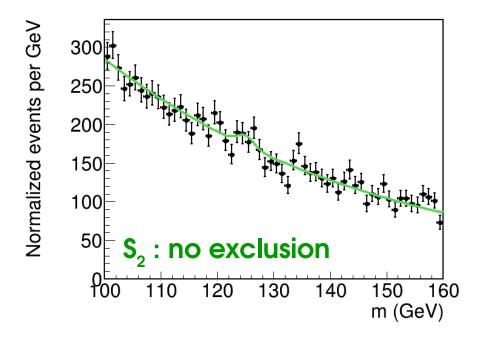
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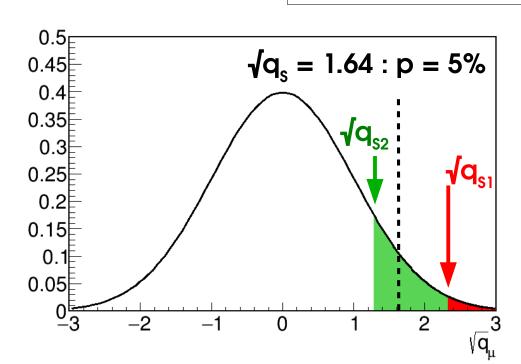
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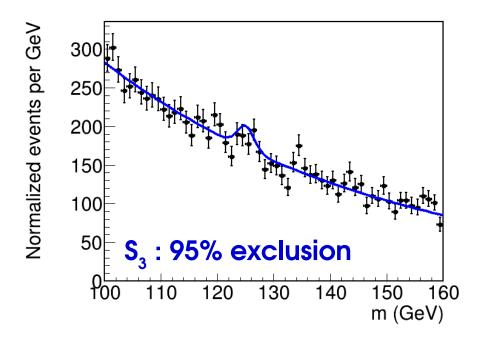
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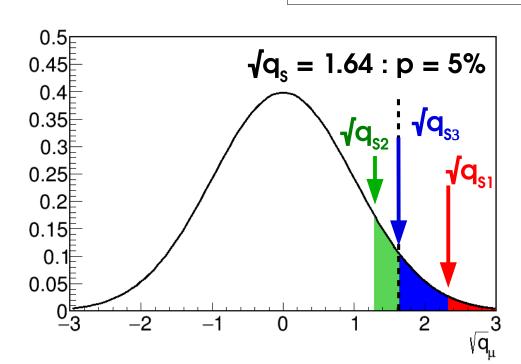
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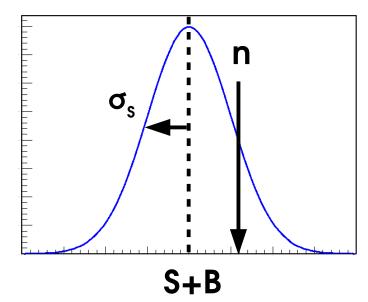




Homework 4: Gaussian Example

Usual Gaussian counting example with known B:

$$L(S;n) = e^{-\frac{1}{2}\left(\frac{n-(S+B)}{\sigma_S}\right)^2}$$
 $\sigma_S \sim \sqrt{B}$ for small S



Reminder: Significance: $Z = \hat{S}/\sigma_s$

- → Compute q_{s0}
- → Compute the 95% CL upper limit on S, S_{up} , by solving $\sqrt{q_{S0}} = 1.64$.

Solution:
$$S_{up} = \hat{S} + 1.64 \sigma_S$$
 at 95 % CL

Upper Limit Pathologies

Upper limit: $S_{up} \sim \hat{S} + 1.64 \sigma_{s}$.

Problem: for negative \$, get **very** good observed limit.

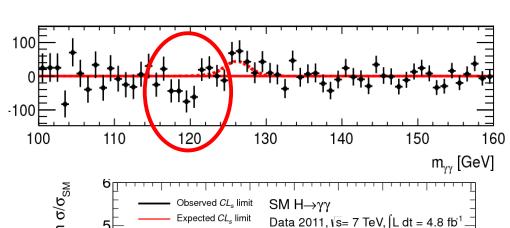
 \rightarrow For \hat{S} sufficiently negative, even $S_{up} < 0$!

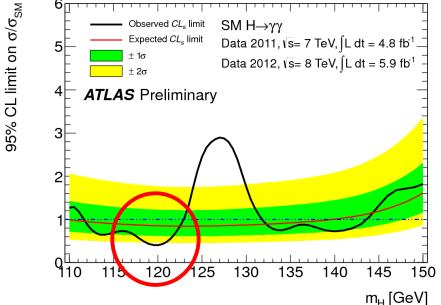
How can this be?

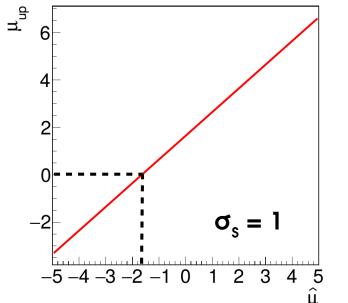
- → Background modeling issue ?... Or:
- → This is a 95% limit \Rightarrow 5% of the time, the limit wrongly excludes the true value, e.g. $S^*=0$.

Options

- \rightarrow live with it: sometimes report limit < 0
- → Special procedure to avoid these cases, since if we assume S must be >0, we know a priori this is just a fluctuation.







The p-value computed



Usual solution in HEP: CL_s.

→ Compute modified p-value

$$p_{CL_s} = \frac{p_{S_0}}{(1 - p_B)}$$
The usual p-value under
$$(1 - p_B)$$

- \Rightarrow **Rescale** exclusion at S₀ by exclusion at S=0.
- → Somewhat ad-hoc, but good properties...

\$ compatible with 0: $p_B \sim O(1)$ $p_{CLs} \sim p_{so} \sim 5\%$, no change.

Far-negative $\hat{\mathbf{S}}$: 1 - $p_R \ll 1$

$$p_{CLs} \sim p_{S0}/(1-p_{B}) \gg 5\%$$

→ lower exclusion ⇒ higher limit, usually >0 as desired

under H(S=0) 95% limit, CL_{s+b} 95% limit, CL $\sigma_s = 1$

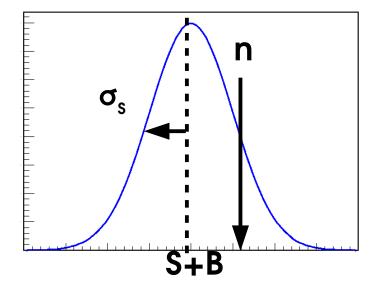
Drawback: overcoverage

 \rightarrow limit is claimed to be 95% CL, but actually >95% CL for small 1-p_R.

Homework 5: CL_s: Gaussian Case

Usual Gaussian counting example with known B:

$$L(S;n) = e^{-\frac{1}{2}\left(\frac{n-(S+B)}{\sigma_S}\right)^2}$$
 $\sigma_S \sim \sqrt{B}$ for small S



Reminder

$$CL_{s+b}$$
 limit: $S_{up} = \hat{S} + 1.64 \sigma_s$ at 95 % CL

CL_s upper limit :

- \rightarrow Compute p_{so} (same as for CLs+b)
- → Compute 1-p_B (hard!)

Solution:
$$S_{up} = \hat{S} + \left[\Phi^{-1}\left(1 - 0.05 \Phi(\hat{S}/\sigma_s)\right)\right]\sigma_s$$
 at 95% CL for $\hat{S} \sim 0$, $S_{up} = \hat{S} + 1.96 \sigma_s$ at 95% CL

Homework 6: CL_s Rule of Thumb for n_{obs}=0

Same exercise, for the Poisson case with $n_{obs} = 0$. Perform an exact computation of the 95% CLs upper limit based on the definition of the p-value:

p-value: sum probabilities of cases at least as extreme as the data

Hint: for $n_{obs}=0$, there are no "more extreme" cases (cannot have n<0!), so

$$p_{s0} = Poisson(n=0 \mid S_0 + B)$$
 and $1 - p_B = Poisson(n=0 \mid B)$

$$S_{\rm up}(n_{\rm obs}=0) = \log(20) = 2.996 \approx 3$$

Solution:

 \Rightarrow Rule of thumb: when $n_{obs} = 0$, the 95% CL_s limit is 3 events (for any B)

Outline

Computing statistical results

Confidence intervals

Upper limits on signal yields

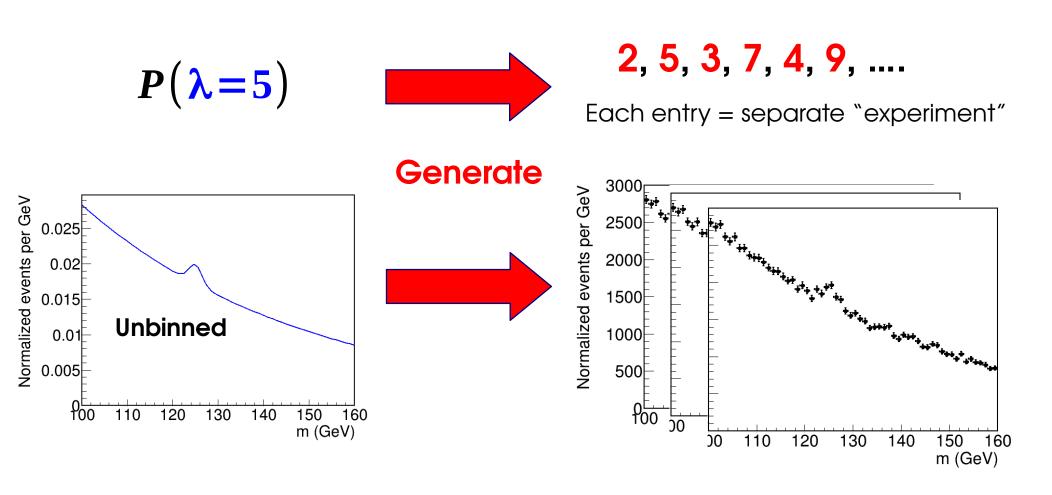
Expected Limits

Generating Pseudo-data

Model describes the distribution of the observable: **P(data; parameters)**

⇒ Possible outcomes of the experiment, for given parameter values

Can draw random events according to PDF: generate pseudo-data



Expected Limits: Toys

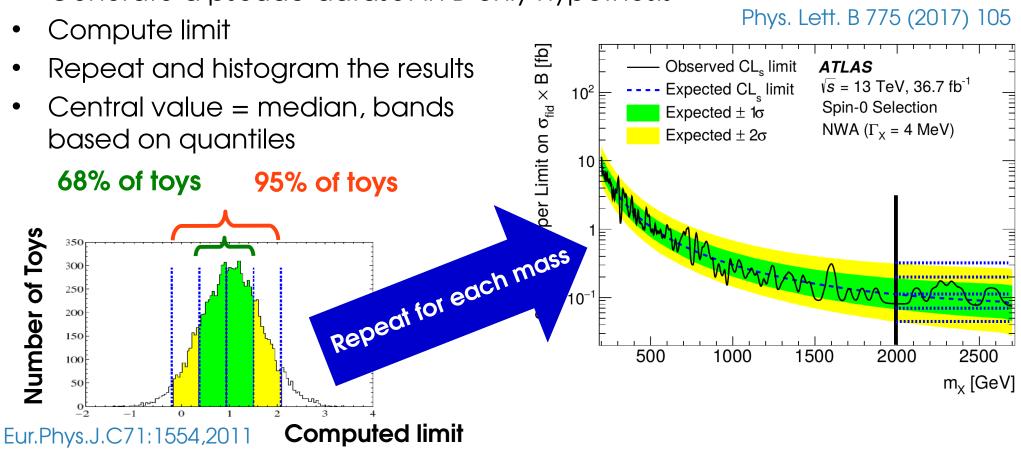
Expected results: median outcome under a given hypothesis

→ usually B-only for searches, but other choices possible.

Two main ways to compute:

→ Pseudo-experiments (toys):

Generate a pseudo-dataset in B-only hypothesis



Expected Limits: Asimov Datasets

Expected results: median outcome under a given hypothesis

→ usually B-only for searches, but other choices possible.

Two main ways to compute:

Strictly speaking, Asimov dataset if

$$X = X_0$$
 for all parameters X ,

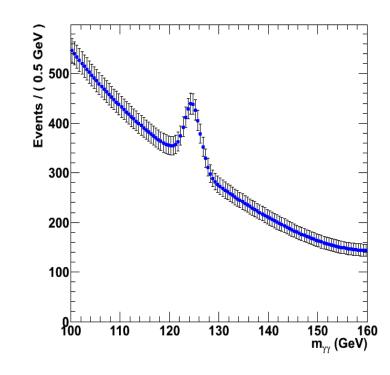
where X_0 is the generation value

→ Asimov Datasets

- Generate a "perfect dataset" e.g. for binned data, set bin contents carefully, no fluctuations.
- Gives the median result immediately:
 median(toy results) ↔ result(median dataset)
- Get bands from asymptotic formulas: Band width

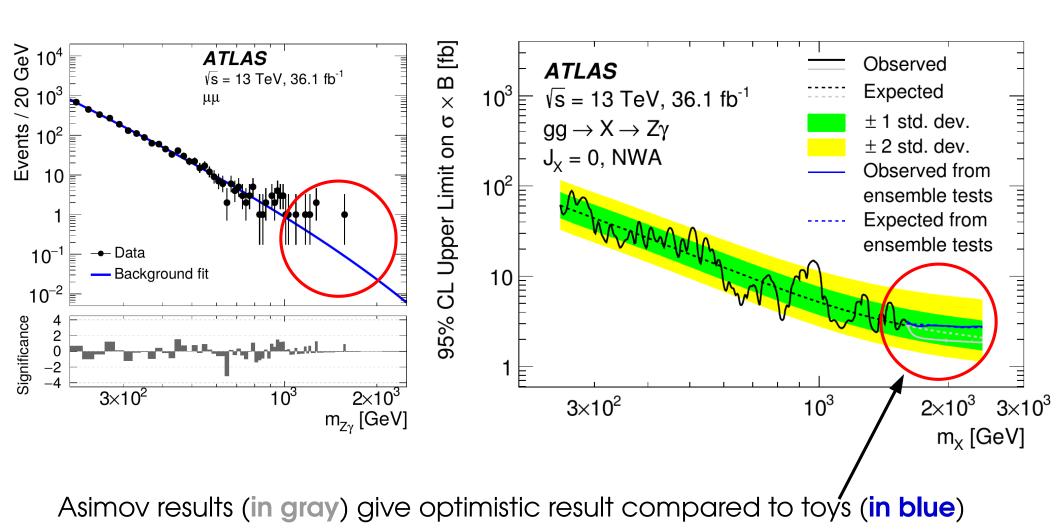
$$\sigma_{S_0,A}^2 = \frac{S_0^2}{q_{S_0}(\text{Asimov})}$$

- Much faster (1 "toy")
- e Relies on Gaussian approximation



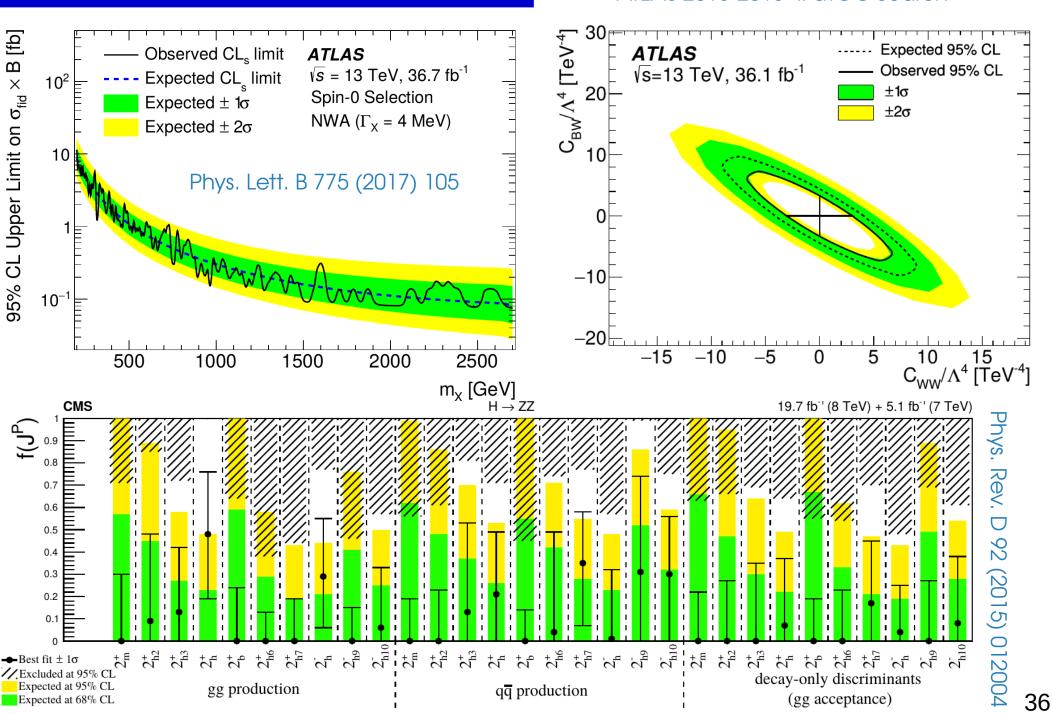
Toys: Example

ATLAS X \rightarrow Z γ Search: covers 200 GeV < m_{χ} < 2.5 TeV \rightarrow for m_{χ} > 1.6 TeV, low event counts \Rightarrow derive results from toys



Upper Limit Examples

ATLAS 2015-2016 4I aTGC Search

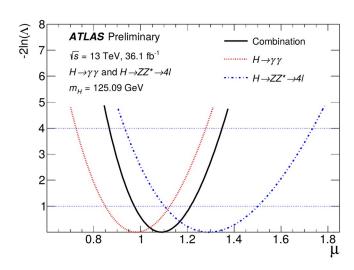


Takeaways

Confidence intervals: use
$$t_{\mu_0} = -2\log\frac{L(\mu = \mu_0)}{L(\hat{\mu})}$$

 \rightarrow Crossings with $t_{\mu 0} = Z^2$ for $\pm Z\sigma$ intervals (in 1D)

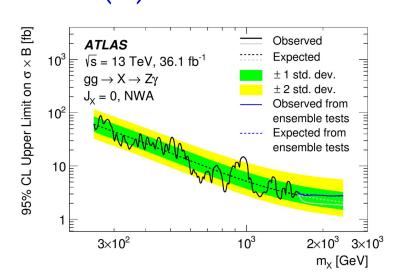
Gaussian regime: $\mu = \hat{\mu} \pm \sigma_{\mu}$ (1 σ interval)



Limits: use LR-based test statistic: $q_{S_0} = -2\log\frac{L(S-S_0)}{L(\hat{S})}$ $S_0 \geq \hat{S}$

→ Use CL, procedure to avoid negative limits

Poisson regime, n=0: $S_{up} = 3$ events



Extra Slides

CL: Gaussian Bands

Usual Gaussian counting example with known B: 95% CL_s upper limit on S:

$$S_{up} = \hat{S} + \left[\Phi^{-1} \left(1 - 0.05 \, \Phi \left(\hat{S} / \sigma_{S} \right) \right) \right] \sigma_{S} \qquad \sigma_{S} = \sqrt{B}$$
Compute expected bands for S=0:

⇒ Asimov dataset
$$\Leftrightarrow \hat{S} = 0$$
: $S_{up,exp}^0 = 1.96 \sigma_S$

 \rightarrow + no bands:

$$S_{\text{up,exp}}^{0} = 1.96 \sigma_{S}$$

$$S_{\text{up,exp}}^{\pm n} = \left(\pm n + \left[1 - \Phi^{-1}(0.05 \Phi(\mp n))\right]\right) \sigma_{S}$$

n	S _{exp} ±n /√B
+2	3.66
+1	2.72
0	1.96
-1	1.41
-2	1.05

CLs:

300

250

150

100

Exents 150

- Positive bands somewhat reduced,
- Negative ones more so

Band width from $\sigma_{S,A}^2 = \frac{S^2}{q_S(\text{Asimov})}$ depends on S, for non-Gaussian cases, different values for each band...

Eur.Phys.J.C71:1554,2011

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Comparison with LEP/TeVatron definitions

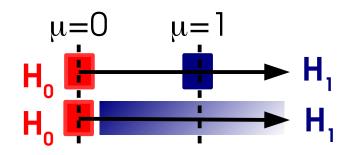
Likelihood ratios are not a new idea:

- $q_{LEP} = -2\log \frac{L(\mu=0,\widetilde{\theta})}{L(\mu=1,\widetilde{\theta})}$
- **LEP**: Simple LR with NPs from MC
 - Compare μ =0 and μ =1
- **Tevatron**: PLR with profiled NPs

$$q_{Tevatron} = -2\log \frac{L(\mu=0, \hat{\theta_0})}{L(\mu=1, \hat{\theta_1})}$$

Both compare to $\mu=1$ instead of best-fit $\hat{\mu}$

LEP/Tevatron IHC



- → Asymptotically:
- **LEP/Tevaton**: q linear in $\mu \Rightarrow \sim Gaussian$
- **LHC**: a quadratic in $\mu \Rightarrow \sim \chi 2$
- → Still use TeVatron-style for discrete cases

