## Statistics for HEP, part I

Nicolas Berger (LAPP Annecy)

## Statistics in Physics

"Statistics" might make you think of this:


## Statistics in Physics

## "Statistics" might make you think of this:

## 직 OECD <br> BETTER POLICIES FOR BETTER LIVES

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| > Productivity statistics |  |

## Or maybe this:



## Statistics in Physics

"Statistics" might make

## Or maybe this:

 you think of this:
## But probably not this



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## Random Processes

- Statistics is the description of random processes. Where does this come into HEP ?


## - Measurement errors



- Quantum Uncertainty



## Measurement Errors : Example

Example: measuring the energy of a photon in a calorimeter


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Example: measuring the energy of a photon in a calorimeter

Measure leakage behind calorimeter


Real life : imperfect measurement


## Measurement Errors

- Best case: measurements imperfections ("bias") can be determined
- Apply correction "event by event", remove effect
- Not always possible
- Too small to be measured reliably
- Impossible to measure
- Next-best solution: describe overall distribution of imperfections
- Typical size
- Probability to reach a given value
$\Rightarrow$ not $\mathrm{m}_{\mathrm{H}}=125 \mathrm{GeV}$ but $m_{H}=125.36+/-0.40 \mathrm{GeV}$
- Need to precisely quantify our uncertainty



## $\mathrm{H} \rightarrow \gamma \gamma$ Example

Phys. Rev. D 90, 112015


## Another Example: $\mathrm{H} \rightarrow \mathrm{ZZ}^{*} \rightarrow 4 \mathrm{I}$

Phys. Rev. D 91, 012006


Rare process: Expect 1 signal event every ~6 days


Quantum randomness: "Will I get an event today ?" - only probabilistic answer Event counts must be described in a probabilistic way

## Contents of the Lectures

- Probability Distributions (short reminder)
- How to build a statistical model
- How to Estimate a parameter value
- How to compute Confidence Intervals (uncertainties on parameters
- Tomorrow:
- Computing a discovery significance
- Setting limits


## Probability Distributions

## Probability Distribution

Probabilistic treatment of possible outcomes $\Rightarrow$ Probability Distribution

- Example: two-coin toss
- Fractions of events in each bin converge to a limit
- Probability distribution :
$p_{i}, i=0,1,2$
- Properties
$-p_{1}>0$
$-\sum p_{i}=1$


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100 trials

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## Probability Distribution

Probabilistic treatment of possible outcomes $\Rightarrow$ Probability Distribution

100000 trials


- Properties
$-p_{i}>0$
$-\sum p_{i}=1$


## Continuous Variables: PDFs

- Continuous variable, can consider binned probability distribution $p_{i}, i=1 . . n_{\text {bins }}$

- Bin size $\rightarrow 0$ :
X


## Probability distribution function $\mathbf{p ( x )}$

- High values $\Leftrightarrow$ high chance to get a measurement here
$-p(x)>0$
$-\int p(x) d x=1$
- Generalizes to multiple variables : $\int p(x, y) d x d y=1$


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Contours: $p(x, y)$

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## PDF Properties: Mean

- Expectation values = expected outcome on average
- $E(X)=$ Mean of $X$

$$
\begin{aligned}
& E(X)=\sum_{i} X_{i} p_{i} \text { or } \\
& E(X)=\int X p(X) d X
\end{aligned}
$$

- Property of the PDF
- If one has a sample $x_{1} \ldots x_{n^{\prime}}$ then can compute Sample Mean:

$$
\bar{x}=\frac{1}{n} \sum_{i} x_{i}
$$

- Property of the sample
- Should approximate PDF mean.



## PDF Properties: Variance

- $\operatorname{Var}(X)=E\left([X-E(X)]^{2}\right)=$ Variance of $X$
- Average square of deviation from mean
$-\operatorname{RMS}(X)=\sqrt{ } \operatorname{Var}(X)$ "root mean square"
- Can be approximated by sample


$$
\sigma^{2}=\frac{1}{n-1} \sum_{i}\left(x_{i}-\bar{x}\right)^{2}
$$

- Covariance of $X$ and $Y$ :
$\operatorname{Cov}(X, Y)=E([X-E(X)][Y-E(Y)])$
- Large if variations of $X, Y$ are "synchronized"

$-\operatorname{Cov}(X, Y)>0$ if $X$ and $Y$ vary in the same direction
$-\operatorname{Cov}(X, Y)<0$ if $X$ and $Y$ vary in opposite direction
$-\operatorname{Cov}(X, Y)=0$ if $X$ and $Y$ vary independently


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$-\operatorname{Cov}(\mathrm{X}, \mathrm{Y})>0$ if X and Y vary in the same direction
$-\operatorname{Cov}(X, Y)<0$ if $X$ and $Y$ vary in opposite direction
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## Example 1 : Gaussian

Gaussian distribution:

$$
G\left(x ; x_{0}, \sigma\right)=\frac{1}{\sigma \sqrt{2 \pi}} e^{-\frac{\left(x-x_{0}\right)^{2}}{2 \sigma^{2}}}
$$

Mean : $x_{0}$
Variance : $\sigma^{2}(\Rightarrow R M S=\sigma)$


- Generalize to $\mathbf{N}$ dimensions:

$$
G\left(X ; X_{0,} C\right)=\frac{1}{(2 \pi|C|)^{n / 2}} e^{-\frac{1}{2}\left(X-X_{0}\right)^{T} C^{-1}\left(X-X_{0}\right)}
$$

Mean (vector) $=X_{0}$
Covariance matrix
$\operatorname{Var}(X)$
$\operatorname{Cov}(X, Y)$
$\underset{\operatorname{Cov}(X, Y)}{\operatorname{Var}(Y)} \mid=C$


## Central Limit Theorem

- For a random variable X with any distribution, one has

$$
\bar{x}=\frac{1}{n} \sum_{i=1}^{n} x_{i} \stackrel{n \rightarrow \infty}{\sim} G\left(\bar{x} ; E(X), \frac{R M S(X)}{\sqrt{n}}\right)
$$

- What this means:
- The average of many measurements is always Gaussian, whatever the distribution for a single measurement
- The mean of the Gaussian is the mean of the single measurements
- the RMS of the Gaussian decreases as $\sqrt{ } \mathrm{n}$ : less fluctuations when averaging over many measurements
- Another version, for the sum:

$$
\sum_{i=1}^{n} x_{i} \stackrel{n \rightarrow \infty}{\sim} G(\bar{x} ; n E(X), \sqrt{n} \sigma(X))
$$

- Mean scales like $n$, but RMS only like $\sqrt{ }$ n


## Central Limit Theorem Example

Draw events from a $x^{2}$ distribution (for illustration only)
$x^{\wedge} 2$


$$
\bar{x}=\frac{1}{n} \sum_{i=1}^{n} x_{i} \longrightarrow
$$



Distribution becomes Gaussian, although very
non-Gaussian originally
Distribution becomes narrower as expected (as $1 / \sqrt{ } n$ )

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& \quad \bar{x}=\frac{1}{n} \sum_{i=1}^{n} x_{i} \longrightarrow \text { Distribution becomes Gaussian, although very }
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Distribution becomes narrower as expected (as $1 / \sqrt{n}$ )

## Central Limit Theorem Example

Draw events from a $x^{2}$ distribution (for illustration only) $x^{\wedge 2}$


$$
\mathrm{n}=12
$$

$$
\begin{aligned}
& \quad \bar{x}=\frac{1}{n} \sum_{i=1}^{n} x_{i} \longrightarrow 0.005 \\
& \text { Distribution becomes Gaussian, although very }
\end{aligned}
$$

non-Gaussian originally
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## Gaussian Integrals

- Probability to be "less than $n \sigma$ " away from the mean:

$$
P\left(\left|x-x_{0}\right|<n \sigma\right)=\int_{x_{0}-n \sigma}^{x_{0}+n \sigma} G\left(x ; x_{0} \sigma\right) d x=\int_{-n}^{+n} N(x) d x
$$

- Used also for other distributions:
"lo error" for $p=68 \%$, etc.
$\begin{aligned} & \text { Standard Normal } \\ & \text { Distribution }\end{aligned} N(x)=\frac{1}{\sqrt{2 \pi}} e^{-\frac{x^{2}}{2}}$

| Number <br> of sigmas | Fraction <br> inside | Fraction <br> outside |
| :--- | :--- | :--- |
| $\mathbf{1}$ | 0.68 | 0.32 |
| $\mathbf{2}$ | 0.955 | 0.045 |
| $\mathbf{3}$ | 0.997 | 0.003 |
| $\mathbf{5}$ | 0.999999 | $6 \times 10^{-7}$ |



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## Example 2 : Counting events

- Consider n trials with probability p. Prob. to get k good events ? Binomial distribution: $P(k ; n, p)=C_{k}^{n} p^{k}(1-p)^{n-k}$

Mean $=\mathrm{np}$
Variance $=n p(1-p)$
n trials


- Not widely used because :
- Suppose $p \ll 1, n \gg 1$, let $\boldsymbol{\lambda}=n p$
- i.e. very rare process, but many trials so still expect events
$\Rightarrow$ Poisson distribution
Mean $=\lambda$
Variance $=\lambda$

$$
p(k ; \lambda)=e_{\uparrow}^{e^{-\lambda}} \frac{\lambda^{k}}{k!}
$$

## Rare Processes?

- HEP : almost always use Poisson distributions.
- ATLAS :
- Collision event rate ~ 1 GHz ( $L \sim 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1} \sim 10 \mathrm{nb}^{-1} / \mathrm{s}, \sigma_{\text {tot }} \sim 10^{8} \mathrm{nb}$, )
- Trigger rate ~ 1 kHz
(Higgs rate ~0.1 Hz)
- $\mathrm{P} \sim 10^{-6}\left(\mathrm{P}_{\text {Higgs }} \sim 10^{-10}\right)$
- A year of data: n ~ $10^{16}$
$\Rightarrow$ Poisson regime!
(Large $\mathrm{n}=$ design requirement, to get not-too-small $\lambda=n \mathrm{p} . .$. )
proton - (anti)proton cross sections



## Poisson Distributions

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



- Discrete distribution (integers only), asymmetric for small $\lambda$
- Central limit theorem : becomes Gaussian for large $\lambda$
- Typical uncertainty (RMS) on $N$ events is $\sqrt{ } \mathbf{N}$, for large $N$


## Poisson Distributions

$$
\lambda=1
$$



## Poisson Distributions



## Poisson Distributions

$$
\lambda=5
$$



## Poisson Distributions



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

$\lambda$ : expected number of events

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## Poisson Distributions



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

$\lambda$ : expected number of events

Mean = $\lambda$
Variance $=\lambda$ RMS $=\sqrt{ } \lambda$

- Discrete distribution (integers only), asymmetric for small $\lambda$
- Central limit theorem : becomes Gaussian for large $\lambda$
- Typical uncertainty (RMS) on $N$ events is $\sqrt{ } \mathbf{N}$, for large $N$


## What we have learned so far (1)

- PDFs: give the probability to obtain each possible value in a random process
- Examples
- Gaussian:

$$
G\left(x ; x_{0,} \sigma\right)=\frac{1}{\sigma \sqrt{2 \pi}} e^{-\frac{\left(x-x_{0}\right)^{2}}{2 \sigma^{2}}}
$$



- To describe a continuous variable
- For large numbers of events, processes become Gaussian
- Poisson :

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

- generally used for counting events



## Building a Statistical Model

## Statistical Model

- Goal: Quantify our knowledge using PDFs:

Build a Statistical Model

- Includes
- Assumptions about what we know (physics, etc.)
- PDFs of random variables: statistical description what we don't know.
- The statements we can make have a probabilistic meaning:
- Not $\mathrm{m}_{\mathrm{H}}=125.5 \mathrm{GeV}$ but $124.95<\mathrm{m}_{\mathrm{H}}<125.77 \mathrm{GeV}$ with $68 \%$ confidence
- Not "there exists a Higgs boson" but "exists with 99.9999\% (5 5 ) confidence"
- For these statements to be correct the PDFs need to correctly describe the distributions of the random variables..
- Not always easy or possible...


## Example: Model for Counting

- Counting experiment:
- observe a number of events n
- describe by a Poisson distribution

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

- With signal and bkg:

$$
P(n ; s, b)=e^{-(s+b)} \frac{(s+b)^{n}}{n!}
$$

- We have assumed a Poisson distribution for n : This is our model, based on physics knowledge.
- Model has parameters (s,b), a priori unknown.
- For example, can assume $\mathbf{b}$ is known.
$\Rightarrow$ Goal: use the measured n to find out about the parameter s .


## Example: Shape Analysis

- Shape analysis experiment
- observe a set of masses $m_{1} \ldots m_{n}$
- Describe shape of $m_{i}$ distribution using
- Gaussian signal $P_{\text {signal }}(m)=G\left(m ; m_{0, \sigma}\right)$
- Exp. background $P_{b k g}(m)=\alpha \exp (-\alpha m)$
- expected yields : s, b
- Overall PDF:



$$
P_{\text {Total }}(m)=\frac{s}{s+b} G\left(m ; m_{H}, \sigma\right)+\frac{b}{s+b} \alpha \exp (-\alpha m)^{m}
$$

- We have assumed
- A signal shape (detector response)
- A background shape (physics)
- Parameters s, b, $\mathrm{m}_{\mathrm{H}} \ldots$ are unknown: measure using the observed $m_{i}$



## Example: Shape Analysis

- Shape
- obse
- Describ
- Gau
- Exp.
- expe
- Overall
- We har
- A sig
- A bo
- Parame



## Monte-Carlo Generation

- Model describes the distribution of the observable: $\Rightarrow$ Possible outcomes of the experiment, for given parameter values
- Can draw random events according to PDF "generate pseudo-data" (a.k.a. "Monte Carlo")



- Useful to design measurement, compute expected results
- Real MC involves realistic physics models, detector response, etc. this is "Toy MC".


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## Inversion

- MC generation: parameter values ( $s, b, m_{H}$ ) as input: model + parameter values $\Rightarrow$ pseudo-dataset
- But what we really want is the other direction:
model + (real) dataset $\Rightarrow$ parameter values



$\Rightarrow$ Parameter Estimation


## What we have learned so far (2)

- Need probabilistic description for some aspects of a measurement.
- Use PDFs as building blocks to construct a model:
- Event counting: use Poisson distribution

$$
P(n ; s, b)=e^{-(s+b)} \frac{(s+b)^{n}}{n!}
$$

- Shape analysis: use PDF shapes that describe the distribution of signal and background.

$$
P_{\text {Total }}\left(m ; \theta_{\text {signal }}, \theta_{\text {bkg }}\right)=\frac{s}{s+b} P_{\text {signal }}\left(m ; \theta_{\text {signal }}\right)+\frac{b}{s+b} P_{b k g}\left(m ; \theta_{b k g}\right)
$$

- Directly usable to generate pseudo-data for given parameter values.
- Goal of the rest of these lectures: how to use data to measure the parameters


## Parameter Estimation

## Likelihood

- Likelihood function: same as PDF, but considered as a function of model parameters, not the random variable
Poisson
PDF

$$
P(n ; \lambda)=e^{-\lambda} \frac{\lambda^{n}}{n!} \rightarrow L(\lambda ; n)=e^{-\lambda} \frac{\lambda^{n}}{n!}
$$

Poisson
Likelihood

- Purely a difference of interpretation!
- PDF: given $\lambda$, how probable to observe $\mathbf{n}$
- Variable : the observed data
- High values of PDF: range of $n$ where data is probable to appear
- Likelihood: Given an observed n,
 how likely was this outcome for some $\lambda$ value?
- Variable : the model parameters.
- High value of the likelihood : value of $\lambda$ for which the data we observed was likely


## Poisson Example

- Assume Poisson distribution with no background:

$$
L(s ; n)=e^{-s} \frac{s^{n}}{n!}
$$

- Say we observed $\mathrm{n}=5$
- Data is fixed, parameter s varies

$$
L(s ; n=5)=e^{-s} \frac{s^{5}}{5!}
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## Maximum Likelihood

- To estimate a parameter $\theta$ : find the value that maximizes $L(\theta)$ The value of $\theta$ for which the data was most likely to occur $\Rightarrow$ Maximum Likelihood Estimator, $\hat{\boldsymbol{\theta}}$
- A function of the data: $\hat{\boldsymbol{\theta}}(\mathbf{n})$ or $\hat{\boldsymbol{\theta}}\left(\mathbf{m}_{1} \ldots . \mathrm{m}_{\mathrm{n}}\right)$
- Not guaranteed that $\hat{\theta}$ is the true value
- sometimes the observed data is unlikely...



Maximum for $\mathrm{s}=5$ : $\widehat{\mathbf{s}}=\mathbf{5}$

## Maximum Likelihood Properties

- Consistent: $\hat{\theta}$ gives the true value on average $E(\hat{\theta})=\theta^{*}$
- Asymptotically Gaussian : for large datasets

$$
P(\hat{\theta}) \sim \exp \left(-\frac{\left(\hat{\theta}-\theta^{*}\right)^{2}}{2 \sigma_{\theta}^{2}}\right) \quad \text { for } n \rightarrow \infty
$$

- Asymptotically Efficient : $\sigma_{\theta}$ is the lowest possible value for an estimator for $\theta$ (in the limit $\mathrm{n} \rightarrow \infty$ )
- Log-likelihood:
- Can also minimize $\boldsymbol{\lambda}=\mathbf{- 2} \log \mathrm{L} \quad \lambda(\theta)=\left(\frac{\hat{\theta}-\theta}{\sigma_{\theta}}\right)^{2}$
- If $L$ is Gaussian, $\lambda$ is parabolic:
- Can drop multiplicative constants in L (additive constants in $\lambda$ )


## Poisson Example

- Event counting with Poisson model, $b=0$

$$
L(s ; n)=e^{-s} s^{n} \quad \leftarrow \text { dropped } n!
$$

- Peak of the poisson is always at $n=s$
-ML estimate: $\hat{\mathbf{S}} \mathbf{=} \mathbf{n}$
- So $\hat{\mathrm{s}}=\mathrm{n}$ is Poisson-distributed
- Properties:
- Consistent $E(\hat{s})=E(n)=s^{*}$
- Gaussian for large n
- Kind of trivial...



## Gaussian Examples

- Gaussian case, one measurement
- We measure $x$
- Likelihood: $L(\theta ; x)=G(x ; \theta, \sigma)$
- What is $\theta$ ? ML estimate : $\hat{\theta}=x$.
- Gaussian case, two measurements

- Measure the same parameter twice - how to combine ?
- Both cases Gaussian, same mean, different resolutions
- Combined likelihood: $\quad L\left(\theta ; x_{1}, x_{2}\right)=G\left(x_{1} ; \theta, \sigma_{1}\right) G\left(x_{2} ; \theta, \sigma_{2}\right)$

Log-likelihood: $\quad \lambda\left(\theta ; x_{1}, x_{2}\right)=\left(\frac{x_{1}-\theta}{\sigma_{1}}\right)^{2}+\left(\frac{x_{2}-\theta}{\sigma_{2}}\right)^{2}$

## Gaussian Examples

- Gaussian case, one measurement
- We measure $x$
- Likelihood: $L(\theta ; x)=G(x ; \theta, \sigma)$
- What is $\theta$ ? ML estimate : $\hat{\theta}=x$.
- Gaussian case, two measurements

- Measure the same parameter twice - how to combine ?
- Both cases Gaussian, same mean, different resolutions
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ML Estimate for $\theta$ :

$$
\hat{\theta}=\frac{\frac{x_{1}}{\sigma_{1}^{2}}+\frac{x_{2}}{\sigma_{2}^{2}}}{\frac{1}{\sigma_{1}^{2}}+\frac{1}{\sigma_{2}^{2}}} \quad \begin{aligned}
& \text { Just average the } \\
& \text { measurements }
\end{aligned}
$$

## Likelihood for a Shape Analysis

- For a single measurement, $\mathbf{L}(\boldsymbol{\theta} ; \mathbf{x})=\mathbf{P}(\mathbf{x} ; \boldsymbol{\theta})$
- For a distribution of $\mathrm{n}_{\text {obs }}$ events, product over events:

$$
L\left(\theta ; x_{1} \ldots x_{n_{\infty \infty}}\right)=\prod_{i=1}^{n_{\infty}} P\left(x_{i} ; \theta\right)
$$

- Also variations for $\mathrm{n}_{\text {obs }}$ : include Poisson term

$$
L\left(N_{\text {exp }}, \theta ; x_{1} \ldots x_{n_{\text {esol }}}\right)=e^{-N_{\text {ep }}} \frac{N_{\text {exp }}^{n_{\text {oxp }}}}{n_{\text {obs }}}!\prod_{i=1}^{n_{\text {exp }}} P\left(x_{i} ; \theta\right)
$$


$\mathbf{N}_{\text {exp }}=$ total number of events expected, model parameter

- If we use $P_{\text {Total }}(m ; s, b, \theta)=\frac{s}{s+b} P_{\text {signal }}(m ; \theta)+\frac{b}{s+b} P_{b k g}(m, \theta)$ then $\mathbf{N}_{\text {exp }}=\mathbf{s}+\mathbf{b}$ and

$$
L\left(s, b, \theta ; m_{1} \ldots m_{n_{\text {obs }}}\right)=e^{-(s+b)} \prod_{i=1}^{n_{\text {obs }}} s P_{\text {signal }}\left(m_{i} ; \theta\right)+b P_{b k g}\left(m_{i}, \theta\right)
$$

## $\mathrm{H} \rightarrow \gamma \gamma$ Example

- Use the $\mathrm{H} \rightarrow \gamma \gamma$-inspired model from before
- Generate 10 k events of pseudo-data with $\mathbf{s}=\mathbf{2 0 0}, \mathbf{m}_{\mathrm{H}}=\mathbf{1 2 5} \mathbf{G e V}$
- Evaluate $\hat{\mathbf{s}}, \mathbf{m}_{\mathrm{H}}$ from the pseudo-data



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## Continuous case, binned

- Previous slide: consider individual events.
- Another option:
- Define a binning
- Consider each bin as a
 counting experiment

$$
L\left(s_{1} \ldots s_{n_{\text {bins }}}, b_{1} \ldots b_{n_{\text {bins }}} ; n_{1} \ldots n_{n_{\text {bins }}}\right)=\prod_{i=1}^{n_{\text {bins }}} e^{-\left(s_{i}+b_{i}\right)} \frac{\left(s_{i}+b_{i}\right)^{n_{i}}}{n_{i}!}
$$

$-s_{i}, b_{i}=$ expected signal and bkg yields in bin $i$.

- For fine enough binning, equivalent to unbinned case
- $\Theta$ depends on binning, can influence the result if not fine enough
- $\oplus$ Binned computations can be much faster for large numbers of events ( $\mathrm{H} \rightarrow \gamma \gamma$ : 100k events, but ~1000 bins enough)


## Summary of Likelihood Definitions

- Method
- Counting • n : measured number - Poisson of events
- Likelihood

$$
L\left(s, b ; n_{i}\right)=e^{-(s+b)} \frac{(s+b)^{n_{\text {oss }}}}{n_{\text {obs }}!}
$$

- b : expected background
- Binned analysis
shape measured events in
- $n_{i}, i=1 . . n_{\text {bins }}$ : each bin.
- Poisson product

$$
L\left(s_{i}, b_{i} ; n_{i}\right)=\prod_{i=1}^{n_{\text {ons }}} e^{-\left(s_{i}+b_{i}\right)} \frac{\left(s_{i}+b_{i}\right)^{n_{\text {nos }}}}{n_{\text {obs }}!}
$$

$f_{i}$ : fraction of signal in each bin
$b_{1}$ : expected background in each bin

- Unbinned - $m_{i}, i=1 . . n_{\text {events }}$ : shape observable value analysis for each event
- Extended Likelihood
$L\left(s, b ; m_{i}\right)=e^{-(s+b)} \prod_{i=1}^{n_{o b s}} s P_{\text {signal }}(m)+b P_{b k g}(m)$
- $\mathrm{P}_{\mathrm{s}^{\prime}} \mathrm{P}_{\mathrm{B}}$ : PDFs for x in signal and background


## What we have learned so far (3)

## Estimating a parameter value

- Build a likelihood for the measurement
- see previous page
- Usually the hard part of the problem!

- Compute the likelinood of the
data $\mathrm{L}_{\text {data }}$ or $\lambda=-2 \log \mathrm{~L}_{\text {data }}$
- Adjust the parameter of the likelihood to maximize $L_{\text {data }}(\theta)$
$\Rightarrow$ Maximum is reached for $\hat{\theta}$.


## Confidence Intervals

## Definition

- What we want : $\boldsymbol{\theta}^{*}=\boldsymbol{\theta}_{0}$
- OK, so what about : $\boldsymbol{\theta}^{*}=\boldsymbol{\theta}_{0} \pm \boldsymbol{\sigma}$, i.e. $\boldsymbol{\theta}_{0}-\sigma<\boldsymbol{\theta}^{*}<\boldsymbol{\theta}_{0}+\boldsymbol{\sigma}$
- Large fluctuations can happen, although unlikely
- But we can have $P\left(\theta_{0}-\sigma<\theta^{*}<\theta_{0}+\sigma\right) \geq 1-\alpha$ for a small $\alpha$. Confidence Interval: a region where $\theta$ is very likely to be
- Usually, use " $1 \sigma$ uncertainties", i.e. $1-\alpha=68 \%$

| $\mathrm{N}_{\text {sigmas }}$ | $1-\alpha$ | $\alpha$ |
| :--- | :--- | :--- |
| 1 | 0.68 | 0.32 |
| 1.645 | 0.90 | 0.10 |
| 1.96 | 0.95 | 0.05 |
| 2 | 0.955 | 0.045 |



## Definition

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## Gaussian case

- If $\hat{\theta}$ is Gaussian, known quantiles :
$P\left(\theta^{*}-\sigma<\hat{\theta}<\theta^{*}+\sigma\right)=68 \%$
- This is a probability for $\hat{\boldsymbol{\theta}}$, not $\boldsymbol{\theta}^{*}$
- But we can invert the relation:

$$
\begin{aligned}
& P\left(\theta^{*}-\sigma<\hat{\theta}<\theta^{*}-\sigma\right)=68 \% \\
& P\left(\left|\hat{\theta}-\theta^{*}\right|<\sigma\right)=68 \% \\
& \mathrm{P}\left(\hat{\boldsymbol{\theta}}-\sigma<\theta^{*}<\hat{\theta}+\sigma\right)=68 \%
\end{aligned}
$$

- This gives the statement on $\theta^{*}$

 we wanted: "if we repeat the experiment many times,
$[\hat{\boldsymbol{\theta}}-\sigma, \hat{\boldsymbol{\theta}}+\sigma$ ] will contain the true value $68 \%$ of the time"
- $\theta_{0}$ is fixed -- actually a statement on the interval $[\hat{\boldsymbol{\theta}}-\boldsymbol{\sigma}, \hat{\boldsymbol{\theta}}+\boldsymbol{\sigma}]$, obtained for each experiment
- Can adjust the probability : $95 \% \rightarrow[\hat{\boldsymbol{\theta}}-1.96 \sigma, \hat{\boldsymbol{\theta}}+\mathbf{1 9 6 \sigma}]$ etc.


## Trivial Application: Gaussian counting

- Suppose a counting experiment measuring $N=S+B$, with
- $B$ is known
$-\mathrm{B} \gg \mathrm{l}$ so N is $\sim$ Gaussian
$-\mathrm{B} \gg \mathrm{S}$ so $\sigma=\sqrt{ }(\mathrm{S}+\mathrm{B}) \sim \sqrt{ } \mathrm{B}$
- Then $\mathrm{L}(\mathbf{S}, \mathrm{B} ; \mathrm{N})=\mathbf{G}(\mathbf{N} ; \mathbf{S}+\mathbf{B}, \sqrt{ } \mathbf{B})$
- Results:

- Best fit signal : Ŝ = N-B
- 68\% confidence interval : [ $\mathbf{S}-\sqrt{B}, \hat{S}+\sqrt{B}$ ]
- Finally : $S=(N-B) \pm \sqrt{ } B$



## General Case: Likelihood intervals

- Gaussian case: $\lambda(\boldsymbol{\theta})-\lambda(\hat{\boldsymbol{\theta}})=(\boldsymbol{\theta}-\hat{\boldsymbol{\theta}})^{2} / \boldsymbol{\sigma}^{2}$
- $68 \%$ interval : $[\hat{\boldsymbol{\theta}}-\sigma, \hat{\boldsymbol{\theta}}+\boldsymbol{\sigma}]$
- So at the interval endpoints $\lambda(\hat{\boldsymbol{\theta}} \pm \sigma)-\lambda(\hat{\boldsymbol{\theta}})=1$
$\Rightarrow$ Find the endpoints by solving:


$$
\lambda(\theta)-\lambda(\hat{\theta})=1
$$

- Also good approximation for non-Gaussian case
- Very easy to apply
- Other interval sizes:

| $\mathrm{N}_{\text {sigmas }}$ |  | $1-\alpha$ |
| :--- | :--- | :--- |
| 1 | $\lambda(\theta)<1$ | 0.68 |
| 1.645 | $\lambda(\theta)<2.71$ | 0.90 |
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- Very easy to apply
- Other interval sizes:



## Example : Back to $\mathrm{H} \rightarrow \gamma \gamma$

- Generate pseudo-data with $\mathrm{s}=200, \mathrm{~m}_{\mathrm{H}}=125 \mathrm{GeV}$
- Measure $\mathbf{s}, \mathbf{m}_{\mathrm{H}}$ in the pseudo-data




$$
\hat{m}_{H}=125.1 \pm 0.3 \mathrm{GeV}
$$

## Coverage \& Toys

- We claim to have computed $\left(\theta_{1}, \theta_{2}\right)$ so that $P\left(\theta_{1}<\theta_{0}<\theta_{2}\right)=68 \%$
- We can check whether this is OK ("good coverage"):
- Generate pseudo-data with $\theta=\theta_{0}$.
- Compute the interval
- Repeat many times, check fraction of cases when we do get $\theta_{1}<\theta_{0}<\theta_{2}$.
- Example on previous slide: run 5 k toys with $\mathrm{s}=200, \mathrm{~m}_{\mathrm{H}}=125 \mathrm{GeV}$
- 134.5 < s < 228.7 : true $3530 / 5 \mathrm{k}=70.6 \%$ of the time
- $124.7<\mathrm{m}_{\mathrm{H}}<125.5 \mathrm{GeV}$ : true $3414 / 5 \mathrm{~K}=68.3 \%$ of the time
- Can also be used to compute ( $\theta_{1}, \theta_{2}$ ) :
- Choose some values, compute coverage
- Adjust $\left(\theta_{1}, \theta_{2}\right.$ ) until coverage is OK.
$\oplus$ No approximations involved $\ominus$ Can be very slow,


## What we have learned so far (4)

## Estimating a parameter

- Build a likelihood $\mathbf{L}(\boldsymbol{\theta})$ for the measurement
- Compute $\lambda(\theta)=-2 \log \mathrm{~L}_{\text {data }}(\theta)$, as a function of $\theta$.

- Find the minimum of $\lambda(\theta)$
$\Rightarrow$ Minimum is reached for $\hat{\boldsymbol{\theta}}$.
- Move the parameter up and down to get $\lambda\left(\hat{\boldsymbol{\theta}}+\sigma_{\mathrm{up}}\right)=\lambda(\hat{\boldsymbol{\theta}})+1$ and $\lambda\left(\hat{\boldsymbol{\theta}}-\sigma_{\text {down }}\right)=\lambda(\hat{\boldsymbol{\theta}})+1$.
Then $\left[\theta-\sigma_{\text {down }}, \theta+\sigma_{\text {up }}\right]$ is a $68 \%$ confidence interval for $\theta: \theta=\hat{\theta}_{-\sigma_{\text {down }}}^{+\sigma_{u p}}$


## Real-Life Case: ATLAS Higgs Mass Measurement

Phys. Rev. D. 90, 052004 (2014)


## Fisher Information

- Gaussian case: $\lambda(\theta)-\lambda(\hat{\boldsymbol{\theta}})=(\theta-\hat{\boldsymbol{\theta}})^{2} / \sigma^{2}$ so $d^{2} \lambda / d \theta^{2}=2 / \sigma^{2}$
- Define the Fisher Information as

$$
I=-E\left|\frac{\partial^{2}}{\partial \theta^{2}} \log L(\theta)\right|
$$

- Measure of the quantity of information in the measurement of $\theta$
- Gaussian case, $\mathrm{I}=\mathbf{1} / \boldsymbol{\sigma}^{2}$ : more information $=>$ smaller uncertainty.
- In general, for any estimator $\hat{\theta}$,
$\operatorname{Var}(\hat{\theta}) \geq 1 / I$ (Cramer-Rao inequality)
(cannot be more precise than information allows.)
- Estimators which reach the bound are efficient - e.g. MLE in the large n limit.


## 2D Contours

- Two correlated parameters:
- Now $\boldsymbol{\lambda}\left(\boldsymbol{\theta}_{1}, \boldsymbol{\theta}_{2}\right)$, Gaussian Likelihood $\Rightarrow$ Paraboloid
- Find 2D maximum
- Find 2D contour :

$$
\lambda\left(\boldsymbol{\theta}_{1}, \boldsymbol{\theta}_{2}\right)=\lambda\left(\hat{\boldsymbol{\theta}}_{1}, \hat{\boldsymbol{\theta}}_{2}\right)+2.30
$$

- Contour values are differen ( $\chi^{2}(n=1)$ vs. $\chi^{2}(n=2)$ )

$\mathrm{N}_{\text {sigmos }} \quad$| For 2 degrees |
| :---: |
| of freedom | $1-\alpha$


$x^{4}$


## Relation with $\chi^{2}$

- $\chi^{2}$ : say you measure $\hat{\theta}_{1} \ldots \hat{\theta}_{\mathrm{n}}$ with means $\theta_{1}^{*} \ldots \theta_{1}^{*}$, uncertainty $\sigma$. Then

$$
\chi^{2}=\sum_{i=1}^{n}\left|\frac{\hat{\theta}_{i}-\theta_{i}^{*}}{\sigma}\right|^{2}
$$

- If good agreement : $\chi^{2} \sim n$.
- If $\hat{\theta}_{i}$ are Gaussian (with same $\theta_{i}^{*}$ and $\sigma$ as in the $\chi^{2}$ expression), then $\chi^{2}$ follows a $\chi^{2}$ distribution with $n$ degrees of freedom, $\chi^{2}{ }_{n}$
- Now go back to the likelihood picture, assume Gaussian measurements:

$$
L=\prod_{i=1}^{n} e^{-\frac{1}{2}\left(\frac{\hat{\theta}_{-}-\theta_{i}}{\sigma}\right)^{2}} \quad \lambda=-2 \log L=\sum_{i=1}^{n}\left|\frac{\hat{\theta}_{i}-\theta_{0}}{\sigma}\right|^{2}
$$

- So
$-\lambda$ is like a $\chi^{2}$
$-L$ is $\exp \left(-\chi^{2} / 2\right)$
$-\lambda$ is $\sim \chi_{n}^{2}$. Quantiles:
- for $\mathbf{n}=1$, same as Gaussian
- For $n>1$, look up the values...

| $\mathrm{N}_{\text {sigmas }}$ | $\chi_{1}^{2}$ | $\chi_{2}^{2}$ | $1-\alpha$ |
| :--- | :--- | :--- | :--- |
| 1 | 1 | 2.30 | 0.68 |
| 1.645 | 2.71 | 4.61 | 0.90 |
| 1.96 | 3.84 | 6.00 | 0.95 |

## Real-Life: $\left(\mu_{g g F}, \mu_{\text {vBF }}\right)$ from $\mathrm{H} \rightarrow \gamma \gamma$

Physics Letters B 740 (2015) 222-242


## ID Contours with Multiple Parameters: Profiling

- What about ID contours, when several parameters are present ? e.g. $\boldsymbol{\lambda}(\boldsymbol{\theta}, \boldsymbol{\alpha})$, , and we want an interval on $\boldsymbol{\theta}$ only.
- Define the profile likelihood $\boldsymbol{\lambda}(\boldsymbol{\theta})=\boldsymbol{\lambda}\left(\boldsymbol{\theta}, \hat{\boldsymbol{\alpha}}_{\theta}\right)$ where $\hat{\boldsymbol{\alpha}}_{\theta}$ is the ML estimate of $\boldsymbol{\alpha}$ for a fixed value of $\boldsymbol{\theta}$.
- Compute intervals as before with

$$
\lambda(\theta)-\lambda(\hat{\boldsymbol{\theta}})=1 \text { i.e. } \lambda\left(\theta, \hat{\boldsymbol{\alpha}}_{\theta}\right)-\lambda(\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\alpha}})=1
$$




## Real-Life: $\mu$ from $\mathrm{H} \rightarrow \gamma \gamma$



FIG. 15. The profile of the negative log-likelihood ratio $\lambda(\mu)$ of the combined signal strength $\mu$ for $m_{H}=125.4 \mathrm{GeV}$. The observed result is shown by the solid curve, the expectation for the SM by the dashed curve. The intersections of the solid and dashed curves with the horizontal dashed line at $\lambda(\mu)=1$ indicate the $68 \%$ confidence intervals of the observed and expected results, respectively.

## Conclusion

- Seen today
-Likelihoods
- Point Estimation
- Interval Estimation
- Tomorrow
-Discovery significance
- Upper Limits
- Further topics


## Exercises

- We perform a counting experiment where $b=400$. We observe 410 events. These counts are large enough so that result is Gaussian
- Write the likelihood
- Compute the best-fit value for s
- Compute the 68\% confidence interval for s.
- Combining two Gaussian measurements
- Recall $L\left(\theta ; x_{1}, x_{2}\right)=G\left(x_{1} ; \theta, \sigma_{1}\right) G\left(x_{2} ; \theta, \sigma_{2}\right)$
- Compute the (68\%) "Combined error" $\hat{\theta}=\frac{\frac{x_{1}}{\sigma_{1}^{2}}+\frac{x_{2}}{\sigma_{2}^{2}}}{\frac{1}{\sigma_{1}^{2}}+\frac{1}{\sigma_{2}^{2}}}$ for this estimate

