## PSI Zuoz Summer School 20

Statistics

Nicolas Berger (LAPP Annecy)

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## Statistics <br> 0 

 4For Physicists

Nicolas Berger (LAPP Annecy)

## Lecture Plan

Statistics basic concepts (Today)
[Basic ingredients (PDFs, etc.)]
Parameter estimation (maximum likelihood, least-squares, ...)
Model testing ( $\chi^{2}$ tests, hypothesis testing, p -values, ...)

Computing statistical results (Today/Tomorrow)
Discovery
Confidence intervals
Upper limits
Systematics and profiling
[Bayesian techniques]

The class will be based on both lectures and hands-on tutorial

## Hands-on sessions

The hands-on session will be based on Jupyter notebooks built using the numpy/scipy/pyplot stack.

If you have a computer with you, please install anaconda before the start of the class. This provides a consistent installation of python, JupyterLab, etc.
$\rightarrow$ Alternatively, you can also install JupyterLab as a standalone package.
$\rightarrow$ Another solution is to run the notebooks on the public jupyter servers at mybinder.org. This will probably be slower but avoids a local install.

| Warmup |  | notebook [solutions] | binder [solutions] |
| :--- | :--- | :--- | :--- |
| Lecture 1 | Lecture Notes | notebook | binder |
| Lecture 2 | Lecture notes | notebook | binder |

The warmup item includes material that will not be covered in detail in the class, as well as an introduction to the notebooks. Please have a look before the beginning of the classes if you are unfamiliar with this.

## Statistics are everywhere

 "There are three types of lies - lies, damn lies, and statistics." - Benjamin Disraeli

Credits: mattbuck / wikimedia

## And Physics ?

"If your experiment needs statistics, you ought to have done a better experiment" - E. Rutherford

## Introduction

Statistical methods play a critical role in many areas of physics

Higgs discovery: "We have $5 \sigma$ "!

## Introduction

Sometimes difficult to distinguish a bona fide discovery from a background fluctuation...


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$7 /$

## Randomness in High-Energy Physics

Experimental data is produced by incredibly complex processes


## Randomness in High-Energy Physics

Experimental data is produced by incredibly complex processes

Muon ——Electron
---. Neutral hadron (e.g. neutron)
__Charged hadron (e.g. pion)
.-..-. Photon

## Randomness in High-Energy Physics

Experimental data is produced by incredibly complex processes

Image Credits:
S. Höche,

SLAC-PUB-16160


Randomness involved in all stages
$\rightarrow$ Classical randomness: detector reponse
$\rightarrow$ Quantum effects in particle production, decay

## Hard scattering

PDFs, Parton shower, Pileup

Decays

Detector response

Reconstruction


## Measurement Errors: Energy measurement

Example: measuring the energy of a photon in a calorimeter


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Cannot predict the measured value for a given event
$\Rightarrow$ Random process $\Rightarrow$ Need a probabilistic description

## Quantum Randomness: $\mathrm{H} \rightarrow \mathrm{ZZ}^{*} \rightarrow 4 \mathrm{I}$



## Quantum Randomness: $\mathrm{H} \rightarrow \mathrm{ZZ}{ }^{*} \rightarrow 4 \mathrm{I}$



Rare process: Expect 1 signal event every ~6 days


View online

## Quantum Randomness: $\mathrm{H} \rightarrow \mathrm{ZZ}^{*} \rightarrow 4 \mathrm{I}$



## Statistical Modeling

## Probability Distributions

Probabilistic treatment of possible outcomes
$\Rightarrow$ Probability Distribution

Example: two-coin toss
$\rightarrow$ Fractions of events in each bin i converge to a limit $p_{i}$

Probability distribution :
$\left\{P_{i}\right\}$ for $i=0,1,2$
Properties

- $P_{i}>0$
- $\quad \Sigma P_{i}=1$


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100 trials


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- $\sum P_{i}=1$

100000 trials


## Continuous Variables: PDFs

Continuous variable: can consider per-bin probabilities $p_{i}, i=1 . . n_{b i n s}$

5 bins


Generalizes to multiple variables:
$P(x, y)>0, \int P(x, y) d x d y=1$

Bin size $\rightarrow 0$ : Probability distribution function $\mathbf{P ( x )}$

High PDF value
$\Rightarrow$ High chance to get a measurement here

$$
P(x)>0, \quad \int P(x) d x=1
$$



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Contours: $\mathrm{P}(\mathrm{x}, \mathrm{y})$
Bin size $\rightarrow 0$ : Probability distribution function $\mathbf{P ( x )}$

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## Random Variables

$\mathrm{X}, \mathrm{Y} .$. are Random Variables (continuous or discrete), aka. observables :
$\rightarrow X$ can take any value $x$, with probability $P(X=x)$.
$\rightarrow P(X=x)$ is the PDF of $X$, a.k.a. the Statistical Model.
$\rightarrow$ The Observed data is one value $\mathrm{x}_{\mathrm{obs}}$ of X , drawn from $P(X=x)$.




## PDF Properties: Mean

$E(X)=\langle X\rangle$ : Mean of $X$ - expected outcome on average over many measurements

$$
\begin{aligned}
\langle X\rangle & =\sum_{i} x_{i} P_{i} \\
\langle X\rangle & =\int x P(x) d x
\end{aligned}
$$

$\rightarrow$ Property of the PDF

For measurements $x_{1} \ldots x_{n}$, then can compute the Sample mean:

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

$\rightarrow$ Property of the sample
$\rightarrow$ approximates the PDF mean.

PDF Mean


PDF Mean Sample Mean


## PDF Properties: (Co)variance

Variance of $X$ :

$$
\operatorname{Var}(X)=\left\langle(X-\langle X\rangle)^{2}\right\rangle
$$

$\rightarrow$ Average square of deviation from mean
$\rightarrow \mathrm{RMS}(\mathrm{X})=\sqrt{ } \operatorname{Var}(\mathrm{X})=\sigma_{\mathrm{x}}$ standard deviation
Can be approximated by sample variance:

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

Covariance of $X$ and $Y$ :

$$
\operatorname{Cov}(\boldsymbol{X}, \boldsymbol{Y})=\langle(\boldsymbol{X}-\langle\boldsymbol{X}\rangle)(\boldsymbol{Y}-\langle\boldsymbol{Y}\rangle)\rangle
$$


$\rightarrow$ Large if variations of $X$ and $Y$ are "synchronized"
Correlation coefficient $\quad \rho=\frac{\operatorname{Cov}(X, Y)}{\sqrt{\operatorname{Var}(X) \operatorname{Var}(Y)}} \quad-1 \leq \rho \leq 1$

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## "Linear" vs. "non-linear" correlations

For non-Gaussian cases, the Correlation coefficient $\rho$ is not the whole story:


Source: Wikipedia
In particular, variables can still be correlated even when $\rho=0$ : "Non-linear" correlations.

## Gaussian PDF

## Gaussian distribution:

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

$\rightarrow$ Mean : $X_{0}$

$\rightarrow$ Variance : $\sigma^{2}(\Rightarrow \mathrm{RMS}=\sigma)$

Generalize to $\mathbf{N}$ dimensions:
$\rightarrow$ Mean : X
$\rightarrow$ Covariance matrix :

$$
\begin{aligned}
C & =\left[\begin{array}{ll}
\operatorname{Var}\left(X_{1}\right) & \operatorname{Cov}\left(X_{1}, X_{2}\right) \\
\operatorname{Cov}\left(X_{2}, X_{1}\right) & \operatorname{Var}\left(X_{2}\right)
\end{array}\right] \\
& =\left[\begin{array}{cc}
\sigma_{1}^{2} & \rho \sigma_{1} \sigma_{2} \\
\rho \sigma_{1} \sigma_{2} & \sigma_{2}^{2}
\end{array}\right]
\end{aligned}
$$

## Gaussian Quantiles

$$
P\left(\left|x-x_{0}\right|>Z \sigma\right)
$$

Consider $\quad z=\left(\frac{\boldsymbol{x}-\boldsymbol{x}_{0}}{\boldsymbol{\sigma}}\right) \quad$ "pull" of $x$
$G\left(x ; x_{0}, \sigma\right)$ depends only on $z \sim G(z ; 0,1)$
Probability $\mathrm{P}\left(\left|\mathrm{x}-\mathrm{x}_{0}\right|>\mathrm{Z} \sigma\right)$ to be away from the mean:
0.317
0.045
0.003
$3 \times 10^{-5}$
$6 \times 10^{-7}$

Gaussian Cumulative Distribution Function (CDF) :

$$
\Phi(z)=\int_{-\infty}^{z} G(u ; 0,1) d u
$$



## Gaussian Quantiles

$Z \quad P\left(\left|x-x_{0}\right|>Z \sigma\right)$

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$$
\begin{equation*}
z=\left(\frac{x-x_{0}}{\sigma}\right) \quad \text { "pull" of } x \tag{2}
\end{equation*}
$$

$$
3
$$

$$
0.003
$$

4
$3 \times 10^{-5}$
$6 \times 10^{-7}$

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## Central Limit Theorem

For an observable X with any ${ }^{\left({ }^{*}\right)}$ distribution, one has

$$
\bar{x}=\frac{1}{n} \sum_{i=1}^{n} x_{i} \stackrel{n \rightarrow \infty}{\sim} G\left(\langle X\rangle, \frac{\sigma_{X}}{\sqrt{n}}\right)
$$

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 average of the single measurements
- The RMS of the Gaussian decreases as $\sqrt{ } \mathbf{n}$ : smaller fluctuations when averaging over many measurements

Another version: $\quad \sum_{i=1}^{n} x_{i} \stackrel{n \rightarrow \infty}{\sim} G\left(n\langle X\rangle, \sqrt{n} \sigma_{X}\right)$
Mean scales like $n$, but RMS only like $\sqrt{ } n$

## Central Limit Theorem in action

Draw events from a parabolic distribution (e.g. decay $\cos \theta^{*}$ )


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

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## Chi-squared

Multiple Independent Gaussian variables $\mathrm{x}_{\mathrm{i}}$ : Define

$$
\chi^{2}=\sum_{i=1}^{n}\left(\frac{x_{i}-x_{i}^{0}}{\sigma_{i}}\right)^{2}
$$

Measures global distance from reference point ( $\mathrm{x}_{1}{ }^{0} \ldots . \mathrm{x}_{\mathrm{n}}{ }^{0}$ )

Distribution depends on n :

Rule of thumb:



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Distribution depends on n :

Rule of thumb:


$\chi^{2} / n$ should be $\lesssim 1$

## Histogram Chi-squared

Histogram $\chi 2$ with respect to a reference shape:

- Assume an independent Gaussian distribution in each bin
- Degrees of freedom = (number of bins) - (number of fit parameters)


BLUE histogram vs. flat reference

$$
\chi^{2}=12.9, \quad \mathrm{p}\left(\chi^{2}=12.9, \mathrm{n}=10\right)=23 \%
$$

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BLUE histogram vs. flat reference $\chi^{2}=12.9, p\left(\chi^{2}=12.9, n=10\right)=23 \%$ RED histogram vs. flat reference $\chi^{2}=38.8, \mathrm{P}\left(\mathrm{x}^{2}=38.8, \mathrm{n}=10\right)=0.003 \%$

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RED histogram vs. flat reference $\chi^{2}=38.8, \mathrm{P}\left(\mathrm{x}^{2}=38.8, \mathrm{n}=10\right)=0.003 \%$

RED histogram vs. correct reference $x 2=9.5, p(x 2=9.5, n=10)=49 \%$

## Error Bars

Strictly speaking, the uncertainty is given by the model :
$\rightarrow$ Bin central value $\sim$ mean of the bin PDF
$\rightarrow$ Bin uncertainty $\sim$ RMS of the bin PDF
The data is just what it is, a simple observed point.
$\Rightarrow$ One should in principle show the error bar on the prediction.
$\rightarrow$ In practice, the usual convention is to have error bars on the data points.


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## Statistical Modeling

## Example 1: Z counting

Measure the cross-section (event rate) of the $Z \rightarrow$ ee process

$$
\sigma^{35000 \pm 187}=\frac{1}{n_{\text {data }}-N_{b k g}} \begin{gathered}
175 \pm 8 \\
C_{\text {fid }} L \\
0.552 \pm 0.006
\end{gathered}
$$



$$
\sigma^{\text {fid }}=0.781 \pm 0.004 \text { (stat) } \pm 0.018 \text { (syst) nb }
$$

Fluctuations in the data counts

Other uncertainties (assumptions, parameter values)

## Example 2: ftH $\rightarrow \mathrm{bb}$



Event counting in different regions:
Multiple-bin counting

## Lots of information available

$\rightarrow$ Potentially higher sensitivity
$\rightarrow$ How to make optimal use of it ?

## Example 3: unbinned modeling



All modeling done using continuous distributions:

$$
\begin{equation*}
\boldsymbol{P}_{\text {total }}\left(m_{\gamma \gamma}\right)=\frac{S}{S+B} P_{\text {signal }}\left(m_{\gamma \gamma} ; m_{H}\right)+\frac{B}{S+B} \boldsymbol{P}_{\mathrm{bkg}}\left(m_{\gamma \gamma}\right) \tag{32}
\end{equation*}
$$

## How to count

Common situation: produce many events N , select a (very) small fraction P
$\rightarrow$ In principle, binomial process
$\rightarrow$ In practice, $P \ll 1, N \gg 1, \Rightarrow$ Poisson approximation.
$\rightarrow$ i.e. very rare process, but very many trials so still expect to see good events
Poisson distribution
$\lambda=0.5$


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

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

For a counting measurement, RMS = $\sqrt{ }$ Mean

Central limit theorem :
becomes Gaussian for large $\lambda$ :

$$
P(\lambda) \xrightarrow{\lambda \rightarrow \infty} G(\lambda, \sqrt{\lambda})
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$$
\begin{array}{ll}
L & (1-P)^{N-n} \stackrel{n \ll N}{\sim}\left(1-\frac{\lambda}{N}\right)^{N} \stackrel{N \ngtr 1}{\sim} e^{-\lambda} \\
\text { Mean }=\lambda & \text { For a counting } \\
\text { Variance }=\lambda & \text { measurement, } \\
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$$
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$$

$\lambda=3$

$$
\square(1-P)^{N-n \stackrel{n}{\aleph} N}\left(1-\frac{\lambda}{N}\right)^{N} \stackrel{N \gg 1}{\sim} e^{-\lambda}
$$

$$
\begin{aligned}
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$\lambda=10$


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$$
\text { L }(1-P)^{N-n} \stackrel{n \ll N}{\sim}\left(1-\frac{\lambda}{N}\right)^{N} \stackrel{N \gtrsim 1}{\sim} e^{-\lambda}
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$$
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\text { Variance }=\lambda
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$$
\square(\mathbf{1}-\boldsymbol{P})^{N-n} \stackrel{n \ll N}{\sim}\left(\mathbf{1}-\frac{\boldsymbol{\lambda}}{N}\right)^{N} \stackrel{N \gg 1}{\sim} \boldsymbol{e}^{-\lambda}
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## Statistical Model for Counting

Observable: number of events $\mathbf{n}$
Typically both Signal and Background present:


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

S:\# of events from signal process
B : \# of events from bkg. processes)

Model has parameters S and B.
B can be known a priori or not (S usually not...)
$\rightarrow$ Example: assume $\mathbf{B}$ is known, use measured n to find out about $\mathbf{S}$.

## Multiple counting bins

Count in bins of a variable $\Rightarrow$ histogram $\mathrm{n}_{1} \ldots \mathrm{n}_{\mathrm{N}}$.
( N : number of bins)
Per-bin fractions (=shapes)
of Signal and Background
$\boldsymbol{P}\left(\left\{n_{i}\right\} ; S, B\right)=\prod_{i=1}^{N} \underbrace{-\left(s f_{s, i}+B f_{p, i}\right)} \frac{\left(\boldsymbol{S f}_{S, i}+\boldsymbol{B} f_{B, i}\right)^{n_{i}}}{n_{i}!}$
Poisson distribution in each bin


Shapes $f$ typically obtained from simulated events (Monte Carlo)
$\rightarrow$ HEP: typically excellent modeling from simulation, although some uncertainties need to be accounted for.

However not always possible to generate sufficiently large MC samples MC stat fluctuations can create artefacts, especially for S < B.

## Model Parameters

Model typically includes:

- Parameters of interest (POIs) : what we want to measure
$\rightarrow \mathrm{S}, \mathrm{m}_{\mathrm{w}}, \ldots$
- Nuisance parameters (NPs) : other parameters needed to define the model
$\rightarrow$ Background levels (B)
$\rightarrow$ For binned data, frig $_{\mathrm{ig}}^{\mathrm{i}}, \mathrm{ffkg}_{\mathrm{i}}$

NPs must be either:
$\rightarrow$ Known a priori (within uncertainties) or
$\rightarrow$ Constrained by the data

## Takeaways

Random data must be described using a statistical model:

| Description | Observable | Likelihood |
| :---: | :---: | :---: |
| Counting | n | Poisson $P(\boldsymbol{n} ; \boldsymbol{S}, \boldsymbol{B})=e^{-(s+\boldsymbol{B})} \frac{(\boldsymbol{S}+\boldsymbol{B})^{n}}{n!}$ |
| Binned shape analysis | $\mathrm{n}_{\mathrm{i}}, \mathrm{i}=1 . . \mathrm{N}_{\text {bins }}$ | Poisson product $P\left(n_{i} ; \boldsymbol{S}, \boldsymbol{B}\right)=\prod_{i=1}^{n_{\mathrm{bins}}} e^{-\left(\boldsymbol{S} f_{i}^{\mathrm{sig}}+\boldsymbol{B} f_{i}^{\mathrm{kgs})}\left(\boldsymbol{S} \boldsymbol{f}_{i}^{\mathrm{sig}}+\boldsymbol{B} f_{i}^{\mathrm{bkg}}\right)^{n_{i}}\right.} \underset{n_{i}!}{ }$ |
| Unbinned shape analysis | $m_{i}, \mathrm{i}=1 . . \mathrm{n}_{\text {evts }}$ | Extended Unbinned Likelihood $P\left(\boldsymbol{m}_{i} ; \boldsymbol{S}, \boldsymbol{B}\right)=\frac{e^{-(\boldsymbol{s}+\boldsymbol{B})}}{\boldsymbol{n}_{\mathrm{evvs}}!} \prod_{i=1}^{n_{\mathrm{ves}}} \boldsymbol{S} P_{\mathrm{sig}}\left(\boldsymbol{m}_{i}\right)+\boldsymbol{B} P_{\mathrm{bkg}}\left(\boldsymbol{m}_{i}\right)$ |

Model can include multiple categories, each with a separate description Includes parameters of interest (POIs) but also nuisance parameters (NPs) Next step: use the model to obtain information on the POIs

## Hypothesis Testing and discovery




## Discovery Testing

We see an unexpected feature in our data, is it a signal for new physics or a fluctuation ?
e.g. Higgs discovery : "We have 5 $\sigma^{\prime}$ !


Phys. Lett. B 716 (2012) 1-29


## Discovery Testing

Say we have a Gaussian measurement with a background $\mathbf{B = 1 0 0}$, and we measure $\mathbf{n}=120$

Did we just discover something ? Maybe :-) (but not very likely)


The measured signal is $S=20$.

$$
\mathrm{S}=\mathrm{n}_{\text {obs }}-\mathrm{B}
$$

Uncertainty on B is $\sqrt{ } \mathrm{B}=10$
$\Rightarrow$ Significance Z $=2$
$\Rightarrow$ we are $\sim 2 \sigma$ away from $S=0$.

## Gaussian quantiles :

$Z=2$ happens $p_{0} \sim 2.3 \%$ of the time if $S=0$
$P$-value:

$$
p_{0}=1-\Phi(Z)
$$

$\Rightarrow$ Rare, but not exceptional

$$
\Phi(Z)=\int_{-\infty}^{Z} G(u ; \mathbf{0}, \mathbf{1}) d u
$$

## Discovery Testing



| $n_{\text {obs }}$ | $s$ | $Z$ | $p_{0}$ |
| :---: | :---: | :---: | :---: |
| 105 | 5 | $0.5 \sigma$ | $31 \%$ |
| 110 | 10 | $1 \sigma$ | $16 \%$ |
| 120 | 20 | $2 \sigma$ | $2.3 \%$ |
| 130 | 30 | $3 \sigma$ | $0.1 \%$ |



Straightforward in this Gaussian case

Need to be able to do the same in more complex cases:

- Determine S

Evidence
Discovery

## Maximum Likelihood Estimation

## What a PDF is for

Model describes the distribution of the observable: P(data; parameters)
$\Rightarrow$ Possible outcomes of the experiment, for given parameter values
Can draw random events according to PDF : generate pseudo-data

$$
P(\lambda=5)
$$




2, 5, 3, 7, 4, 9,
Each entry = separate "experiment"



## What a PDF is also for: Likelihood

Model describes the distribution of the observable: P(data; parameters)
$\Rightarrow$ Possible outcomes of the experiment, for given parameter values
We want the other direction: use data to get information on parameters

$$
P(\lambda=\text { ? })
$$



2



Likelihood: L(parameters) = P(data; parameters)
$\rightarrow$ same as the PDF, but seen as function of the parameters

## Maximum Likelihood Estimation

To estimate a parameter $\mu$, find the value $\hat{\boldsymbol{\mu}}$ that maximizes $L(\mu)$
Maximum Likelihood

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



MLE: the value of $\mu$ for which this data was most likely to occur The MLE is a function of the data - itself an observable No guarantee it is the true value (data may be "unlikely") but sensible estimate

## Gaussian case



## Gaussian case



## Gaussian case



## Multiple Gaussian bins


-2 log Likelihood:

$$
\lambda(\mu)=-2 \log L(\mu)=\sum_{i=1}^{N_{\text {bins }}}\left(\frac{n_{i}-\mu_{i}}{\sigma_{i}}\right)^{2}
$$

Maximum likelihood $\Leftrightarrow$ Minimum $\chi^{2}$
$\Leftrightarrow$ Least-squares minimization

However typically need to perform non-linear minimization in other cases.

HEP practice:

- MINUIT (C++ library within ROOT, numerical gradient descent)
- scipy.minimize - using NumPy/TensorFlow/PyTorch/... backends
$\rightarrow$ Many algorithms - gradient-based, etc.


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\begin{aligned}
& \qquad \lambda(\mu)=-2 \log L(\mu)=\sum_{i=1}^{N_{\text {bins }}}\left(\frac{n_{i}-\mu_{i}}{\sigma_{i}}\right)^{2} \\
& \text { Maximum likelihood } \Leftrightarrow \text { Minimum } \chi^{2} \\
& \Leftrightarrow \\
& \\
& \\
& \text { Least-squares } \\
& \text { minimization }
\end{aligned}
$$

However typically need to perform non-linear minimization in other cases.

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## Hypothesis Testing

Null Hypothesis: assumption on POIs, say value of $S$ (e.g. $\mathbf{H}_{0}: \mathbf{S}=\mathbf{0}$ )
$\rightarrow$ Goal : decide if $\mathrm{H}_{0}$ is favored or disfavored using a test based on the data

| Possible <br> outcomes: | Data disfavors $H_{0}$ <br> (Discovery claim) | Data favors $H_{0}$ <br> (Nothing found) |
| :--- | :--- | :--- |
| $H_{0}$ is false <br> (New physics!) | Discovery! | Missed <br> discovery |
| $H_{0}$ is true <br> (Nothing new) | False <br> discovery |  |

"... the null hypothesis is never proved or established, but is possibly disproved, in the course of experimentation. Every experiment may be said to exist only to give the facts a chance of disproving the null hypothesis." - R. A. Fisher

## Hypothesis Testing

Hypothesis：assumption on model parameters，say value of $S\left(e . g . H_{0}: S=0\right)$

|  | Data disfavo （Discovery c | Data favors $\mathrm{H}_{0}$ （Nothing found） |  |
| :---: | :---: | :---: | :---: |
| $\mathrm{H}_{0}$ is false （New physics！） | Discovery！ | Type－II error （Missed discovery） |  |
| $\mathrm{H}_{0}$ is true （Nothing new） | Type－I error （False discovery） | No new physics， none found | 可到四 |

Lower Type－I errors $\Leftrightarrow$ Higher Type－II errors and vice versa：cannot have everything！
$\rightarrow$ Goal：test that minimizes Type－II errors for a given level of Type－I error．


## ROC Curves

## "Receiver operating characteristic"

 (ROC) Curve:$\rightarrow$ Shows Type-I vs Type-II rates for different selections
$\rightarrow$ All curves monotonically decrease from $(0,1)$ to $(1,0)$
$\rightarrow$ Better discriminators more bent towards (1,1)

$\rightarrow$ Goal: test that minimizes Type-II errors for given level of Type-l error.
$\rightarrow$ Usually set predefined level of acceptable Type-I error (e.g. " $5 \sigma$ ")

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Need to be able to do the same in more complex cases:

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## Testing for Evidence in Gaussian counting



## Testing for Evidence in Gaussian counting



## Hypothesis Testing with Likelihoods

## Neyman-Pearson Lemma

When comparing two hypotheses $H_{0}$ and $H_{1}$, the optimal discriminator is the Likelihood ratio (LR)
$\frac{L\left(H_{1} ; \text { data }\right)}{L\left(H_{0} ; \text { data }\right)}$
e.g. $\frac{L(S=5 ; \text { data })}{L(S=0 ; \text { data })}$

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.
$\rightarrow$ Always need an alternate hypothesis to test against the null.
$\rightarrow$ Minimizes Type-II uncertainties for given level of Type-I uncertainties
$\rightarrow$ 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 :

- $\mathrm{H}_{0}$ : background only $(\mathrm{S}=0)$ against

- $\mathrm{H}_{1}$ : presence of a signal $(\mathbf{S}>0)$
$\rightarrow$ For $\mathrm{H}_{1}$, any $\mathrm{S}>0$ is possible, which to use ? The one preferred by the data, $\hat{\mathbf{S}}$.
$\Rightarrow$ Use Likelihood ratio: $\frac{L(S=0)}{L(\hat{S})}$
$\rightarrow$ In fact use the test statistic $q_{0}=-2 \log \frac{L(S=0)}{L(\hat{S})}$

Note: for $\hat{S}<0$, set $\mathrm{q}_{0}=0$ to reject negative signals ("one-sided test statistic") ${ }_{\text {/ }}^{54}$

## Discovery p-value

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

data
$\Rightarrow$ observed S is far from 0
$\Rightarrow \mathrm{H}_{0}(\mathrm{~S}=0)$ disfavored compared to $\mathrm{H}_{1}(\mathrm{~S} \neq 0)$.
$\Rightarrow$ Large S !

Compute $p$-value in the tail of the distribution
 to exclude $\mathbf{H}_{0}$ (... and claim a discovery!)

$$
p_{0}=\int_{q_{0}^{\text {obs }}}^{\infty} f\left(q_{0} \mid S=0\right) d q_{0}
$$

Need to know $f\left(q_{0} \mid S=0\right)$, the distribution of the test statistic...

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## Asymptotic distribution of $\mathrm{q}_{0}$

Gaussian regime for $\hat{\mathbf{S}}$ (e.g. large $\mathrm{n}_{\text {evts }}$, Central-limit theorem) :
Wilk's Theorem: $\mathbf{q}_{0}$ distributed as $\chi^{2}\left(n_{\text {par }}\right)$ for $S=0$
$\Rightarrow \mathrm{n}_{\mathrm{par}}=1: \sqrt{ } \mathrm{q}_{0}$ is distributed as a Gaussian
$\Rightarrow$ Can compute p -values from Gaussian quantiles

$$
p_{0}=1-\Phi\left(\sqrt{q_{0}}\right)
$$

$\Rightarrow$ Even more simply, the significance is:

$$
Z=\sqrt{q_{0}}
$$

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


## Homework 1: Gaussian Counting

## Count number of events $\mathbf{n}$ in data

$\rightarrow$ Assume n large enough so process is Gaussian
$\rightarrow$ Assume $B$ is known, and we measure $S$

Likelihood :

$$
L\left(S ; \boldsymbol{n}_{\mathrm{obs}}\right)=\boldsymbol{e}^{-\frac{1}{2}\left(\frac{n_{\mathrm{abs}}-(S+B)}{\sqrt{S+B})^{2}}\right.}
$$


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

## Homework 2: Poisson Counting

Same problem but now not assuming Gaussian behavior:

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

$\rightarrow$ As before, compute $\hat{\mathrm{S}}$, and $\mathrm{q}_{0}$
(Can remove the n ! constant since we're only dealing with $L$ ratios)
$\rightarrow$ Compute $\mathrm{Z}=\sqrt{ } \mathrm{a}_{0}$, assuming asymptotic behavior

## Solution:

$$
Z=\sqrt{2\left\lfloor\left.(\hat{S}+B) \log \left(1+\frac{\hat{S}}{B}\right)-\hat{S} \right\rvert\,\right.}
$$

Exact result can be obtained using pseudo-experiments $\rightarrow$ close to $\sqrt{ } \mathrm{q}_{0}$ 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


## Discovery Thresholds

Evidence : $3 \sigma \Leftrightarrow p_{0}=0.3 \% \Leftrightarrow 1$ chance in 300

Discovery: $5 \sigma \Leftrightarrow p_{0}=310^{-7} \Leftrightarrow 1$ chance in 3.5 M
Why so high thresholds? (from Louis Lyons):

- Look-elsewhere effect: searches typically cover multiple independent regions $\Rightarrow$ Higher chance to have a fluctuation "somewhere"
$N_{\text {trials }} \sim 1000$ : local $5 \sigma \Leftrightarrow \mathrm{O}\left(10^{-4}\right)$ more reasonable
- Mismodeled systematics: factor 2 error in syst-dominated analysis $\Rightarrow$ factor 2 error on Z...

- History: $3 \sigma$ and $4 \sigma$ excesses do occur regularly, for the reasons above

Extraordinary claims require extraordinary evidence!

## Extra Slides

## Rare Processes?

HEP : almost always use Poisson distributions. Why ?

## ATLAS :

- Event rate ~ 1 GHz

$$
\left(\mathrm{L} \sim 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1} \sim 10 \mathrm{nb}^{-1} / \mathrm{s}, \sigma_{\mathrm{tot}} \sim 10^{8} \mathrm{nb},\right)
$$

- Trigger rate ~ 1 kHz
(Higgs rate $\sim 0.1 \mathrm{~Hz}$ )
$\Rightarrow \mathrm{p} \sim 10^{-6} \ll 1\left(\mathrm{p}_{\mathrm{H} \rightarrow \mathrm{W}} \sim 10^{-13}\right)$
A day of data: $\mathrm{N} \sim 10^{14} \gg 1$
$\Rightarrow$ Poisson regime! Similarly true in many other physics situations.



## Unbinned Shape Analysis

Observable: set of values $m_{1} \ldots m_{n}$, one per event
$\rightarrow$ Describe shape of the distribution of $m$
$\rightarrow$ Deduce the probability to observe $m_{1} \ldots m_{n}$

## $\mathrm{H} \rightarrow \mathrm{\gamma} \mathrm{\gamma}$-inspired example:

- Gaussian signal $\quad P_{\text {signal }}(m)=G\left(m ; m_{H}, \sigma\right)$
- Exponential bkg $\quad \boldsymbol{P}_{\text {bkg }}(m)=\alpha \boldsymbol{e}^{-\alpha m}$

Expected yields: S, B
$\Rightarrow$ Total PDF for a single event:
$P_{\text {total }}(m)=\frac{S}{S+B} G\left(m ; m_{H}, \sigma\right)+\frac{B}{S+B} \alpha e^{-\alpha m}$
$\Rightarrow$ Total PDF for a dataset
Probability to observe the value $\mathrm{m}_{\mathrm{i}}$




Probability to observe n events $p(\{m)$
$P\left(\left\{m_{i}\right\}_{i=1 \ldots n}\right)=e^{-(S+B)} \frac{(S+B)^{n}}{n!} \prod_{i=1}^{n} \frac{S}{S+B} G\left(m_{i} ; m_{H}, \sigma\right)+\frac{B}{S+B} \alpha e^{-\alpha m_{i}}$

## Poisson Example

Assume Poisson distribution with $\mathrm{B}=0: \quad \underset{\text { Say we observe } \mathrm{n}=5 \text {, want to infer information on the parameter } \mathrm{S}}{\boldsymbol{P}(n ; S)=} e^{-s} \frac{\boldsymbol{S}^{\boldsymbol{n}}}{n!}$
$\rightarrow$ Try different values of $S$ for a fixed data value $\mathrm{n}=5$
$\rightarrow$ Varying parameter, fixed data: likelihood

$$
L(S ; n=5)=e^{-S} \frac{S^{5}}{5!}
$$



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$$
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$$



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## MLEs in Shape Analyses

## Binned shape analysis:

$$
L\left(\boldsymbol{S} ; \boldsymbol{n}_{\boldsymbol{i}}\right)=P\left(\boldsymbol{n}_{i} ; \boldsymbol{S}\right)=\prod_{i=1}^{N} \operatorname{Pois}\left(\boldsymbol{n}_{i} ; \boldsymbol{S} \boldsymbol{f}_{i}+B_{i}\right)
$$

Maximize global L(S) (each bin may prefer a different $\mathbf{S}$ ) In practice easier to minimize


$$
\lambda_{\text {Poi }}(S)=-2 \log L(S)=-2 \sum_{i=1}^{N} \log \operatorname{Pois}\left(n_{i} ; \boldsymbol{S} f_{i}+B_{i}\right) \quad \text { Needs a computer... }
$$ In the Gaussian limit

$$
\lambda_{\text {Gas }}(\boldsymbol{S})=\sum_{i=1}^{N}-2 \log G\left(\boldsymbol{n}_{i} ; \boldsymbol{S} f_{i}+B_{i}, \sigma_{i}\right)=\sum_{i=1}^{N}\left|\frac{\boldsymbol{n}_{i}-\left(\boldsymbol{S} f_{i}+B_{i}\right)}{\sigma_{i}}\right|^{2} \quad x^{2} \text { formula! }
$$

$\rightarrow$ Gaussian MLE (min $x^{2}$ or min $\lambda_{\text {Gus }}$ ): Best fit value in a $x^{2}$ (Least-squares) fit $\rightarrow$ Poisson MLE (min $\lambda_{\text {polis }}$ : Best fit value in a likelihood fit (in ROOT, fit option "L") In RooFit, $\boldsymbol{\lambda}_{\text {Pis }} \Rightarrow$ RooAbsPdf: :fyi to(), $\boldsymbol{\lambda}_{\text {Gus }} \Rightarrow$ RooAbsPdf::chi2FitTo().

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

$$
L\left(\boldsymbol{S}, \boldsymbol{B} ; \boldsymbol{m}_{i}\right)=e^{-(\boldsymbol{s}+\boldsymbol{B})} \prod_{i=1}^{n_{\text {vs }}} \boldsymbol{S} P_{\text {sig }}\left(\boldsymbol{m}_{i}\right)+\boldsymbol{B} P_{\text {bkg }}\left(\boldsymbol{m}_{\boldsymbol{i}}\right)
$$



Estimate the MLE $\hat{S}$ of ?
$\rightarrow$ Perform (likelihood) best-fit of model to data
$\Rightarrow$ fit result for S is the desired $\hat{\mathrm{S}}$.

In particle physics, often use the MINUIT minimizer within ROOT.

## MLE Properties

- Asymptotically Gaussian and unbiased $\langle\hat{\mu}\rangle=\mu^{*}$ for $n \rightarrow \infty$ $\underset{\operatorname{P}(\hat{\mu})}{ } \propto \exp \left|-\frac{\left(\hat{\mu}-\mu^{*}\right)^{2}}{2 \sigma_{\hat{\mu}}^{2}}\right|$ for $n \rightarrow \infty$
Standard deviation of the distribution of $\hat{\mu}$ for large enough datasets
- Asymptotically Efficient : $\sigma_{\mathrm{p}}$ is the lowest possible value (in the limit $\mathrm{n} \rightarrow \infty$ ) among consistent estimators.
$\rightarrow$ MLE captures all the available information in the data
- Also consistent: $\hat{\mu}$ converges to the true value for large n ,

- Log-likelihood: Can also minimize $\lambda=-2 \log \mathrm{~L}$
$\rightarrow$ Usually more efficient numerically
$\rightarrow$ For Gaussian $L, \lambda$ is parabolic:
- Can drop multiplicative constants in L(additive constants in $\lambda$ )


## Extra: Fisher Information

Fisher Information:

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

Measures the amount of information available in the measurement of $\mu$.

Gaussian likelihood: $\quad I(\mu)=\frac{1}{\sigma_{\text {Gauss }}^{2}}$
$\rightarrow$ smaller $\sigma_{\text {Gauss }} \Rightarrow$ more information.

$$
\operatorname{Var}(\tilde{\mu}) \geq \frac{1}{I(\mu)}
$$

## Gaussian case:

- For a Gaussian estimator $\tilde{\mu}$

$$
P(\tilde{\mu}) \propto \exp \left(-\frac{\left(\tilde{\mu}-\mu^{*}\right)^{2}}{2 \sigma_{\tilde{\mu}}^{2}}\right)
$$

- MLE: $\operatorname{Var}(\hat{\mu})=\sigma_{\hat{\mu}}{ }^{2}$

Cramer-Rao: $\operatorname{Var}(\tilde{\mu}) \geq \sigma_{\text {Gauss }}{ }^{2}=\sigma_{\tilde{\mathrm{H}}}{ }^{2}$

For any estimator $\tilde{\mu}$.
$\rightarrow$ cannot be more precise than allowed by information in the measurement.
Efficient estimators reach the bound : e.g. MLE in the large dataset limit.

## Some Examples

High-mass X $\boldsymbol{\text { WY S Search: JHEP } 0 9 \text { (2016) } 1}$

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



## Upper Limit Pathologies

Upper limit: $\quad \mathrm{S}_{\mathrm{up}} \sim \hat{\mathbf{S}}+1.64 \sigma_{\mathrm{s}}$.
Problem: for negative Ŝ, get very good observed limit.
$\rightarrow$ For $\widehat{S}$ sufficiently negative, even $\mathrm{S}_{\mathrm{up}}<0$ !

How can this be ?
$\rightarrow$ Background modeling issue ?... Or:
$\rightarrow$ 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
$\rightarrow$ Special procedure to avoid these cases, since if we assume $S$ must be $>0$, we know a priori this is just a fluctuation.




Usual solution in HEP : $\mathrm{CL}_{\mathrm{s}}$.
$\rightarrow$ Compute modified p-value

$$
\begin{aligned}
& \boldsymbol{p}_{C L_{s}}={\frac{\boldsymbol{p}_{S_{0}}{ }^{\circ}}{\left(1-\boldsymbol{p}_{B}\right)}}_{\text {The } \mathrm{H}\left(\mathrm{~S}=\mathrm{S}_{0}\right)(=5 \%)}^{\text {The } \mathrm{p} \text {-value computed }} \\
& \text { under } \mathrm{H}(\mathrm{~S}=0)
\end{aligned}
$$

$\Rightarrow$ Rescale exclusion at $S_{0}$ by exclusion at $\mathrm{S}=0$.
$\rightarrow$ Somewhat ad-hoc, but good properties...
Ŝ compatible with $0: p_{B} \sim O(1)$
$p_{\mathrm{cls}} \sim p_{\mathrm{so}} \sim 5 \%$, no change.

Far-negative $\widehat{S}$ : $1-p_{B} \ll 1$
$p_{\mathrm{Cls}} \sim \mathrm{p}_{\mathrm{s} 0} /\left(1-\mathrm{p}_{\mathrm{B}}\right) \gg 5 \%$
$\rightarrow$ lower exclusion $\Rightarrow$ higher limit, usually >0 as desired


Drawback: overcoverage
$\rightarrow$ limit is claimed to be $95 \% \mathrm{CL}$, but actually $>95 \% \mathrm{CL}$ for small $1-\mathrm{p}_{\mathrm{B}}$.

## $\mathrm{CL}_{\mathrm{s}}$ : Gaussian Bands

Usual Gaussian counting example with known B: $95 \% \mathrm{CL}_{\mathrm{s}}$ upper limit on S :

$$
S_{\mathrm{up}}=\hat{S}+\left[\boldsymbol{\Phi}^{-1}\left(1-0.05 \Phi\left(\hat{S} / \sigma_{S}\right)\right)\right] \sigma_{S} \quad \begin{gathered}
\text { with } \\
\sigma_{S}=\sqrt{B}
\end{gathered}
$$

Compute expected bands for $\mathrm{S}=0$ :
$\rightarrow$ Asimov dataset $\Leftrightarrow \hat{\mathbf{S}}=\mathbf{0}$

$$
S_{\mathrm{up}, \exp }^{0}=1.96 \sigma_{s}
$$


$\rightarrow \pm$ no bands:

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

| n | $S_{\text {exp }}{ }^{ \pm n} / \sqrt{\text { B }}$ |
| :---: | :---: |
| +2 | 3.66 |
| +1 | 2.72 |
| 0 | 1.96 |
| -1 | 1.41 |
| -2 | 1.05 |

## CLs :

- Positive bands somewhat reduced,
- Negative ones more so

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

## Comparison with LEP/TeVatron definitions

Likelihood ratios are not a new idea:

- LEP: Simple LR with NPs from MC

$$
\begin{aligned}
q_{L E P} & =-2 \log \frac{L(\mu=0, \widetilde{\theta})}{L(\mu=1, \widetilde{\theta})} \\
q_{\text {Tevarron }} & =-2 \log \frac{L\left(\mu=0, \hat{\hat{\theta}_{0}}\right)}{L\left(\mu=1, \hat{\hat{\theta}_{1}}\right)}
\end{aligned}
$$

- Compare $\mu=0$ and $\mu=1$
- Tevatron: PLR with profiled NPs

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

LEP/Tevatron LHC


$\rightarrow$ Asymptotically:

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



## Probability Distributions

Probabilistic treatment of possible outcomes
$\Rightarrow$ Probability Distribution

Example: two-coin toss
$\rightarrow$ Fractions of events in each bin i converge to a limit $p_{i}$

Probability distribution :
$\left\{P_{i}\right\}$ for $i=0,1,2$
Properties

- $P_{i}>0$

- $\quad \sum P_{i}=1$


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## Continuous Variables: PDFs

Continuous variable: can consider per-bin probabilities $p_{i}, i=1 . . n_{b i n s}$
5 bins


Bin size $\rightarrow 0$ :
Probability distribution function $P(x)$
$\rightarrow$ High values $\Leftrightarrow$ high chance to get a measurement here

$$
P(x)>0, \int P(x) d x=1
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## Random Variables

$\mathrm{X}, \mathrm{Y} .$. are Random Variables (continuous or discrete), aka. observables :
$\rightarrow X$ can take any value $x$, with probability $P(X=x)$.
$\rightarrow P(X)$ is the PDF of $X$, a.k.a. the Statistical Model.
$\rightarrow$ The Observed data is one value $x_{\text {obs }}$ of $X$, drawn from $P(X)$.


500 bins

y


## PDF Properties: Mean

$E(X)=\langle X\rangle$ : Mean of $X$ - expected outcome on average over many measurements

$$
\langle\boldsymbol{X}\rangle=\sum \boldsymbol{x}_{\boldsymbol{i}} \boldsymbol{P}_{\boldsymbol{i}} \quad \text { or }
$$

$\rightarrow$ Property of the PंDF

$$
\langle X\rangle=\int x P(x) d x
$$

For measurements $x_{1} \ldots x_{n}$, then can compute the Sample mean:
$\rightarrow$ Property of the sample
$\rightarrow$ approximates $\frac{1}{n} \sum_{i} \boldsymbol{X}_{\boldsymbol{i}}$

PDF Mean


PDF Mean Sample Mean


## PDF Properties: (Co)variance

Variance of X :

$$
\operatorname{Var}(\boldsymbol{X})=\left\langle(\boldsymbol{X}-\langle\boldsymbol{X}\rangle)^{2}\right\rangle
$$

$\rightarrow$ Average square of deviation from mean
$\rightarrow \mathrm{RMS}(\mathrm{X})=\sqrt{ } \operatorname{Var}(\mathrm{X})=\sigma_{\mathrm{x}}$ standard deviation
Can be approximated by sample variance:


Covariance of $X$ and $Y$ :

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

$\rightarrow$ Large if variations of $X$ and $Y$ are "synchronized"

$$
\operatorname{Cov}(X, Y)=\langle(X-\langle X\rangle)(\boldsymbol{Y}-\langle\boldsymbol{Y}\rangle)\rangle
$$



Correlation coefficient

$$
\begin{equation*}
\rho=\frac{\operatorname{Cov}(X, Y)}{\sqrt{\operatorname{Var}(X) \operatorname{Var}(Y)}} \quad-1 \leq \rho \leq 1 \tag{77}
\end{equation*}
$$

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## ＂Linear＂vs．＂non－linear＂correlations

For non－Gaussian cases，the Correlation coefficient $\rho$ is not the whole story：

| $\rho$ | 1 | 0.8 | 0.4 | 0 | －0．4 | －0．8 | －1 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  |
| $\rho$ | 1 | 1 | 1 |  | －1 | －1 | －1 |
|  |  |  | － | ．－．－ | － | $X$ | $\quad \tan 2 \alpha=\frac{2 \rho \sigma_{1} \sigma_{2}}{\sigma_{1}^{2}-\sigma_{2}^{2}}$ |
| $\rho$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
|  |  |  |  |  |  |  | 縭潮 W变变 |

Source：Wikipedia
In particular，variables can still be correlated even when $\rho=0$ ：＂Non－linear＂correlations．

## Gaussian PDF

## Gaussian distribution:

$\rightarrow \operatorname{Med}\left(\mathrm{X}:, X_{0}^{X_{0}}, \sigma\right)=\frac{1}{\sigma \sqrt{2 \pi}} e^{-\frac{\left(x-X_{0}\right)^{2}}{2 \sigma^{2}}}$
$\rightarrow$ Variance : $\sigma^{2}(\Rightarrow$ RMS $=\sigma)$


Generalize to $\mathbf{N}$ dimensions:
$\rightarrow$ Mean : X
$\rightarrow$ Covariance matrix :

$$
\begin{gathered}
G\left(x ; X_{0}, C\right)=\frac{1}{\left[(2 \pi)^{N}|C|\right]^{1 / 2}} e^{-\frac{1}{2}\left(x-X_{0}\right)^{T} C^{-1}\left(x-x_{0}\right)} \\
x_{2}{ }^{15}\left[W \left\lvert\, W(W) W W=\frac{2 \rho \sigma_{1} \sigma_{2}}{\sigma_{1}^{2}-\sigma_{2}^{2}}\right.\right.
\end{gathered}
$$

$$
\begin{aligned}
C & =\left[\begin{array}{ll}
\operatorname{Var}\left(X_{1}\right) & \operatorname{Cov}\left(X_{1}, X_{2}\right) \\
\operatorname{Cov}\left(X_{2}, X_{1}\right) & \operatorname{Var}\left(X_{2}\right)
\end{array}\right] \\
& =\left[\begin{array}{cc}
\sigma_{1}^{2} & \rho \sigma_{1} \sigma_{2} \\
\rho \sigma_{1} \sigma_{2} & \sigma_{2}^{2}
\end{array}\right]
\end{aligned}
$$

## Gaussian Quantiles

$P\left(\left|x-x_{0}\right|>Z \sigma\right)$

Consider $\quad z=\left(\frac{x-x_{0}}{\sigma}\right) \quad$ "pull" of $x$
2
0.317
0.045
0.003
$G\left(x ; x_{0}, \sigma\right)$ depends only on $z \sim G(z ; 0,1)$

Probability $\mathrm{P}\left(\left|\mathrm{X}-\mathrm{x}_{0}\right|>\mathrm{Z} \mathrm{\sigma}\right)$ to be away from the mean:

Gaussian Cumulative Distribution Function (CDF) :

$$
\Phi(z)=\int_{-\infty}^{z} G(u ; 0,1) d u
$$



## Gaussian Quantiles

| $Z$ | $P\left(\left\|X-x_{0}\right\|>Z \sigma\right)$ |
| :--- | :---: |
| 1 | 0.317 |
| 2 | 0.045 |
| 3 | 0.003 |
| 4 | $3 \times 10^{-5}$ |
| 5 | $6 \times 10^{-7}$ |

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## Central Limit Theorem

(*) Assuming $\sigma_{x}<\infty$ and other regularity conditions

For an observable $X$ with any distribution, one has( ${ }^{*}$ )
What this means: $\bar{X}=\frac{1}{n} \sum_{i=1}^{n} x_{i} \stackrel{n \rightarrow \infty}{\sim} G\left(\langle X\rangle, \frac{\sigma_{X}}{\sqrt{n}}\right)$

- The average of many measurements is always Gaussian, whateVer the distribution for a single measurement
- The mean of the Gaussian is the average of the single measurements
- The RMS of the Gaussian decreases as $\sqrt{ } \mathrm{n}$ : smaller fluctuations when averaging over many measurements

Another version:

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

$$
\sum_{i=1}^{n} x_{i} \stackrel{n \rightarrow \infty}{\sim} G\left(n\langle X\rangle, \sqrt{n} \sigma_{X}\right)
$$

## Central Limit Theorem in action

Draw events from a parabolic distribution (e.g. decay $\cos \theta^{*}$ )


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

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Draw events from a parabolic distribution (e.g. decay $\cos \theta^{*}$ )


$$
\mathrm{n}=12
$$

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## Chi-squared

Multiple Independent Gaussian variables $\mathrm{x}_{\mathrm{i}}$ : Define

$$
\chi^{2}=\sum_{i=1}^{n}\left(\frac{x_{i}-x_{i}^{0}}{\sigma_{i}}\right)^{2}
$$

Measures global distance from reference point ( $\mathrm{x}_{1}{ }^{0} \ldots . . \mathrm{x}_{\mathrm{n}}{ }^{0}$ )

Distribution depends on n :

Rule of thumb:
$\chi^{2} / n$ should be $\mathfrak{\Sigma} 1$



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## Histogram Chi-squared

Histogram X2 with respect to a reference shape:

- Assume an independent Gaussian distribution in each bin
- Degrees of freedom = (number of bins) - (number of fit parameters)


BLUE histogram vs. flat reference $\mathrm{X}^{2}=12.9, \mathrm{P}\left(\mathrm{X}^{2}=12.9, \mathrm{n}=10\right)=23 \%$

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RED histogram vs. flat reference $\mathrm{X}^{2}=38.8, \mathrm{P}\left(\mathrm{X}^{2}=38.8, \mathrm{n}=10\right)=0.003 \% \mathrm{X}$

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RED histogram vs. flat reference $X^{2}=38.8, ~ P\left(X^{2}=38.8, n=10\right)=0.003 \% X$

RED histogram vs. correct reference $x^{2}=9.5, p(x 2=9.5, n=10)=49 \%$

## Error Bars

Strictly speaking, the uncertainty is given by the model :
$\rightarrow$ Bin central value ~ mean of the bin PDF
$\rightarrow$ Bin uncertainty $\sim$ RMS of the bin PDF
The data is just what it is, a simple observed point.
$\Rightarrow$ One should in principle show the error bar on the prediction.
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