## Basic concepts - part 2

SOS 2018 May 28 - June 1, La Londe les Maures

## Samples and parameter estimation

A random variable $X$ can be described by its p.d. $f(x)$
$f$ depends of (generally unknown) parameters $\vec{\theta}=\left\{\theta_{1}, \ldots, \theta_{p}\right\} \rightarrow f(x, \vec{\theta})$
An experiment measuring X provides a sample of values $\vec{x}=\left\{x_{1}, \ldots, x_{N}\right\}$
One can construct a function of $\vec{x}$ to infer the properties of the p.d.f

- This function is called an estimator
- The estimator for a parameter $\boldsymbol{\theta}$ is often written: $\widehat{\boldsymbol{\theta}}$
- Parameter fitting: estimate $\boldsymbol{\theta}$ using estimator $\widehat{\boldsymbol{\theta}}$ and data $\overrightarrow{\boldsymbol{x}}$
- $\widehat{\boldsymbol{\theta}}(\overrightarrow{\boldsymbol{x}})$ is itself a random variable following a p.d.f $\boldsymbol{g}(\widehat{\boldsymbol{\theta}} ; \boldsymbol{\theta})$

A good estimator should be
Consistent: $\widehat{\boldsymbol{\theta}}$ converges to $\boldsymbol{\theta}$ for infinite sample $(N \rightarrow+\infty)$
Unbiased: average of $\widehat{\boldsymbol{\theta}}$ for infinite number of measurements is $\boldsymbol{\theta}$
$\rightarrow$ that is: $\boldsymbol{E}[\widehat{\boldsymbol{\theta}}(\overrightarrow{\boldsymbol{x}})]-\boldsymbol{\theta}=\boldsymbol{b}=\mathbf{0}$

## Basic estimators

Consider a sample of size N of a random variable $\mathrm{X}: \overrightarrow{\boldsymbol{x}}=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{N}\right\}$ X follows a p.d.f $f(x)$ of truth mean $\boldsymbol{\mu}$ and variance $\boldsymbol{\sigma}^{2}$
A simple estimator is the arithmetic mean of values $x_{i}: \bar{x}=\frac{1}{N} \sum_{i=1}^{N} x_{i}$

$$
E[\bar{x}]=\frac{1}{N} \sum_{i=1}^{N} E\left[x_{i}\right]=\mu \quad \rightarrow \text { Unbiased estimator of } \mu
$$

$$
V[\bar{x}]=\boldsymbol{E}\left[\bar{x}^{2}\right]-\boldsymbol{E}[\bar{x}]^{2}=\frac{\boldsymbol{\sigma}^{2}}{\boldsymbol{N}} \quad \begin{aligned}
& \text { This implies that the uncertainty } \\
& \text { on the sample mean } \bar{x} \text { is: } \sigma / \sqrt{N}
\end{aligned}
$$

Estimator of the variance: $v=\frac{1}{N} \sum_{i=1}^{N}\left(x_{i}-\bar{x}\right)^{2}=\overline{x^{2}}-\bar{x}^{2}$
Expected value of the estimator: $E[v]=\sigma^{2}-\frac{\sigma^{2}}{N}=\frac{N-1}{N} \sigma^{2}$
$\rightarrow$ Biased estimator of $\sigma^{2}!$

## Basic estimators

Consider a sample of size N of a random variable $\mathrm{X}: \overrightarrow{\boldsymbol{x}}=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{N}\right\}$ X follows a p.d.f $f(x)$ of truth mean $\boldsymbol{\mu}$ and variance $\boldsymbol{\sigma}^{2}$
A simple estimator is the arithmetic mean of values $x_{i}: \bar{x}=\frac{1}{N} \sum_{i=1}^{N} x_{i}$

$$
E[\bar{x}]=\frac{1}{N} \sum_{i=1}^{N} E\left[x_{i}\right]=\mu \quad \rightarrow \text { Unbiased estimator of } \mu
$$

$$
V[\bar{x}]=\boldsymbol{E}\left[\bar{x}^{2}\right]-\boldsymbol{E}[\bar{x}]^{2}=\frac{\boldsymbol{\sigma}^{2}}{\boldsymbol{N}} \quad \begin{aligned}
& \text { This implies that the uncertainty } \\
& \text { on the sample mean } \bar{x} \text { is: } \sigma / \sqrt{N}
\end{aligned}
$$

Estimator of the variance: $v=\frac{1}{N-1} \sum_{i=1}^{N}\left(x_{i}-\bar{x}\right)^{2}=\frac{N}{N-1}\left(\overline{x^{2}}-\bar{x}^{2}\right)$
Expected value of the estimator: $E[v]=\sigma^{2}$
$\rightarrow$ Unbiased estimator of $\sigma^{2}!$

## Maximum Likelihood estimator (ML)

Suppose a random variable $\mathbf{X}$ distributed according to a p.d.f $\boldsymbol{f}(\boldsymbol{x} ; \overrightarrow{\boldsymbol{\theta}})$

- The form of $f$ being know but not the parameters $\vec{\theta}=\left\{\theta_{1}, \ldots, \theta_{P}\right\}$
- Consider a sample of $X$ of $N$ values: $\vec{x}=\left\{x_{1}, \ldots, x_{N}\right\}$

The method of ML is a technique to estimate $\overrightarrow{\boldsymbol{\theta}}$ given data $\overrightarrow{\boldsymbol{x}}$

Joint likelihood function (the $x_{i}$ are fixed here)

$$
L(\vec{\theta})=\prod_{i=1}^{N} f\left(x_{i} ; \vec{\theta}\right)
$$

The estimators $\widehat{\theta}_{i}$ are given by: $\frac{\partial L}{\partial \theta_{i}}=0, i=1 \ldots P$

## Notes:

- maximizing the likelihood provides and estimate of parameters $\theta$
- In practice the log of $L$ (log likelihoood) is often used
- The likelihood is not a p.d.f !
- Bayesian do transform the likelihood in a p.d.f


## Simple examples

Exponential distribution $f(x ; \tau)=\frac{1}{\tau} e^{-\frac{x}{\tau}}$
Likelihood: $L(\tau)=\prod_{i=1}^{N} \frac{1}{\tau} e^{-\frac{x_{i}}{\tau}}$
Log-likelihood:
$\log L(\tau)=\sum_{i=1}^{N} \log f\left(x_{i} ; \tau\right)=-N \log \tau-\sum_{i=1}^{N} \frac{x_{i}}{\tau}$
Estimator: $\frac{d \log L}{d \tau}=0 \Leftrightarrow \tau=\hat{\boldsymbol{\tau}}=\frac{1}{\boldsymbol{N}} \sum_{i=1}^{\boldsymbol{N}} \boldsymbol{x}_{\boldsymbol{i}}$

$$
E[\hat{\tau}]=\tau \quad \text { (unbiased estimator) }
$$

$$
N=200
$$



## Simple examples

Gaussian distribution $f(x ; \mu, \sigma)=\frac{1}{\sqrt{2 \pi} \sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^{2}}, \log L(\vec{\theta})=\sum_{i=1}^{N} \log f\left(x_{i} ; \mu, \sigma\right)$ Estimators:
$E[\hat{\mu}]=\mu \quad$ (unbiased)
$\frac{\partial \log L}{\partial \sigma^{2}}=0 \Leftrightarrow \widehat{\boldsymbol{\sigma}^{\mathbf{2}}}=\frac{\mathbf{1}}{\boldsymbol{N}} \sum_{i=1}^{N}\left(\boldsymbol{x}_{\boldsymbol{i}}-\widehat{\boldsymbol{\mu}}\right)^{2} \quad E\left[\widehat{\sigma^{2}}\right]=\frac{N-1}{N} \sigma^{2}$ (biased)

$$
N=1000
$$




## Interlude : (Linear) regression



## Simple example: polynomial curve fitting

## Training dataset

- $N$ observations of $x=\left(x_{1}, \ldots, x_{N}\right)^{\top}$ : uniformly spaced in $[0,1]$
- Target values $\mathbf{t}=\left(\mathrm{t}_{1}, \ldots, \mathrm{t}_{\mathrm{N}}\right)^{\top}: \sin (2 \pi x)+$ Gaussian noise



## Polynomial curve fitting

## Fit function

- Polynomial function of degree $\mathbf{M}$, with coefficients $\mathbf{w}=\left(w_{1}, \ldots, w_{M}\right)^{\top}$

$$
y(x, \mathbf{w})=w_{0}+w_{1} x+w_{2} x^{2}+\ldots+w_{M} x^{M}=\sum_{j=0}^{M} w_{j} x^{j}
$$

- Non-linear function of $x$, but linear function of $\mathbf{w} \rightarrow$ linear model
- Values of coefficient obtained by minimizing an error function
- Common choice: sum of the square of the errors $E(w)$

$$
E(\mathbf{w})=\frac{1}{2} \sum_{n=1}^{N}\left\{y\left(x_{n}, \mathbf{w}\right)-t_{n}\right\}^{2}
$$



Fitted weights w*
$E\left(w^{*}\right)$


## Linear basis function models

## Basis functions

$$
y(\mathbf{x}, \mathbf{w})=w_{0}+\sum_{j=1}^{M-1} w_{j} \phi_{j}(\mathbf{x}) \quad \begin{aligned}
& \mathrm{w}_{0}: \text { offset } \\
& \varphi_{j}(\mathrm{x}): \text { basis function }
\end{aligned}
$$

$$
\begin{aligned}
y(\mathbf{x}, \mathbf{w}) & =\sum_{j=0}^{M-1} w_{j} \phi_{j}(\mathbf{x})=\mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}) \quad \text { with } \varphi_{0}(\mathrm{x})=1 \\
\mathbf{w} & =\left(w_{0}, \ldots, w_{M-1}\right)^{\mathrm{T}} \quad \phi=\left(\phi_{0}, \ldots, \phi_{M-1}\right)^{\mathrm{T}}
\end{aligned}
$$

By using nonlinear basis functions, we allow the function $y(\mathbf{x}, \mathbf{w})$ to be a non-linear function of the input vector $\mathbf{x}$. These functions are called linear models, however, because they are linear in $\mathbf{w}$.
For high number of dimensions linear models suffer from limitations, and other approaches (as NN) are more suited.

## Likelihood and regression

## Likelihood

Consider $\mathbf{N}$ measurements of x distributed along a given probability law $\mathrm{p}(\mathrm{x})$.

$$
\mathbf{x}=\left(\mathrm{x}_{1}, \ldots, \mathrm{x}_{N}\right)^{\top}
$$

where values $x_{i}$ are independent and identically distributed (i.i.d).
Ex: Normal (a.k.a Gaussian) law with 2 parameters: mean $\mu$ and variance $\sigma^{2}$


$$
\mathcal{N}\left(x \mid \mu, \sigma^{2}\right)=\frac{1}{\left(2 \pi \sigma^{2}\right)^{1 / 2}} \exp \left\{-\frac{1}{2 \sigma^{2}}(x-\mu)^{2}\right\}
$$

## Likelihood and regression

## Likelihood and parameter estimation

Since the variables x are i.i.d we can write the joint probability distribution, therefore the likelihood of the dataset, given $\mu$ and $\sigma$ is:

$$
p\left(\mathbf{x} \mid \mu, \sigma^{2}\right)=\prod_{n=1}^{N} \mathcal{N}\left(x_{n} \mid \mu, \sigma^{2}\right)
$$

To estimate $\mu$ and $\sigma$ given $\mathbf{x}$ one maximizes $p$ w.r.t these parameters. In practice often maximize $\ln (p)$ or minimize $-\ln (p)$.

$$
\ln p\left(\mathbf{x} \mid \mu, \sigma^{2}\right)=-\frac{1}{2 \sigma^{2}} \sum_{n=1}^{N}\left(x_{n}-\mu\right)^{2}-\frac{N}{2} \ln \sigma^{2}-\frac{N}{2} \ln (2 \pi)
$$

$$
\left\{\begin{array}{l}
\frac{\partial\left(\ln p\left(\mathbf{x} \mid \mu, \sigma^{2}\right)\right)}{\partial \mu}=0 \rightarrow \mu_{\mathrm{ML}}=\frac{1}{N} \sum_{n=1}^{N} x_{n} \\
\frac{\partial\left(\ln p\left(\mathbf{x} \mid \mu, \sigma^{2}\right)\right)}{\partial \sigma}=0 \rightarrow \sigma_{\mathrm{ML}}=\frac{1}{N} \sum_{n=1}^{N}\left(x_{n}-\mu_{\mathrm{ML}}\right)^{2}
\end{array}\right.
$$

Expected values

$$
\mathbb{E}\left[\mu_{\mathrm{ML}}\right]=\mu
$$

$$
\mathbb{E}\left[\sigma_{\mathrm{ML}}^{2}\right]=\left(\frac{N-1}{N}\right) \sigma^{2}
$$

## Likelihood and regression

## Curve fitting with noise

Assume target variable in training dataset is subject to Gaussian noise

$$
p(t \mid x, \mathbf{w}, \beta)=\mathcal{N}\left(t \mid y(x, \mathbf{w}), \beta^{-1}\right)
$$

where $\beta=1 / \sigma^{2}$ is a precision parameter.


## Likelihood and regression

## Predictive probabilistic model

By maximizing the likelihood on the training dataset we obtain a probabilistic predictive model for $t$ (instead of a single point estimate):

$$
p\left(t \mid x, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}\right)=\mathcal{N}\left(t \mid y\left(x, \mathbf{w}_{\mathrm{ML}}\right), \beta_{\mathrm{ML}}^{-1}\right)
$$

where $\mathbf{w}_{n}$ is obtained by minimizing the sum of square error $E(\mathbf{w})$

$$
E(\mathbf{w})=\frac{1}{2} \sum_{n=1}^{N}\left\{y\left(x_{n}, \mathbf{w}\right)-t_{n}\right\}^{2}
$$

and $\beta_{\mathrm{ML}}$ is given by

$$
\frac{1}{\beta_{\mathrm{ML}}}=\frac{1}{N} \sum_{n=1}^{N}\left\{y\left(x_{n}, \mathbf{w}_{\mathrm{ML}}\right)-t_{n}\right\}^{2}
$$



## Chi-square method

Consider N independent variables $\mathbf{y}_{\mathrm{i}}$ function of a another variable $\mathbf{x}_{i}$

- The $y_{i}$ are Gaussian distributed of mean $\boldsymbol{\mu}_{\mathrm{i}}$ and (known) std $\boldsymbol{\sigma}_{\mathrm{i}}$
- Suppose that $\mu=f(x ; \overrightarrow{\boldsymbol{\theta}})$ with unknow parameters $\overrightarrow{\boldsymbol{\theta}}$


Likelihood: $L(\vec{\theta})=\prod_{i=1}^{N} \frac{1}{\sqrt{2 \pi} \sigma_{i}} e^{-\frac{1}{2}\left(\frac{y_{i}-f\left(x_{i} \vec{\theta}\right)}{\sigma_{i}}\right)^{2}}$
Maximizing $\log L(\vec{\theta})$ to estimate parameters $\vec{\theta}$ is equivalent to minimize:

$$
\chi^{2}(\vec{\theta})=\sum_{i=1}^{N}\left(\frac{y_{i}-f\left(x_{i} ; \vec{\theta}\right)}{\sigma_{i}}\right)^{2}
$$

## Simple example

Fit data with a line $f(x ; a, b)=a x+b$


Simple linear regression: minimize the variance of $y_{i}-f\left(x_{i} ; a, b\right)$
$w(a, b)=\sqrt{\frac{1}{n} \sum_{i}\left(y_{i}-\left(a x_{i}+b\right)\right)^{2}}$

$$
\left\{\begin{array}{l}
\frac{\partial w(a, b)}{\partial a}=0 \\
\frac{\partial w(a, b)}{\partial b}=0
\end{array}\right.
$$

$$
\left\{\begin{aligned}
a & =\frac{\operatorname{cov}(x, y)}{\operatorname{var}(x)}=r \frac{\sigma(y)}{\sigma(x)} \\
b & =\bar{y}-r \frac{\sigma(y)}{\sigma(x)} \bar{x}
\end{aligned}\right.
$$

(r: correlation factor between x and y )

## Simple example

Fit data with a line $f(x ; a, b)=a x+b$
Chi-square fit: minimize $\chi^{2}(a, b)$

$a=\frac{A E-D C}{B E-C^{2}} \quad b=\frac{D B-A C}{B E-C^{2}}$
$A=\sum_{i} \frac{x_{i} y_{i}}{\left(\Delta y_{i}\right)^{2}}, B=\sum_{i} \frac{x_{i}^{2}}{\left(\Delta y_{i}\right)^{2}}, C=\sum_{i} \frac{x_{i}}{\left(\Delta y_{i}\right)^{2}}, D=\sum_{i} \frac{y_{i}}{\left(\Delta y_{i}\right)^{2}}, E=\sum_{i} \frac{1}{\left(\Delta y_{i}\right)^{2}}$

## Uncertainty of ML estimator



## Uncertainty of ML estimator

Variance of estimator, $V[\hat{\tau}]$ can be tricky to estimate. Several methods exist:

1) Analytical method

For example for the previous exponential distribution

$$
\hat{\tau}=\frac{1}{N} \sum_{i=1}^{N} x_{i} \quad \text { and } \quad V[\hat{\tau}]=(\ldots)=\frac{\tau^{2}}{N}
$$

2) Monte-Carlo method

Very useful for complex cases (multiparameters, systematic uncertainties)
Ex: generate samples distributed exponentially

$$
N_{\text {sample }}=200
$$


$N_{\text {experiments }}=500$


## Uncertainty of ML estimator

## 3) Cramér-Rao bound

Gives a lower bound on any estimator variance (not only ML)

$$
V[\theta] \geq \frac{\left(1+\frac{\partial b}{\partial \theta}\right)^{2}}{E\left[-\frac{\partial^{2} \log L}{\partial \theta^{2}}\right]},(b: \text { bias })
$$

Equality: estimator is efficient ML are asymptotically efficient

For multiple parameters $\vec{\theta}=\left\{\theta_{1}, \ldots, \theta_{P}\right\}: \quad\left(V^{-1}\right)_{i j}=E\left[-\frac{\partial^{2} \log L}{\partial \theta_{i} \partial \theta_{j}}\right]$
(and assuming efficiency and $\mathrm{b}=0$ )
For large samples: an estimate of the inverse covariant matrix $\mathrm{V}^{-1}$ is:

$$
\left(\widehat{V^{-1}}\right)_{i j}=-\frac{\partial^{2} \log L}{\partial \theta_{i} \partial \theta_{j}}(\theta=\hat{\theta})
$$

1 parameter:

$$
\widehat{\sigma^{2}}=\frac{-1}{\frac{\partial^{2} \log L}{\partial \theta^{2}}(\hat{\theta})}
$$

## Uncertainty of ML estimator

## 4) Graphical method

Taylor expansion of $\log L$ on estimate :

$$
\begin{aligned}
\log L(\theta) & =\log L(\hat{\theta})+(\theta-\hat{\theta}) \frac{\partial \log L}{\partial \theta}(\hat{\theta})+\frac{1}{2}(\theta-\hat{\theta})^{2} \frac{\partial^{2} \log L}{\partial \theta^{2}}(\hat{\theta}) \\
& =\log L_{\max }-\frac{1}{2 \widehat{\sigma}^{2}}(\theta-\hat{\theta})^{2}
\end{aligned}
$$

$$
\Rightarrow \log L(\hat{\theta} \pm \hat{\sigma})=\log L_{\max }-\frac{1}{2}
$$

$\hat{\boldsymbol{\tau}} \pm \widehat{\sigma_{\tau}}$ corresponds to a 68.3\% confidence interval


$$
\begin{aligned}
\Delta \log L & =0.5: 68.3 \% \mathrm{CI} \\
\Delta \log L & =2: 95.4 \% \mathrm{CI} \\
\Delta \log L & =4.5: 99.7 \% \mathrm{CI}
\end{aligned}
$$

## Error ellipse

## Case for 2 parameters $\boldsymbol{\theta}_{1}$ and $\boldsymbol{\theta}_{2}$ :



## Error ellipse

## Case for 2 parameters $\boldsymbol{\theta}_{1}$ and $\boldsymbol{\theta}_{2}$ :



## Chi-square: generalization

If $\mathbf{y}_{\mathbf{i}}$ measurements are not independent but related by their cov. matrix $\mathrm{V}_{\mathrm{ij}}$

$$
\log L(\vec{\theta})=-\frac{1}{2} \sum_{i, j=1}^{N}\left(y_{i}-f\left(x_{i} ; \vec{\theta}\right)\right)\left(V^{-1}\right)_{i j}\left(y_{j}-f\left(x_{j} ; \vec{\theta}\right)\right)+\text { additive terms }
$$

$\log L(\vec{\theta})$ is maximized by minimizing:

$$
\chi^{2}(\vec{\theta})=\sum_{i, j=1}^{N}\left(y_{i}-f\left(x_{i} ; \vec{\theta}\right)\right)\left(V^{-1}\right)_{i j}\left(y_{j}-f\left(x_{j} ; \vec{\theta}\right)\right.
$$

Written in matrix notation: $\chi^{2}(\vec{\theta})=(\vec{y}-\vec{f})^{T} V^{-1}(\vec{y}-\vec{f})$
If $f\left(x_{i} ; \vec{\theta}\right)$ is linear in the parameters $\vec{\theta}: 1-\sigma$ uncertainty contour given by:

$$
\chi^{2}(\vec{\theta})=\chi^{2}(\overrightarrow{\hat{\theta}})+1=\chi_{\text {min }}^{2}+q
$$

| N param. | 1 | 2 | 3 |
| :--- | :--- | :--- | :--- |
| q | 1.00 | 2.30 | 3.53 |



## Test hypothesis

Testing compatibility of observed data against a model

- model = background predictions (for simplicity)
$\rightarrow n_{b}$ events: follows Poisson distribution of mean $v_{b}$
$\rightarrow \mathrm{n}_{\text {obs }}$ observed events
To quantify degree of compatibility of $\mathrm{n}_{\text {obs }}$ with the background-only hypothesis we calculate how likely it is to find $\mathrm{n}_{\text {obs }}$ or more events of background
p-value: probability that the expected number of event (background) is at least as high as the number of observed data

$$
\mathrm{p}-\text { value }=P\left(n \geq n_{o b s}\right)=1-P\left(n<n_{o b s}\right)
$$

$$
=\sum_{n=n_{o b s}}^{+\infty} \frac{e^{-v_{b}} v_{b}^{n}}{n!}=1-\sum_{n=0}^{n_{o b s}^{-1}} \frac{e^{-v_{b}} v_{b}^{n}}{n!}
$$

$$
\left[\text { for } v_{b}<n_{o b s}\right]
$$



## Test hypothesis

For the case where $\mathbf{v}_{\mathbf{b}}>\mathbf{n}_{\text {obs }}$ one can define:

$$
\mathrm{p} \text {-value }=\sum_{n=0}^{n_{\text {obs }}} \frac{e^{-v_{b}} v_{b}^{n}}{n!}
$$



The previous sums can be simplified using incomplete Gamma functions:

$$
\sum_{n=n_{o b s}}^{+\infty} \frac{e^{-v_{b}} v_{b}^{n}}{n!}=\frac{1}{\Gamma\left(n_{o b s}\right)} \int_{0}^{v_{b}} t^{n_{o b s}-1} e^{-t} d t=\Gamma\left(v_{b}, n_{o b s}\right)
$$

$$
\text { with } \left.\Gamma\left(n_{o b s}\right)=\int_{0}^{\infty} t^{n_{o b s}-1} e^{-t} d t=\left(n_{o b s}-1\right)!\text { (if } n_{o b s} \text { integer }\right)
$$

## Significance

It is customary to transform the $p$-value into a Z-value using the integral of the Gaussian distribution:

$$
\int_{-\infty}^{Z} \operatorname{Gaus}(x, \mu=0, \sigma=1) d x=\int_{-\infty}^{Z} \frac{1}{\sqrt{2 \pi}} e^{-\frac{x^{2}}{2}} d x=1-\text { pvalue }
$$

Z-value = number of standard deviation, used as a measure of the significance of an excess (or a deficit) w.r.t the (background) hypothesis.



## Significance

In practice one uses the inverse cumulative distribution function of the Gaussian distribution to compute the significance:

$$
Z=\sqrt{2} \operatorname{Erf}^{-1}(1-2 \times \mathrm{p} \text {-value })
$$



| $p$-value | $Z$ |
| :--- | :--- |
| 0.159 | $1 \sigma$ |
| $2.28 \times 10^{-2}$ | $2 \sigma$ |
| $1.35 \times 10^{-3}$ | $3 \sigma$ |
| $3.15 \times 10^{-5}$ | $4 \sigma$ |
| $2.85 \times 10^{-7}$ | $5 \sigma$ |

## Example: BumpHunter algorithm

Software used to search for excess or deficit in a spectrum.

- No assumptions are made on the signal shape or yield
- Just test data against background-only hypothesis
$\rightarrow$ Compute the p -value for all possible intervals.
$\rightarrow$ Select the interval with smallest p-value.

This gives the local $p$-value: $p_{\text {min }}^{\text {local }}$


## Example: BumpHunter algorithm

Since many intervals are considered there is a increasing probability that an excess is found due to statistical fluctuations

- This is the (in)famous (and misnamed) Look Elsewhere Effect: LEE
- To cope for this effect a global p-value is calculated
$\rightarrow$ The global $p$-value is extracted by comparing $-\log \left(p_{\min }^{\text {local }}\right)$ to a set of $-\log \left(\mathrm{p}_{\min }^{\text {local }}\right)$ generated using background-only pseudo-experiments

$\mathrm{p}^{\text {global }}$ : fraction of PE that gives a result higher than the one observed
${ }_{\mathrm{P}} \mathrm{global}=$ fraction of $\left(\mathrm{P}_{\mathrm{min}}^{\mathrm{PE}}>\mathrm{P}_{\mathrm{min}}^{\mathrm{obs}}\right)$


## Hypothesis test: CLs method

Test of two hypothesis $\mathbf{H}_{0}$ and $\mathbf{H}_{1}$ using data

- Likelihood of data given an hypothesis: $\mathrm{L}\left(\right.$ data| $\mathrm{H}_{0}$ ) or $\mathrm{L}\left(\right.$ data $\left.\mid \mathrm{H}_{1}\right)$ $\begin{aligned} & \text { Neyman-Pearson lemma: optimal test statistics for } \\ & \text { hypothesis testing is given by }(\log ) \text { likelihood ratio }\end{aligned} \quad L L R=-2 \log \frac{L\left(\text { data } \mid H_{0}\right)}{L\left(\text { data } \mid H_{1}\right)}$


$$
\begin{aligned}
& \int_{L L R_{o b s}}^{\infty} f\left(t \mid H_{0}\right) d t=\mathrm{CL}_{s+b} \\
& \int_{-\infty}^{L L R_{o b s}} f\left(t \mid H_{1}\right) d t=1-\mathrm{CL}_{b}
\end{aligned}
$$

$$
\mathrm{H}_{0} \text { rejected at }(1-\alpha) \quad \mathrm{CL}_{s+b}<\alpha
$$

$$
\text { More robust test } \mathrm{CL}_{s}=\frac{\mathrm{CL}_{s+b}}{\mathrm{CL}_{b}}<\alpha
$$

## Hypothesis test: CLs method

Testing signal strenght ( $\mu$ ):

- Express number of event of signal as $s=\mu \times S_{\text {nominal }}$
- CLs test can be performed for increasing values of $\mu$
- Exclusion limit on $\mu$ when CLs $<\alpha$






## Combining measurements



## BLUE method

## Best Linear Unbiased Estimator: L.Lyons et al. NIM A270 (1988) 110

- Find linear (unbiased) combination of results: $x=\Sigma w_{i} x_{i}$
with weights $w_{i}$ that give minimum possible variance $\sigma_{x}{ }^{2}$
- Account properly of correlations between measurements
- For Gaussian errors: method equivalent to $\chi^{2}$ minimization
- Two measurements: $\mathrm{x}_{1} \pm \sigma_{1}, \mathrm{x}_{2} \pm \sigma_{2}$ with correlation $\rho$
- The weights that minimize the $\chi^{2}$ : Cov. matrix

$$
\left.\chi^{2}=\left(\begin{array}{ll}
x_{1}-x & x_{2}-x
\end{array}\right)\left(\begin{array}{cc}
\sigma_{1}^{2} & \rho \sigma_{1} \sigma_{2} \\
\rho \sigma_{1} \sigma_{2} & \sigma_{2}^{2}
\end{array}\right)\right]^{-1}\binom{x_{1}-x}{x_{2}-x}
$$

are:

$$
w_{1}=\frac{\sigma_{2}^{2}-\rho \sigma_{1} \sigma_{2}}{\sigma_{1}^{2}-2 \rho \sigma_{1} \sigma_{2}+\sigma_{2}^{2}} \quad w_{2}=\frac{\sigma_{1}^{2}-\rho \sigma_{1} \sigma_{2}}{\sigma_{1}^{2}-2 \rho \sigma_{1} \sigma_{2}+\sigma_{2}^{2}} \quad\left(\mathrm{w}_{1}+\mathrm{w}_{2}=1\right)
$$

## BLUE method

## Best Linear Unbiased Estimator: L.Lyons et al. NIM A270 (1988) 110

- Find linear (unbiased) combination of results: $x=\Sigma w_{i} x_{i}$ with weights $w_{i}$ that give minimum possible variance $\sigma_{x}{ }^{2}$
- Account properly of correlations between measurements
- For Gaussian errors: method equivalent to $X^{2}$ minimization
- Two measurements: $\mathrm{x}_{1} \pm \sigma_{1}, \mathrm{x}_{2} \pm \sigma_{2}$ with correlation $\rho$
- The combined result is:

$$
x=w_{1} x_{1}+w_{1} x_{2}
$$

- And the uncertainty on the combined measurement is:

$$
\sigma_{x}=\sqrt{\frac{\sigma_{1}^{2} \sigma_{2}^{2}\left(1-\rho^{2}\right)}{\sigma_{1}^{2}-2 \rho \sigma_{1} \sigma_{2}+\sigma_{2}^{2}}}
$$

## BLUE method

## Iterative method

- Biases could appear when uncertainties depend on central value of each measurement (L. Lyons et al., Phys. Rev. D41 (1990) 982985)
- Reduced if covariance matrix determined as if the central value is the one obtained from combination
- Rescale uncertainties to combined value
ex: for measurement 1 , and category i : $\sigma_{\mathrm{i}, 1}{ }^{\text {rescaled }}=\sigma_{\mathrm{i}, 1} \cdot \mathrm{x}_{1} / \mathrm{x}_{\text {blue }}$
- Iterate until central value converges to stable value


## Single-top t-channel 8 TeV results

ATLAS [ATLAS-CONF-2012-132, $\left.5.8 \mathrm{fb}^{-1}\right]$ :
$\sigma_{\mathrm{t}}(\mathrm{t}-\mathrm{ch})=.95 \pm 2$ (stat.) $\pm 18$ (syst.) pb $=95 \pm 18 \mathrm{pb}$

- Multivariate analysis with limited assumptions on simulations
- Fit of NN distribution in the data in e/ $\mu+2 / 3$ jet events, with 1-btag

CMS [CMS PAS TOP-12-011, $5.0 \mathrm{fb}^{-1}$ ]:
$\sigma_{\mathrm{t}}(\mathrm{t}-\mathrm{ch})=.80.1 \pm 5.7$ (stat.) $\pm 11.0$ (syst.) $\pm 4.0$ (lumi.) pb $=80.1 \pm 12.8 \mathrm{pb}$

- Cut-based analysis, data-driven background estimates (shapes, rates)
- Fit $|\boldsymbol{\eta}|$ distribution of forward jet in $\boldsymbol{\mu}+2$ jet events, with 1-btag


CMS Preliminary, $5.0 \mathrm{fb}^{-1}, \sqrt{\mathrm{~s}}=8 \mathrm{TeV}$


## Uncertainties categories and correlations

## 6 categories of uncertainties. Correlation factor between ATLAS/CMS estimated for each.

| Category | ATLAS |  | CMS |  | $\rho$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Statistics | Stat. data Stat. sim. | $\begin{aligned} & 2.4 \% \\ & 2.9 \% \end{aligned}$ | Stat. data Stat. sim. | $\begin{aligned} & \hline 7.1 \% \\ & 2.2 \% \end{aligned}$ | 0 |
| Total |  | 3.8\% |  | 7.5\% | 0 |
| Luminosity | Calibration <br> Long-term stability | $\begin{aligned} & \hline \hline 3.0 \% \\ & 2.0 \% \end{aligned}$ | Calibration Long-term stability | $\begin{aligned} & \hline \hline 4.1 \% \\ & 1.6 \% \end{aligned}$ | 1 |
| Total |  | 3.6\% |  | 4.4\% | 0.78 |
| Simulation and modelling | $\begin{array}{\|l\|} \hline \text { ISR/FSR } \\ \text { PDF } \\ \text { t-ch. generator } \\ \mathrm{tt} \text { generator } \\ \text { Parton shower/had. } \\ \hline \end{array}$ | $\begin{aligned} & \hline \hline 9.1 \% \\ & 2.8 \% \\ & 7.1 \% \\ & 3.3 \% \\ & 0.8 \% \end{aligned}$ | $\begin{aligned} & \hline \hline Q^{2} \text { scale } \\ & \text { PDF } \\ & \text { t-ch. generator } \end{aligned}$ | $\begin{aligned} & \hline \hline 3.1 \% \\ & 4.6 \% \\ & 5.5 \% \end{aligned}$ | 1 1 1 0 0 |
| Total | 12.3\% |  | 7.8\% |  | 0.83 |
| Jets | JES <br> Jet res. \& reco. | $\begin{aligned} & \hline 7.7 \% \\ & 3.0 \% \end{aligned}$ | JES <br> Jet res. | $\begin{aligned} & \hline \hline 6.8 \% \\ & 0.7 \% \end{aligned}$ | 0 |
| Total | 8.3\% |  | 6.8\% |  | 0 |
| Backgrounds | Norm. to theory <br> Multijet (data-driven) | $\begin{aligned} & \hline \hline 1.6 \% \\ & 3.1 \% \end{aligned}$ | Norm. to theory <br> Multijet (data-driven) <br> W+jets, tt (data-driven) | $\begin{aligned} & \hline \hline 2.1 \% \\ & 0.9 \% \\ & 4.5 \% \end{aligned}$ | 1 0 0 |
| Total | 3.5\% |  | , 5.0\% |  | 0.19 |
| Detector modelling | b-tagging <br> $E_{\mathrm{T}}^{\text {miss }}$ <br> Jet Vertex fraction <br> lepton eff. <br> lepton res. <br> lepton scale | $\begin{aligned} & \hline \hline 8.5 \% \\ & 2.3 \% \\ & 1.6 \% \\ & 4.1 \% \\ & 2.2 \% \\ & 2.1 \% \end{aligned}$ | b-tagging Unclustered $E_{\mathrm{T}}^{\text {miss }}$ <br> pile up <br> $\mu$ trigger + reco. | $\begin{aligned} & 4.6 \% \\ & 1.0 \% \\ & \\ & 0.5 \% \\ & \\ & 5.1 \% \end{aligned}$ | $\begin{array}{r}0.5 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \hline\end{array}$ |
| Total | 10.3\% |  | 6.9\% |  | 0.27 |
| Total uncert. | 19.2\% |  | 16.0\% |  | 0.38 |

## Combined t-channel single-top cross section

Sum covariance matrices in each category to obtain total covariance matrix.

$$
\begin{gathered}
\mathbf{C}=\left(\begin{array}{cc}
\sigma_{1}^{2} & \rho \sigma_{1} \sigma_{2} \\
\rho \sigma_{1} \sigma_{2} & \sigma_{2}^{2}
\end{array}\right) \\
\\
\Sigma
\end{gathered}
$$

| Source | Uncertainty (pb) |
| :--- | :---: |
| Statistics | 4.1 |
| Luminosity | 3.4 |
| Simulation and modelling | 7.7 |
| Jets | 4.5 |
| Backgrounds | 3.2 |
| Detector modelling | 5.5 |
| Total systematics (excl. lumi) | 11.0 |
| Total systematics (incl. lumi) | 11.5 |
| Total uncertainty | 12.2 |

$$
\mathbf{C}=\left(\begin{array}{cc}
269 & 84 \\
84 & 182
\end{array}\right) \mathrm{pb}^{2}
$$

Breakdown of uncertainties

$$
\sigma_{i}^{2}=w_{1}^{2} \sigma_{i, 1}^{2}+2 w_{1} w_{2} \rho_{i} \sigma_{i, 1} \sigma_{i, 2}+w_{2}^{2} \sigma_{i, 2}^{2}
$$

$$
\sigma_{\text {t-ch. }}=85.3 \pm 4.1 \text { (stat.) } \pm 11.0 \text { (syst.) } \pm 3.4 \text { (lumi.) } \mathrm{pb}=85.3 \pm 12.2 \mathrm{pb}
$$

With $\mathrm{w}_{\text {AtLAS }}=0.35$ and $\mathrm{w}_{\text {СмS }}=0.65, \mathrm{X}^{2}=0.79 / 1$
Overall correlation of measurements is $\rho_{\text {tot }}=0.38$.

## ATLAS+CMS Preliminary, $\sqrt{s}=8 \mathrm{TeV}$



