# Some More Statistical Concepts & Terms Relevant in Gamma-Ray Astronomy\*

# Ullrich Schwanke Humboldt-Universität zu Berlin



#### **Motivation**

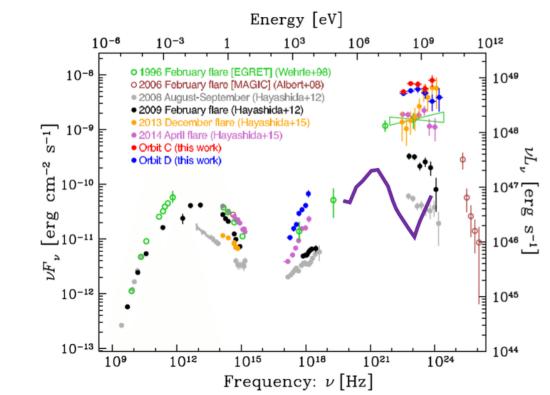
- Glen's lectures have introduced unbinned maximum-likelihood estimators and their uses in
  - Point estimation
  - Interval estimation
  - Hypothesis testing
- In the end, the likelihood of an experiment encodes all the information – but it is not always accessible for outside people
- Would like to elaborate on a few concepts and terms that are also relevant for gamma-ray astronomy (and the workshop starting tomorrow)

#### **Content**

- Error propagation/change of variables
- Statistical and systematic errors
- Binned maximum likelihood and model testing
- Trial factors /look-elsewhere effect

#### **Content**

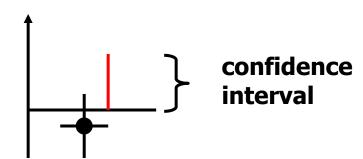
- Error propagation/change of variables
- Statistical and systematic errors
- Binned maximum likelihood and model testing
- Trial factors /look-elsewhere effect



### **Variance and Confidence Intervals**

#### Flux (true flux non-negative!)

Measurements within $\pm 1\sigma$ around mean	
Gauss	68.3%
Exponential	86.5%
Uniform distribution	57.7%

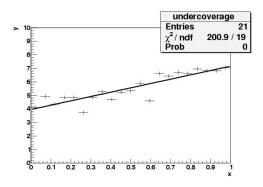


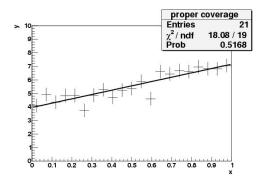
$$V(x) = E[(x-E(x))^2]$$

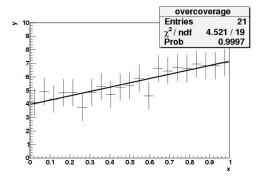
PDF  $f(x,16)$ 

- Lecture 1: sqrt(Variance) as measure of the width of a PDF
- This "error" is not accurate enough ("Probability content" depends on shape/type of PDF)
- A confidence interval (CI) should (i) include the true value of a parameter with some probability (degree of belief, Bayesian) or (ii) belong to an ensemble of CIs a certain fraction of which (confidence level) includes the true value (Frequentist)

### **Confidence Intervals: Coverage**



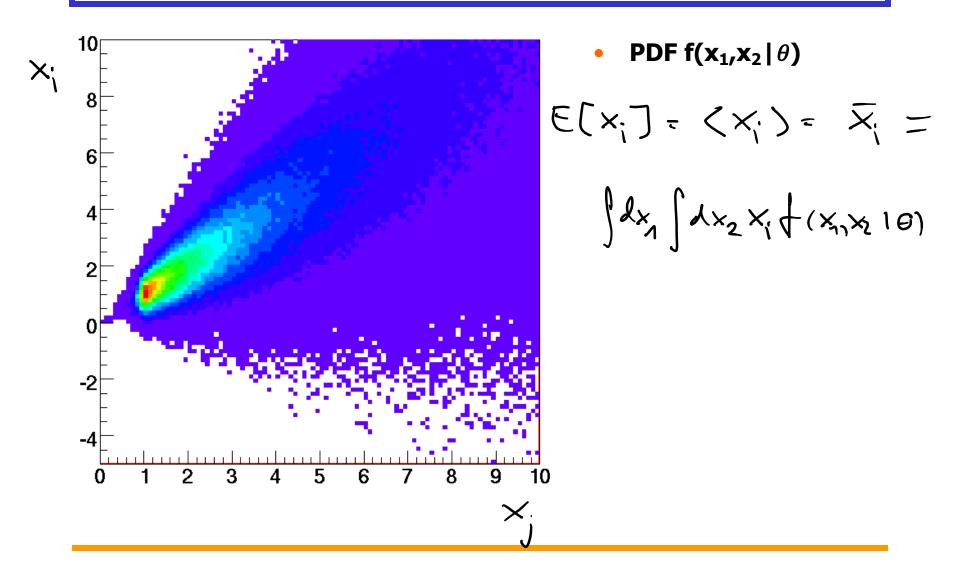




- Confidence intervals too narrow "undercoverage"
- Measurement appears more precise than it is (should be avoided)
- Correct coverage

- Confidence intervals too broad (i.e. too conservative) "overcoverage"
- Excludes fewer (wrong) hypotheses
- Proper coverage of calculated confidence intervals can be tested with the help of Monte Carlo simulations (see appendix for pseudo codes for the Frequentist and Bayesian case)

### **Variance and Covariance**



#### Variance and Covariance

PDF 
$$f(X_1,X_2|\vec{6})$$
  
 $(OV(X_1,X_2) = E[(X_1 - \overline{X_1})(X_1 - \overline{X_2})]$ 

$$\forall (x_1) = \left[ \left( x_1 - E(x_1)^2 \right) \right] = \langle ov(x_1, x_2)$$

- If PDF f(x<sub>1</sub>,x<sub>2</sub>) factorizes as f(x<sub>1</sub>,x<sub>2</sub>) = f<sub>1</sub>(x<sub>1</sub>) f<sub>2</sub>(x<sub>2</sub>) the random variables are mutually independent and their covariance is 0
- Important: The converse statement is not true (i.e. one cannot claim that two variables are independent if their covariance vanishes)
- For N variables, cov(x<sub>1</sub>,...,x<sub>N</sub>) is a symmetric NxN matrix that is called covariance matrix/variance matrix/error matrix

#### **Correlation Coefficient**

$$\begin{cases} \chi_{1} & \dots & \chi_{n} \\ \vdots & \vdots \\ \vdots & \vdots$$

### **Covariance Matrix (1/2)**

$$V[\widehat{\theta}] \geq \left(1 + \frac{\partial b}{\partial \theta}\right)^{2} / E\left[-\frac{\partial^{2} \ln L}{\partial \theta^{2}}\right] = MVB \quad \text{(Minimum Variance Bound)}$$

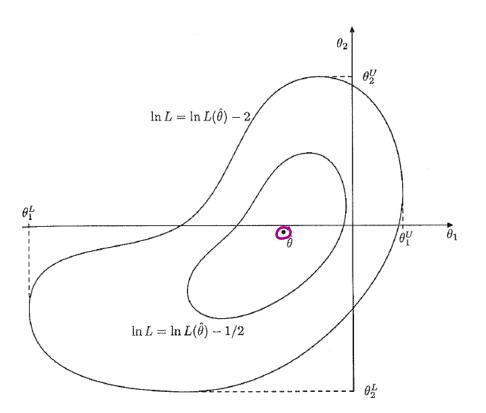
$$e.g. 2 \quad \text{parameters} \quad \text{i)} = 1...2$$

$$V(\widehat{\theta}_{ij}) = - \left[\frac{32 \ln L}{36 \Omega G_{j}}\right]$$

$$= - \frac{32 \ln L}{30 \Omega \Theta_{j}} |_{G_{i}} = \widehat{\theta}_{i}, \quad \Theta_{j} = \widehat{\theta}_{j}$$

- In the ML scheme, the covariance matrix can be estimated (often numerically) from the Hessian Matrix of 2nd derivatives
- Strictly valid (only) in the limit of large N
- PDF of the estimate is then a multivariate Gaussian, no bias

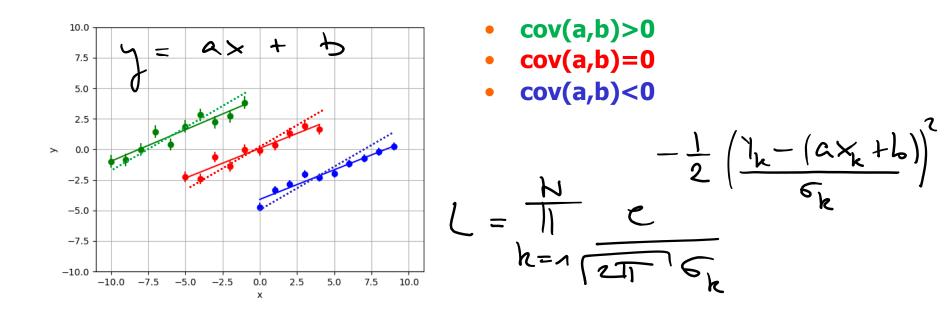
### **Covariance Matrix (2/2)**



- The estimate of the covariance matrix from the derivatives near the optimal parameter values is an approximation
- Approximation will be bad when the likelihood is still non-Gaussian
- The likelihood encodes more information than the covariance matrix (unless N→∞)

Contours at confidence levels of 39.9% and 86.5%

### Removing Correlation (1/2)



- Cov(i,j)-terms (i≠j) can be brought to zero by a suitable transformation
- The transformation will introduce new parameters that one has to cite in connection with revised covariance matrix
- Common application: decorrelation energy when fitting spectral models (flux as a function of energy)

### Removing Correlation (2/2)

$$-\ln L = \frac{1}{2} \sum_{k} \left[ \frac{1}{k} - \frac{(\alpha \times k + b)}{6k} \right]^{2} + const.$$

$$-\frac{\partial enL}{\partial a} = \sum_{k} \left[ \frac{1}{k} - \frac{(\alpha \times k + b)}{6k} \right] \left( -\frac{x_{k}}{6k} \right)$$

$$-\frac{\partial^{2}enL}{\partial b \partial a} = \sum_{k} \left( -\frac{a}{6k} \right) \left( -\frac{x_{k}}{6k} \right) = \sum_{k} \frac{x_{k}}{6k}$$

$$+ \text{ranstormation}:$$

$$\frac{x_{k}^{2}}{6k} = \frac{x_{k}}{6k} - \frac{1}{N} \sum_{k} \frac{x_{k}}{6k}$$

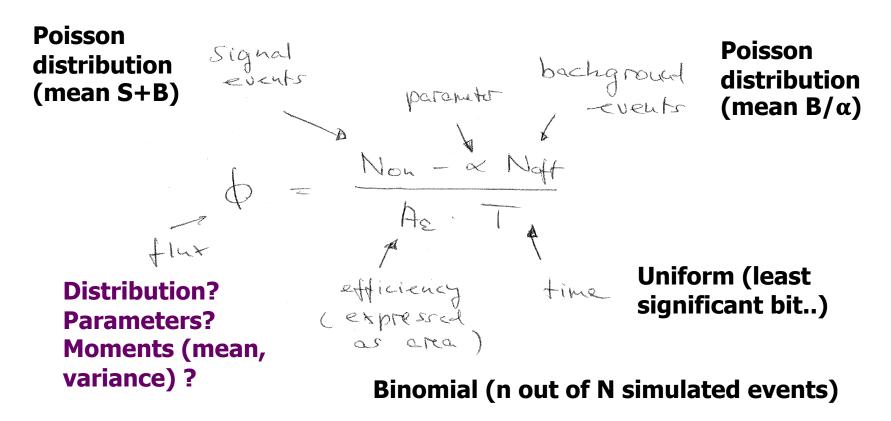
- ML and Least Squares are equivalent when the PDF is Gaussian
- Recall: Inverting a symmetric 2D matrix scales the off-diagonal element and changes its sign

### **Change of Variables**

Transformation (RV=random variable)	New PDF
Sum of N $x_i^2$ when $x_i$ is RV from Norm(0,1)	$\chi^2(N)$
Sum of N $\alpha_i x_i$ when $x_i$ from Norm(0,1), $\alpha_i$ constant	Gaussian
Quotient of $x_1$ and $x_2$ , both from Norm(0,1)	Cauchy distribution
Sum of two RV from U(0,1)	Triangular distribution

- Suppose x follows PDF  $f_x(x | \theta)$  and we apply y = f(x)
- Would like to know the PDF f<sub>y</sub>(y | θ`) for y and the mapping from θ to θ`
- Old and new PDF are known for some cases (→table), and the concept of a characteristic function and transformation formulae are helpful when deriving the new PDF
- In (experimental) practice, the x is a vector of variables and the PDF will anyway be quite complicated when one folds in effects like (energy, space) resolution and acceptance

### **Error Propagation**



- Error propagation is a term used by experimentalists
- Error propagation is approximate change of variables

# **Approximate Error Propagation**

$$y = f(x_1 - x_N) = [(x_1 - x_1) + \sum_{i=1}^{N} dx_i]_{x_i} (x_i - x_i)$$

$$V(y_1) = [(y_1 - E(y_1)^2)] = \sum_{i=1}^{N} dx_i]_{x_i} dx_j \left[ E(x_i - x_1)(x_i - x_i) \right]$$

$$V(y_1) = [(y_1 - E(y_1)^2)] = \sum_{i=1}^{N} dx_i]_{x_i} dx_j \left[ E(x_i - x_1)(x_i - x_i) \right]$$

$$V(y_1) = [(y_1 - E(y_1)^2)] = \sum_{i=1}^{N} dx_i]_{x_i} dx_j \left[ x_i - x_1(x_i - x_i) \right]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_1)^2] = [(x_1 - x_1)^2]$$

$$V(y_1) = [(x_1 - x_$$

# **Approximate Error Propagation**

$$y_{2} = f_{2}(x_{1}...x_{N}) \quad E[x_{1}] = M.$$

$$y_{2} = f_{2}(x_{1}...x_{N}) + \sum_{i=1}^{N} df_{i}(x_{i}-y_{i}) ...$$

$$y_{2} = f_{2}(x_{1}...x_{N}) + \sum_{i=1}^{N} df_{i}(x_{i}-y_{i}) ...$$

$$y_{2} = E[y_{2}](y_{2} - E[y_{2}]) = \sum_{i=1}^{N} df_{i}df_{i}E[(x_{i}-y_{i})(x_{i}+y_{i})]$$

$$y_{2} = f_{2}(x_{1}...x_{N}) + \sum_{i=1}^{N} df_{i}(x_{i}-y_{i}) ...$$

$$y_{3} = f_{2}(x_{1}...x_{N}) + \sum_{i=1}^{N} df_{i}(x_{i}-y_{i}) ...$$

$$y_{4} = f_{2}(x_{1}...x_{N}) + \sum_{i=1}^{N} df_{i}(x_{i}-y_{i}) ...$$

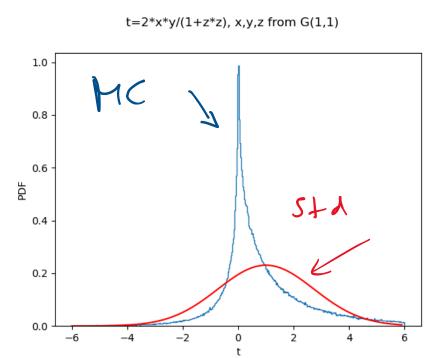
$$y_{5} = f_{5}(x_{1}...x_{N}) + \sum_{i=1}^{N} df_{i}(x_{i}-y_{i}) ...$$

$$y_{6} = f_{6}(x_{1}...x_{N}) + \sum_{i=1}^{N} df_{i}(x_{i}-y_{i}) ...$$

$$y_{7} = f_{7}(x_{1}...x_{N}) + \sum_{i=1}^{N} df_{i}(x_{i}-y_{i}) ...$$

$$y_{8} = f_{6}(x_{1}...x_{N}) + \sum_{i=1}^{N$$

### **MC Error Propagation**



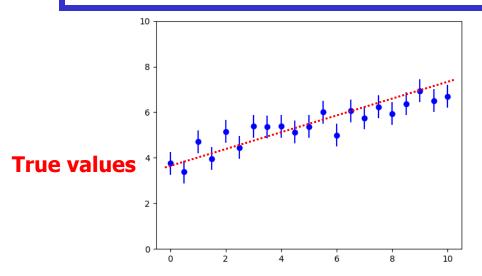
Example: 
$$E = \frac{2x_1}{1+x_2}$$
  
 $x_1y_1z_1$  from  $G(1n_1n_1)$   
 $\frac{df}{dx}\Big|_{x_1} = \frac{df}{dx}\Big|_{x_2} = 1$   
 $\frac{df}{dx}\Big|_{x_1} = \frac{1}{1+x_2}$ 

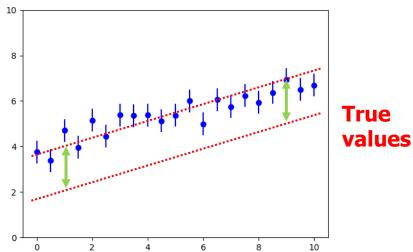
- Standard error propagation is only approximate except in the linear case
- Sampling the input distribution with MC techniques is often an alternative

#### **Content**

- Error propagation/change of variables
- Statistical and systematic errors
- Binned maximum likelihood and model testing
- Trial factors /look-elsewhere effect

### **Errors: Statistical vs Systematic**



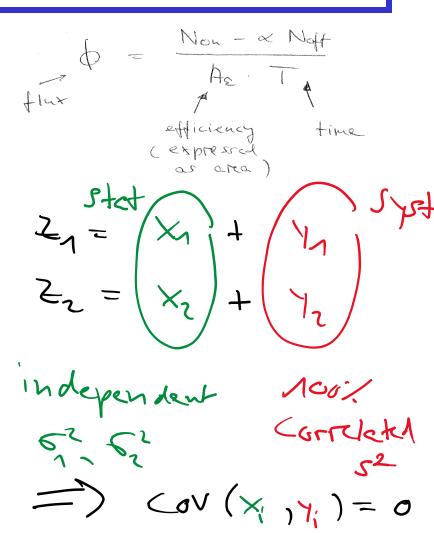


- Statistical errors:
- Deviations to lower and higher values
- Precision improves with 1/sqrt(N)
- PDF (mostly) known

- **Systematic errors:**
- Deviations into the same direction
- Repeated measurements (at the same point) are not independent; central limit theorem does not apply
- In fact, all measurements are correlated
- PDF (mostly) unknown

### **Systematic Errors**

- Statistical errors can become systematic ones
- Systematic errors can become statistical ones (randomizing the sequence of data)
- There are obvious techniques to avoid systematic errors (e.g. to measure ratios)
- Can be identified with suitable methods (conservation laws, measure a quantity as a function of a variable it should not depend on)
- Systematic errors and statistical error occur independently
- Systematic errors can be treated with the usual statistical methods



### **Example (1/2)**

$$C = (Stat + (JASt = (Stat + JAST)) = S^{2} + JA$$

$$C = (Stat + (JASt = (Stat + JAST)) = S^{2}$$

$$C = (Stat + (JAST) + (JAST)) = S^{2}$$

$$C = (Stat + (JAST) + (JAST)) = S^{2}$$

$$C = (Stat + (JAST) + (JAST)) = S^{2}$$

$$C = (Stat + (JAST) + (JAST)) = S^{2}$$

$$C = (Stat + (JAST) + (JAST)) = S^{2}$$

$$C = (Stat + (JAST) + (JAST) + (JAST)) = S^{2}$$

$$C = (Stat + (JAST) + (JAST) + (JAST) + (JAST))$$

$$C = (Stat + (JAST) + (JAST) + (JAST) + (JAST) + (JAST)$$

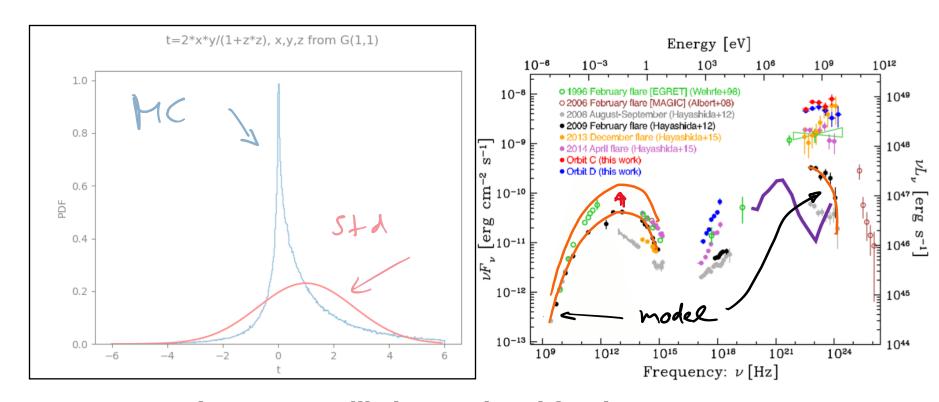
$$C = (Stat + (JAST) + (JAST) + (JAST) + (JAST) + (JAST) + (JAST)$$

$$C = (Stat + (JAST) + ($$

# **Example (2/2)**

$$V(z_1 \pm z_2) = 5_1^2 + 6_2^2 + 2(5^2 \pm 5^2)$$

### **MC Error Propagation: Systematics**



- Systematic errors are likely correlated for the same experiment/observatory but not between different experiments/observatories
- Vary all points of an experiment in the same direction....

### **Including Systematics**

- The presence of systematic errors ("nuisance parameters") must broaden confidence intervals
- There are a number of Bayesian/Frequentist/hybrid procedures the (Frequentist) coverage of which is tested with the help of simulations
- Maximum Likelihood errors with the profile likelihood method have become a standard

Signal events parameter bachground

Parameter events

Non - & Noft

As: The efficiency time

(expressed as area)

### **Profile Likelihood**

- CI for single parameters of interest (e.g. π) can be obtained by constructing a likelihood ratio that depends only on this parameter (1 degree of freedom)
- All others parameters  $\theta_{1}$ , ...,  $\theta_{k}$  are maximised at all times for the given value  $\pi = \pi_{0}$
- Of course, this also works for a parameter space  $\pi_{1,...}$ ,  $\pi_{n}$

**Parameters of interest (mass, flux)** 

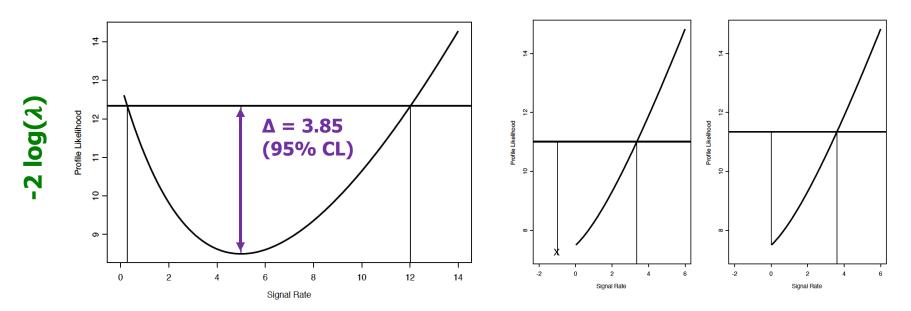
$$L(\boldsymbol{\pi}, \boldsymbol{\theta}|X) = \prod_{i=1}^{n} f(X_i|\boldsymbol{\pi}, \boldsymbol{\theta})$$

nuisance parameters (efficiency, constants)

#### **Profile likelihood:**

$$\lambda(\boldsymbol{\pi}_0|X) = \frac{\sup \{L(\boldsymbol{\pi}_0, \boldsymbol{\theta}|X); \boldsymbol{\theta}\}}{\sup \{L(\boldsymbol{\pi}, \boldsymbol{\theta}|X); \boldsymbol{\pi}, \boldsymbol{\theta}\}}$$

### **Profile Likelihood**

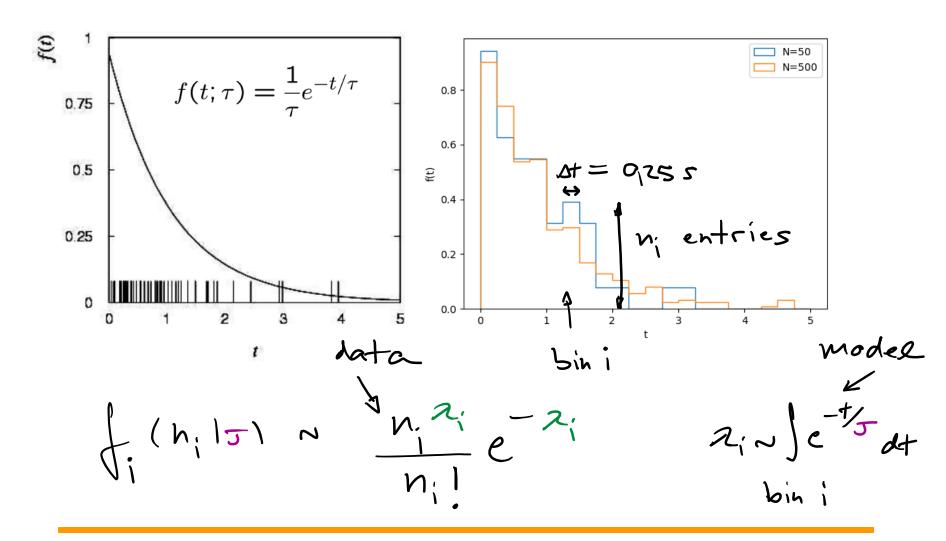


- Ad-hoc prescriptions when (i) the minimum is in the unphysical range or (ii) when the required increase leads into the unphysical range
- Important for small N, when log(L) can be highly non-Gaussian
- Software tuned to give proper coverage; provides several PDFs for data and efficiency etc (see e.g. arXiv:0403059)

#### **Content**

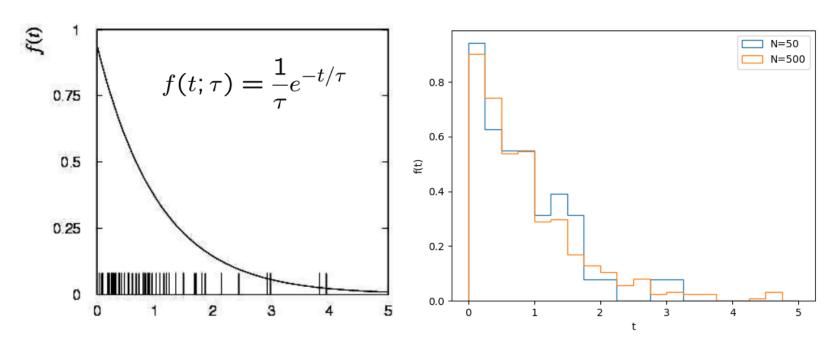
- Error propagation/change of variables
- Statistical and systematic errors
- Binned maximum likelihood and model testing
- Trial factors /look-elsewhere effect

#### **ML: Unbinned vs Binned**



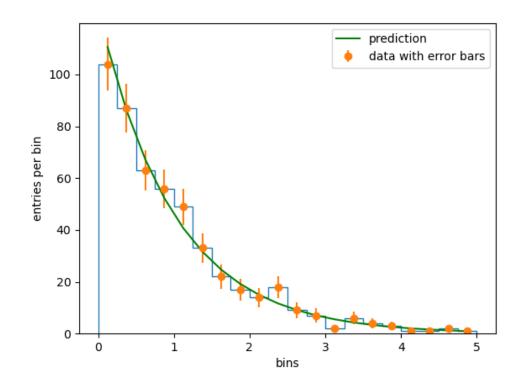
2; average number of counts expected in bin i

### **ML: Unbinned vs Binned**



- No loss of information due to binning effects
- Number of terms in L ~ events
- Goodness of fit testing might require a binning anyway
- Loss of information due to binning effects (horrible in this example!)
- Number of terms in L ~ bins
- Goodness of fit testing basically straightforward

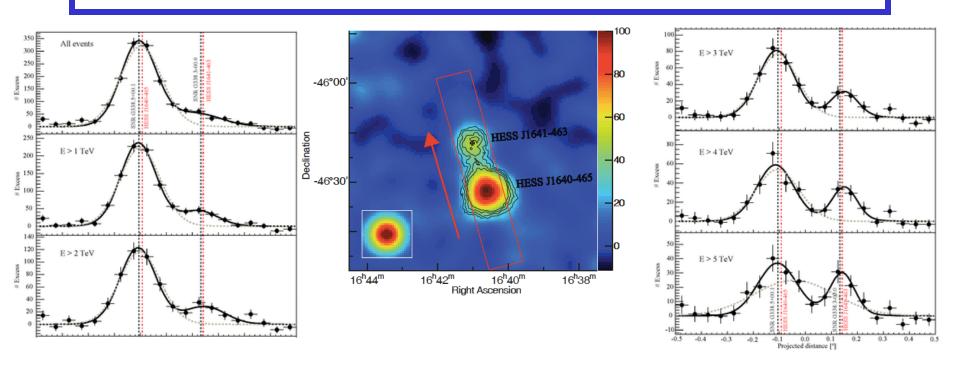
#### **Goodness of Fit**



$$\chi^2 = \sum_{i=1}^{\text{bins}} \left( \frac{n_i - n_i}{5_i} \right)^2$$

- Number of degrees of freedom (Ndof) is number of histogram bins if the prediction (=model) is completey defined
- Ndof is decreased by M if M model parameters are estimated from the binned data
- Ndof unclear when the M model parameters are estimated by unbinned ML
- Note: Assume that the bin content is "high enough" for Gaussian approximation

### **Binned Maximum Likelihood**



- Binned ML is popular due to a high number of bins (spatial bins, energy bins), the desire for automatization (e.g. catalogue production and data modelling) and the intimate relation with GOF
- The value of -2 log(likelihood) at the maximum is asymptotically Chi<sup>2</sup> distributed and can be used in tests immediately

### **Binned Maximum Likelihood**

#### Binned Maximum Likelihood

$$-2 \log L = \sum_{i} \left(\frac{2i-hi}{hi}\right)^{2}$$

$$\Rightarrow \frac{1}{h_{i}} = \frac{1}{2i+h(-2i)} = \left(\frac{1}{2i} - \frac{(h_{i}-2i)}{2i^{2}}\right)$$

$$= \frac{1}{2i} \left(1 - \frac{h_{i}}{2i} + 1\right)$$

$$= \frac{1}{2i} \left(1 - \frac{h_{i}}{2i} + 1\right)$$

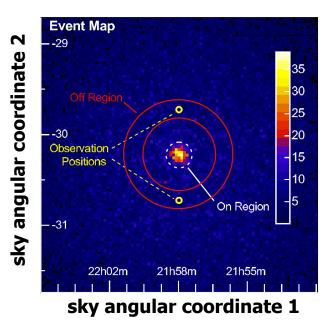
$$= \frac{1}{2i} \left(1 - \frac{h_{i}}{2i} + 1\right)$$

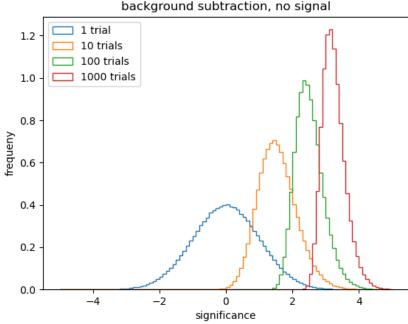
This value (called CSTAT) is used as test statistic in model comparisons

#### **Content**

- Error propagation/change of variables
- Statistical and systematic errors
- Binned maximum likelihood and model testing
- Trial factors /look-elsewhere effect

#### **Trials**





- Signal searches are often applied repeatedly to several data sets (e.g. transient events) or in many locations (slices/bins in energy/mass/ space) of the same (fixed) data set
- Estimators like the detection significance have to be corrected for the number of trials
- Remark: a full judgement (i.e. interpretation) of the result can depend on measurements conducted by others or earlier

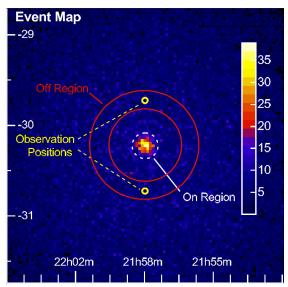
### (Naive) Correction for Trials

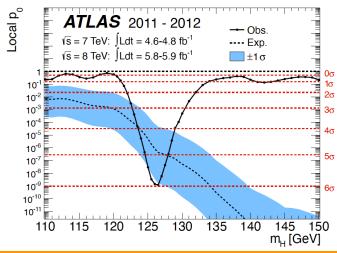
$$(\Lambda - P)^{N} = \Lambda - P_{N}$$

Probality that signal level S was not reached in any of the N trials

- p: probability that some signal level S (e.g. number of events) is reached in a single trial (pre-trial probability)
- p<sub>N</sub>: probability that one gets a signal level S after N identical trials (post-trial probability)
- P values can be converted to Gaussian significances as explained in lecture 1
- Remark: Expect numerical problems when evaluating the formula above directly (see appendix for a more stable version)

### **Complications**





- The naive formula assumed identical trials which is often not the case
- Trials are often not independent (e.g. due to overlapping background or signal regions)
- Trial factors also occur when an extended parameter space (e.g. mass) is covered
- The number of trials N is hard to estimate; one is then usually conservative and avoids underestimating N
- MC simulations are straightforward but have computing demands (O(10<sup>7</sup>) simulations for 5sigma effect!)

# **Thanks**

### **Testing Coverage**

#### **Frequentist MC**

```
CL = 0.9 //confidence level
N = 1000 //experiments
mu1 = mu2 = 0
for( every possible true mu0 ){
  //test coverage for this mu0
  coverage = 0
  //simulate experiments
  for(i=0;i<N;i=i+1){
    x0 \sim p(x | mu0)
    FreqLimit(CL,x0,mu1,mu2)
    if( mu1<=mu0<=mu2 )
      coverage = coverage + 1
 coverage = coverage/N
 //coverage should equal CL
```

#### **Bayesian MC**

```
CL = 0.9 //confidence level
N = 1000 //attempts
mu1 = mu2 = 0
for( every possible x0 ){
  //test coverage for this x0
  coverage = 0
  BayesLimit(CL,x0,mu1,mu2)
 //sample posterior
 for(i=0;i<N;i=i+1){
    mu0 \sim p(mu|x0)p(mu)/p(x0)
    if( mu1<=mu0<=mu2 )
     coverage = coverage + 1
 coverage = coverage/N
 //coverage should equal CL
```

x,mu: random variables x0,mu0: drawn from PDF

#### **Trial Correction**

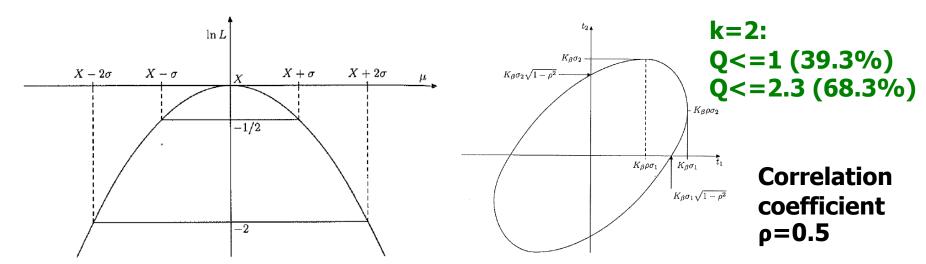
$$p_n = 1 - (1 - p)^n = 1^n - (1 - p)^n = (p + (1 - p))^n - (1 - p)^n$$

$$= \sum_{j=0}^n \binom{n}{j} p^j (1 - p)^{n-j} - (1 - p)^n = \sum_{j=1}^n \binom{n}{j} p^j (1 - p)^{n-j}$$

#### Approximation for small p: just keep the first two terms in the sum

$$p_n = np(1-p)^{n-1} + \frac{n(n-1)}{2}p^2(1-p)^{n-2}$$

#### Likelihood-based CI



- In L( $\mu$ )=In L( $\mu_{max}$ )-1/2 for 1 parameter
- In  $L(\mu_1, ..., \mu_k) = In L(\mu_{max,1}, ..., \mu_{max,k}) 1/2 F(k,CL)$
- F(k,CL) is a constant factor
- Integral from 0 to F(k,CL) over a χ²-distribution with k degrees of freedom gives CL
  - F(1,68.3%)=1
  - F(2,39.3%)=1, F(2,68.3%)=2.3
  - F(3,68.3%)=3.53

#### **Multivariate Gaussian**

$$f(\mathbf{X}) = \frac{1}{(2\pi)^{k/2} |\mathcal{X}|^{\frac{1}{2}}} \exp\left[-\frac{1}{2}(\mathbf{X} - \boldsymbol{\mu})^{\mathrm{T}} \mathcal{X}^{-1} (\mathbf{X} - \boldsymbol{\mu})\right]$$

$$\mathcal{X} = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \cdots & \rho_{1N}\sigma_1\sigma_N \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & & \vdots \\ \vdots & & \ddots & & \\ \vdots & & & \ddots & \vdots \\ \rho_{1N}\sigma_1\sigma_N & \cdots & \cdots & \cdots & \sigma_N^2 \end{pmatrix}$$

- k Gaussian random variables
- Vector of RV X = (x<sub>1</sub>, ..., x<sub>k</sub>)
- Vector of means  $\mu = (\mu_1, ..., \mu_k)$
- Correlated unless covariance matrix V is diagonal
- V has k(k-1)/2 (off diagonal) + k (diagonal) = k(k+1)/2 independent parameters
- V is positive definite
- Bell-shaped in k dimensions

#### **Multivariate Gaussian in 2D**

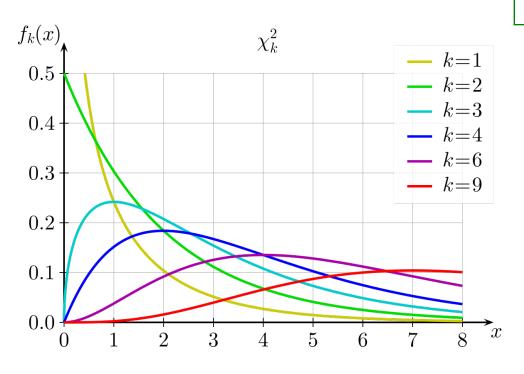
$$f(X,Y) = \frac{1}{2\pi\sigma_X \sigma_Y \sqrt{(1-\rho^2)}} \times \exp\left[-\frac{1}{2(1-\rho^2)} \left\{ \frac{(X-\mu_X)^2}{\sigma_X^2} - 2\rho \frac{(X-\mu_X)(Y-\mu_Y)}{\sigma_X \sigma_Y} + \frac{(Y-\mu_Y)^2}{\sigma_Y^2} \right\} \right]$$

$$\mathcal{X} = \begin{pmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 \end{pmatrix}$$

- k=2 Gaussian random variables X and Y
- 2 means μ<sub>x</sub> and μ<sub>k</sub>
- 2x2 covariance matrix (3 parameters)

#### **Covariance Form**

$$f(\mathbf{X}) = \frac{1}{(2\pi)^{k/2} |\mathcal{Y}|^{\frac{1}{2}}} \exp\left[-\frac{1}{2} (\mathbf{X} - \boldsymbol{\mu})^{\mathrm{T}} \mathcal{Y}^{-1} (\mathbf{X} - \boldsymbol{\mu})\right]$$
Covariance form Q



- **Contours of constant** probability are given by Q=constant
- Q is distributed as  $\chi^2(\mathbf{k})$ , (independent of  $\mu!$ )
- Can estimate the probability content of a hyperellipsoid by integrating over the  $\chi^2(k)$  distribution