Spectral Analysis & Statistics

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Overview

1. Ideal experiment / X-ray Astrophysics

2. Spectral analysis

3. Questions to be answered by the spectra

4. Statistical tests

5. The large view

6. Golden rules of statistics

Ideal Experiment

- **expected spectrum: either from theory or short test measurement**
- **resolution of detector >> intrinsic line-width**
- **effective area: known per resolution element**
- **background: either known or short test measurement**
- **optimization of experiment:**
  - **exposure time per resolution element: such that constant signal/noise ratio is expected**

X-ray Astrophysics

- spectrum and flux:
  - generally not known with sufficient accuracy to plan observation accurate
- resolution vs. line-with:
  - pn < MOS << RGS
    - in general:
      - line-width < resolution,
      - redistribution
- background:
  - not well known in advance and variable
- observation optimization:
  - only partly possible

Ideal Experiment

- reconstruction of spectrum:
- data [counts]:
  - Y1, Y2, Y3, Y4 …. Y2000
- effective area:
  - a1, a2, a3, a4 ….a2000
- exposure time:
  - t1, t2, t3 ..t2000
- spectra [photons/sec/cm²] :
  - f1=Y1/ t1/ a1 + 0 x Y2/ t1/a1
  - f2=Y2/ t2/ a2 + 0 x Y1/t1 ..
  - f3=Y3/ t3/ a3 + 0 x Y1/….

- start with the spectrum:
- input spectrum [photons/sec]:
  - P1(E1), P2(E2), P3, P4 …
- registered with a certain probability: effective area
  - a1x t1, a2 x t2, …
- redistributed with respect of counts channels:
- Y1(e1) = P1(E1) x a1(E1) x t1(E1) + P2(E2) X 0

X-ray Astrophysics

- reconstruction of spectrum:

- data [counts]:
  - Y1, Y2, Y3, Y4 …. Y2000

- effective area [cm2]:
  - a1, a2, a3, a4 ….a2000

- exposure time:
  - t1, t2, t3 ..t2000

- spectra [photons/sec/cm²] :
  - f1=Y1/ t1/ a1 + b x Y2/ t1/a1
  - f2=Y2/ t2/ a2 + c x Y1/t1 ..
  - f3=Y3/ t3/ a3 + c x Y1/….

- start with the spectrum:

- input spectrum [photons/sec/cm²]:
  - f1(E1), f2(E2), f3, f4 …

- registered with a certain probability: effective area
  - a1x t1, a2 x t2, ….

- redistributed with respect of counts channels:

- Y1(e1) = f1(E1) x a1(E1) x t1(E1) + P2(E2) X b

X-ray Astrophysics

- reconstruction of spectrum:
- data [counts]:
  - Y1, Y2, Y3, Y4 …. Y2000
- effective area [cm²]:
  - a1, a2, a3, a4 ….a2000
- exposure time:
  - t1, t2, t3 ..t2000
- spectra [counts/sec/cm²] :
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- start with the spectrum:
- input spectrum [photons/sec/cm²]:
  - P1(E1), P2(E2), P3, P4 …
- registered with a certain probability: effective area
  - a1x t1, a2 x t2, a3, a3
- redistributed with respect of counts channels:
- Y1(e1) = P1(E1) x a1(E1) x t1(E1)
  + P2(E2) X b ….

Redistribution and Resolution

- **the channels in the spectra reflect a purely mathematical sorting**
- **a count in a channel, which corresponds to an energy k, can not be identified with a photon of energy k**
- **physical sampling, “real” channels, “independent bins”, resolution:**
  - **simplest case: (Abbe, 1820-1830) what is the minimum distance between two point which can be resolved with a given resolution?**
  - **today more complex: Shannon information theorem, Nyquist criteria**
  - **information content of a given spectra does not increase if the sampling goes below FWHM/3**
- **most of the spectra provided in X-ray missions are over-sample**

Concept Of Spectral Analysis

1. physically motivated model spectra which is a function of parameters (x1,x2..xi) and energy (e1, e2,..)
   - Example:
     - thermal emission of a blackbody (BB),
       – with parameters: temperature (T) and norm (N)
     - BB(T,N,e_i)

2. multiplication with effective area (a1, a2, ..): expected flux (f) as function of energy and model
   - F (BB(T,N), e_i) = BB(T,N,e_j) * a_{ij}, (i=j a_{ij} = k_j, i not j a_{ij}=0)

3. folding with redistribution matrix (Detector Response Matrix (bij)) and multiplication with exposure time (t): counts as function of channel (ki) and model:
   - counts(c_j) = F(BB(T,N),e_i) * b_{ij}

4. statistical analysis
   - is model true?
     - hypothesis tests
   - can the description of the spectra be improved?
     - new loop with changed parameter of model

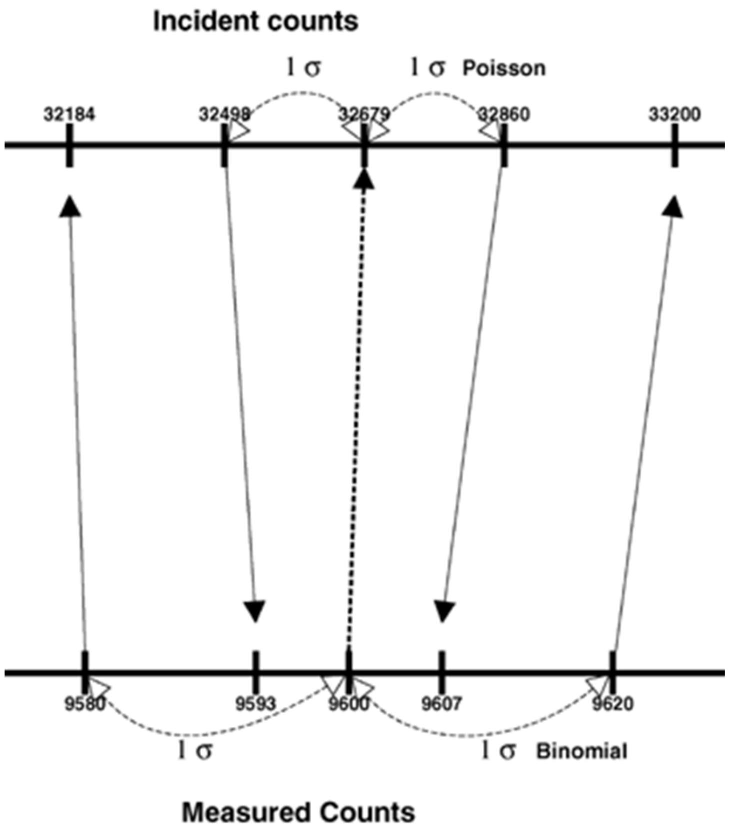
Standard Questions

- given a data set the most common questions are:
  - distributions
    - 50 counts are measured. What is there distribution?
  - hypothesis test:
    - ASCA showed a power law with Γ=2.1 and flux =1.5 ➔ does this model describe the pn data?
  - estimate of parameters:
    - the data can be described with a power law. What is the index and the normalization?
  - estimate of confidence level:
    - what is the error of the power law and what is the error of the normalization?
  - hypothesis test:
  - comparison between two fits:
    - is a power-law or a power-law + emission line a better description of the data

Statistical Methods

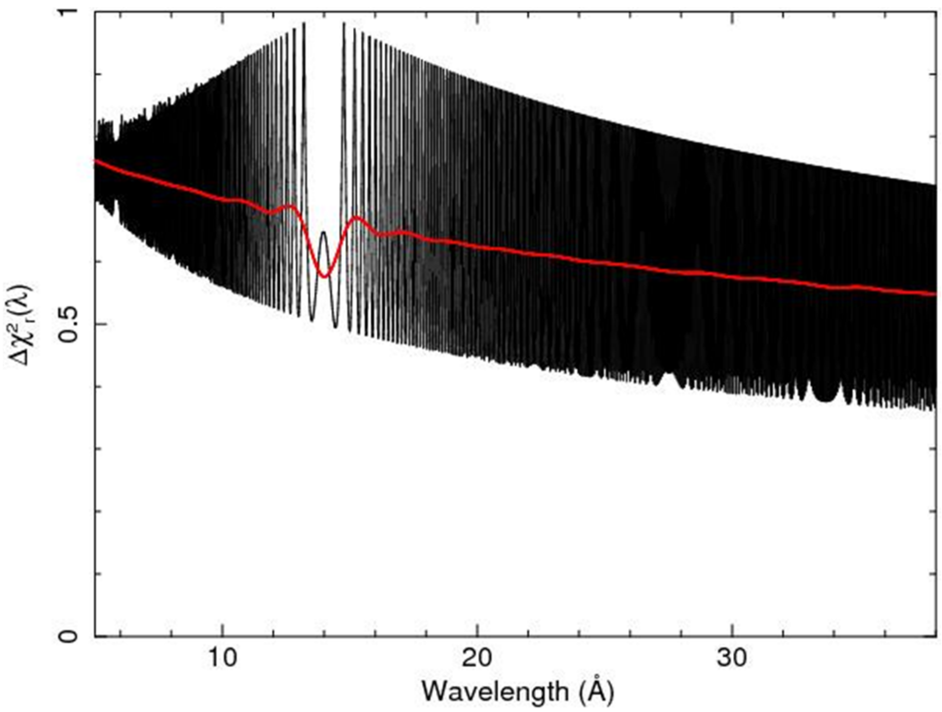
- statistical methods to answer the questions (provided in xspec):
  - distributions
    - Poisson distribution versus binomial distribution
  - hypothesis test:
    - χ^2 hypothesis test
  - estimate of parameters
    - modified minimum χ^2 method
    - minimize C value (C-statistics)
  - estimate of confidence level
    - determine parameter for $\chi^2 = \chi^2_{\text{minimum}} + \Delta \chi^2$
  - comparison between two fits
    - F-test

Comments to Distributions I: OM



- Kuin & Rosen, 2008, MNRAS 383, 383
- Fordham et al., 2000, MNRAS 312, 83

Comments to Distributions II: RGS



Relative contribution per wavelength bin to the reduced χ2. Calculated and shown is the ratio Var [Yi] /E [Yi] (see text). The thick line is a low-resolution spline approximation showing the trends in the average value. (From Kaastra, J. S. et, al., 2011, A&A 534, A37)

- **J. S. Kaastra et al. 2011, A&A 534, A37**

- **Study of 600 ks RGS spectrum of Mrk 509 with excellent quality**
- **Fluxed Spectrum:**

  > 400 coutns per bin

  Expectaion: reduced χ2 >> 1

  But: reduced χ2 ≈ 0.6

  ➔Counts are not χ2 distributed

  ➔ use rescaled χ2

  ➔ Small number of counts in fluxed RGS spectra do follow the C-statistic

Statistical Functions

- χ^2 is defined as: $\chi^2 = \Sigma (Y_m - Y_e)^2 / (Y_e)$
  - for $n \rightarrow \infty$
  - and requires:
    - Gaussian errors of individual data points
    - independence of data points

- modified χ^2 is defined as: $\chi^2_{mod} = \Sigma (Y_m - Y_e)^2 / (\Delta Y_m)^2$
  - assumption for $n \rightarrow \infty$ $\chi^2_{mod} \rightarrow \chi^2$
  - only valid if: $(\Delta Y_m)^2 \approx Y_e$
  - requirements of χ^2 are fulfilled

- C-statistics is defined as: $C = 2 \Sigma (Y_e - Y_m \ln Y_e)$
  - W. Cach, 1979, Apj 228, 939
  - assumption for $n \rightarrow \infty$ $C \rightarrow \chi^2 + K$
  - Uses:
    - Poisson errors of individual data points

- F-test is defined as: $F = \chi^2_1 * d.o.f_2 / \chi^2_2 / d.o.f._1$

Independence Of Data Points

- the measurement of each Yi is statistically independent
- but the Yi are correlated (over-sampling in provided spectra, resolution)

- statistically independent but correlated data points

- all (presented) test methods require independent data points
  - (small sentence at the beginning of each text book)

- never sample with a bin-size < FWHM/3, this provides
  - complete spectral information
  - avoids over-sampling

Independence Of Data Points

- example: same spectra, same signal/noise for each bin:

1. sampling without considering the resolution:
   - reduced chi-squared = 0.8191388
   - for 3364 degrees of freedom
   - null hypothesis probability = 1.00

2. sampling with bin-size > FWHM/3:
   - reduced chi-squared = 1.094959
   - for 138 degrees of freedom
   - null hypothesis probability = 0.210

Asymptotic Distributed …

- all quantities used for the statistical analysis, are itself of statistical nature, i.e. they have an error
  - example: r.m.s.(χ^2) = √(2(d.o.f.))

- all statistical proofs and theorems are valid for n→∞

- but we have often not an infinite number of counts
  - Example:
  - χ^2 tests requires:
    - signal to noise ≥ 5 for central Y_i and
    - signal to noise ≥ 4 for Y_1 and Y_{last}
    - number of Y ≥ 5

Parameter Estimation

- intrinsic correlation between error and data!

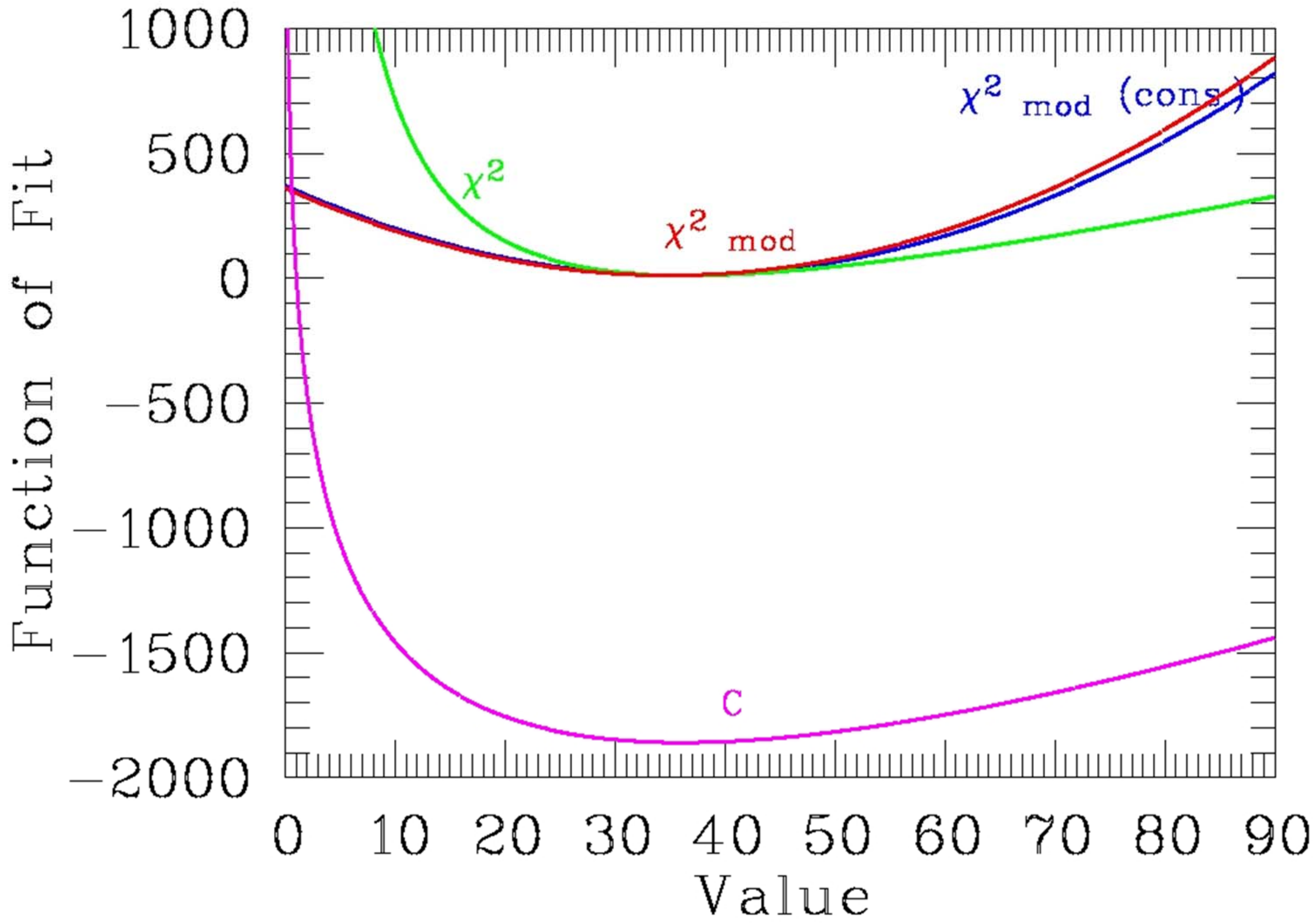
- example:
    - <Y>=36,
    - 10 data points Y1, Y2 ….: 30, 42, 24, 48, 33, 39, 34, 38, 36 , 36
    - error of Y1 = √Y1
  - mean Y = 360 / 10 = 36
  - minimum of χ^2 = ?
  - minimum of χ^2_{mod} = ?
  - minimum of C =?

Parameter Estimation

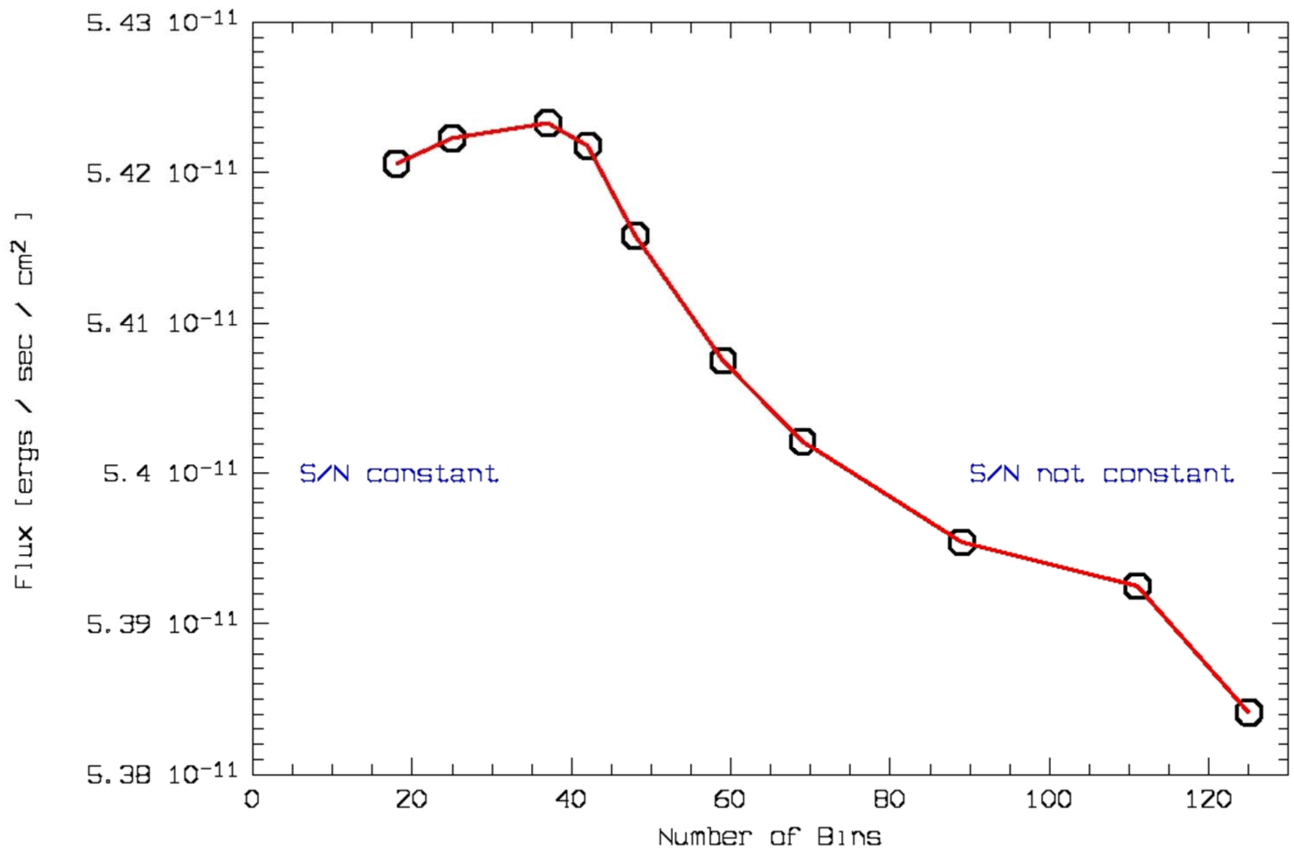
- **intrinsic correlation between error and data!**

- **example:**
    - **<Y>=36,**
    - **10 data points Y1, Y2 …: 30, 42, 24, 48, 33, 39, 34, 38, 36, 36**
    - **Error of Y1 = √Y1**
  - **Mean Y = 360 / 10 = 36.0**
  - **Minimum of χ^2 = 36.5**
  - **Minimum of χ^2_{mod} = 34.9**
  - **Minimum of C = 36.0**
  - **Minimum of χ^2_{mod} (constant error) = 36.0**

Parameter Estimation



Real Example



Parameter Estimation

our data show a correlation between data points and their error: $\Delta Y \approx \sqrt{(Y)}$

bias for parameter estimation!

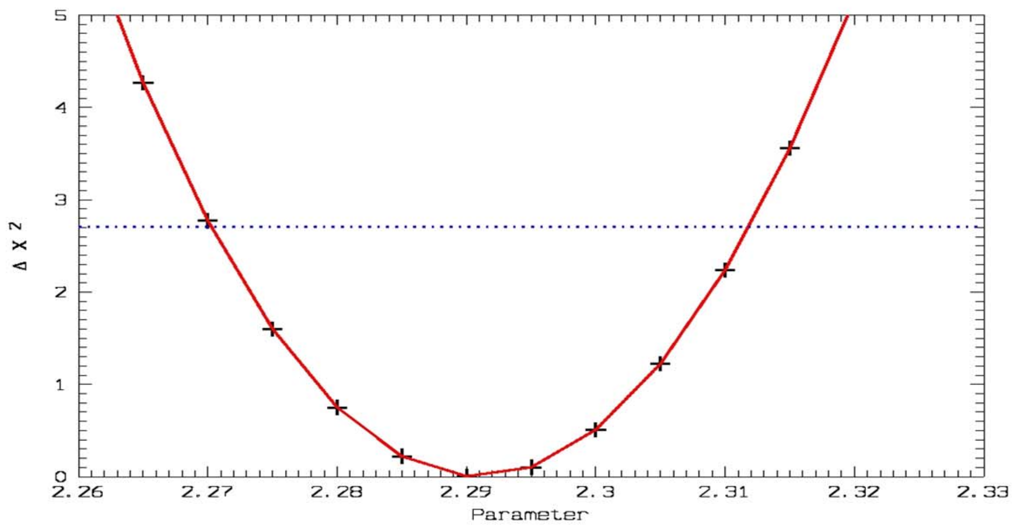
possible solutions:

- estimator which is independent of error,
  - e.g. C-statistics
- ensure, that data points have equal errors,
  - e.g. binning with constant signal/noise

the higher the numbers of counts the less important are bias effects!

Estimation Of Errors

- **method:** **search for the value of the parameter which corresponds to a certain confidence level, i.e. $\Delta\chi^2$**
  - **example:**
    - **90 % confidence level of one interesting parameter =>**
    - **$\Delta\chi^2 = 2.71$ ($\chi^2 = \chi^2$minimum + 2.71)**



Estimation Of Errors

- **be careful:**

- **$\Delta\ \chi^2$ (parameter) is in general not a smooth function with a single minimum**
  - **plot $\Delta\ \chi^2$ as function of the parameter**

- **the interesting parameter is often not independent from other parameters**
  - **plot two-dimensional $\Delta\ \chi^2$ contours**

Hypothesis Test

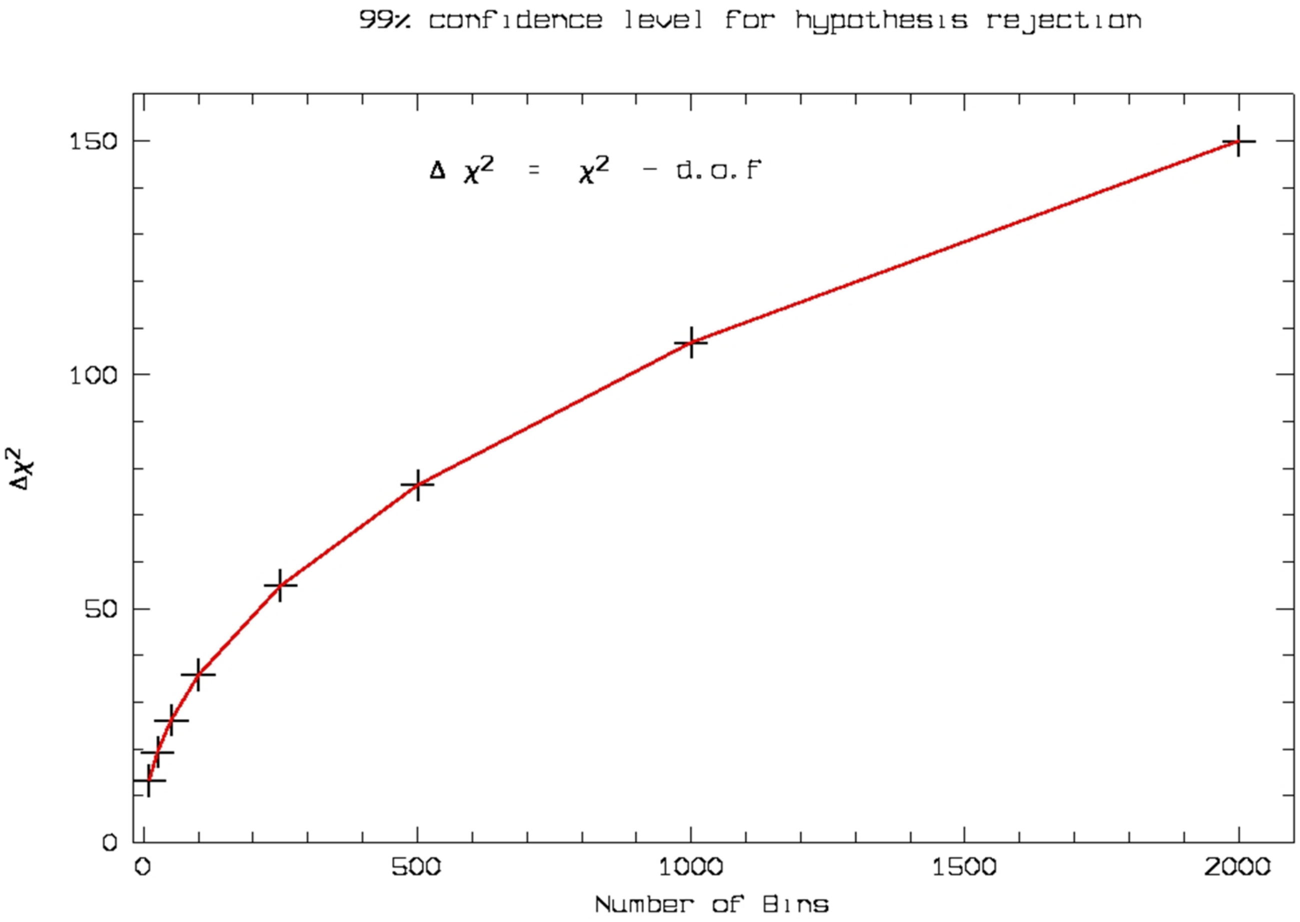
- **Literature: J. Kaastra in X-ray spectroscopy in astrophysics, 1999, p 276**

- **correct model:**
  - $\chi^2 = n - m$ **(n: number of data points, m:=number of free parameters**
  - **r.m.s.**$(\chi^2) = \sqrt{(2(n-m))}$

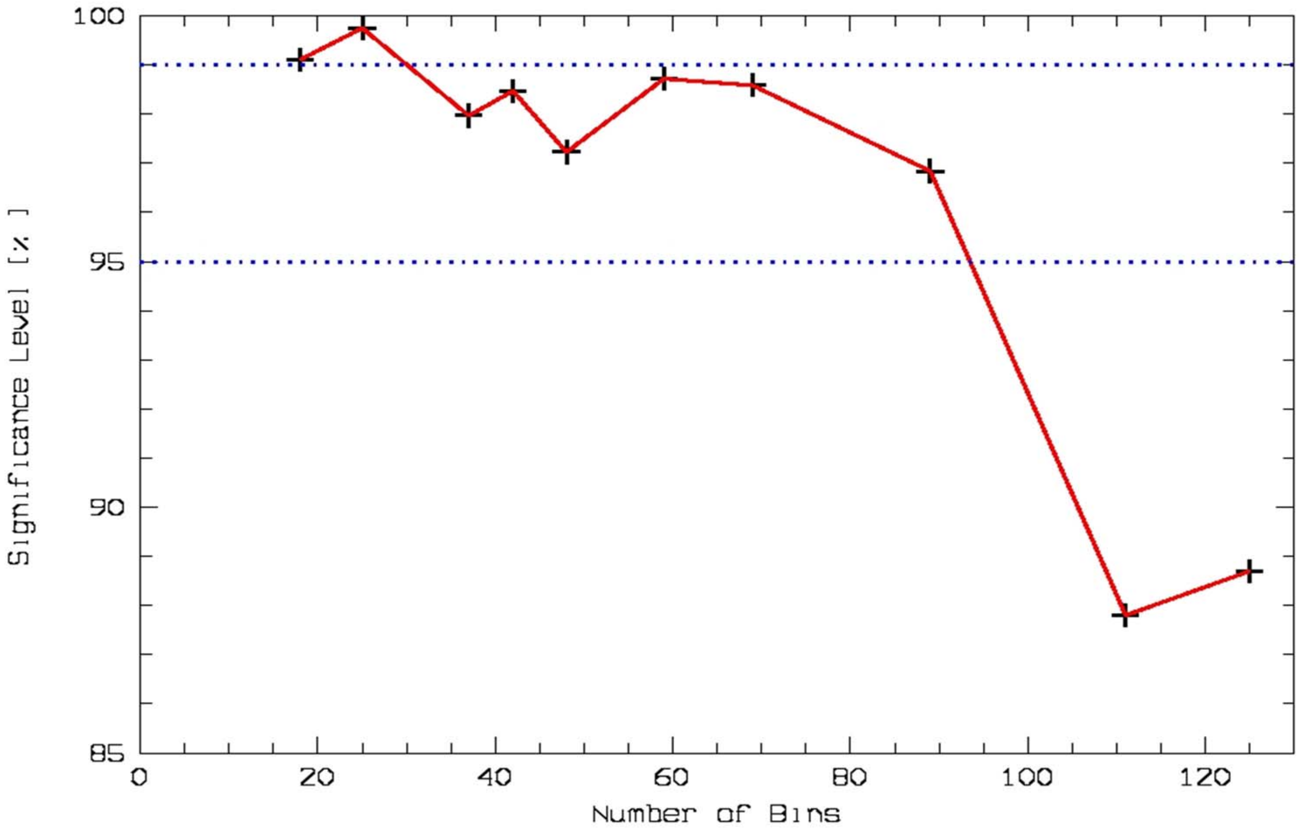
- **false model:**
  - $\chi^2 = n - m + r$
  - **r~number of photons (but independent from n)**

- **rejection of model**
  - $\chi^2 \geq n - m + f \sqrt{(2(n-m))} \rightarrow r > \sqrt{(2(n-m))}$

Hypothesis Test



Real Example



F-Test

- literature: J. Kaastra in X-ray spectroscopy in astrophysics, 1999, p 276

- F is defined as:
  - $F = \chi^2_1 \text{ d.o.f}_2 \ / \ \chi^2_2 \text{ d.o.f.}_1$
  - $F = \chi^2_1(n\text{-}m_2) \ / \ \chi^2_2(n\text{-}m_1)$
  - where
    - n number of data points
    - m number of fitted parameters

- F is a statistical quantity!
  - For large n:
  - $\text{r.m.s (F)} = 2 / \sqrt{(n)}$
  - $F = 1 + (r_1+r_2)/n$

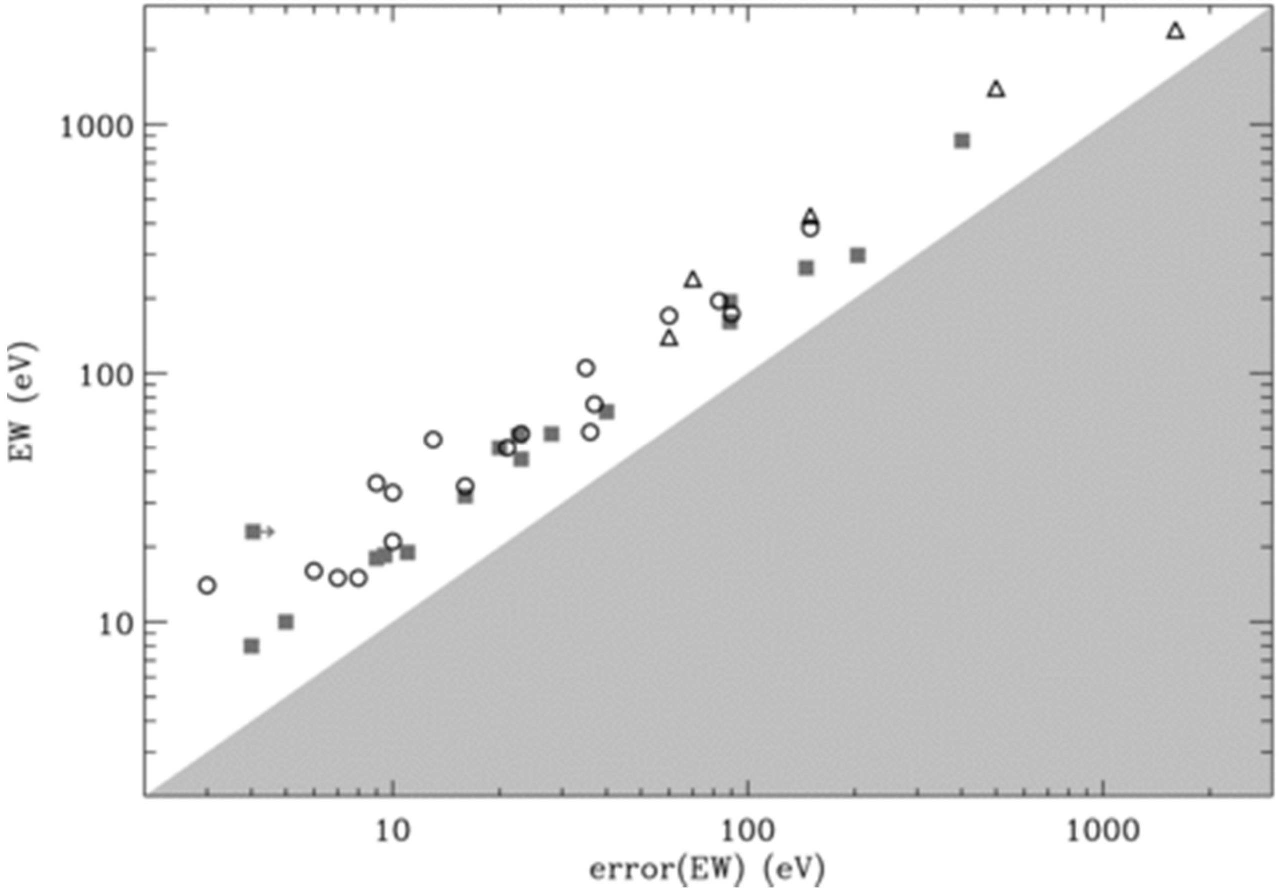
F-Test

- **Example:**
  - $r_1 + r_2 = 15$ (independent from n)
  - $m_1=3$,
  - $m_2=6$,

- **n = 40,**
  - d.o.f.$_1$=37, $\chi^2_1 = 52$, d.o.f.$_2$=34 χ^2_2=34
  - R.m.s.(F) = 0.3162
  - Probability of improvement:
    - F => 99.951897%
    - F+R.m.s(F) => 99.997780%
    - F-R.M.S(F) => 98.051537%

- **n = 100,**
  - d.o.f.$_1$=97, $\chi^2_1 = 112$, d.o.f.$_2$=94 χ^2_2=94
  - R.m.s.(F) = 0.2
  - Probability of improvement:
    - F => 99.912766%
    - F+R.m.s(F) => 99.999939%
    - F-R.M.S(F) => NO, model 1 is better than model 2

The Large View



Vaughan, S.; Uttley, P., 2008, MNRAS 390, 421

Golden Recipe Of The Statistical Analysis

1. golden Recipe of the statistical analysis does not exist.

2. every scientific question is a new statistical challenge and often requires a new concepts

3. In general:
   1. never over-sample a spectra
   2. a bin-width < 1/3 FWHM does not add any spectral information, but increases the d.o.f.
   3. if possible bin with constant signal/noise

4. every spectral analysis requires a new optimal solution depending on the analyzed spectra and on the specific scientific question