X-Ray Spectral Analysis

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Goal of this presentation

Providing you with a reference for topics relevant to spectroscopy of low-resolution (*i.e.* CCD) spectra:

- How do we fit spectra?
  - [and, by the way, what does it mean "*fitting a spectrum*"?]
- Which files do we need? what are they?
- How do we turn the fitting wheel?

If I make things too messy, *no panic*! Look at (*e.g.*):

http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/manual/XspecSpectralFitting.html

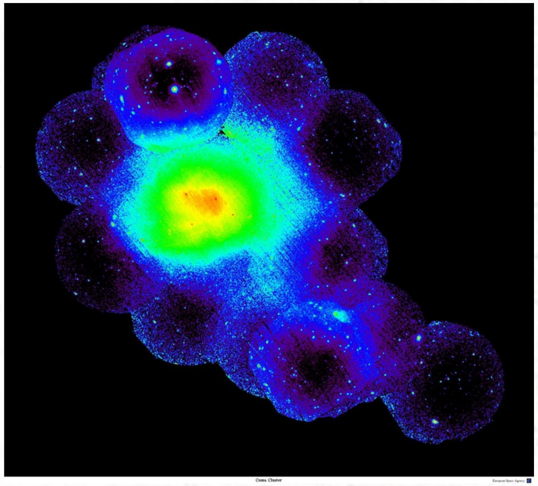
You Tube videos by Javier Garcia on our Slack Channel

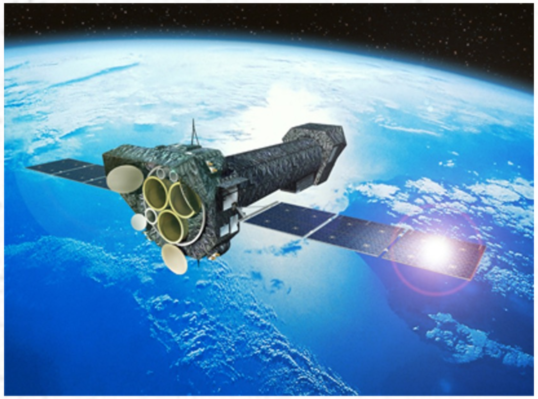
Out ultimate goal is ...

Intrinsic source spectrum s(E) ...

… seen through IGM/ISM absorption a(E) ...

… detected as observed counts C(PHA)





We measure C(PHA). We want to determine S(E) - occasionally A(E). Easy, isn't it?

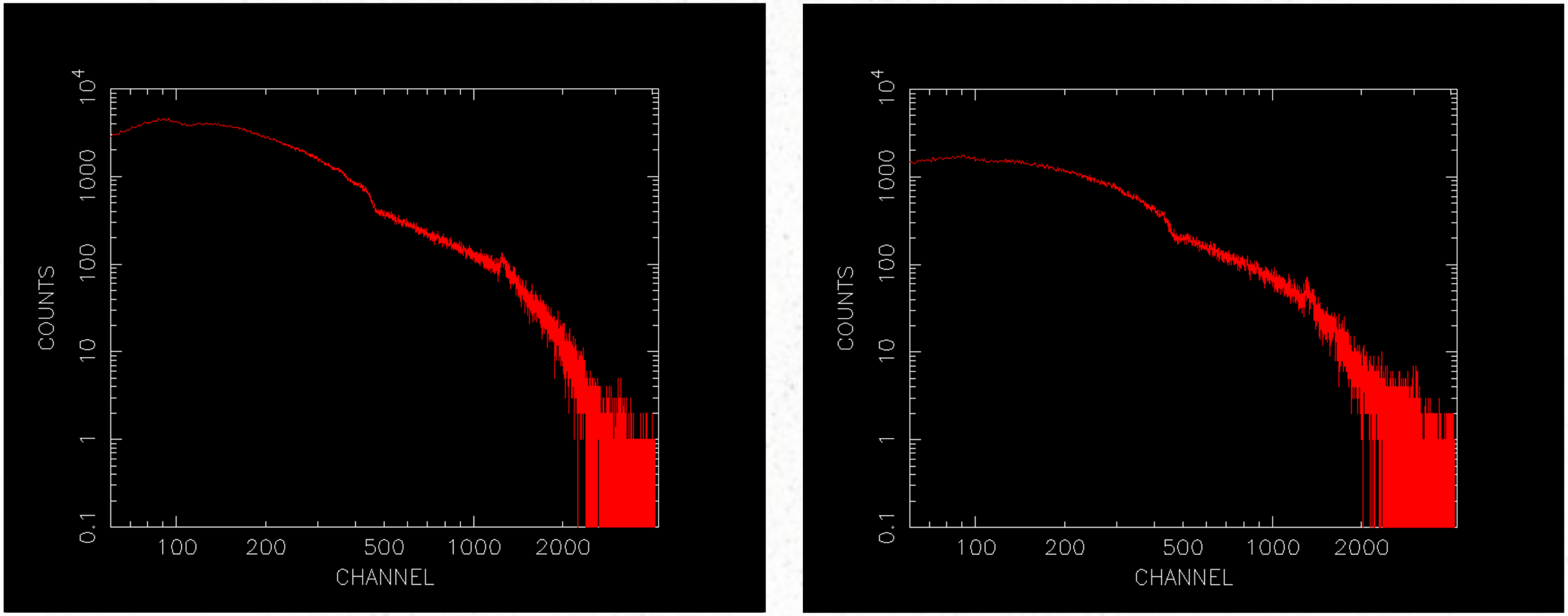
(Coma Cluster as seen by XMM-Newton: courtesy P.Rodriguez-Pascual)

(IGM simulation: courtesy G.Becker)

(Horsehead Nebula: courtesy M.Richmond)

When all candles be out, all cats are grey

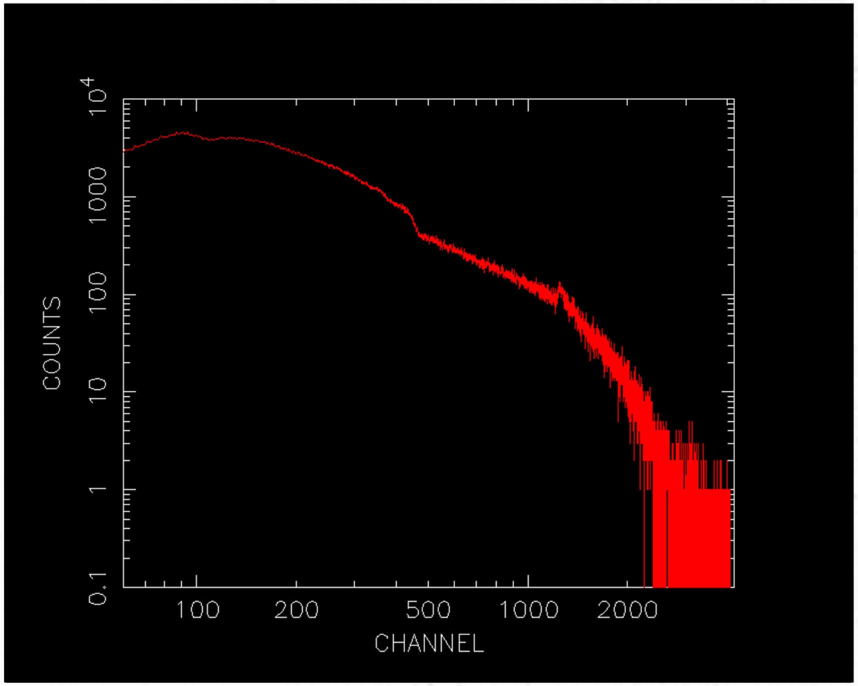
CCD spectra extracted by `dmextract`, `xmm`/`evselect`, or `xselect` look like this:



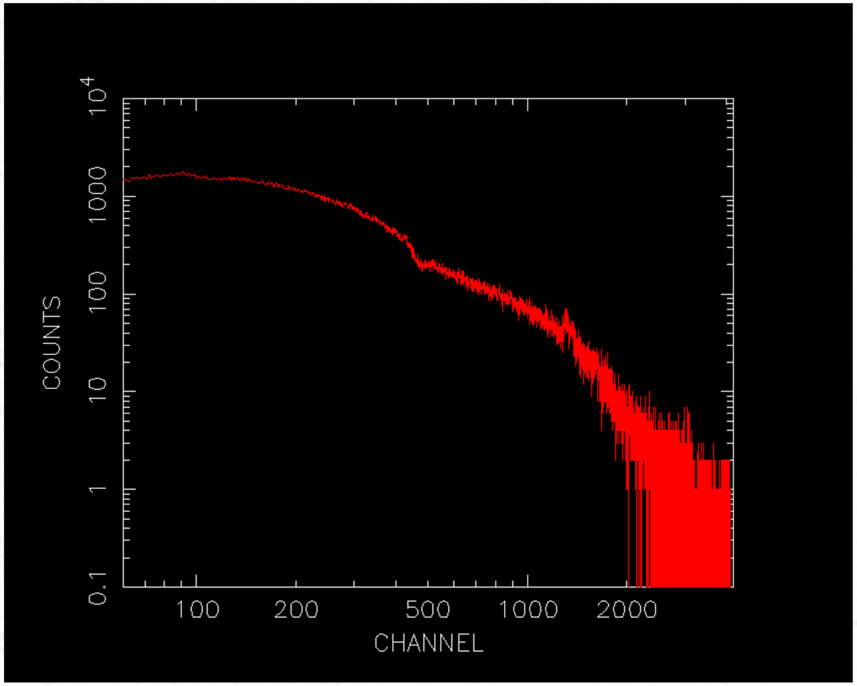
When all candles be out, all cats are grey

CCD spectra extracted by `dmextract`, `xmm`/`evselect`, or `xselect` look like this:

Ark120 – EPIC-pn (AGN)



Coma – EPIC-pn (Galaxy Cluster)



These are “`COUNTS` per bin”, not flux!

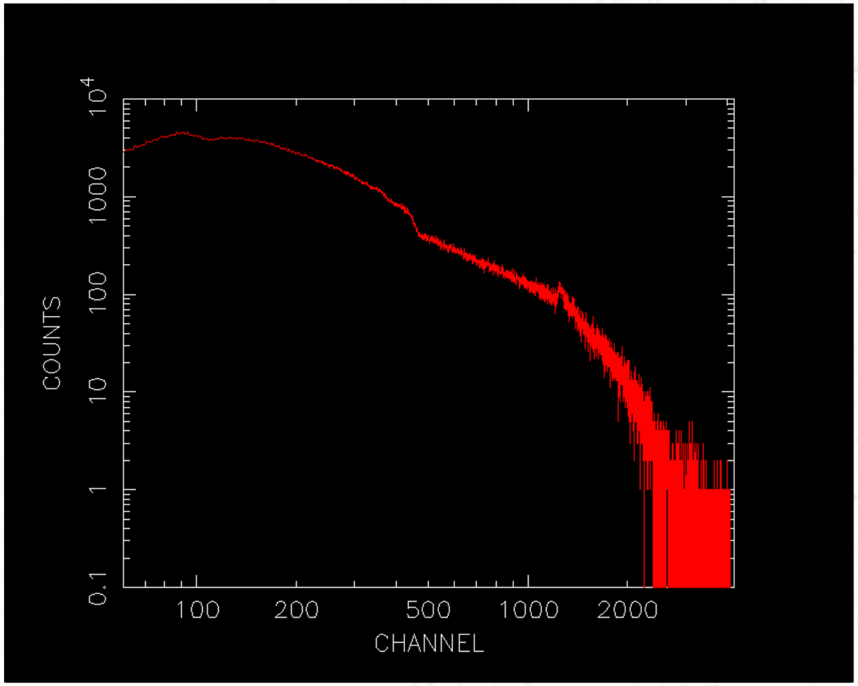
These are “`CHANNEL`s”, not energy!

First problem: spectral extractors produce spectra in instrumental quantities

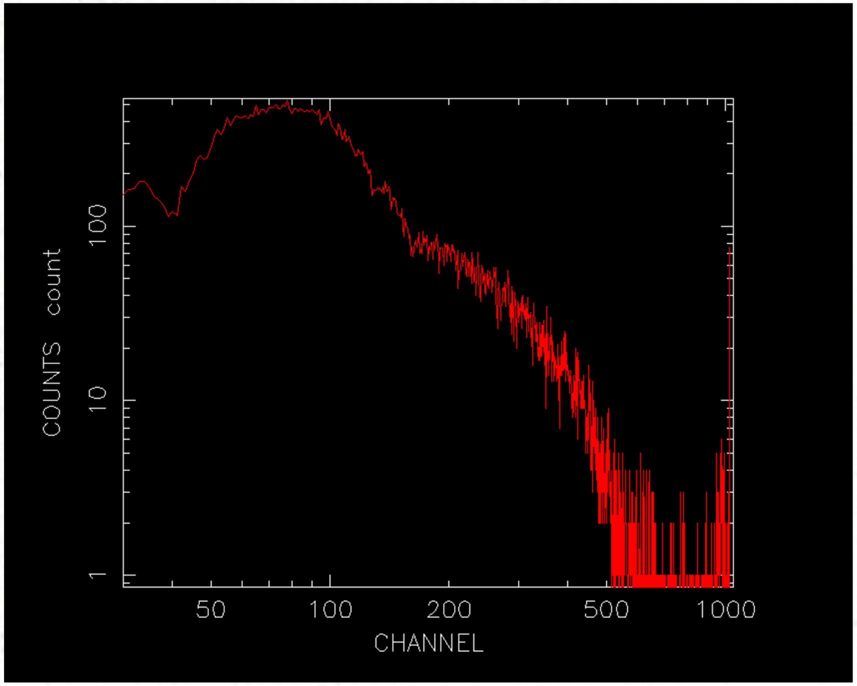
When all candles be out, all cats are grey

"*And now, for something completely different: the larch …*" (Monty Python, 1968)

Ark120 – EPIC-pn (AGN)



Ark120 – SIS (AGN)



Second problem: the shape of the count spectra is dominated by the transfer function of the telescope+detector: we must "decode" it

The spectral equation

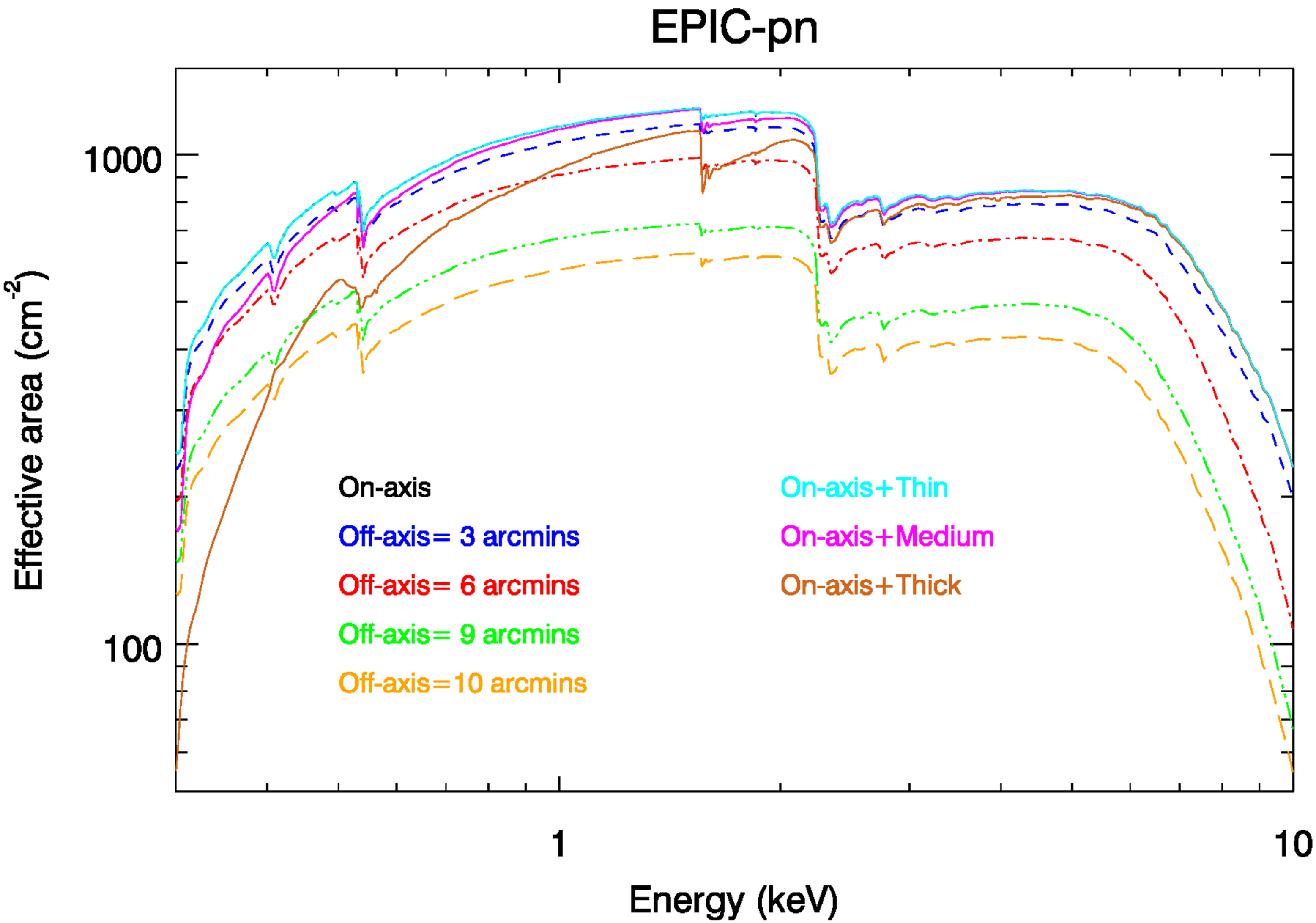
$$C(h) = (N\tau)\int dE\, R(h,\, E)A(E)s(E)$$

- *(Nτ)* = exposure time
- *C(h)* = observed spectrum, in units of *counts per spectral bin*
- *R(h,E)* = redistribution matrix (a.k.a. “RMF file”), typically normalised to 1
- *A(E)* = effective area (a.k.a. “ARF” or “ancillary file”) in units of *area*
- *s(E)* = intrinsic spectrum (to be determined)
- *h* = spectral channels, in units of *Pulse Height Analysis* (`PHA`) or *Pulse Invariant* (`PI`): digital instrumental quantities only loosely related to energy

We would need to invert this equation to get *s(E)*
However, in general this is not possible. Why?

(Davis, 2001, ApJ, 562, 575)

The effective area A(E)

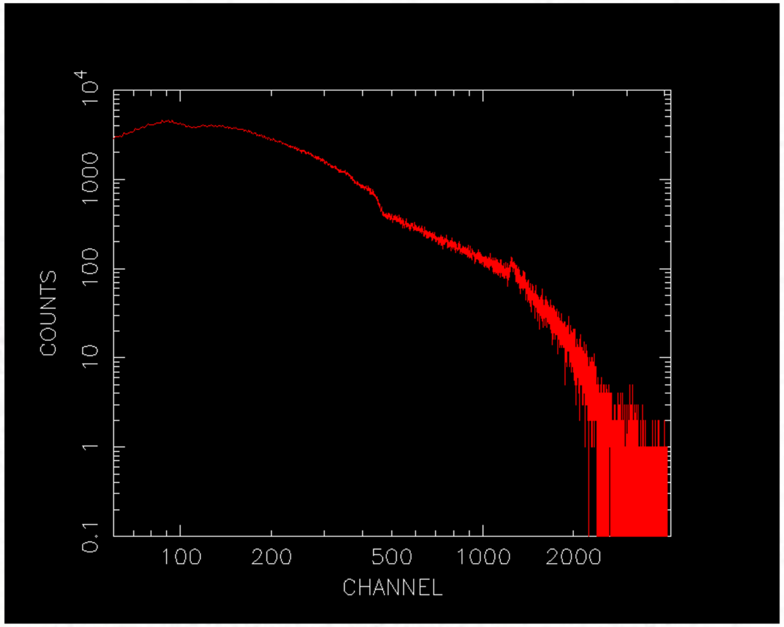


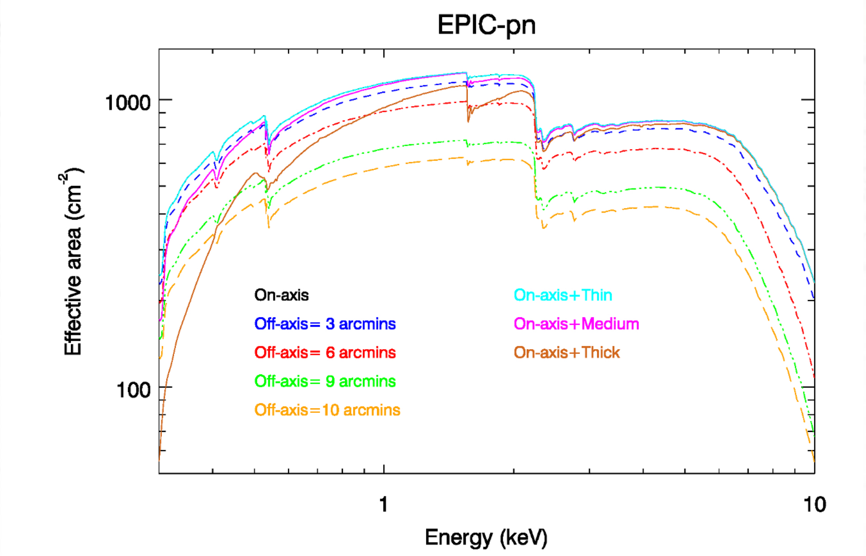
Measure (conventionally expressed in units of “*area*”) of the collecting power of telescope+filter+detector. It depends on energy and position (“off-axis”)

[Beware: not all observatories carry “*optical photon blocking filters*”]

Can I obtained the source spectrum by simple division?

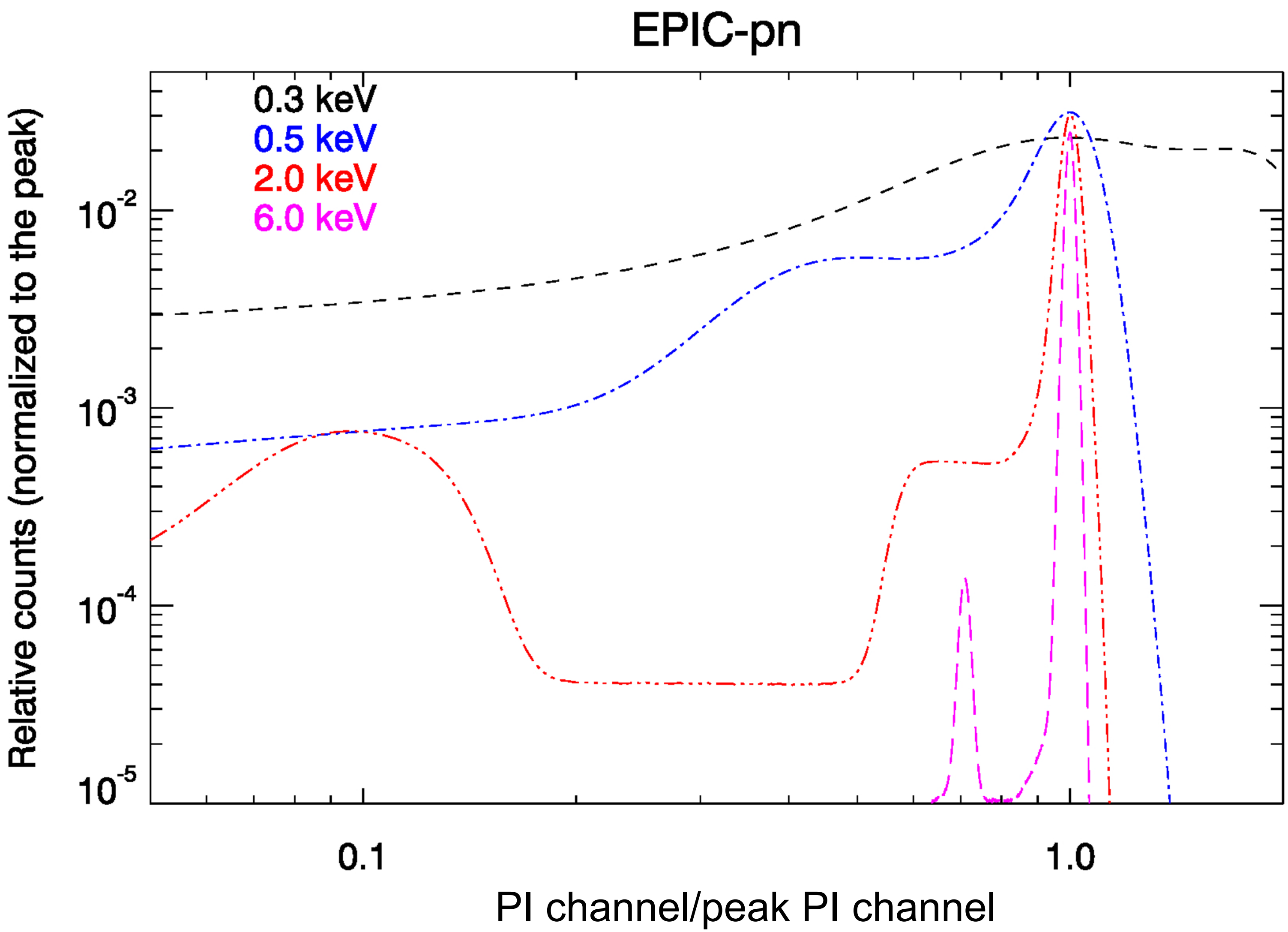
Source spectrum (E) =





?

Redistribution matrix R(E)



Response of the detector to a monochromatic line. Highly dependent on the energy
The width of the core defines the instrument resolution

Inverting the spectral equation?

The redistribution is sampled at discrete spectral channels:

$$R^i_{hE} = \frac{\int_{E_{j-1}}^{E_j} R(i, E')dE'}{(E_j - E_{j-1})}$$

The whole spectral equation is a discrete matrix equation:

$$C_h = T\Sigma_i \Sigma_E R^i_{hE} A^i_E S^i_E dE$$

The R^i_{hE} matrix cannot be inverted.

Alternative: **Forward-folding approach**

Forward-folding approach

1) Assume a model with its defining parameters

2) Define a set of parameter values

3) Convolve the model with the instrument response

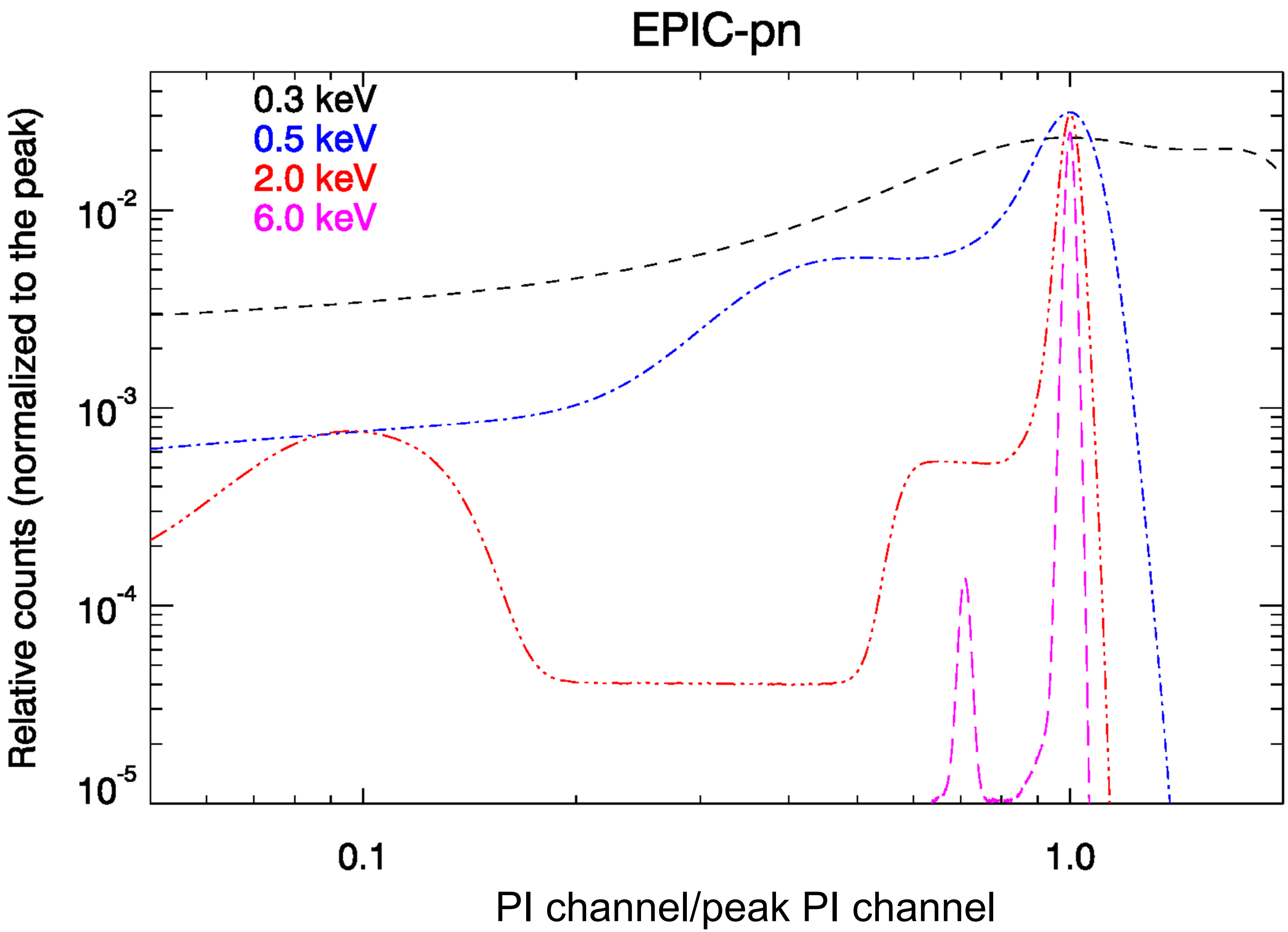
4) Compare the (dis)agreement between the observed spectrum and the folded model through a *goodness-of-fit* statistical test

5) Change the parameter values to minimize the goodness-of-fitness test ≡ **fit**

6) Once the best-fit is found, calculate the confidence intervals on the best-fit parameters

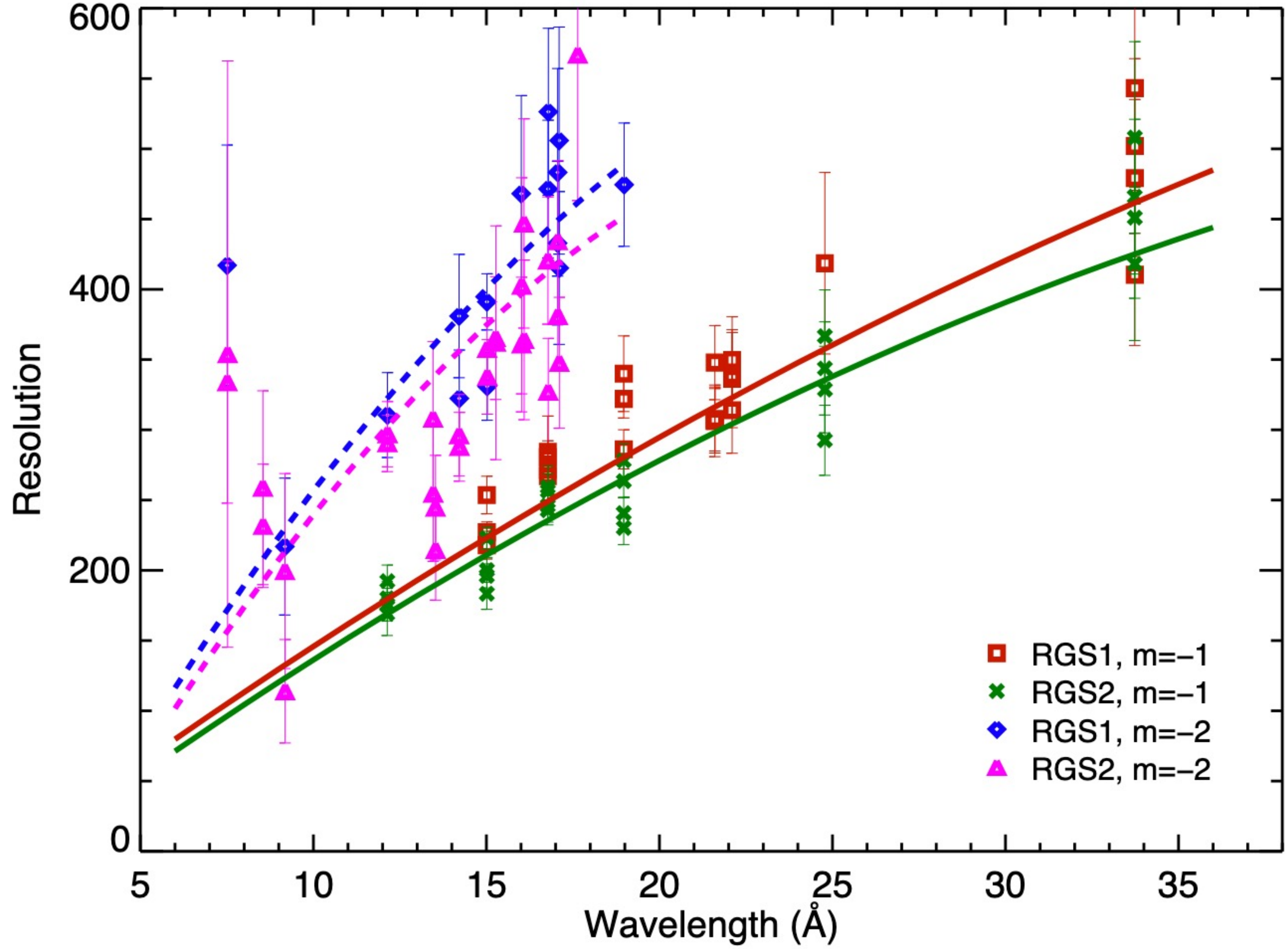
Spectral packages are looping machines through the steps above (+ a few other cosmetic features)

Redistribution matrix R(E)



Response of the detector to a monochromatic line. Highly dependent on the energy
The width of the core defines the instrument resolution

What about high-resolution instruments (e.g. RGS in XMM-Newton)?

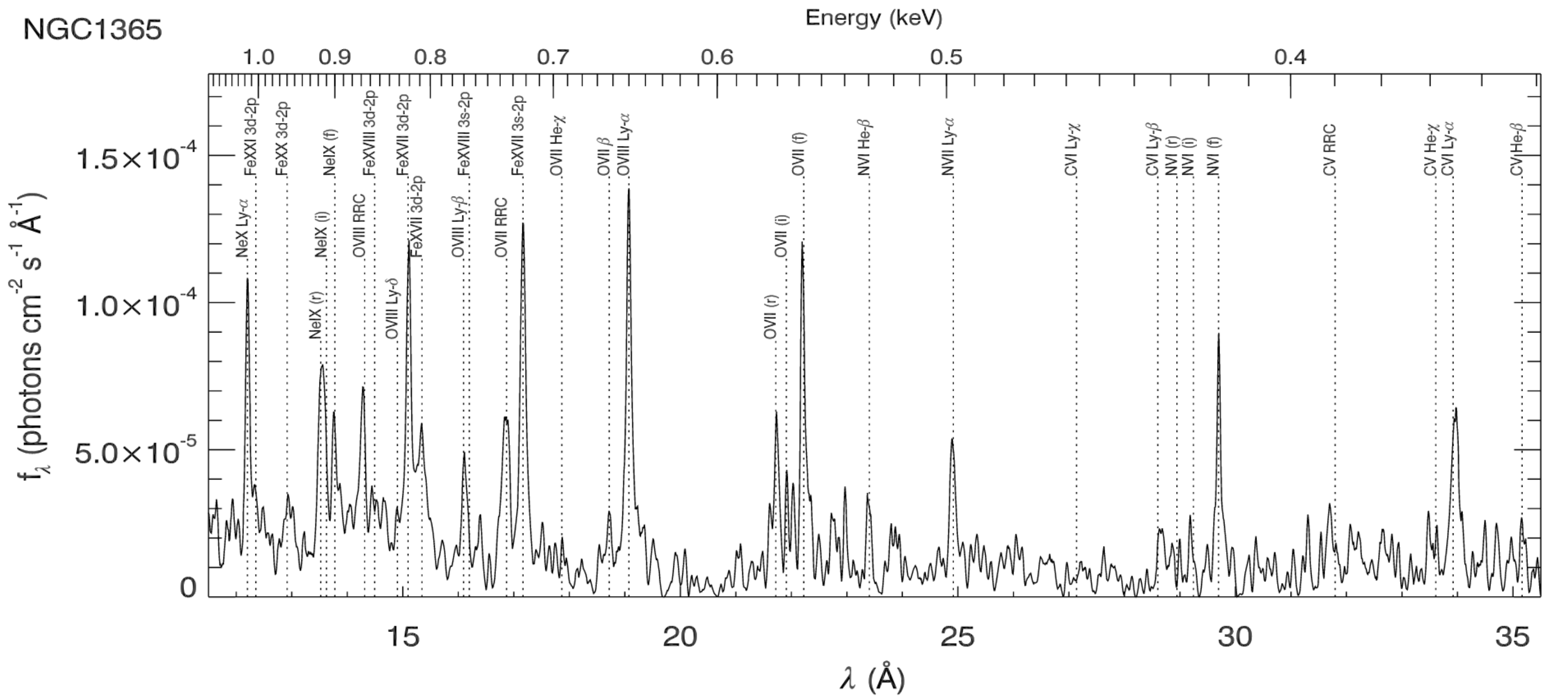


The resolving power of the EPIC cameras at 1 keV (~12.4Å) is ~15

(Gonzalez-Riestra et al., 2021, XMM-SOC-CAL-TN-0030)

rgsfluxer

```
setenv SPECTRA *SRSPEC*
setenv BKGs    *BGSPEC*
setenv RMFs    *RSPMAT*
rgsfluxer pha="$SPECTRA" bkg="$BKGs" rmf="RMFs" file=HR1099.RGS.spectrum
```



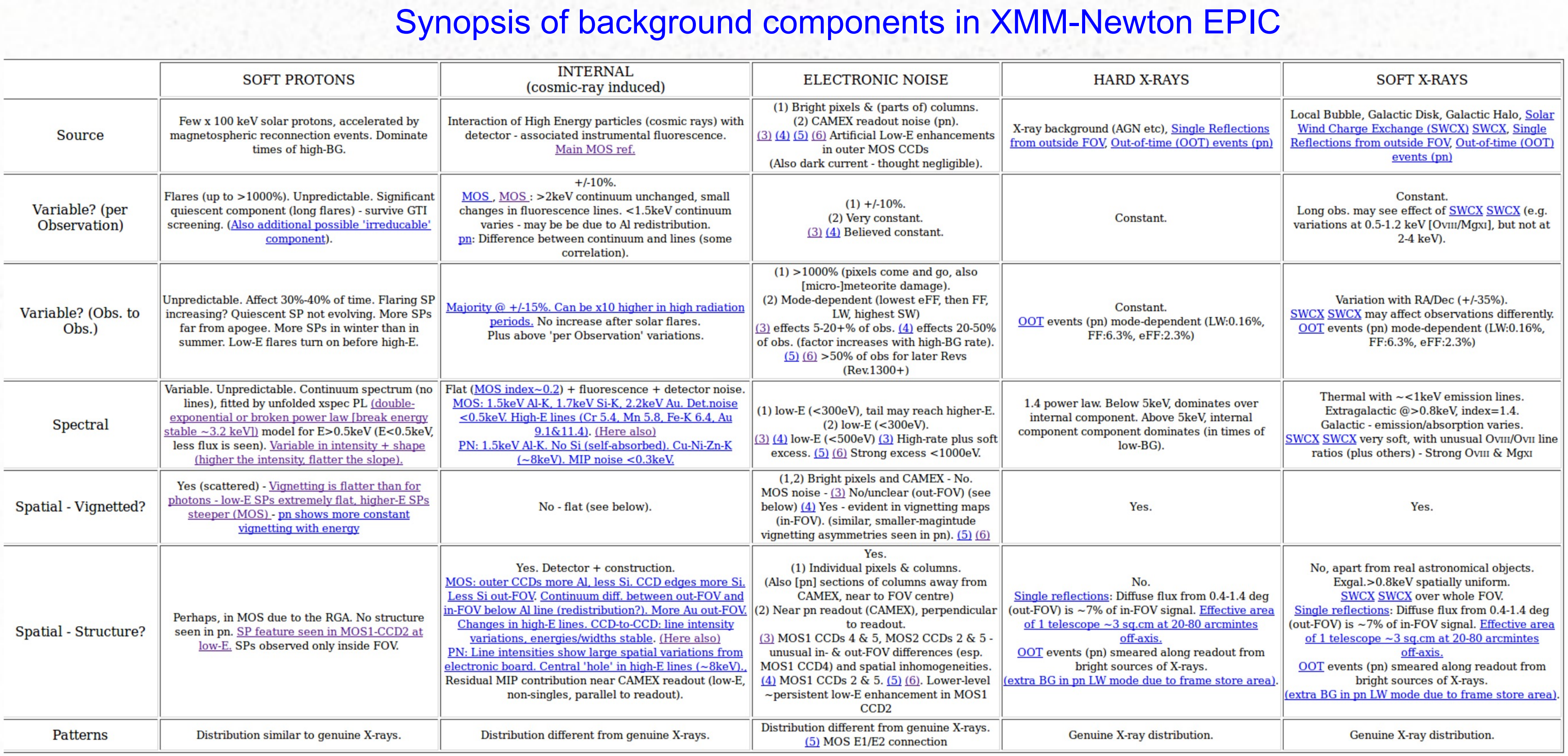
To be used only as "quick-look" only – *not for quantitative analysis*

(Guainazzi & Bianchi, 2007, MNRAS, 374, 1290)

Background spectra

The *inevitable background* is due to various component:

- Space environment
- Instrument
- Astrophysical sources



Synopsis of background components in XMM-Newton EPIC

	SOFT PROTONS	INTERNAL (cosmic-ray induced)	ELECTRONIC NOISE	HARD X-RAYS	SOFT X-RAYS
Source	Few x 100 keV solar protons, accelerated by magnetospheric reconnection events. Dominate times of high-BG.	Interaction of High Energy particles (cosmic rays) with detector - associated instrumental fluorescence. Main MOS ref.	(1) Bright pixels & (parts of) columns. (2) CAMEX readout noise (pn). (3) (4) (5) (6) Artificial Low-E enhancements in outer MOS CCDs (Also dark current - thought negligible).	X-ray background (AGN etc), Single Reflections from outside FOV, Out-of-time (OOT) events (pn)	Local Bubble, Galactic Disk, Galactic Halo, Solar Wind Charge Exchange (SWCX) SWCX, Single Reflections from outside FOV, Out-of-time (OOT) events (pn)
Variable? (per Observation)	Flares (up to >1000%). Unpredictable. Significant quiescent component (long flares) - survive GTI screening. (Also additional possible 'irreducable' component).	+/-10%. MOS , MOS : >2keV continuum unchanged, small changes in fluorescence lines. <1.5keV continuum varies - may be be due to Al redistribution. pn: Difference between continuum and lines (some correlation).	(1) +/-10%. (2) Very constant. (3) (4) Believed constant.	Constant.	Constant. Long obs. may see effect of SWCX SWCX (e.g. variations at 0.5-1.2 keV [OVIII/MgXI], but not at 2-4 keV).
Variable? (Obs. to Obs.)	Unpredictable. Affect 30%-40% of time. Flaring SP increasing? Quiescent SP not evolving. More SPs far from apogee. More SPs in winter than in summer. Low-E flares turn on before high-E.	Majority @ +/-15%. Can be x10 higher in high radiation periods. No increase after solar flares. Plus above 'per Observation' variations.	(1) >1000% (pixels come and go, also [micro-]meteorite damage). (2) Mode-dependent (lowest eFF, then FF, LW, highest SW) (3) effects 5-20+% of obs. (4) effects 20-50% of obs. (factor increases with high-BG rate). (5) (6) >50% of obs for later Revs (Rev.1300+)	Constant. OOT events (pn) mode-dependent (LW:0.16%, FF:6.3%, eFF:2.3%)	Variation with RA/Dec (+/-35%). SWCX SWCX may affect observations differently. OOT events (pn) mode-dependent (LW:0.16%, FF:6.3%, eFF:2.3%)
Spectral	Variable. Unpredictable. Continuum spectrum (no lines), fitted by unfolded xspec PL (double-exponential or broken power law [break energy stable ~3.2 keV]) model for E>0.5keV (E<0.5keV, less flux is seen). Variable in intensity + shape (higher the intensity, flatter the slope).	Flat (MOS index~0.2) + fluorescence + detector noise. MOS: 1.5keV Al-K, 1.7keV Si-K, 2.2keV Au. Det.noise <0.5keV. High-E lines (Cr 5.4, Mn 5.8, Fe-K 6.4, Au 9.1&11.4). (Here also) PN: 1.5keV Al-K. No Si (self-absorbed). Cu-Ni-Zn-K (~8keV). MIP noise <0.3keV.	(1) low-E (<300eV), tail may reach higher-E. (2) low-E (<300eV). (3) (4) low-E (<500eV) (3) High-rate plus soft excess. (5) (6) Strong excess <1000eV.	1.4 power law. Below 5keV, dominates over internal component. Above 5keV, internal component component dominates (in times of low-BG).	Thermal with ~<1keV emission lines. Extragalactic @>0.8keV, index=1.4. Galactic - emission/absorption varies. SWCX SWCX very soft, with unusual OVIII/OVII line ratios (plus others) - Strong OVIII & MgXI
Spatial - Vignetted?	Yes (scattered) - Vignetting is flatter than for photons - low-E SPs extremely flat, higher-E SPs steeper (MOS) - pn shows more constant vignetting with energy	No - flat (see below).	(1,2) Bright pixels and CAMEX - No. MOS noise - (3) No/unclear (out-FOV) (see below) (4) Yes - evident in vignetting maps (in-FOV). (similar, smaller-magintude vignetting asymmetries seen in pn). (5) (6)	Yes.	Yes.
Spatial - Structure?	Perhaps, in MOS due to the RGA. No structure seen in pn. SP feature seen in MOS1-CCD2 at low-E. SPs observed only inside FOV.	Yes. Detector + construction. MOS: outer CCDs more Al, less Si. CCD edges more Si. Less Si out-FOV. Continuum diff. between out-FOV and in-FOV below Al line (redistribution?). More Au out-FOV. Changes in high-E lines. CCD-to-CCD: line intensity variations, energies/widths stable. (Here also) PN: Line intensities show large spatial variations from electronic board. Central 'hole' in high-E lines (~8keV)., Residual MIP contribution near CAMEX readout (low-E, non-singles, parallel to readout).	Yes. (1) Individual pixels & columns. (Also [pn] sections of columns away from CAMEX, near to FOV centre) (2) Near pn readout (CAMEX), perpendicular to readout. (3) MOS1 CCDs 4 & 5, MOS2 CCDs 2 & 5 - unusual in- & out-FOV differences (esp. MOS1 CCD4) and spatial inhomogeneities. (4) MOS1 CCDs 2 & 5. (5) (6). Lower-level ~persistent low-E enhancement in MOS1 CCD2	No. Single reflections: Diffuse flux from 0.4-1.4 deg (out-FOV) is ~7% of in-FOV signal. Effective area of 1 telescope ~3 sq.cm at 20-80 arcmintes off-axis. OOT events (pn) smeared along readout from bright sources of X-rays. (extra BG in pn LW mode due to frame store area).	No, apart from real astronomical objects. Exgal.>0.8keV spatially uniform. SWCX SWCX over whole FOV. Single reflections: Diffuse flux from 0.4-1.4 deg (out-FOV) is ~7% of in-FOV signal. Effective area of 1 telescope ~3 sq.cm at 20-80 arcmintes off-axis. OOT events (pn) smeared along readout from bright sources of X-rays. (extra BG in pn LW mode due to frame store area).
Patterns	Distribution similar to genuine X-rays.	Distribution different from genuine X-rays.	Distribution different from genuine X-rays. (5) MOS E1/E2 connection	Genuine X-ray distribution.	Genuine X-ray distribution.

This implies that some components are focused by the telescope. Others aren't

(Courtesy A.Read: `http://www.star.le.ac.uk/~amr30/BG/BGTable.html`))

How to deal with background spectra

$$C_h = T[\Sigma_i \Sigma_E R^i_{hE} A^i_E (s^i_E + b^{i,f}_E) dE + b^{i,u}_E]$$

focused

not focused

Three approaches are possible:

- Ignore the background. Wrong

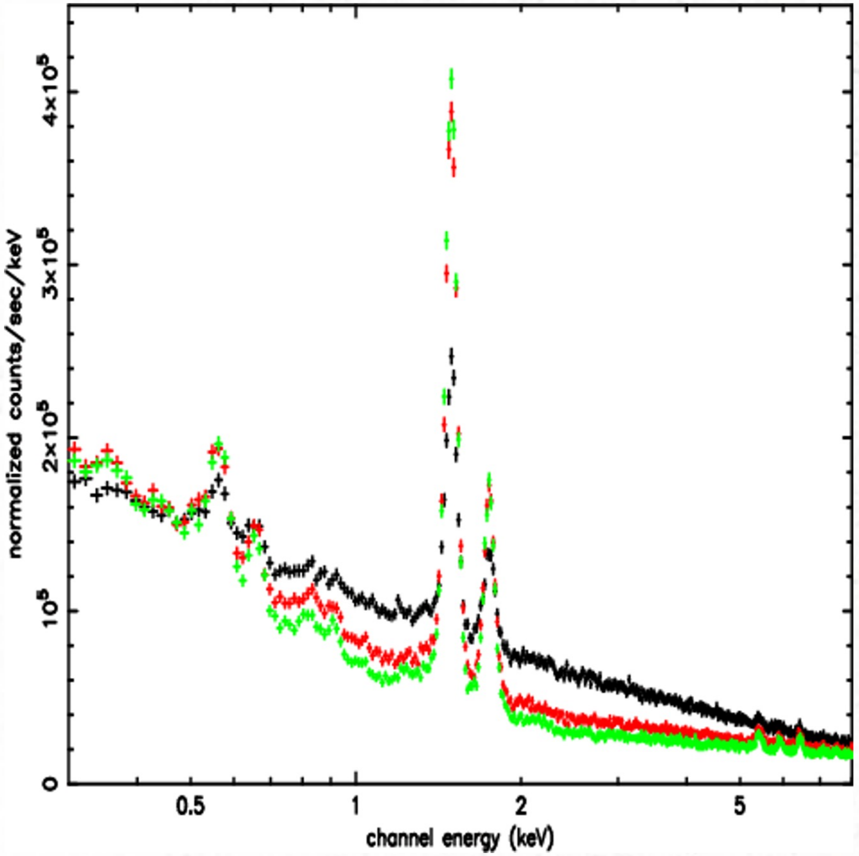
- Subtract the background. Easy, but:
- "It reduces the amount of statistical information in the analysis [..]
- The background subtracted data are not Poisson-distributed;
- [For example, subtracting a background can give negative counts; this is definitely not Poissonian!
- Fluctuations, particularly in the vicinity of localized features, can adversely affect analysis"

- Model and fit simultaneously the source and the background. Appealing, but:
- The background spectra is often awfully complex, time- and detector-position
- dependent, sometimes not known at all

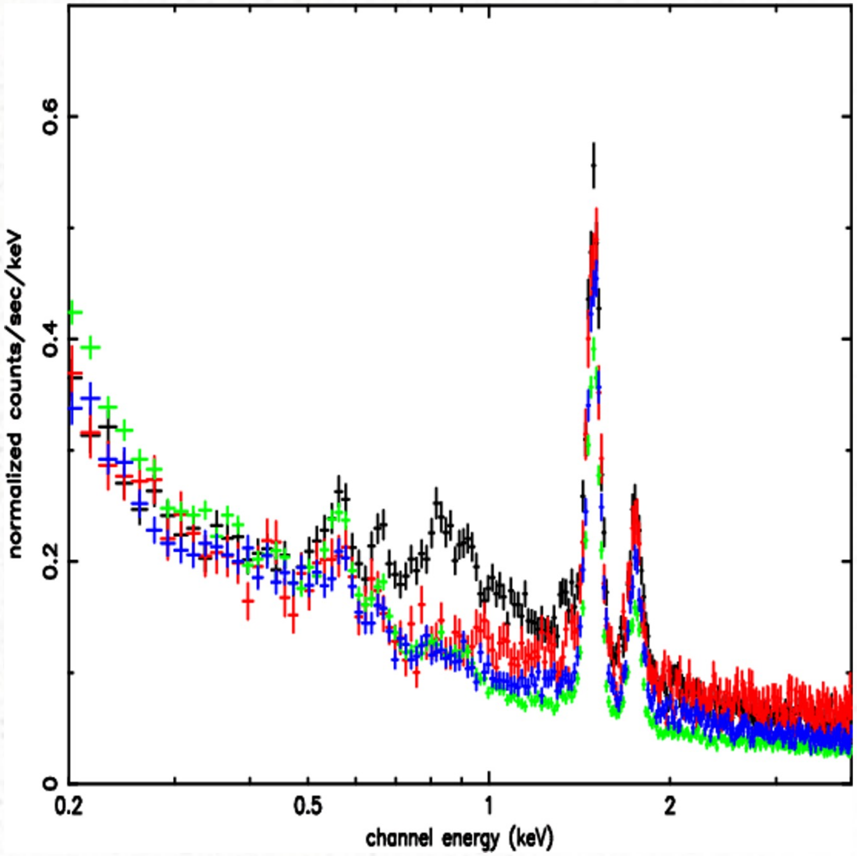
(Verbatim extracted from the *Sherpa* manual)

Goodness-of-fit statistical tests

EPIC-MOS background spectra
as a function of count rate

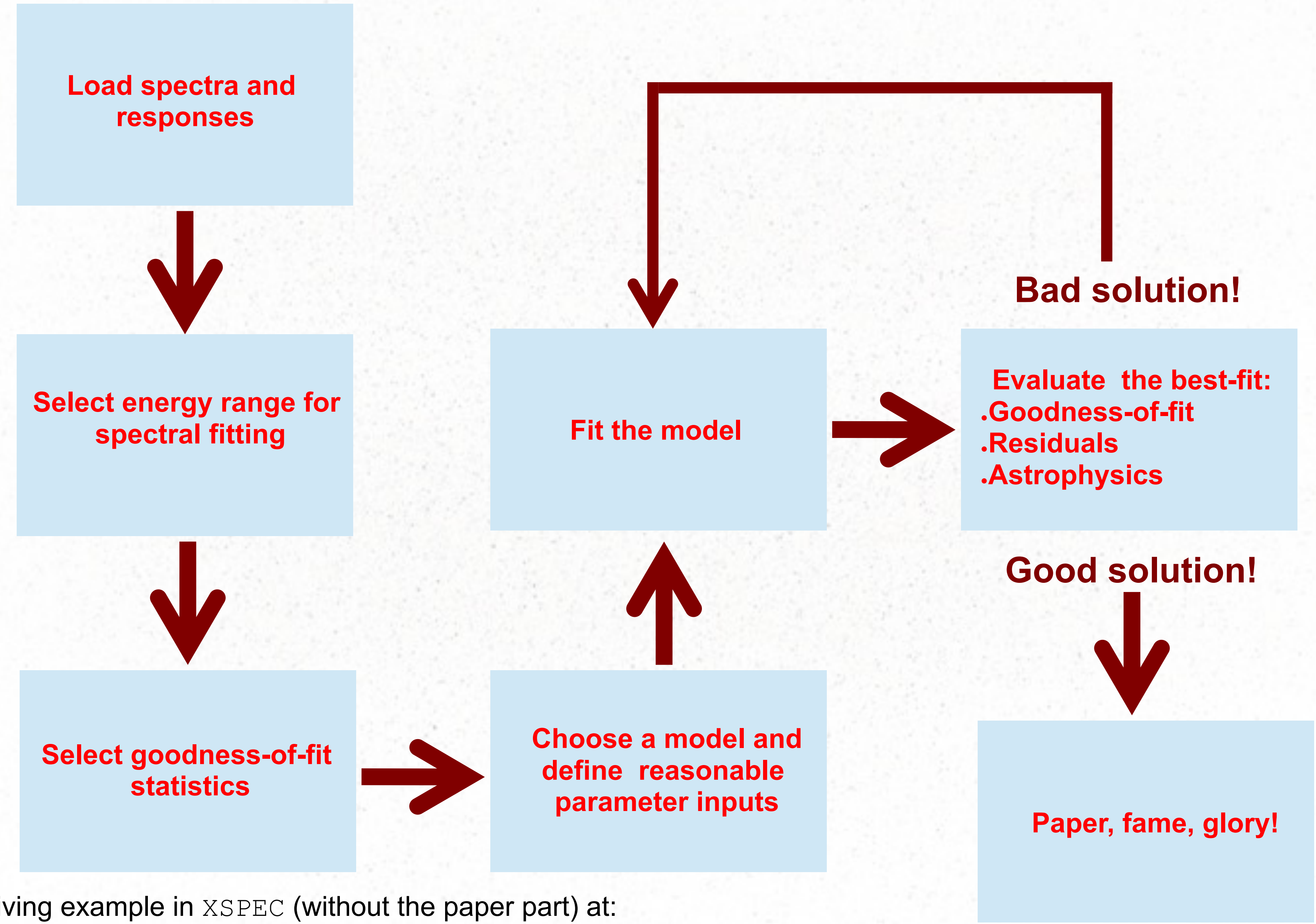


EPIC-MOS background spectra along
different line-of-sights



(Carter & Read, 2007, A&A, 464, 1155)

Forward-folding in action



Load spectra and responses

Select energy range for spectral fitting

Select goodness-of-fit statistics

Choose a model and define reasonable parameter inputs

Fit the model

Evaluate the best-fit:
.Goodness-of-fit
.Residuals
.Astrophysics

Bad solution!

Good solution!

Paper, fame, glory!

Living example in `XSPEC` (without the paper part) at:
http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/manual/XspecWalkthrough.html

Important questions to ask before starting

1. How do I quantitative compare models and data?
2. Is the numbet of channels in my spectrum adequate to constrain S(E)?

Goodness-of-fit tests

$$\chi^2 = \sum_{k=1}^{n} \frac{(O_k - E_k)^2}{\sigma_k^2}$$

O_k = Observer counts
E_k = Expected counts
σ_k = Statistical error

$$\chi^2 / dof \approx 1$$ ✓

However, the chi-squared is the maximum likelihood for the Gaussian distribution. The distribution of photon-counting detectors is Poissoniasm. The corresponding maximum likelihood is the Cash statistics

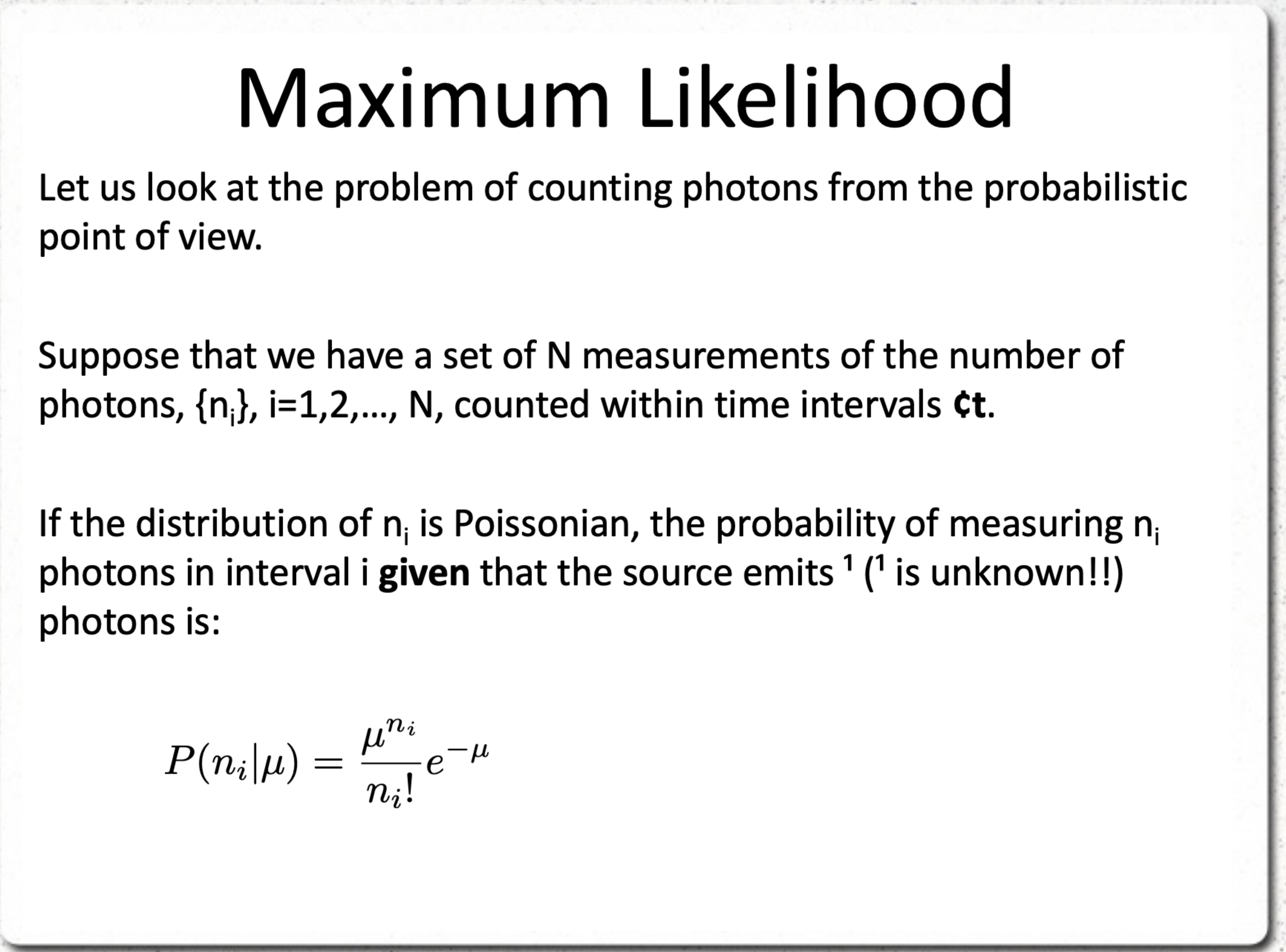
$$C = 2 \sum_{i=1}^{n} s_i - N_i + N_i \ln(N_i / s_i).$$

The Cash statistic is implemented in all spectral packages (`statistic cstat` in XSPEC)
It does not provide a *measurement of the absolute quality of a fit* -> Monte-Carlo approach

More in Mendez' lecture on statistics

(see Arnaud et al., "Fitting low count spectra", https://astrophysics.gsfc.nasa.gov/XSPECwiki/low_count_spectra) (Cash, 1976, ApJ, 52, 307)

Refresher on the concept of maximum likelihood – I.



Maximum Likelihood

Let us look at the problem of counting photons from the probabilistic point of view.

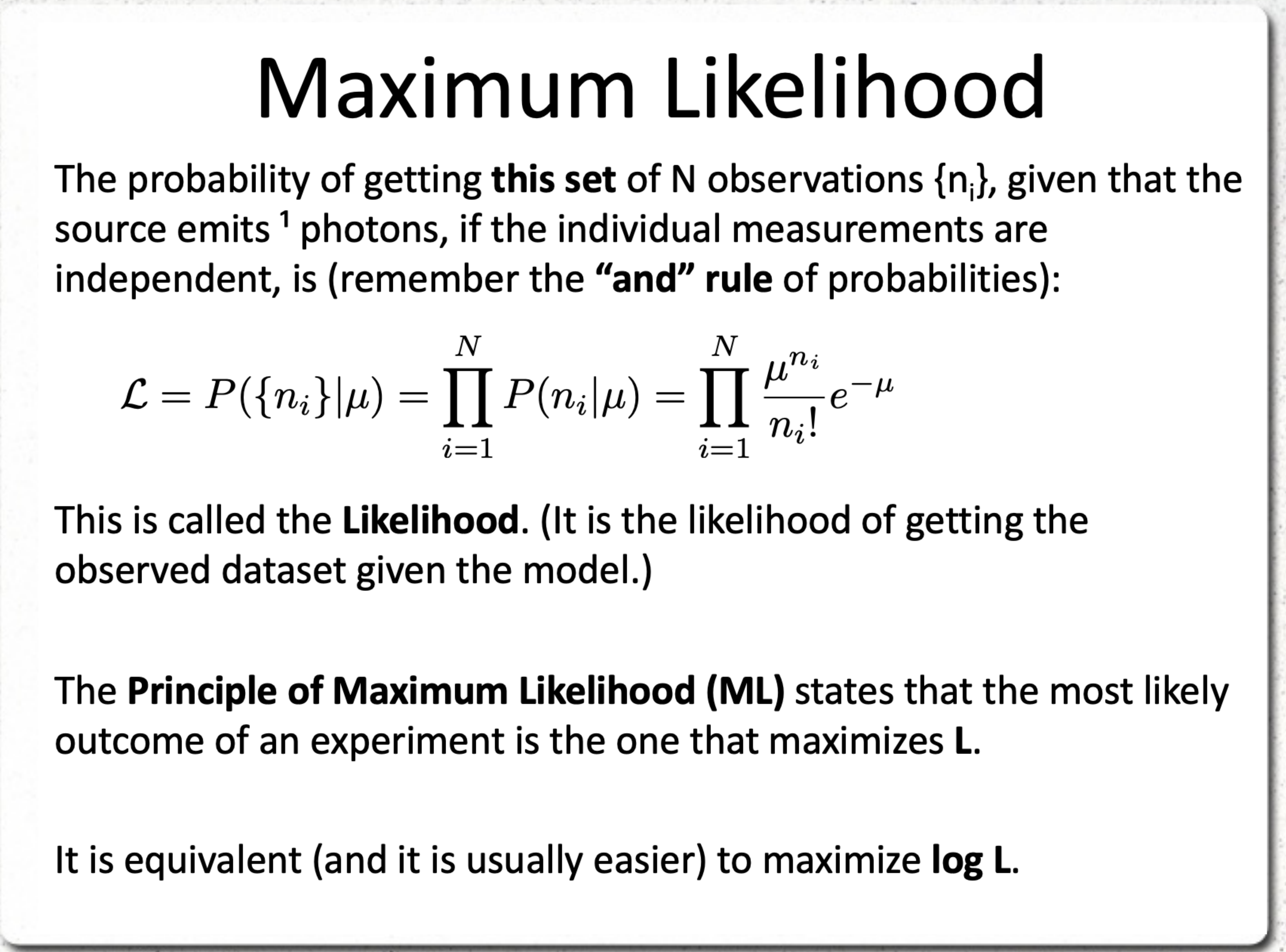
Suppose that we have a set of N measurements of the number of photons, $\{n_i\}$, i=1,2,…, N, counted within time intervals **¢t**.

If the distribution of n_i is Poissonian, the probability of measuring n_i photons in interval i **given** that the source emits ¹ (¹ is unknown!!) photons is:

$$P(n_i|\mu) = \frac{\mu^{n_i}}{n_i!}e^{-\mu}$$

(cf. M. Mendez presentation on statistics)

Refresher on the concept of maximum likelihood – II.



Maximum Likelihood

The probability of getting **this set** of N observations {n_i}, given that the source emits ^{1} photons, if the individual measurements are independent, is (remember the **“and” rule** of probabilities):

$$\mathcal{L} = P(\{n_i\}|\mu) = \prod_{i=1}^{N} P(n_i|\mu) = \prod_{i=1}^{N} \frac{\mu^{n_i}}{n_i!} e^{-\mu}$$

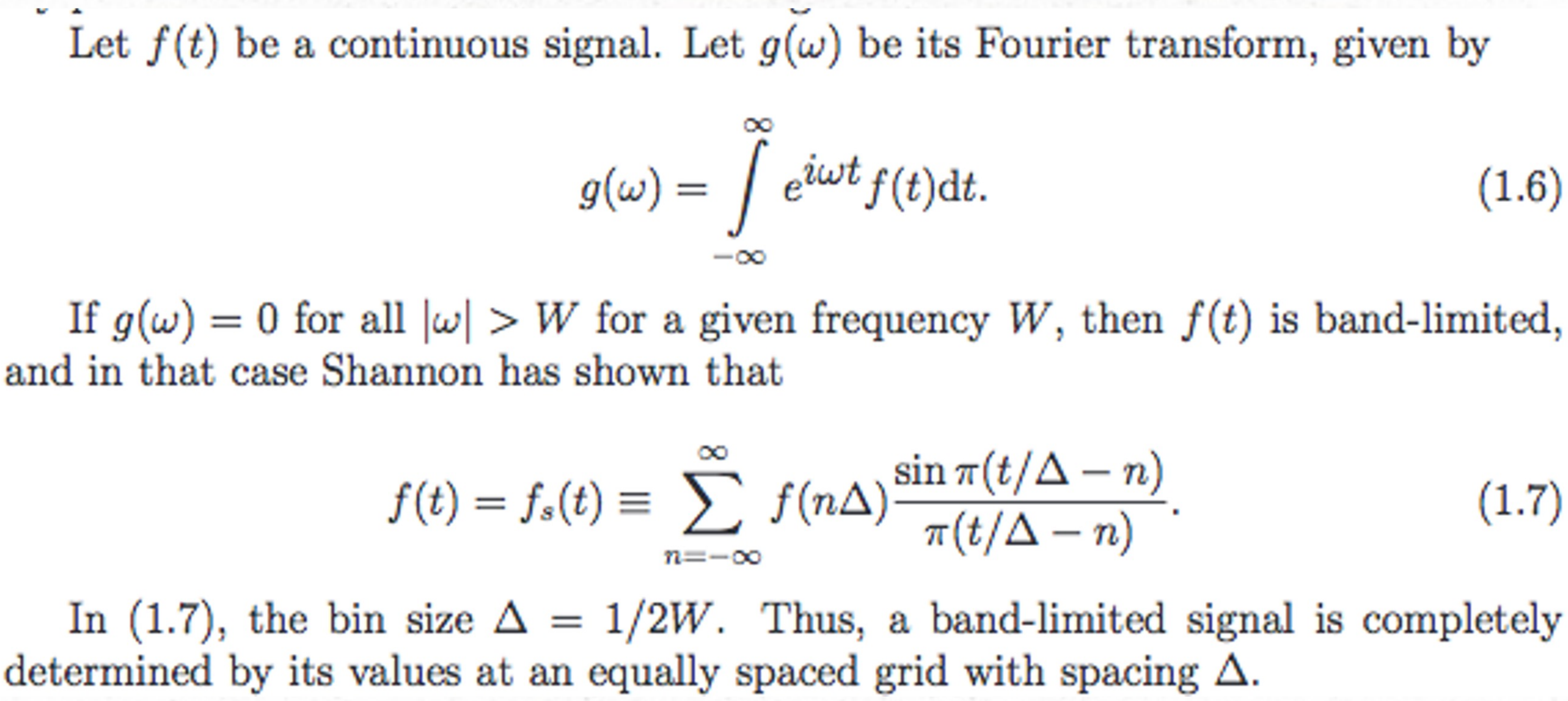
This is called the **Likelihood**. (It is the likelihood of getting the observed dataset given the model.)

The **Principle of Maximum Likelihood (ML)** states that the most likely outcome of an experiment is the one that maximizes **L**.

It is equivalent (and it is usually easier) to maximize **log L**.

(cf. M. Mendez presentation on statistics)

Shannon theorem



Let $f(t)$ be a continuous signal. Let $g(\omega)$ be its Fourier transform, given by

$$g(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} f(t) \mathrm{d}t. \tag{1.6}$$

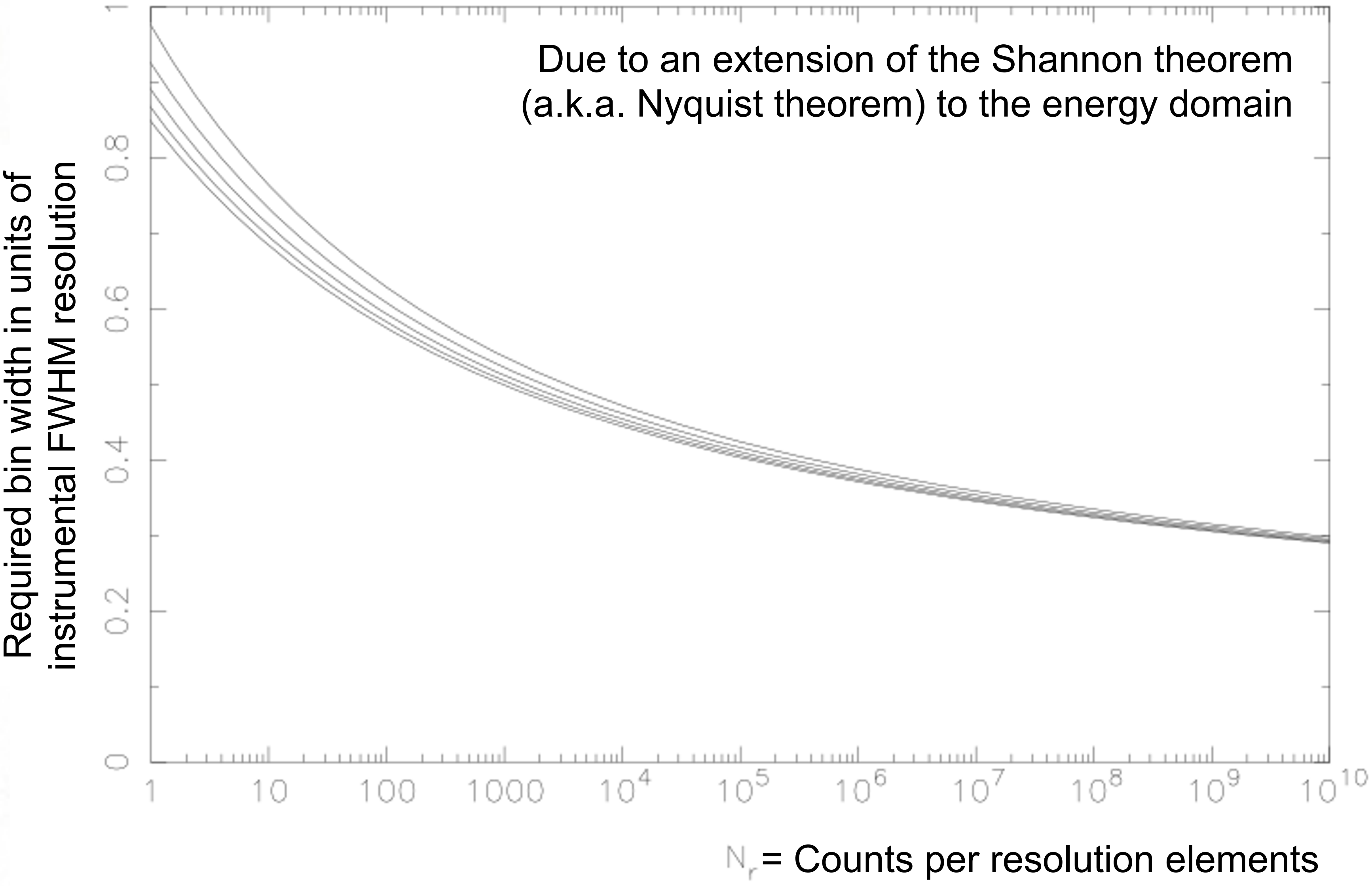
If $g(\omega) = 0$ for all $|\omega| > W$ for a given frequency W, then $f(t)$ is band-limited, and in that case Shannon has shown that

$$f(t) = f_s(t) \equiv \sum_{n=-\infty}^{\infty} f(n\Delta) \frac{\sin \pi(t/\Delta - n)}{\pi(t/\Delta - n)}. \tag{1.7}$$

In (1.7), the bin size $\Delta = 1/2W$. Thus, a band-limited signal is completely determined by its values at an equally spaced grid with spacing Δ.

(from J.Kaastra's and F.Verbunt's lecture notes on high-energy astrophysics, 2008)

The rigorous rebinning strategy



Due to an extension of the Shannon theorem (a.k.a. Nyquist theorem) to the energy domain

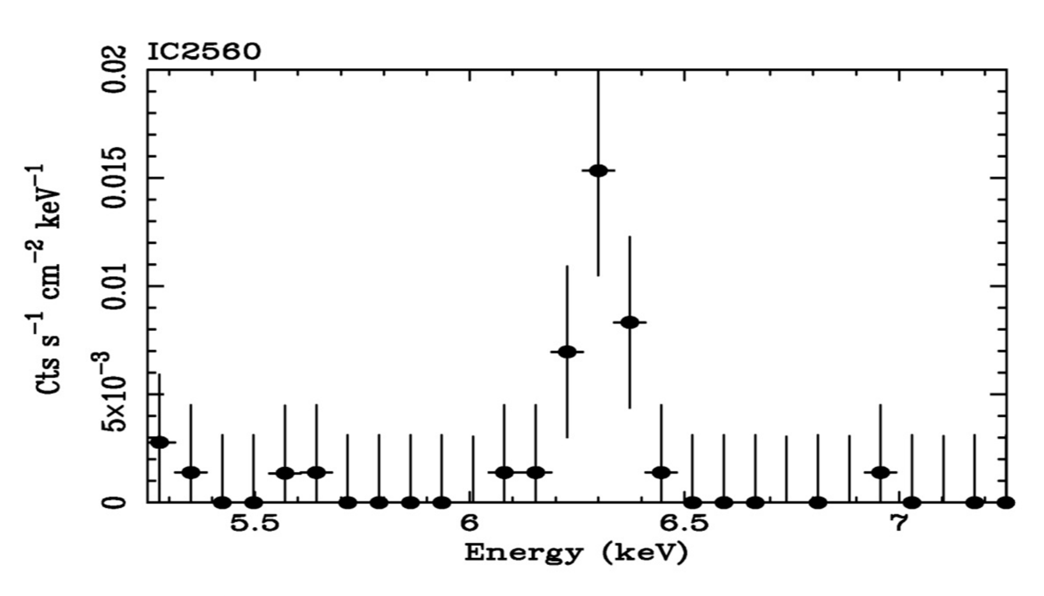
`ftgrouppha` in LEASHOFT implements this (and other rebinning schemes)

(Kaastra & Bleeker, 2016, A&A, 587, 151)

To (re)bin or not to (re)bin?

- Rebin your spectra is pure evil, may lead to loss of scientific information:

Photons in the line: 21



Photons in the continuum: 9

- However, a minimum level of spectral rebinning is required to avoid oversampling the intrinsic resolution of the instrument

(Guainazzi et al., 2005, MNRAS; 356, 295)

X-ray fitting packages

- XSPEC: http://heasarc.nasa.gov/xanadu/xspec/
- ISIS: http://space.mit.edu/cxc/isis/
- SHERPA: http://cxc.harvard.edu/sherpa4.4/index.html
- SPEX: http://www.sron.nl/spex

Models

Most software packages include the same suite of astrophysical models (~10^2):

- Additive:

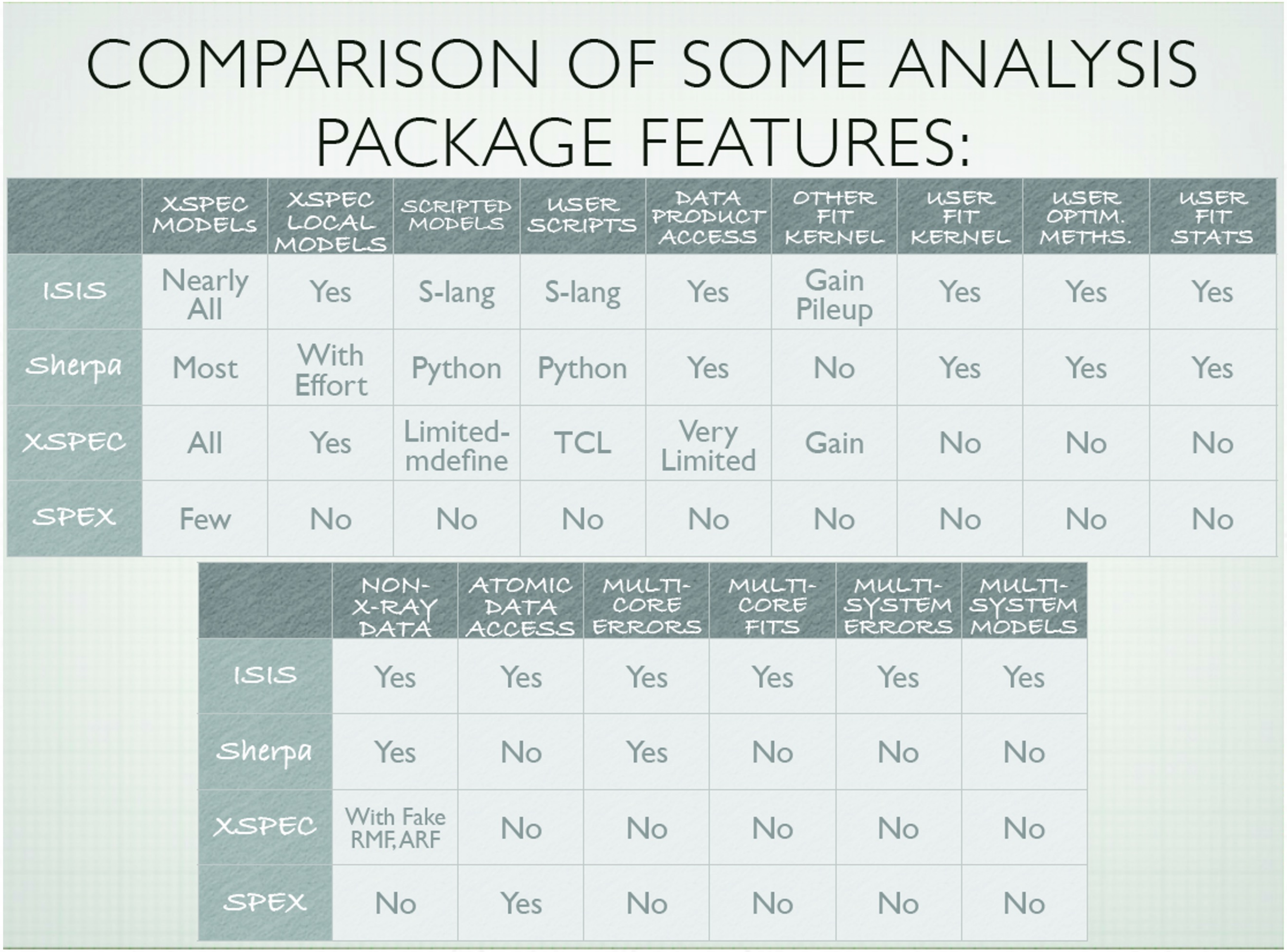
blackbody Gaussian profile
power-law bremsstrahlung

  - Phenomenological: `po`, `bb`, `brems`, `gauss`
  - Astrophysical: `comptt`, `diskbb`, `apec`, `relxill`

Comptonization Thermal plasma
Accretion disk blackbody Relativistic accretion disk emissiom

- Multiplicative:
  - Absorption, cut-off ...
- Convolution:
  - Kernels, flux calculation …
- Mixing
  - Surface brigthness, deprojection …
- Colleagues in the community contribute their own (“external model”), either as functions or as FITS table
- You can create your own (it does not require a software guru)!

Features of the existing X-Ray fitting packages



COMPARISON OF SOME ANALYSIS PACKAGE FEATURES:

	XSPEC MODELS	XSPEC LOCAL MODELS	SCRIPTED MODELS	USER SCRIPTS	DATA PRODUCT ACCESS	OTHER FIT KERNEL	USER FIT KERNEL	USER OPTIM. METHS.	USER FIT STATS
ISIS	Nearly All	Yes	S-lang	S-lang	Yes	Gain Pileup	Yes	Yes	Yes
Sherpa	Most	With Effort	Python	Python	Yes	No	Yes	Yes	Yes
XSPEC	All	Yes	Limited-mdefine	TCL	Very Limited	Gain	No	No	No
SPEX	Few	No	No	No	No	No	No	No	No

	NON-X-RAY DATA	ATOMIC DATA ACCESS	MULTI-CORE ERRORS	MULTI-CORE FITS	MULTI-SYSTEM ERRORS	MULTI-SYSTEM MODELS
ISIS	Yes	Yes	Yes	Yes	Yes	Yes
Sherpa	Yes	No	Yes	No	No	No
XSPEC	With Fake RMF, ARF	No	No	No	No	No
SPEX	No	Yes	No	No	No	No

(Courtesy M.Nowak)