X-Ray Spectrum Analysis I.
Low-resolution Spectra

Matteo Guainazzi

European Space Astronomy Centre
European Space Agency
Villafranca del Castillo, Spain
Matteo.Guainazzi@sciops.esa.int

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 min "*fitting a spectrum*"?]
- What files do we need? what are they?
- How do we turn the fitting wheel?
- How do we deal with calibration uncertainties?

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

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

Outline

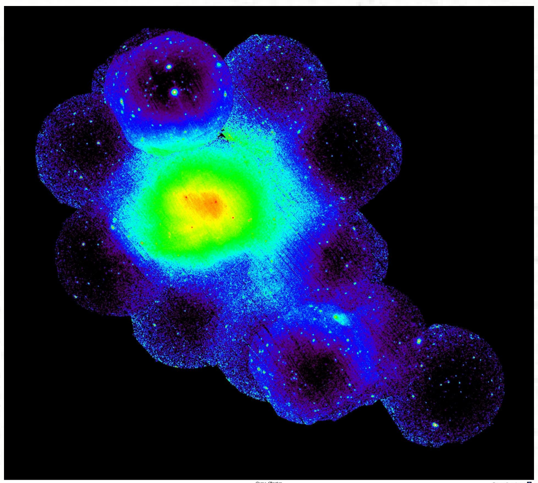
- This talk is primarily intended for users of CCD spectra:
  - ASCA/SIS
  - *Chandra*/ACIS
  - Swift/XRT
  - *Suzaku*/XIS
  - XMM-Newton/EPIC (-MOS and -pn)
- However, some basic principles can be applied to instruments with even lower resolution:
  - ROSAT/PSPC, ASCA/GIS, BeppoSAX, RXTE, Suzaku/HXD, NuSTAR …
- [Bias: *Many examples refer to the EPIC cameras, but only because I am paid to ensure that they work ...*]

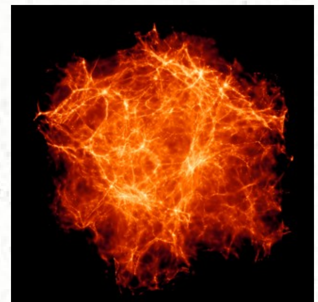
Out ultimate goal is ...

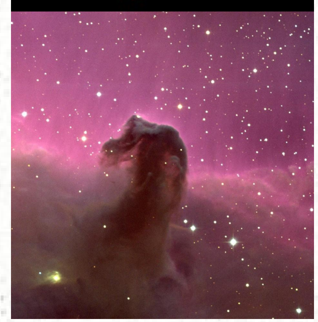
Intrinsic source spectrum s(E) ...

... 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?

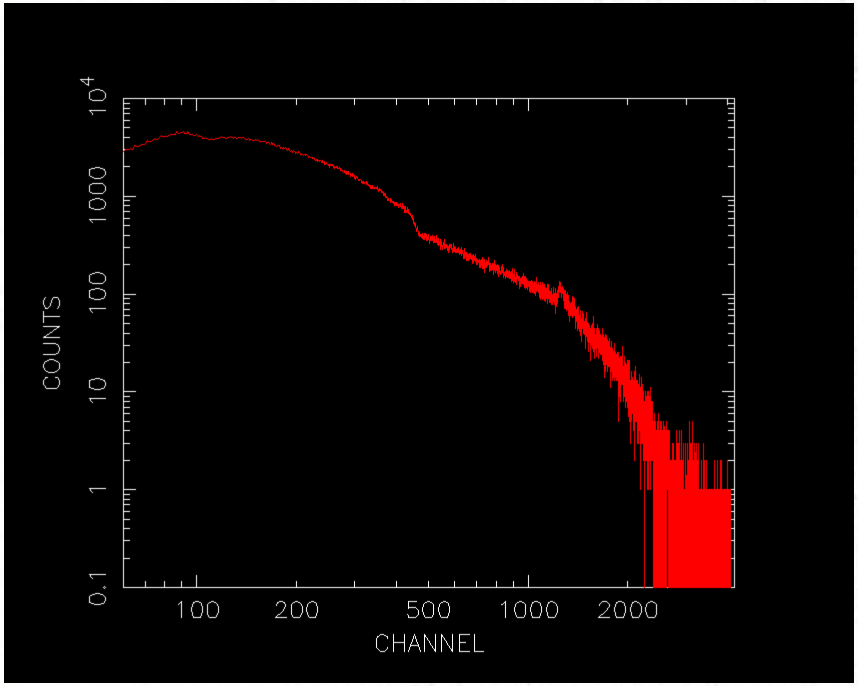
(Coma Cluster as seen by XMM-Newton: courtesy P.Rodriguez-Pascual)

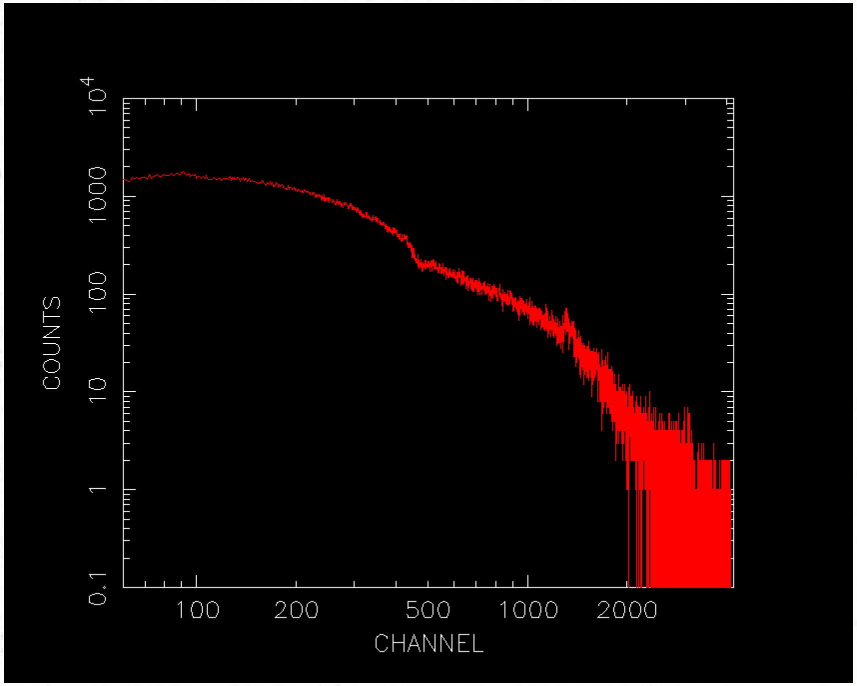
(IGM simulation: courtesy G.Becker)

(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:

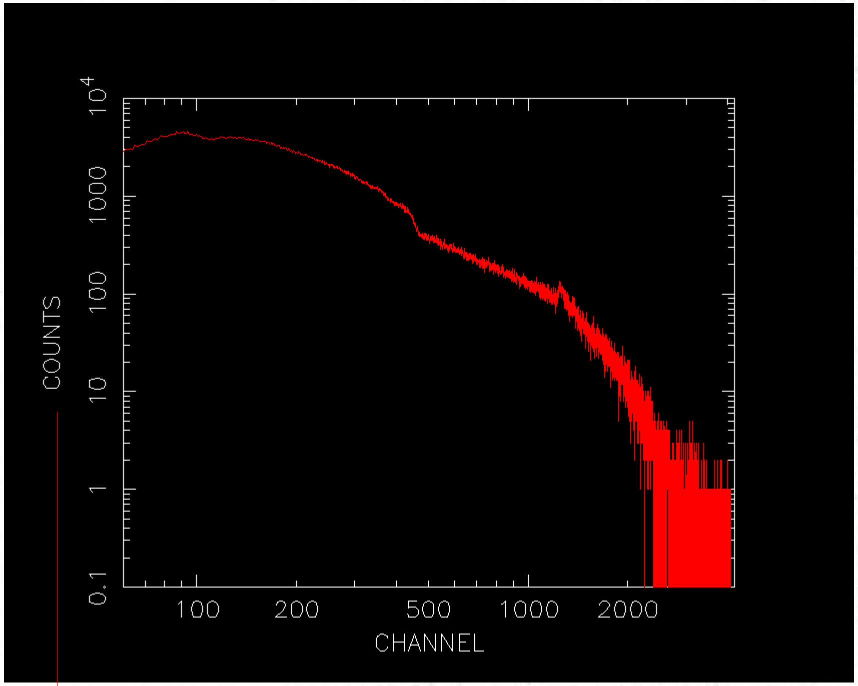




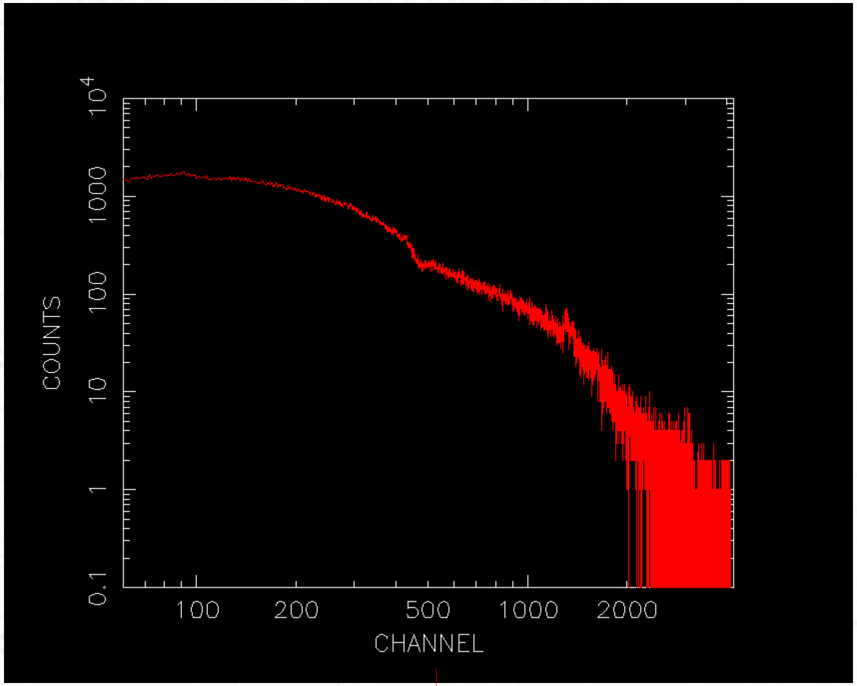
When all candles be out, all cats are grey

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!

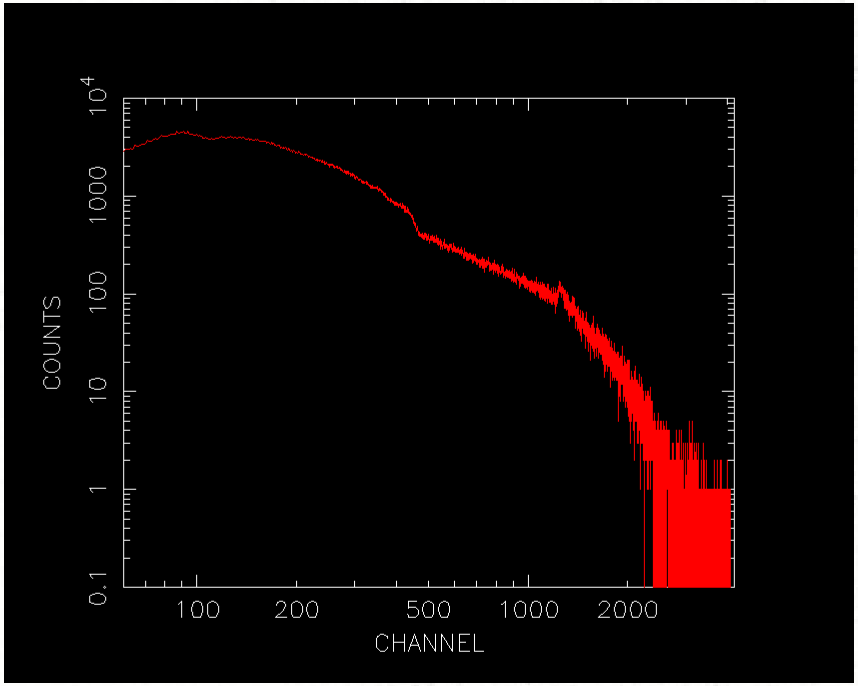
These are "CHANNELs", not energy!

First problem: spectral extractors produce spectra in instrumental quantities

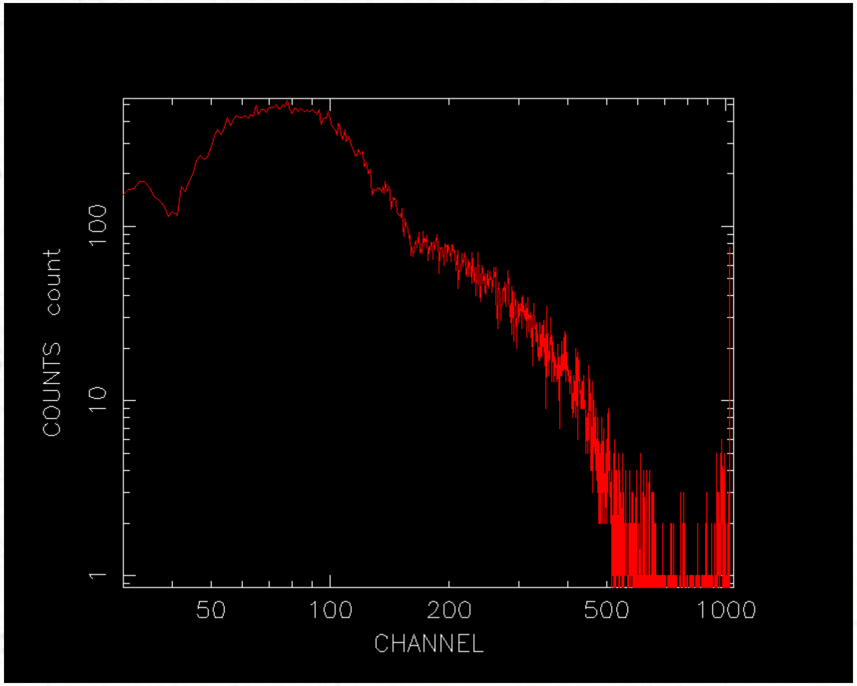
When all candles be out, all cats are grey

"*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

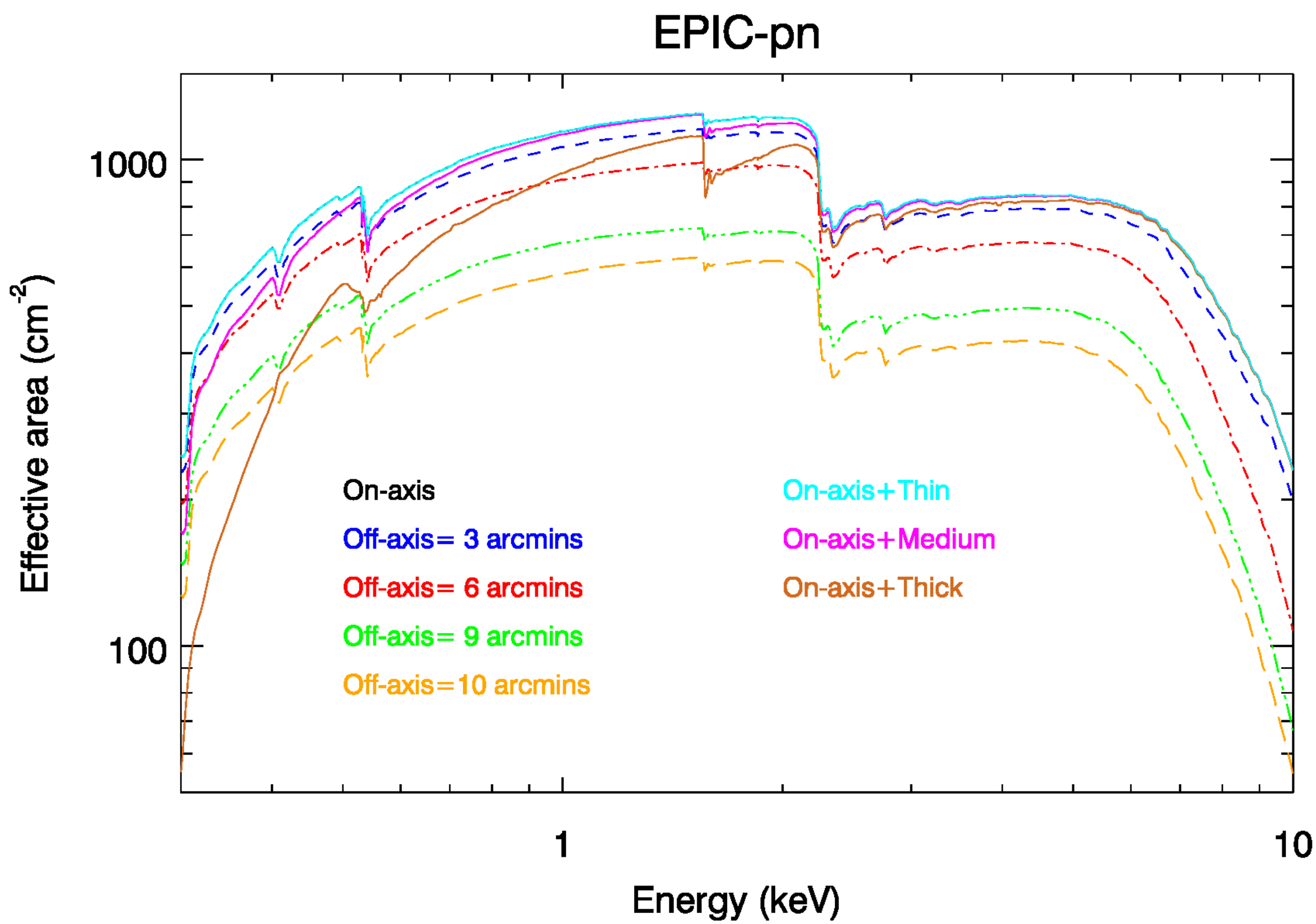
$$C(h) = (N\tau)\int dE\, R(h, E)A(E)s(E)$$

- $(N\tau)$ = 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)

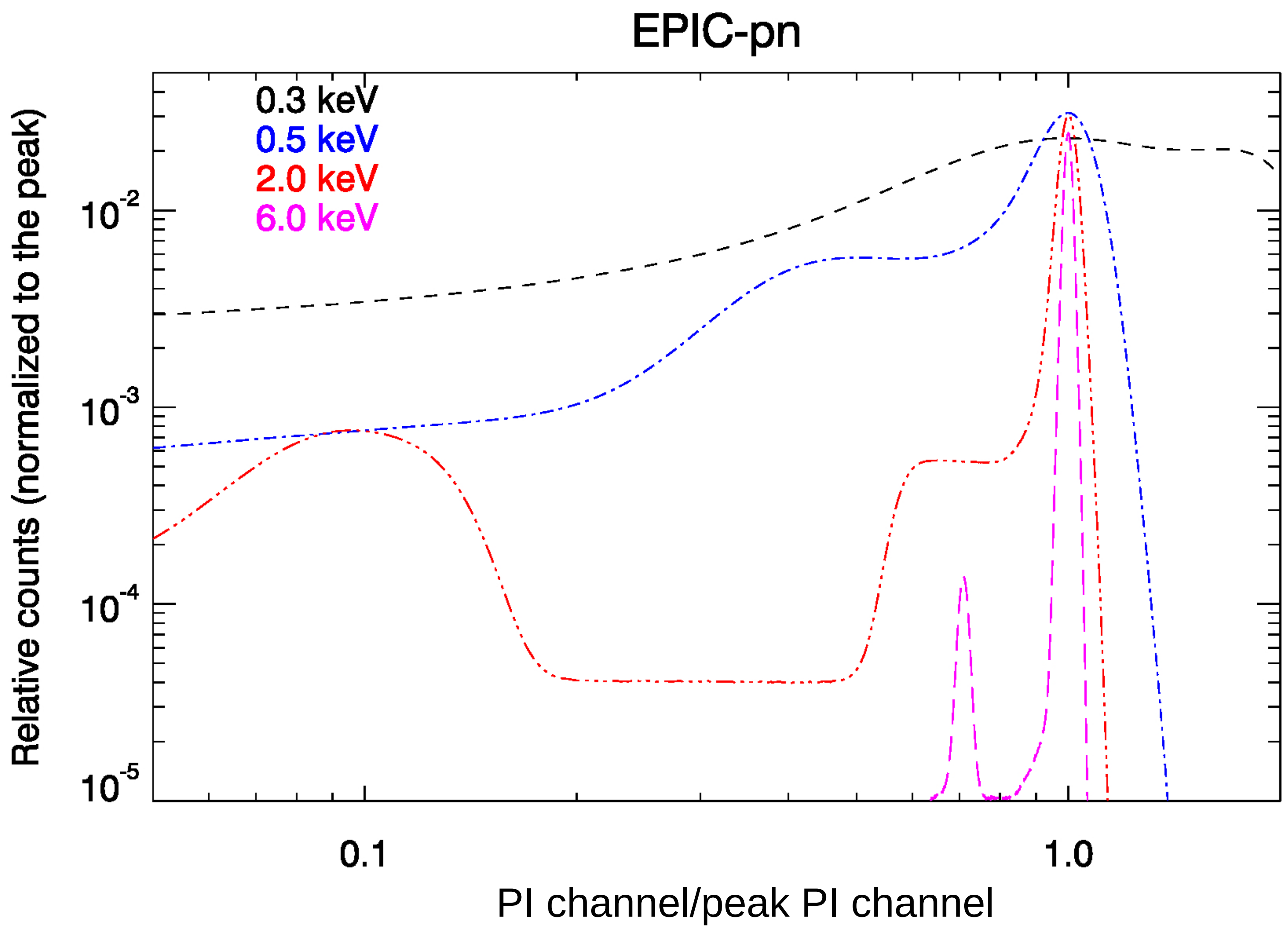
The effective area A(E)



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*”]

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:

$\boldsymbol{\sigma_{PHA} = [n^2+fE]^{0.5}}$ ($n^2 \rightarrow$ noise term)

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 spectra matrix is actually a discrete matrix equation:

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

The cross-talk among different energies prevents the R^i_{hE} matrix from being inverted.

<u>Alternative</u>: **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)

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

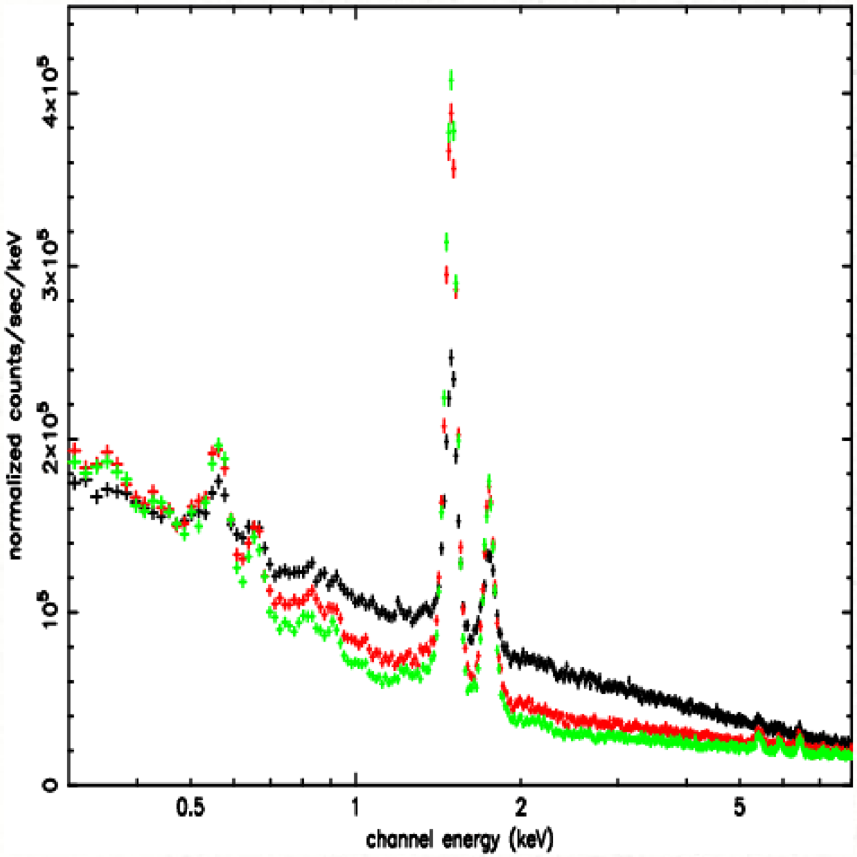
Three approaches are possible:

- <u>Ignore the background</u>. Wrong, even if in *Chandra* it is often very low
- <u>Subtract the background</u>. 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”
- <u>Model and fit simultaneously</u> the source and the background. Appealing, but:
  - The background spectra is often awfully complex, time- and detector-position dependent, sometimes not known at all

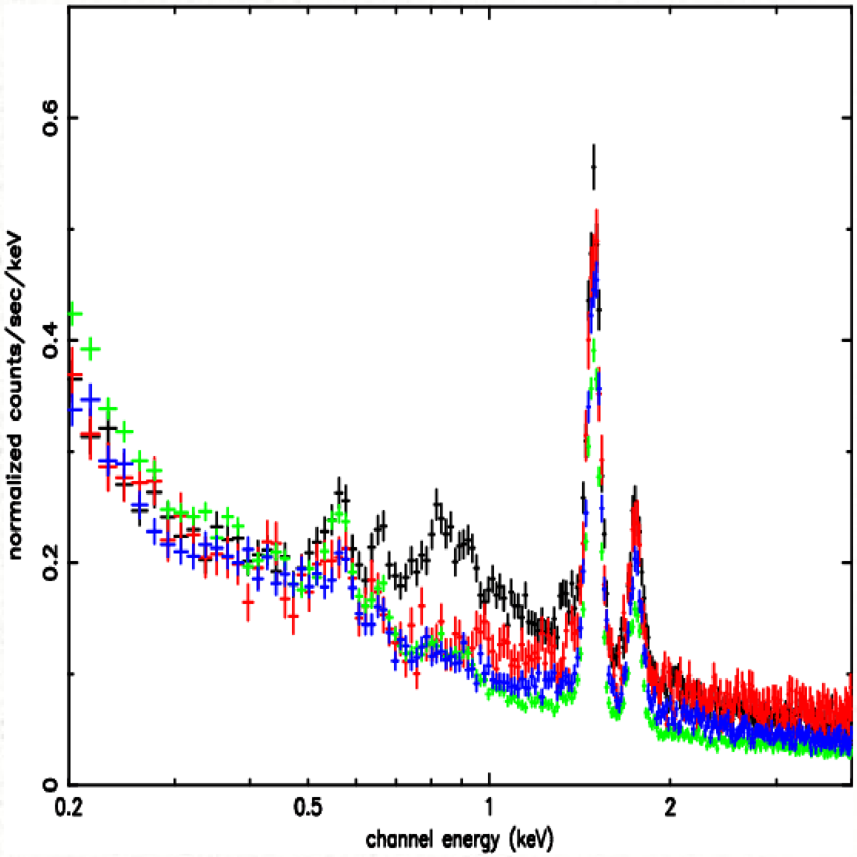
(Verbatim extracted from the *Sherpa* manual)

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)

Models

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

- Additive:
  - Phenomenological: po, bb, brems, gauss

    (power-law, blackbody, bremsstrahlung, Gaussian profile)
  - Astrophysical: comptt, diskbb, apec, diskline

    (Comptonization, Accretion disk blackbody, Thermal plasma, Relativistic line emission)
- 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)!

A detour on presentation skills

Never write a slide with more words than you can read in 30 seconds

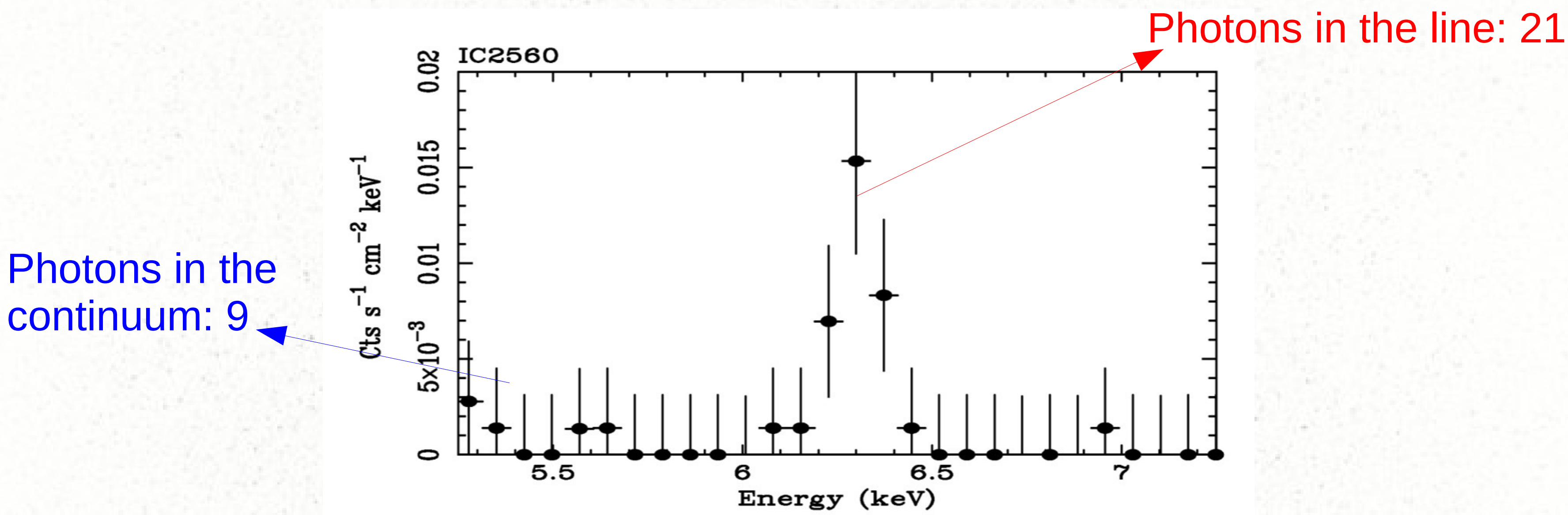
Goodness-of-fit tests

- The most common goodness-of-fit statistics test is the "chi-squared" (χ^2): $$\chi^2 = \sum \frac{(\text{observed} - \text{expected})^2}{\text{expected}}$$
  - It requires that the distribution of background-subtracted counts in each spectral channel is well approximated by a Gaussian (*5-10 counts*)
  - Different alternatives for the denominator: the XSPEC default is biased. Use `weight churazov`, or `weight model` instead
- Alternatively, one can use the Cash (C-)statistics $$C = 2\sum_{i=1}^{n} s_i - N_i + N_i \ln(N_i/s_i).$$
  - Applicable to data following the Poissonian statistics only (i.e.: non-background subtracted spectra).
  - XSPEC implements a flavour (the "W-statistics") which can be directly applied to background-subtracted spectra
  - [*issue with spectra with very low number of counts: K.Arnaud recommends to rebin the spectra to ensure that each channel has got at least one count – reason unknown*]
  - It does not yield a metrics of the absolute quality of a a fit (one need to use Monte-Carlo simulations in this case)
- XSPEC version 12.8 allows you to use different statistics to calculate the best-fit parameters, and the absolute quality of the fit. Recommendations: C-statistics for the former, χ^2 for the latter

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

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

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



- 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)

Shannon theorem

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

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

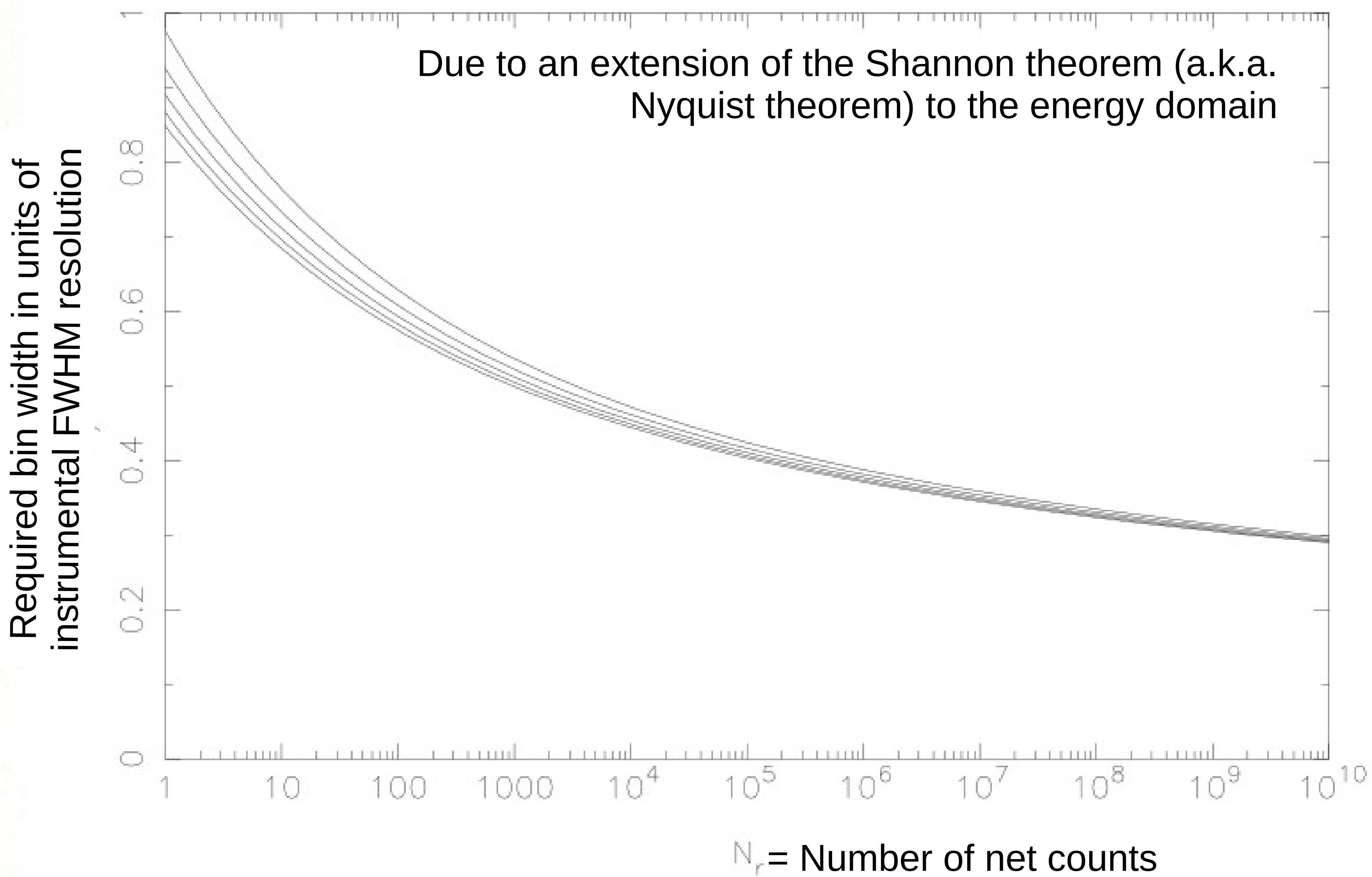
If $g(\omega) = 0$ for all $|\omega| > W$ for a given frequency W, then $f(t)$ is band-limited, and in that case Shannon has shown that

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

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)

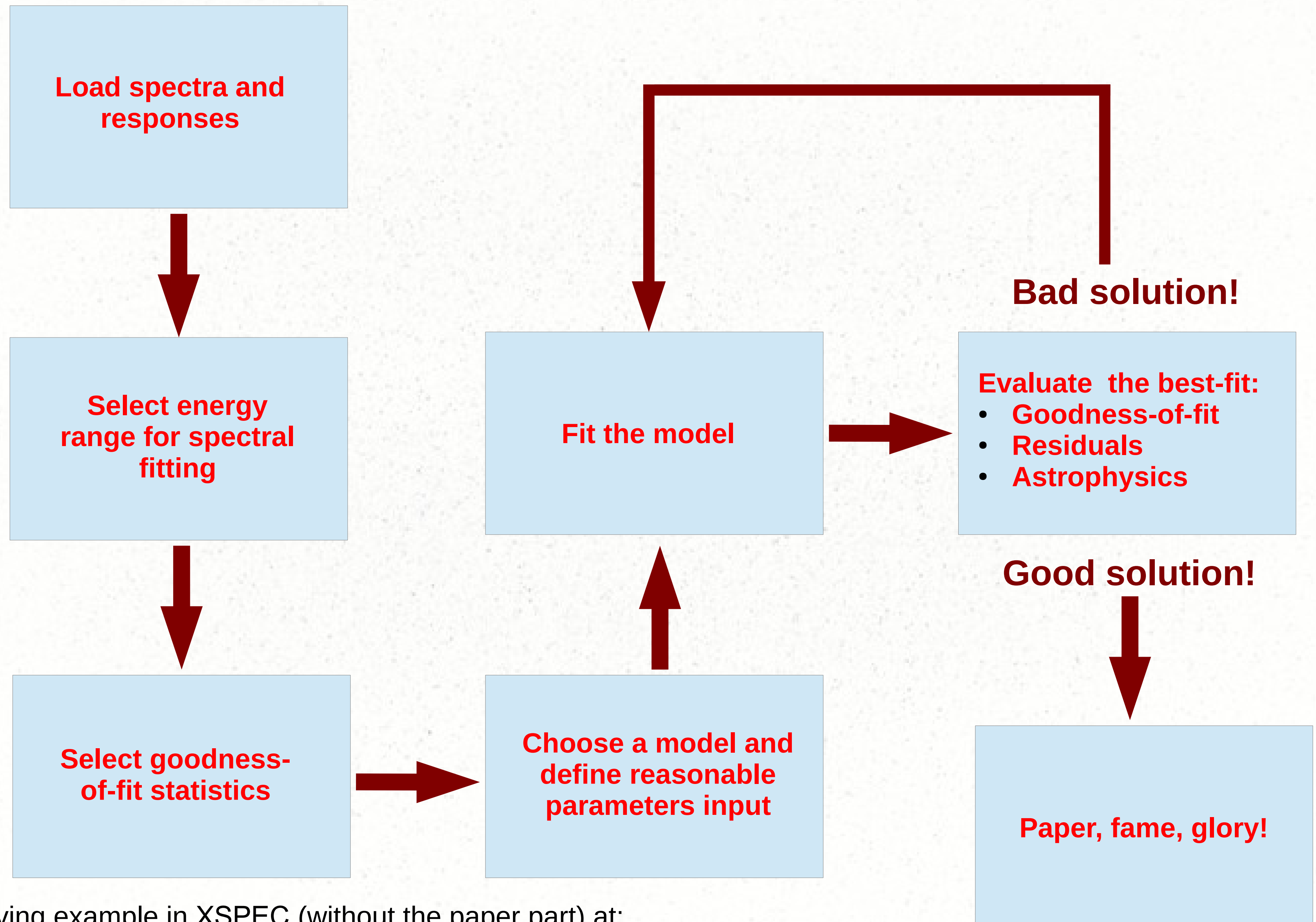
An ideal rebinning strategy



specgroup in SAS implements this, and many other spectral rebinning schemes

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

Forward-folding in action



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