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Combining Statistical and Systematic Uncertainties for High Count Spectra

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Abstract

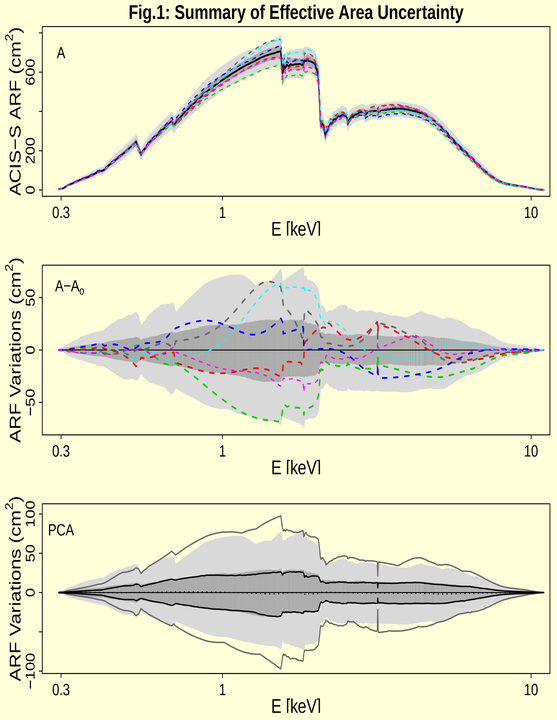
Instrument effective areas affect spectral fitting results, and the derived parameter values will depend on the particular effective area chosen for the analysis. This is an issue for high-counts, high-quality data more than low-counts spectra because systematic uncertainties may produce a larger variance in the parameters than statistical uncertainties, whereas statistical uncertainties dominate for low counts spectra.

With plausible effective areas that span the systematic variations, we show that their effect can be easily computed using existing tools like Sherpa. Here we describe that the variances due to statistical and systematic uncertainties can be combined with the well-known multiple imputation combining rule. We demonstrate its effectiveness with simulation examples using typical variations expected of ACIS-S effective areas. We show that approximately 20 full-fledged spectral fits, carried out with different effective areas, are needed to capture the full extent of calibration uncertainty in the parameter error estimate. We apply this technique to a set of observed AGN spectra and directly demonstrate the relevance of such calculations.

Effective Area Uncertainty

Best fit parameters and errors depend on the choice of a calibration file. A set of effective areas can be synthesized by calibration scientists and its information must be aggregated into spectral fitting analysis. Fig. 1 illustrates a set of 1000 effective area curves $\{\mathbf{A}\}$ showing the systematic uncertainty in the nominal ACIS-S effective areas (Drake et al. 2006; see also Drake et al. 2009 [C.11]). The top panel shows the set of effective areas, the middle panel shows the deviations from the nominal, and the bottom panel shows the same set reconstructed from a small subset of its Principal Components. Some illustrative curves are shown in the middle panel. The dark gray areas cover 68% of the variations.

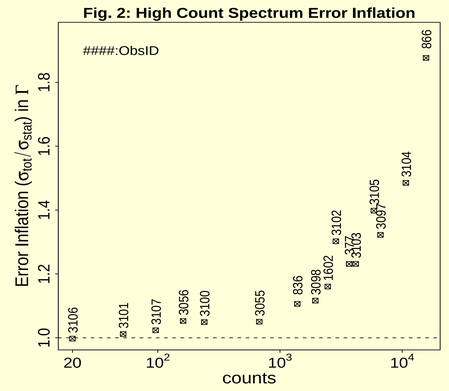
Fig.1: Summary of Effective Area Uncertainty



Importance of Calibration Uncertainties

Fig. 2 shows the importance of systematic uncertainty in high count spectra. With marked ObsIDs in 3-4 digits, 16 radio loud QSO spectra (Siemiginowska et al. 2008) are fit with an absorbed power-law spectrum using an MCMC algorithm (BLoCXS, van Dyk et al. 2001, Lee et al. 2009). Fits were carried out both **with** and **without** including the systematic uncertainties in the effective areas. As the number of counts in the spectra increase, the statistical error σ_{stat} decreases, but the systematic error is unaffected. Thus, the total error σ_{tot} is inflated relative to σ_{stat}.

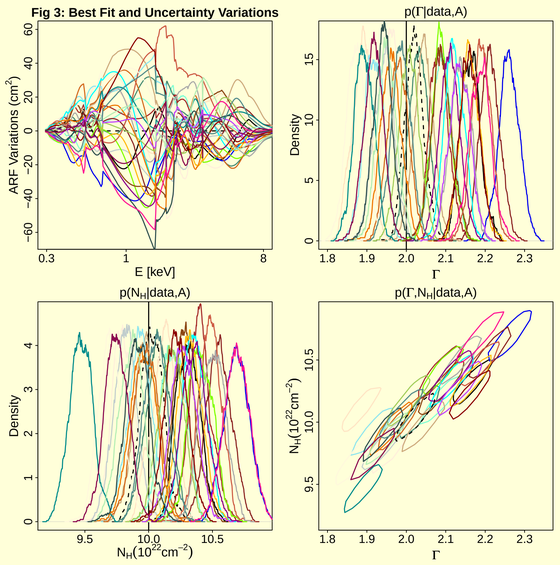
Fig. 2: High Count Spectrum Error Inflation



Calibration Uncertainty & Inference

Without considering calibration uncertainty, best fit parameters are subject to be biased and error bars are underestimated. Fig. 3 shows the behavior of posterior probability densities (ppd) conditioning on different effective area from fitting a $powerlaw*wabs$ fakeit spectrum ($\Gamma = 2, N_H = 10^{23} cm, \sim 10^5$ counts). The center and width of each ppd indicates best fit and statistical error. The ellipses are 90% contours. Colors identify 30 arbitrary selected effective areas and matching best fits and errors. These systematic variations due to calibration uncertainty are difficult to be quantified independent of model and data.

Fig 3: Best Fit and Uncertainty Variations



How to combine Errors

Given a set of effective areas, $\{\mathbf{A}_i : i = 1, ..., m\}$, Sherpa can compute a series of best fit parameters $\{\hat{\theta}_i\}$ and associated statistical error bars $\{\sigma_i\}$. The average of $\{\sigma_i\}$ is an estimate of the statistical error σ_{stat}. The spread in $\{\hat{\theta}_i\}$ represents the variations due to systematic error. These two can be added in quadrature to get the combined error on the best fit.

We use the multiple imputation combining rule (Schafer 1999) to achieve this. The average statistical error, also called the **within variance** W_m, is

$$W_m = \frac{1}{m}\sum_{i=1}^{m}\sigma_i^2,$$

and the variance in the best fits, also called the **between variance** B_m, is

$$B_m = \frac{1}{m-1}\sum_{i=1}^{m}(\hat{\theta}_i - \bar{\theta})^2.$$

The **total variance** T_m is

$$T_m = W_m + (1 + 1/m)B_m. \quad (1)$$

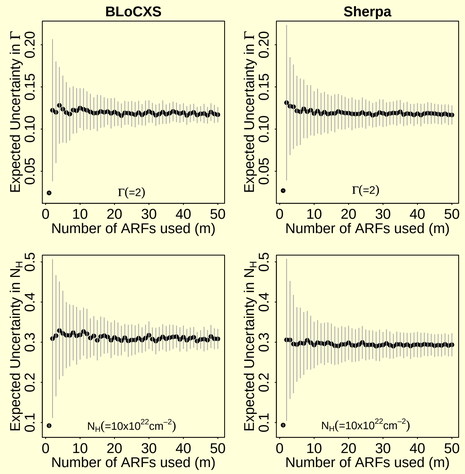
Then, the best parameter fit $\overline{\theta}$ is the average of $\{\hat{\theta}_i\}$ and the combined error σ_{tot} is $\sqrt{T_m}$. Note that $(1 + 1/m)B_m$ estimates the increase in variance due to the effective area uncertainty. This combining rule approximates the sampling distribution of θ by t distribution

$$T_m^{-1/2}(\theta - \overline{\theta}) \sim t_\nu$$

with the degree of freedom $\nu = (m-1)(1 + \frac{W}{(1+1/m)B})^2$. The confidence interval from this t distribution results in an error bar of statistical and systematic uncertainties combined.

How many calibration files?

Fig. 4 shows $m \approx 20$ to fit the same $powerlaw*wabs$ model of Fig. 3 with calibration uncertainty by choosing m random $\mathbf{A}$ to compute T_m for 100 times. The average and sample std. dev. of 100 T_m is marked by dots and vertical lines.



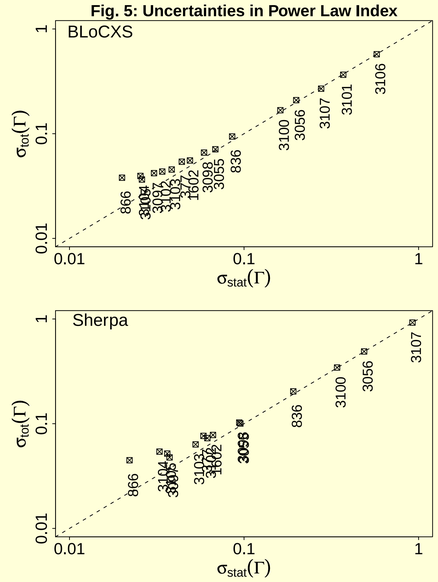
Limitations of the Combining Rule

1. Parameter uncertainties are assumed to be Gaussian distributed.
2. No well defined rules for choosing m.
3. Therefore, Monte Carlo simulation type experimental design studies are required for every model and data.

Example

The same QSO spectra in Fig. 2 are fit to compare uncertainties from BLoCXS and Sherpa/combining rule ($m = 50$). Simply applying the combining rule within existing tools like Sherpa can handle calibration uncertainties in spectral fitting analysis.

Fig. 5: Uncertainties in Power Law Index



Procedure

- spectrum, ARF, RMF, information of effective area uncertainty.
- set spectral model
- fit: get confidence intervals
- **for** $i = 1, ..., m$
  - sample and update effective area.
  - fit: get best fit parameter θ_i and statistical error σ_i.

  end
- apply the combining rule Eq.(1) on $\{\theta_i\}$ and $\{\sigma_i\}$ for $\overline{\theta}$ and σ_{tot}.

Summary

- Calibration uncertainties inflate errors in best fit parameters of high count spectra.
- Eq.(1) provides a simple rule of combining systematic and statistical uncertainties.
- This combining rule can be adapted to other types of calibration uncertainties simultaneously as long as the sample or the summary covers the full span of variations.
- Plausible samples of calibration uncertainties will be provided through ciao/Sherpa distribution to be incorporated into spectral analysis as described in Procedure.

References

Drake, J. et al. (2006) Proc. SPIE, 6270, p.49
Drake, J. et al. (2009) [C.10]
Lee, H. et al.(2009) in prep.
Schafer, J.L. (1999) SMMR, 8, p.3
Siemiginowska, A. et al.(2008) ApJ, 684, p.811
van Dyk, D. et al. (2001) ApJ, 548(1), p.224 (BLoCXS)

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