



pyblocxs

Bayesian Low-Counts X-ray Spectral Analysis in Sherpa

Aneta Siemiginowska

Harvard-Smithsonian Center for Astrophysics

Vinay Kashyap (CfA), David Van Dyk (UCI), Alanna Connors (Eureka), T.Park(Korea)+CHASC
Brian Refsdal (CfA) + CXC Data System



Outline

- Motivation and Statistical Introduction
- MCMC algorithm and Python Implementation
- Application - include calibration uncertainties
- Summary

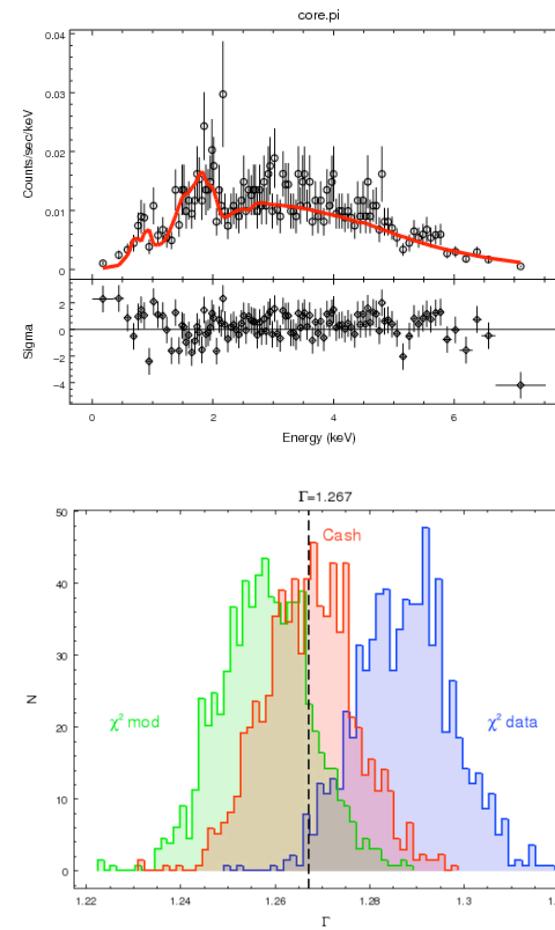
*“Analysis of Energy Spectra with Low Photon Counts
via Bayesian Posterior Simulations”* -

Van Dyk, Connors, Kashyap & Siemiginowska 2001, ApJ. 548, 224



Low Counts X-ray Data

- Standard X-ray analysis in XSPEC or Sherpa
- Parameterized Forward Fitting of the data
- Assuming statistics - typically χ^2
- Modified/weight χ^2 to account for low counts
- Bias when the distributions are not normal.
- Poisson data - need to use the Poisson likelihood (e.g. Cash)
- MCMC methods probe the entire parameter space and do not get stuck in local minima (i.e. it can get out).





Statistical Model For Low Counts Data

Bayesian Framework

$$p(\theta|d,I) = \frac{\text{likelihood}}{\text{prior}} p(d|\theta,I) p(\theta|I)$$

Posterior distribution

constant

θ - model parameters
d - observed data
I - initial information

Poisson Likelihood

$$p(d|\lambda_s, \lambda_b, I) = \frac{\exp^{-(\lambda_s + \lambda_b)} (\lambda_s + \lambda_b)^d}{d!}$$

data source background



Statistical Model For Low Counts Data

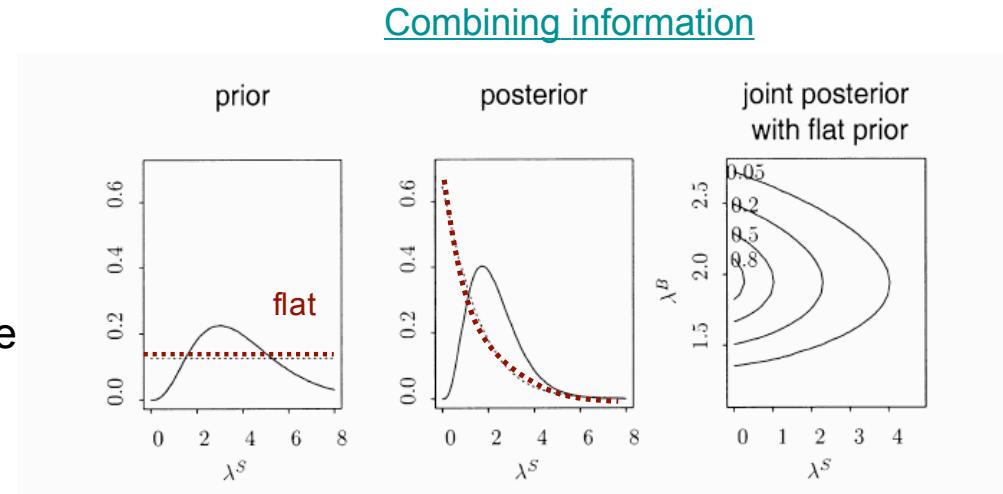
Model Predicted X-ray Spectra

$$\text{Predicted Intensity} = \text{Instrument Response} \left(\text{Source Model Intensity}_{\theta_s \text{ parameters}} \times \text{Effective Area} \right) + \text{Background}_{\theta_b \text{ parameters}}$$

Model
 $\lambda_s(\theta_s) + \lambda_b(\theta_b)$

Prior

- allows us to include a priori knowledge, e.g. range of parameters
- non-informative - e.g. flat within the range
- normal, log-normal, γ - gamma etc.





Simulations from Posterior

- Example:

- An absorbed power law model => $M_j(a, \Gamma, N_H) = a^* E_j^{-\Gamma} * f_j(N_H)$
- Poisson Likelihood:

$$\text{Log-likelihood} \quad \sum_j -M_j + d_j \log(M_j) \quad (\text{similar to Cash})$$
$$\prod_{j=1}^J \frac{e^{-M_j} M_j^{d_j}}{d_j!}$$

Gaussian distributions are typical prior distributions for (a, Γ, N_H) and
Log Posterior Distribution is then:

$$\sum_j [-M_j + d_j \log(M_j)] + [\log G(\log(a), \mu_a, \sigma_a) + \log G(\Gamma, \mu_\Gamma, \sigma_\Gamma) + \log G(N_H, \mu_N, \sigma_N)]$$



Simulations from Posterior

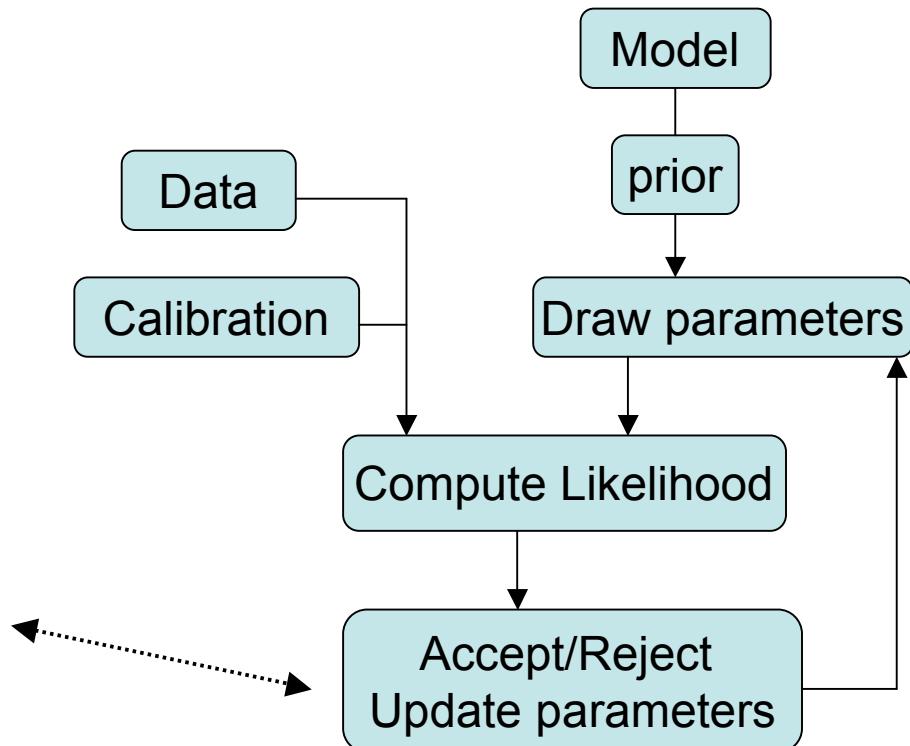
$$\sum_j [-M_j + d_j \log(M_j)] + [\log G(\log(a), \mu_a, \sigma_a) + \log G(\Gamma, \mu_\Gamma, \sigma_\Gamma) + \log G(N_H, \mu_N, \sigma_N)]$$

↑
prior

Likelihood

Simulation from the posterior distribution requires careful and efficient algorithms:

Draw parameters from a "proposal distribution", calculate likelihood and posterior probability of the "proposed" parameter value given the observed data, use a Metropolis-Hastings criterion to accept or reject the "proposed" values.





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Python Implementation in Sherpa

- **Sherpa** is a general fitting and modeling application written in Python. It provides a library of models, statistics and optimization methods.
<http://cxc.harvard.edu/contrib/sherpa/> - Python package
<http://cxc.harvard.edu/sherpa/index.html> - in CIAO
- It can accommodate Python code that extends the initial functionality.
- We use **Sherpa** to fit the data at the initial step and estimate the scale for setting priors and use the **Sherpa** statistics (Cash) to calculate the likelihood.



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Python Implementation in Sherpa

- <http://hea-www.harvard.edu/AstroStat/pyBLoCXS/index.html> - documentation and downloads
- **pyblocxs** - samples from a multivariate t-distribution with a multivariate scale determined by Sherpa covar() function, at the best fit values.
- It has two samplers:
 - Metropolis-Hastings:
 - » centered on the best fit values
 - Metropolis-Hastings mixed with Metropolis jumping rule:
 - » centered on the current draw of parameters
 - » the scale can be specified as a scalar multiple of covar()
- **pyblocxs:**
 - ✓ Explores parameter space and summarized the full posterior or profile posterior distributions.
 - ✓ Computed parameter uncertainties can include calibration errors.
 - ✓ Simulates replicate data from the posterior predictive distributions.
 - ✓ Tests for added spectral components by computing the Likelihood Ratio Statistic on replicate data and the ppp-value.



Running it!

Usage

The primary way to run pyBLoCXS within *Sherpa* is to call the function `pyblocxs.get_draws()`

First read in the spectrum:

```
load_phd("pha.fits")
```

and define the model:

```
set_model(xsphabs.abs1*powlaw1d.p1)
```

and carry out a regular fit to define the covariance matrix:

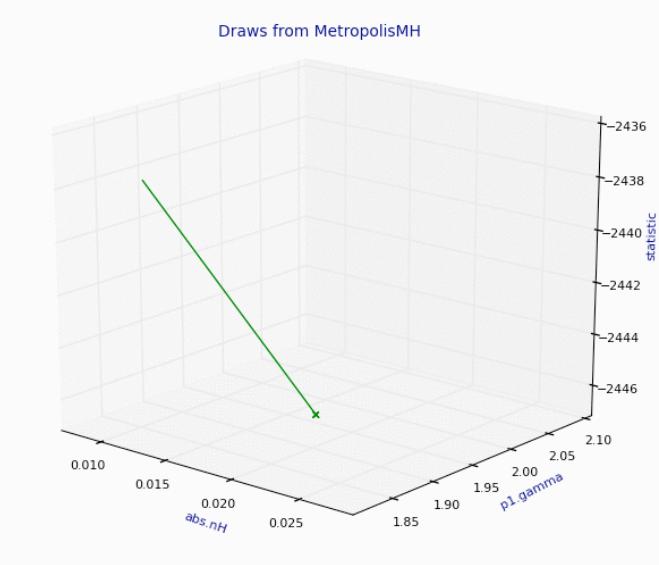
```
set_stat("cash")
fit()
covar()
```

then invoke pyBLoCXS with MetropolisMH as follows:

```
import pyblocxs
pyblocxs.set_sampler("MetropolisMH")
stats, accept, params = pyblocxs.get_draws(niter=1e4)
```

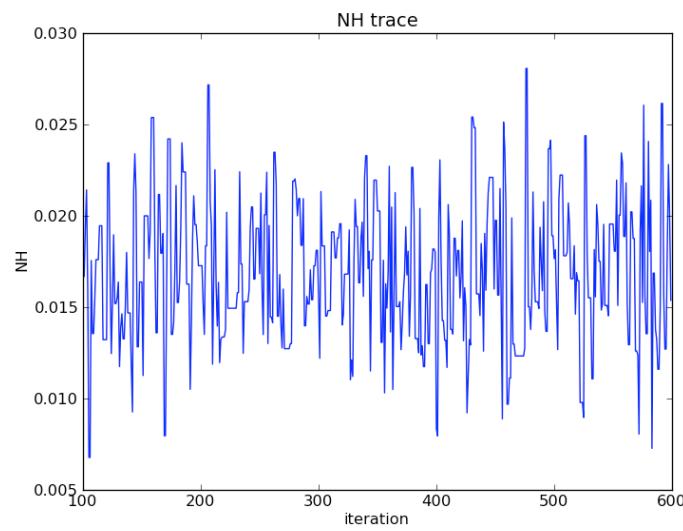
to change to MH:

```
pyblocxs.set_sampler("MH")
stats, accept, params = pyblocxs.get_draws(niter=1e4)
```

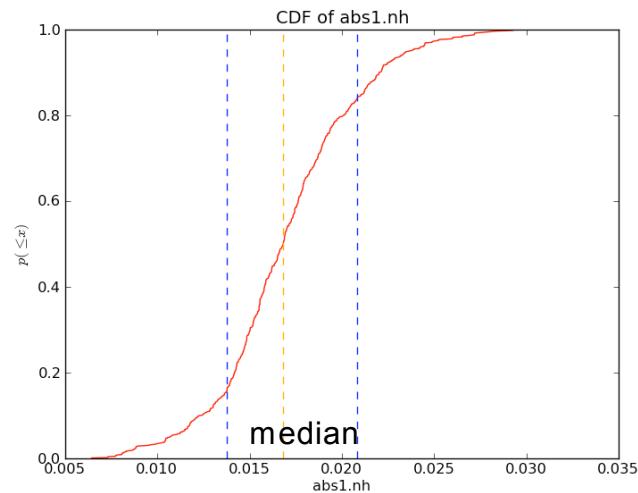




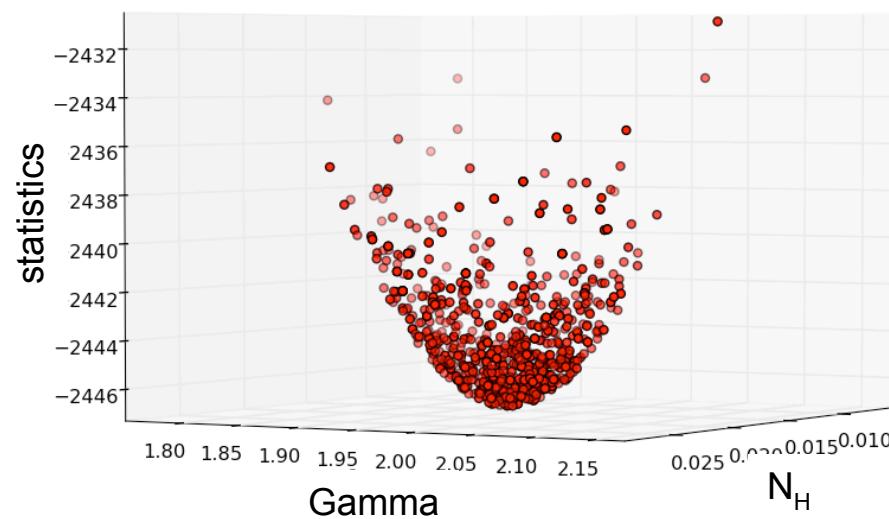
Trace of a parameter during MCMC run



Cummulative distribution of a parameter



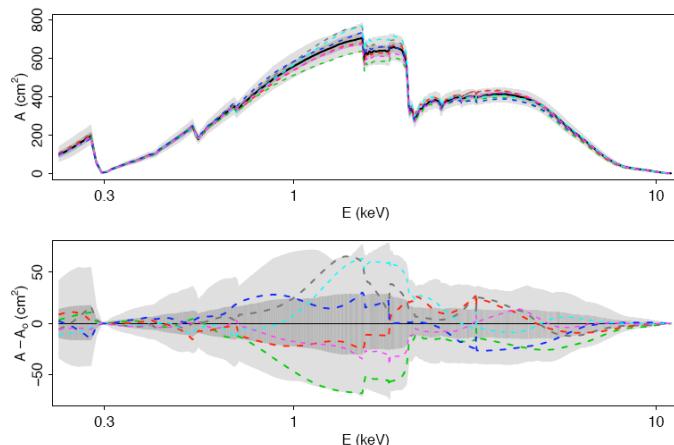
3D Parameter space probed with MCMC





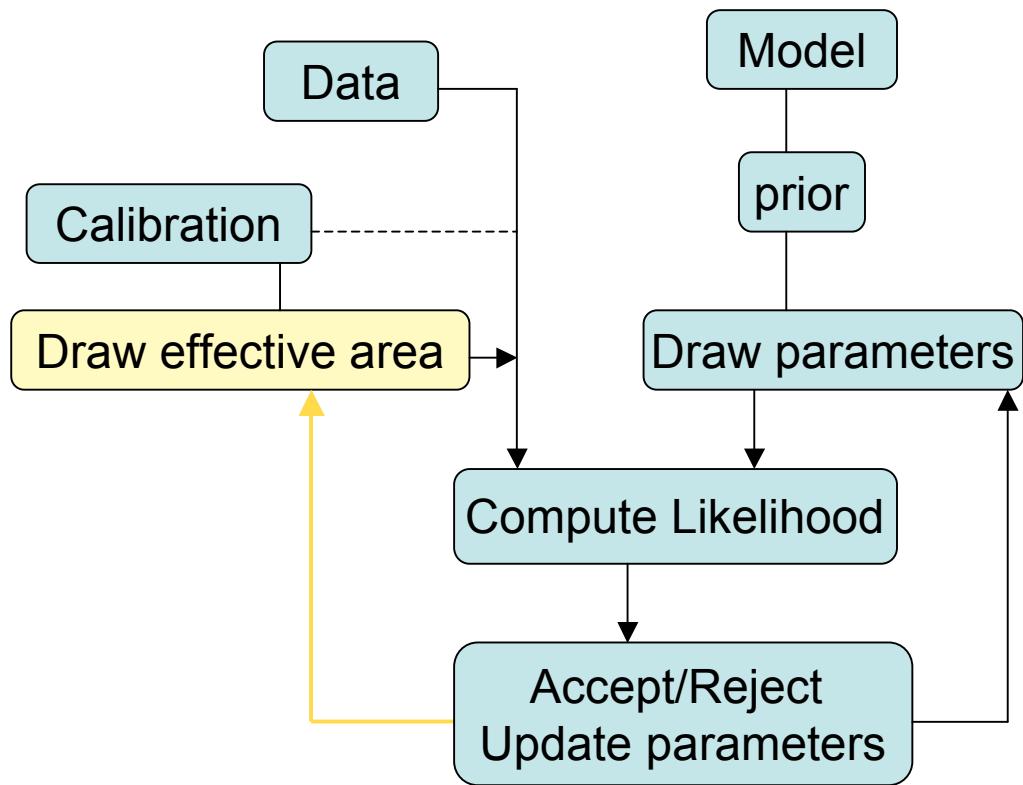
Application: Calibration Uncertainties

Chandra ACIS-S Effective Area



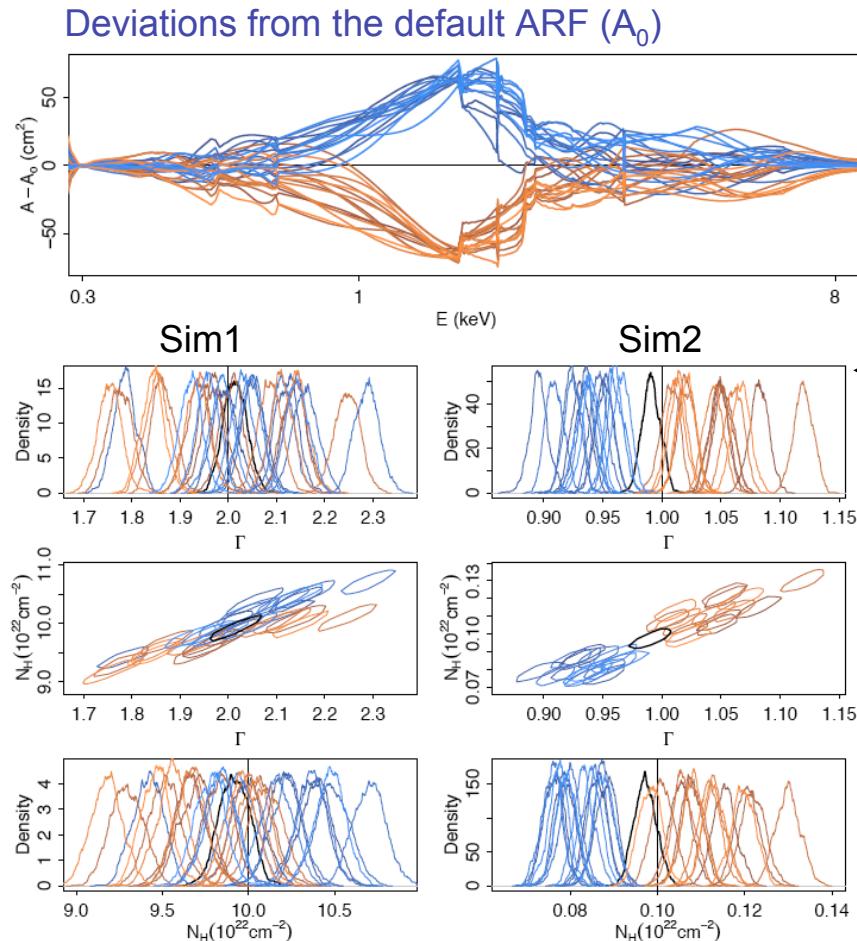
Drake et al. 2006 Proc. SPIE, 6270, 49

- Non-linear errors cannot simply add to stats errors.
- Include a draw from an ensemble of effective area curves in the simulations.





Application: Calibration Uncertainties



Simulations of 10^5 counts
Sim1: $\Gamma=2$ $N_H=1\text{e}23$
Sim2: $\Gamma=1$ $N_H=1\text{e}21$



Summary

- **pyblocxs** can be used for the Poisson X-ray data.
- Provides the MCMC simulations to explore parameter space of models applied to observed data.
- Caveats:
 - Needs Sherpa
 - Tested on simple models only!
 - Parameter space can be complex for composite models with different modes.
- Available as a Sherpa Python extension at

<http://hea-www.harvard.edu/AstroStat/pyBLoCXS/index.html>

Focus Demo at 3.30pm by Brian Refsdal on
Advanced Python scripting using Sherpa

Check **CIAO booth**, talk to developers and get personal demos of the software!