



# pyblocxs

## Bayesian Low-Counts X-ray Spectral Analysis in Sherpa

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Brian Refsdal (CfA) + CXC Data System

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# Outline

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

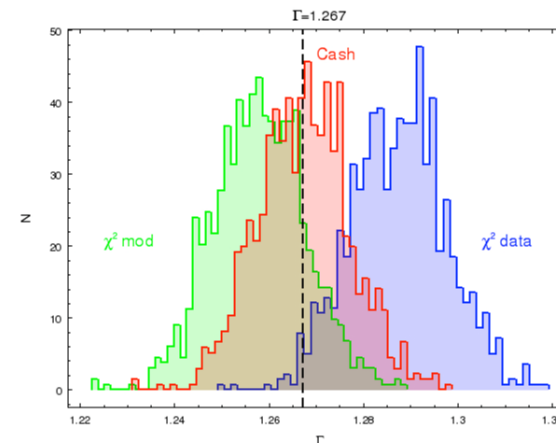
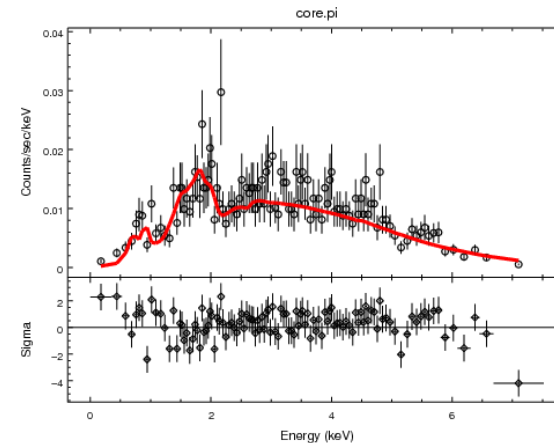
*“Analysis of Energy Spectra with Low Photon Counts  
via Bayesian Posterior Simulations” -*

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  $\chi^2$
- Modified/weight  $\chi^2$  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

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

$\theta$  - 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 →  $d$   
 source →  $\lambda_s$   
 background →  $\lambda_b$



# Statistical Model For Low Counts Data

## Model Predicted X-ray Spectra

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

$\theta_s$  parameters       $\theta_b$  parameters

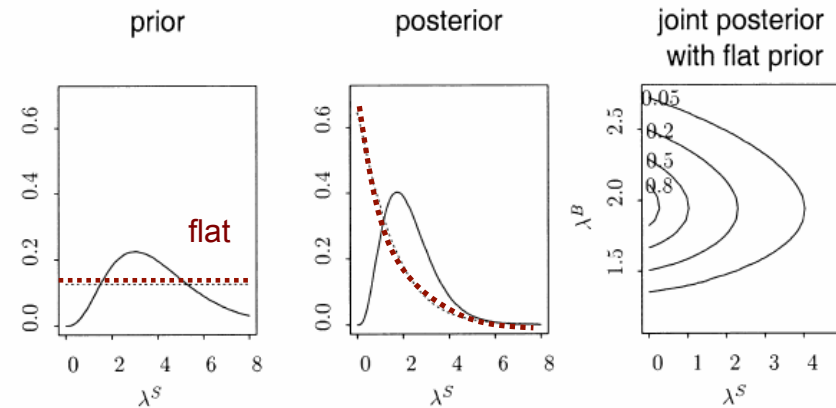
Model

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

### Prior

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

### Combining information





# 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:

$$\prod_{j=1}^J \frac{e^{-M_j} M_j^{d_j}}{d_j!}$$

Log-likelihood  $\sum_j -M_j + d_j \log(M_j)$  (similar to Cash)

Gaussian distributions are typical prior distributions for  $(a, \Gamma, N_H)$  and **Log Posterior Distribution** is then:

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



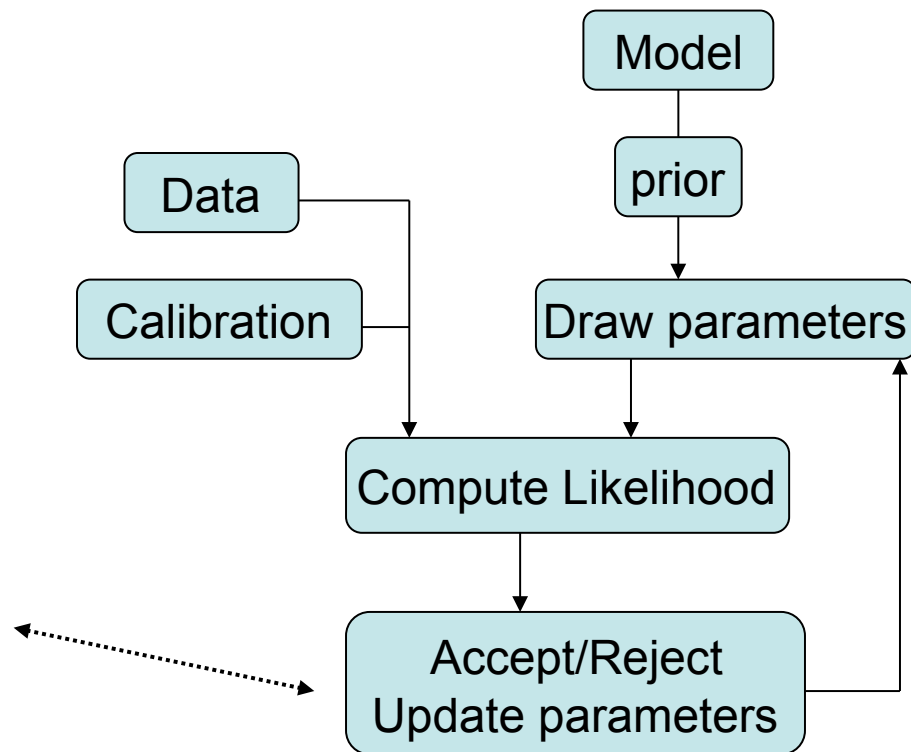
# Simulations from Posterior

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

← Likelihood
← prior

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.





# pyblocxs

## 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.





# pyblocxs

## 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_pha("pha.fits")
```

and define the model:

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

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

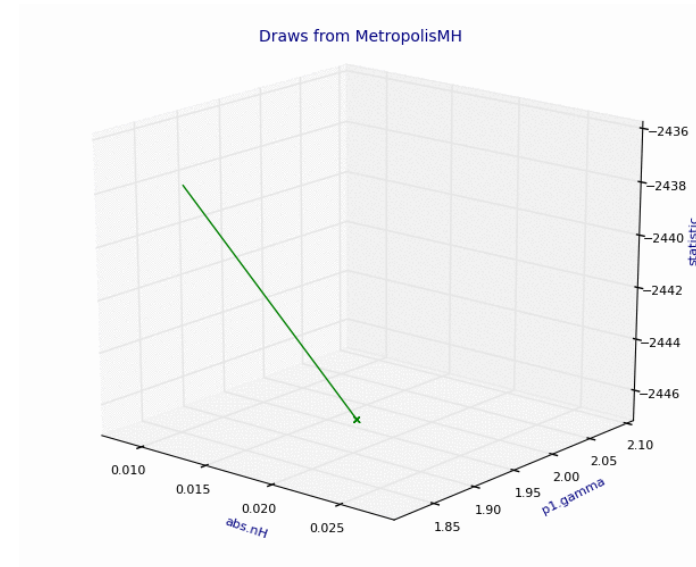
```
set_stat("cash")  
fit()  
covar()
```

then invoke pyBLoCXS with MetropolisMH as follows:

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

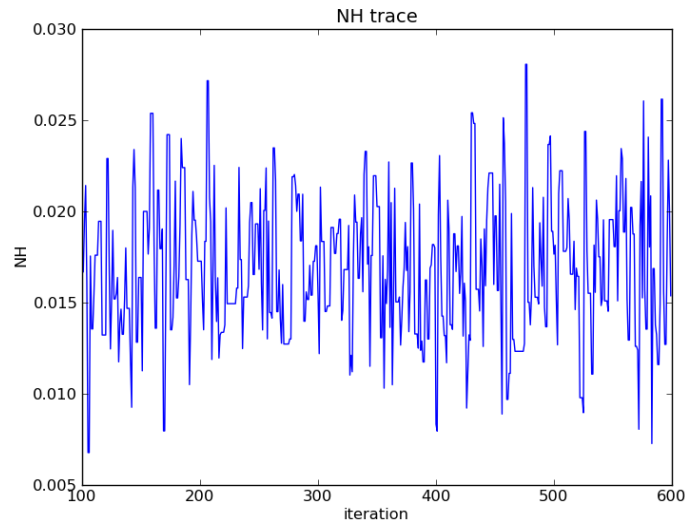
to change to MH:

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

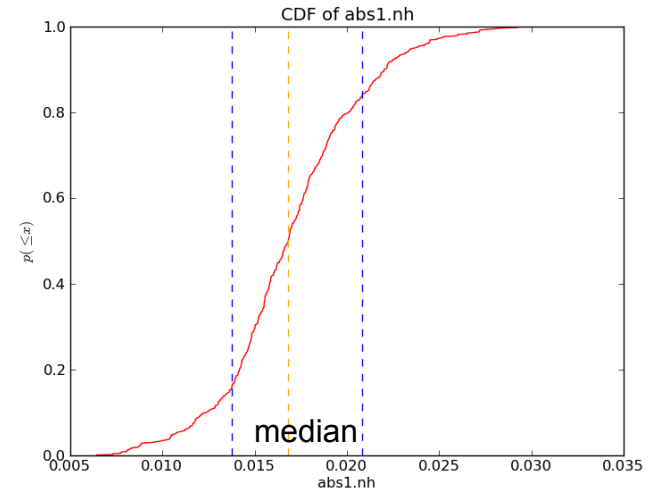




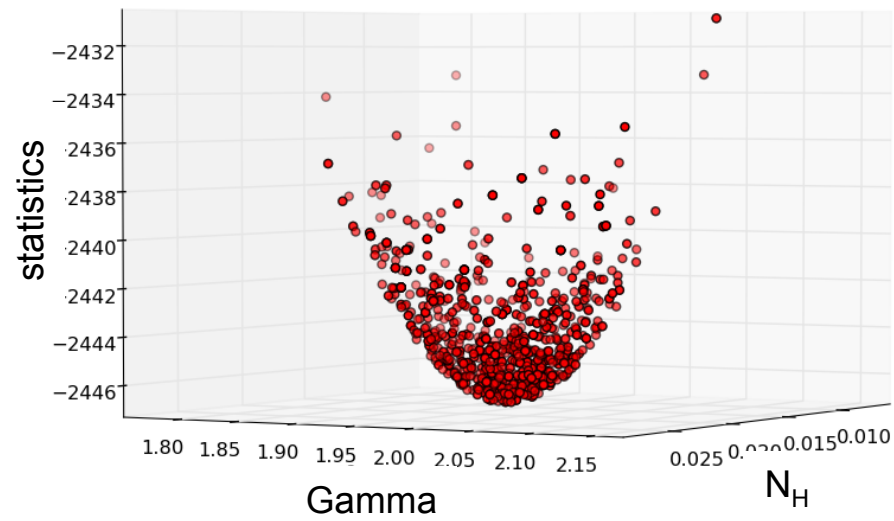
Trace of a parameter during MCMC run



Cumulative distribution of a parameter



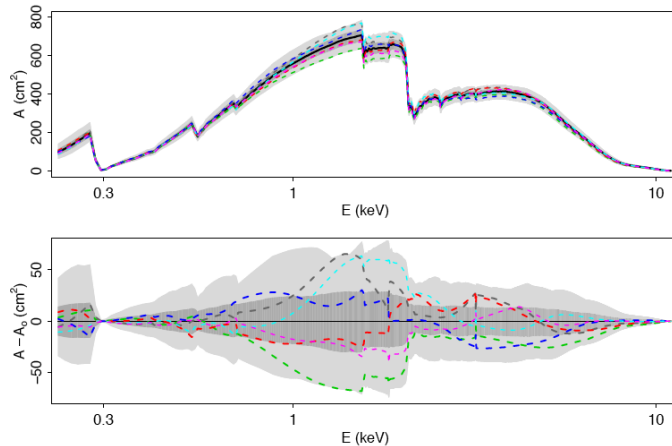
3D Parameter space probed with MCMC





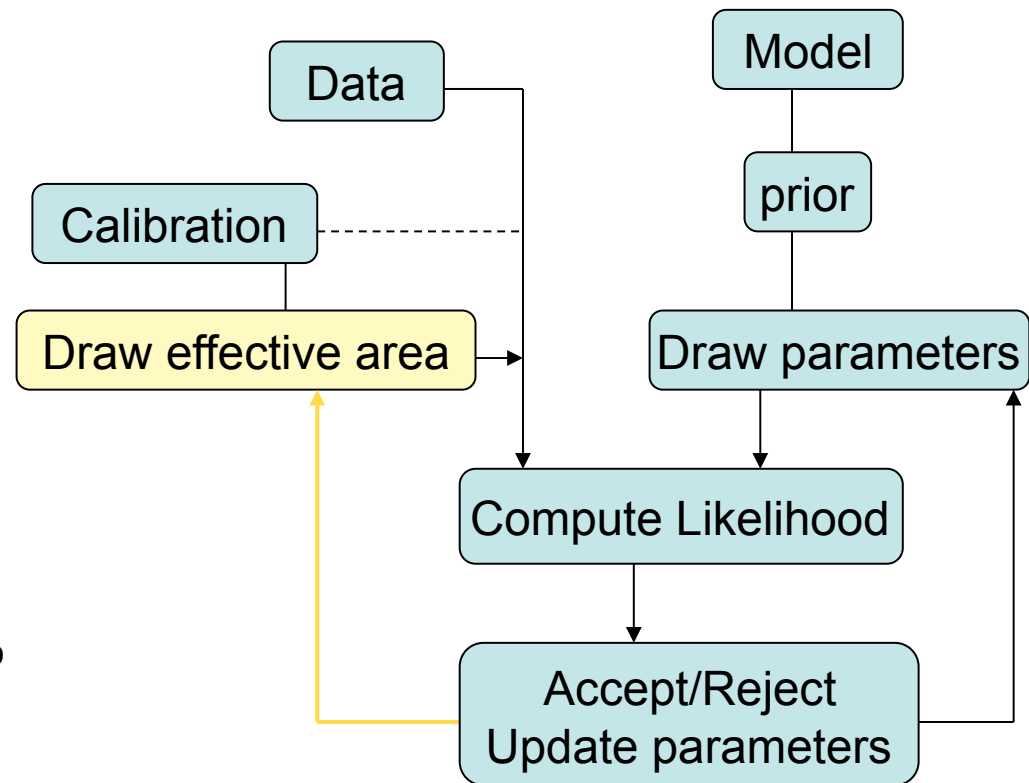
# Application: Calibration Uncertainties

Chandra ACIS-S Effective Area



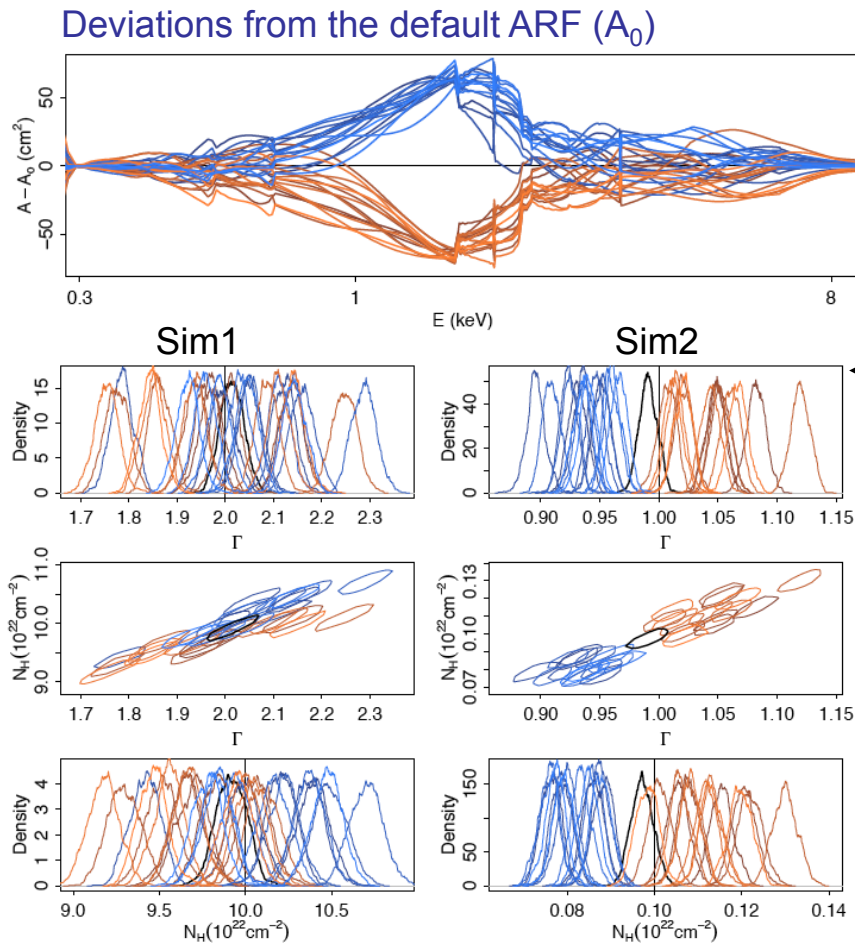
Drake et al. 2006 Proc. SPIE, 6270,49

- 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



Lee et al 2010, ApJ, submitted



# 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!