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

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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” - 
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

\[ p(\theta | d, I) = \frac{p(d | \theta, I)p(\theta | I)}{p(d | I)} \]

- Posterior distribution
- likelihood
- prior

Poisson Likelihood

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

- data
- source
- background

\( \lambda \) - model parameters
\( d \) - observed data
\( I \) - initial information
Statistical Model For Low Counts Data

Model Predicted X-ray Spectra

Predicted Intensity = Instrument Response \left( \begin{array}{c}
\text{Source Model Intensity} \\
\text{Effective Area}
\end{array} \right) + \text{Background}

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.
Simulations from Posterior

- Example:
  - An absorbed power law model \( M_j(a, \Gamma, N_H) = a^*E_j^{-\Gamma} \cdot f_j(N_H) \)
  - Poisson Likelihood:
    \[
    \prod_{j=1}^{J} \frac{e^{-M_j} M_j^{d_j}}{d_j!} \]
    
    Log-likelihood
    \[
    \sum_j -M_j + d_j \log(M_j) \quad \text{(similar to Cash)}
    \]

Gaussian distributions are typical prior distributions for \((a, \Gamma, N_H)\) and

**Log Posterior Distribution** is then:

\[
\sum_j [-M_j + d_j \log(M_j)] + \left[ \log G(\log(a), \mu_a, \sigma_a) + \log G(\Gamma, \mu_\Gamma, \sigma_\Gamma) \right. \\
\left. + \log G(N_H, \mu_N, \sigma_N) \right]
\]
Simulations from Posterior

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

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](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:

```python
load_pha("pha.fits")
```

and define the model:

```python
set_model(xsphsbe.abs1*powlaw1d.pl)
```

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

```python
set_stat("cash")
fit()
ocovar()
```

then invoke pyBLoCXS with MetropolisMH as follows:

```python
import pyblocxs
pyblocxs.set_sampler("MetropolisMH")
stats, accept, params = pyblocxs.get_draws(niter=100)
```

to change to MH:

```python
pyblocxs.set_sampler("MH")
stats, accept, params = pyblocxs.get_draws(niter=100)
```
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

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

Drake et al. 2006 Proc. SPIE, 6270,49
Application: Calibration Uncertainties

Effects of ARF uncertainty on parameters

Simulations of $10^5$ counts
Sim1: $\Gamma=2$ $N_H=1e23$
Sim2: $\Gamma=1$ $N_H=1e21$

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](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!