Accounting for Calibration Uncertainty in Spectral Analysis

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Outline

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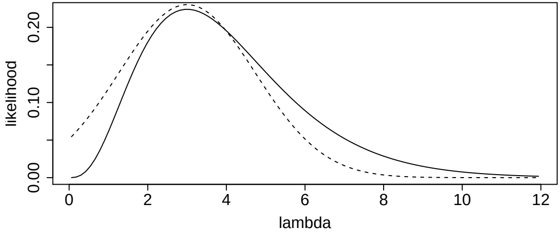
Bayesian Statistical Analyses: Likelihood

Likelihood Functions: The distribution of the data given the model parameters. E.g., $Y \stackrel{\text{dist}}{\sim} \text{Poisson}(\lambda_S)$:

$$\text{likelihood}(\lambda_S) = e^{-\lambda_S} \lambda_S^Y / Y!$$

Maximum Likelihood Estimation: Suppose $Y = 3$



The likelihood and its normal approximation.

Can estimate λ_S and its error bars.

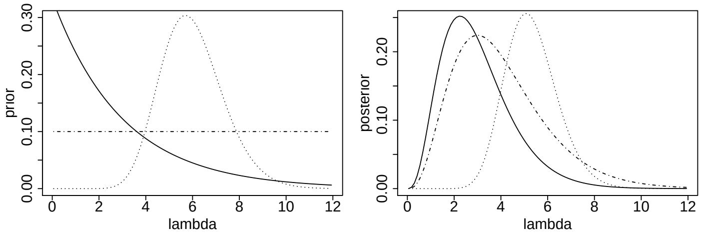
Bayesian Analyses: Prior and Posterior Dist'ns

Prior Distribution: Knowledge obtained *prior* to current data.

Bayes Theorem and Posterior Distribution:

$$\text{posterior}(\lambda) \propto \text{likelihood}(\lambda) \times \text{prior}(\lambda)$$

Combine past and current information:



Bayesian analyses rely on probability theory

Multi-Level Models

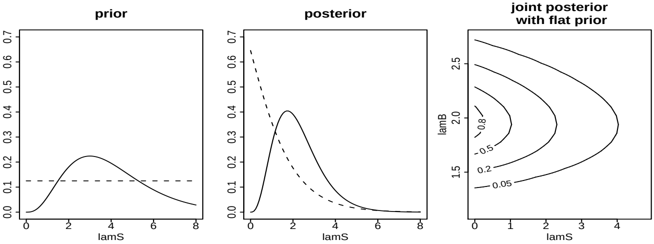
A Poisson Multi-Level Model:

LEVEL 1: $Y | Y_B, \lambda_S \overset{\text{dist}}{\sim} \text{Poisson}(\lambda_S) + Y_B,$

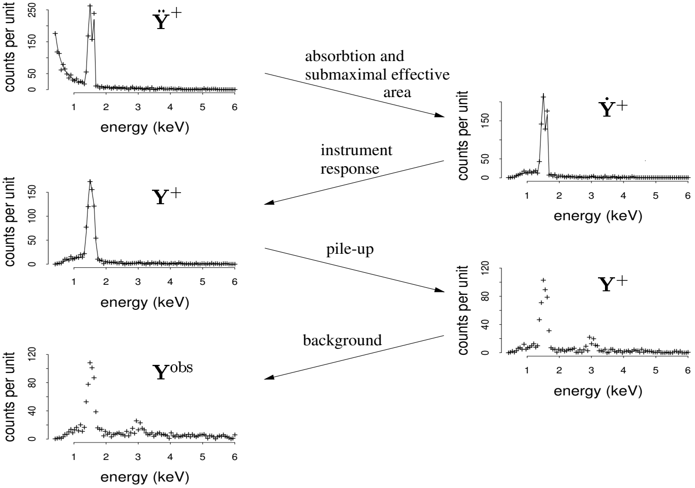
LEVEL 2: $Y_B | \lambda_B \overset{\text{dist}}{\sim} \text{Pois}(\lambda_B)$ and $X | \lambda_B \overset{\text{dist}}{\sim} \text{Pois}(\lambda_B \cdot 24),$

LEVEL 3: specify a prior distribution for λ_B, λ_S.

Each level of the model specifies a dist'n given unobserved quantities whose dist'ns are given in lower levels.



Multi-Level Models: X-ray Spectral Analysis



PyBLoCXS: Bayesian Low-Count X-ray Spectral Analysis

Embedding Calibration Uncertainty into a Statistical Model

We aim to include calibration uncertainty as a component of the multi-level statistical model fit in PyBLoCXS.

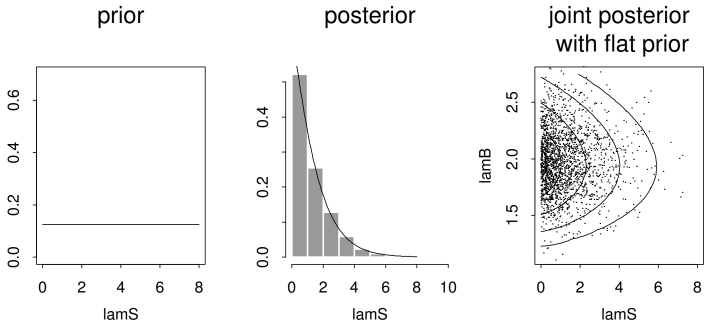
Build a multi-level model

- In addition to spectral parameters, calibration products are treated as unknown quantities.
- Calibration products are high dimensional unknowns.
- Calibration scientists provide valuable prior information about these quantities.
- We must quantify this information into a *prior distribution*.

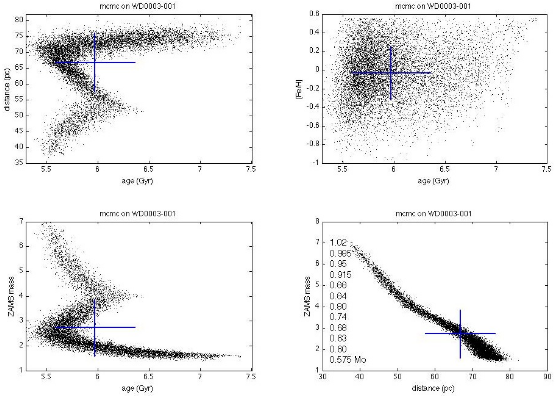
Computation becomes a real issue!

Markov Chain Monte Carlo

Exploring the posterior distribution via Monte Carlo.

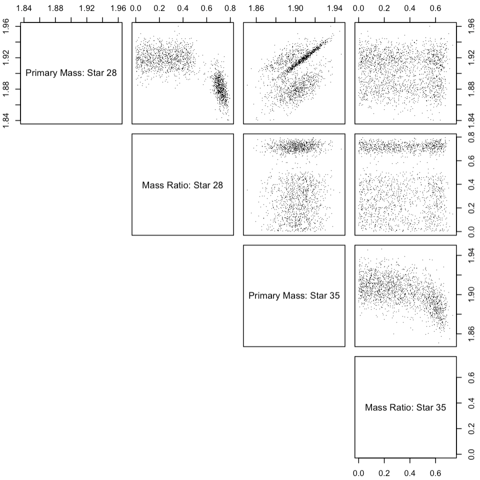


Model Fitting: Complex Posterior Distributions



Highly non-linear relationship among parameters.

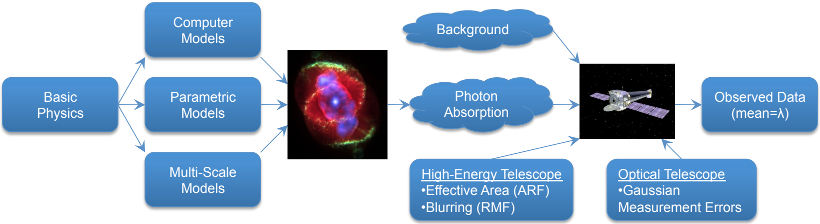
Model Fitting: Complex Posterior Distributions



The classification of certain stars as field or cluster stars can cause multiple modes in the distributions of other parameters.

Outline

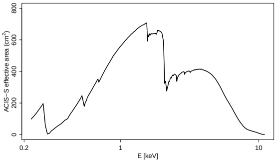
The Basic Statistical Model



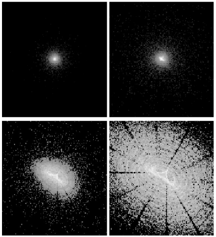
- Embed physical models into multi-level statistical models.
- Must account for complexities of data generation.
- State of the art computational techniques enable us to fit the resulting highly-structured model.

Calibration Products

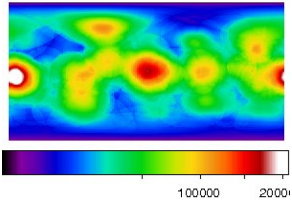
- Analysis is highly dependent on *Calibration Products:*
  - Effective Area Cuves
  - Energy Redistribution Matrices
  - Exposure Maps
  - Point Spread Functions
- In this talk we focus on uncertainty in the effective area.



A *Chandra* effective area.



Sample Chandra psf's
(Karovska et al., ADASS X)

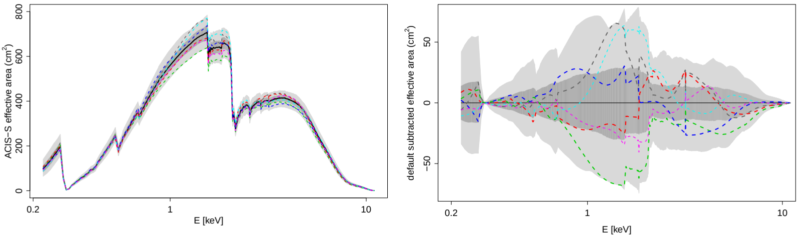


EGRET exposure map
(area $\times$ time)

Calibration Sample

Calibration sample of 1000 representative curves[1]

- Sample exhibits complex variability.
- Requires storing many high dimensional calibration products.



[1] Thanks to Jeremy Drake and Pete Ratzlaff.

Generating Calibration Products on the Fly

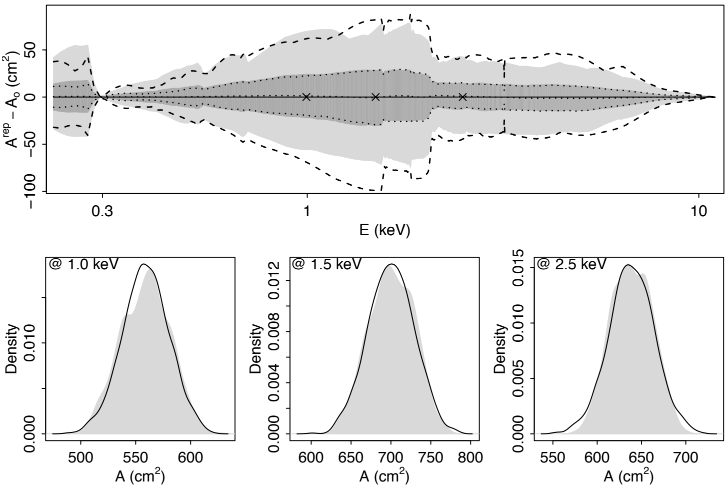
We use *Principal Component Analysis* to represent uncertainty:

$$A \sim A_0 + \bar{\delta} + \sum_{j=1}^{m} e_j r_j \boldsymbol{v}_j,$$

A_0: default effective area,
$\bar{\delta}$: mean deviation from A_0,
r_j and $\boldsymbol{v}_j$: first m principle component eigenvalues & vectors,
e_j: independent standard normal deviations.

Capture 99% of variability with $m = 18$.

Checking the PCA Emulator



The Simulation Studies

Simulated Spectra

- Spectra were simulated using an absorbed power law,

$$f(E_j) = \alpha e^{-N_H \sigma(E_j)} E_j^{-\Gamma},$$

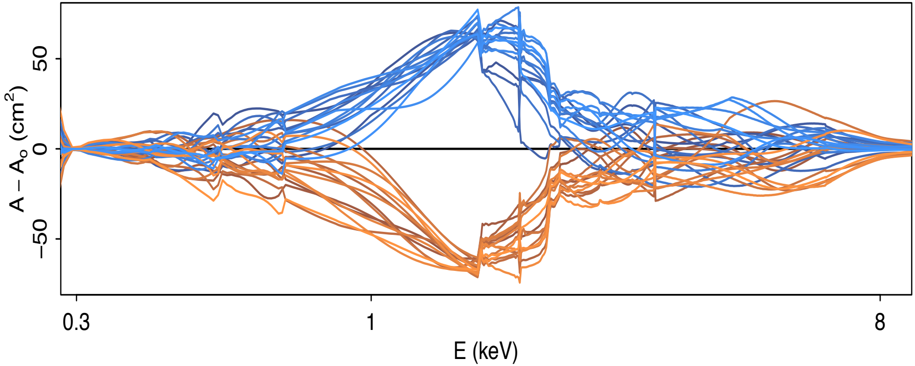
  accounting for instrumental effects; E_j is the energy of bin j.
- Parameters (Γ and N_H) and sample size/exposure times:

	Effective Area		Nominal Counts		Spectal Model	
	Default	Extreme	10^5	10^4	Harder†	Softer‡
SIM 1	X		X		X	
SIM 2	X		X			X
SIM 3	X			X	X	

†An absorbed powerlaw with $\Gamma = 2$, $N_{\rm H} = 10^{23}/{\rm cm}^2$

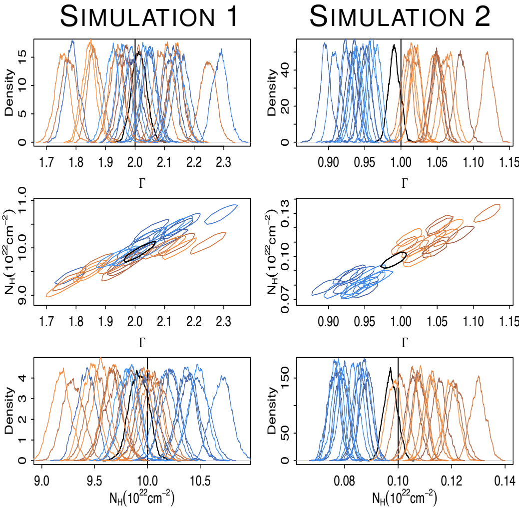
‡An absorbed powerlaw with $\Gamma = 1$, $N_{\rm H} = 10^{21}/{\rm cm}^2$

30 Most Extreme Effective Areas in Calibration Sample



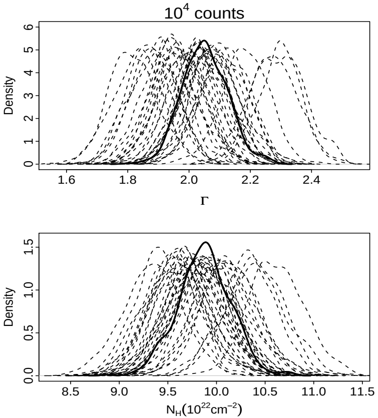
15 largest and 15 smallest determined by maximum value

The Effect of Calibration Uncertainty



- Columns represent two simulated spectra.
- True parameters are horizontal lines.
- Posterior under default calibration is plotted in black.
- The posterior is highly sensitive to the choice of effective area!

The Effect of Sample Size



The effect of Calibration Uncertainty is more pronounced with larger sample sizes.

Outline

Accounting for Calibration Uncertainty

We consider inference under:

A PRAGMATIC BAYESIAN TARGET: $\pi_0(A, \theta) = p(A)p(\theta|A, Y)$.

THE FULLY BAYESIAN POSTERIOR: $\pi(A, \theta) = p(A|Y)p(\theta|A, Y)$.

Here:

$p(\theta|A, Y)$: PyBLoCXS posterior with known effective area, A.

$p(A|Y)$: The *posterior distribution* for A.

$p(A)$: The *prior distribution* for A.

Should we let the current data inform inference for calibration products?

Two Possible Target Distributions

We consider inference under:

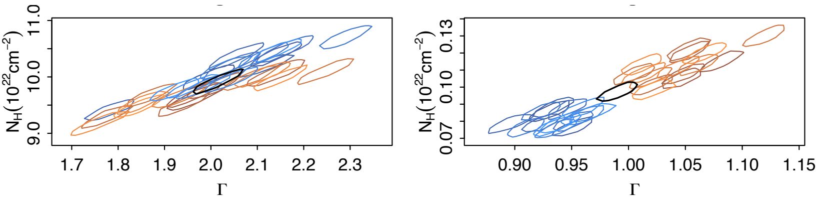
A PRAGMATIC BAYESIAN TARGET: $\pi_0(A, \theta) = p(A)p(\theta|A, Y)$.

THE FULLY BAYESIAN POSTERIOR: $\pi(A, \theta) = p(A|Y)p(\theta|A, Y)$.

Concerns:

- **Statistical** Fully Bayesian target is “correct”.
- **Cultural** Astronomers have concerns about letting the current data influence calibration products.
- **Computational** Both targets pose challenges, but pragmatic Bayesian target is easier to sample.
- **Practical** How different are $p(A)$ and $p(A|Y)$?

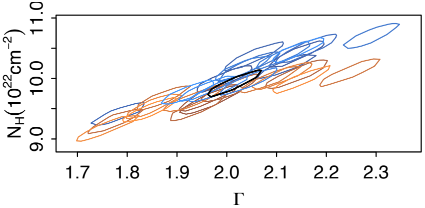
Using Multiple Imputation to Account for Uncertainty



MI is a simple, but approximate, method:

- Fit the model $M \ll 1000$ times, each with random effective area curve from the calibration sample.
- Estimate parameters by averaging the M fitted values.
- Estimate uncertainty by combining the within and between fit errors.

The Multiple Imputation Combining Rules



$$\hat{\theta} = \frac{1}{M}\sum_{m=1}^{M}\hat{\theta}_m, \qquad W = \frac{1}{M}\sum_{m=1}^{M}\mathrm{Var}(\hat{\theta}_m),$$

$$B = \frac{1}{M-1}\sum_{m=1}^{M}(\hat{\theta}_m - \hat{\theta})(\hat{\theta}_m - \hat{\theta})^{\top}, \quad T = W + \left(1 + \frac{1}{M}\right)B.$$

The total variance combines the variances within and between the M analyses.

Accounting for Calibration Uncertainty with MCMC

When using MCMC in a Bayesian setting we can:

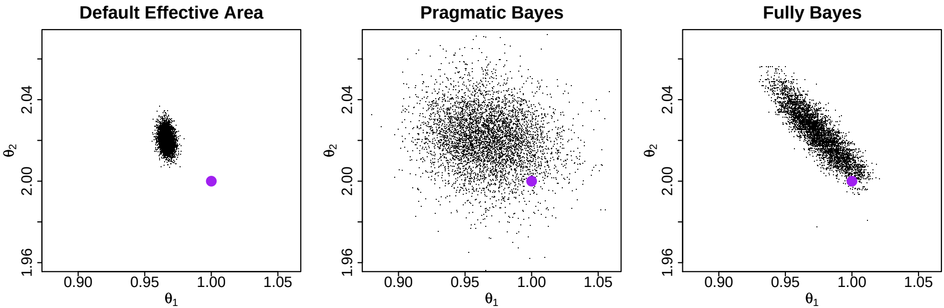
- Sample a different effective area from the calibration sample at each iteration according to:

  Pragmatic Bayes: $p(A)$
  Fully Bayes: $p(A|Y)$
- Computational challenges arise in both cases.
- We focus on comparing the results of the two methods.

A Simulation.

- Sampled 10^5 counts from a power law spectrum: E^{-2}.
- $A_{\rm true}$ is 1.5σ from the center of the calibration sample.

Sampling From the Full Posterior

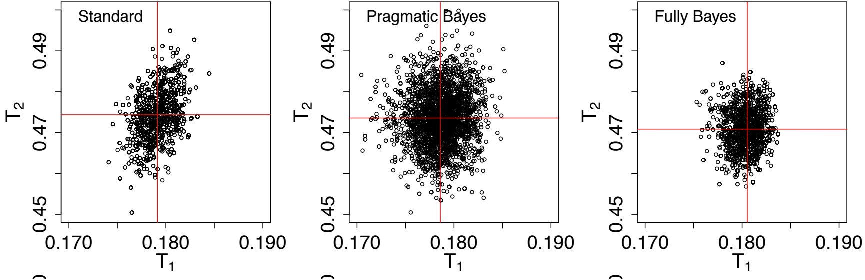


Spectral Model (purple bullet = truth):

$$f(E_j) = \theta_1 e^{-\theta_1 \sigma(E_j)} E_j^{-\theta_2}$$

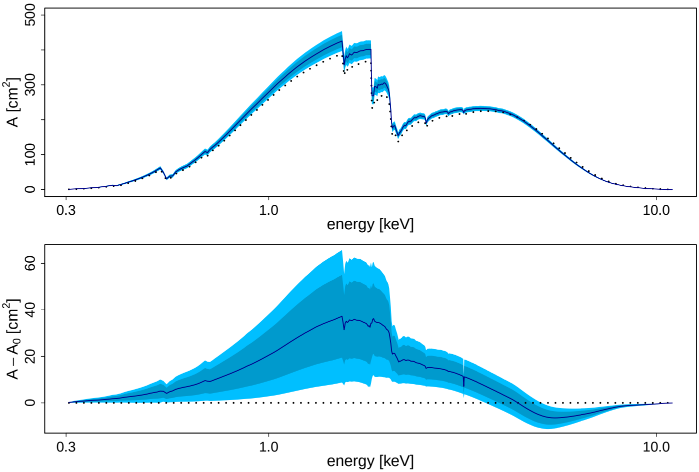
Pragmatic Bayes is clearly better than current practice, but a Fully Bayesian Method is the ultimate goal.

The Effect in the Analysis of a Binary System

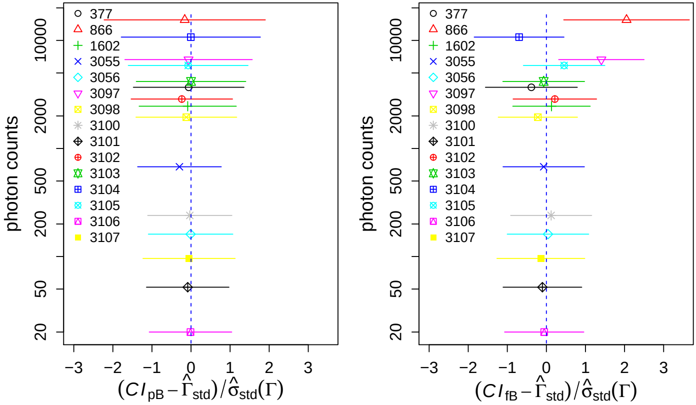


Fitting ζ Ori with a Multithermal Spectral Model

Learning the Effective Area



Results: 95% Intervals Standardized by Standard Fit



With high counts calibration uncertainty swamps statistical error and fully Bayes identifies A and shifts interval.

Thanks...

Collaborative work with:

- Vinay Kashyap
- Jin Xu
- Alanna Connors
- Hyunsook Lee
- Aneta Siegminowska
- California-Harvard Astro-Statistics Collaboration

If you want more details...

Lee, H., Kashyap, V., van Dyk, D., Connors, A., Drake, J., Izem, R., Min, S., et al.
Accounting for Calibration Uncertainties in X-ray [Spectral] Analysis
The Astrophysical Journal, **731**, 126–144, 2011.

Xu, J., van Dyk, D., Kashyap, V., Siemiginowska, A., Connors, A., Drake, J., et al.
A Fully Bayesian Method for Jointly Fitting Calibration and X-ray Spectral Models
The Astrophysical Journal, **794**, 97, 2014.