

Accounting for Calibration Uncertainty in Spectral Analysis

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Joint work with

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Outline

- 1 Bayesian Statistical Methods
 - Components of a Statistical Model
 - Statistical Computation
- 2 Calibration Uncertainty
 - The Calibration Sample
 - The Effect of Calibration Uncertainty
- 3 Bayesian Analysis of Calibration Uncertainty
 - Pragmatic and Fully Bayesian Solutions
 - Empirical Illustration

Outline

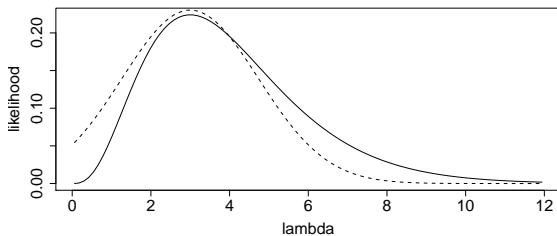
- 1 **Bayesian Statistical Methods**
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Bayesian Statistical Analyses: Likelihood

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.

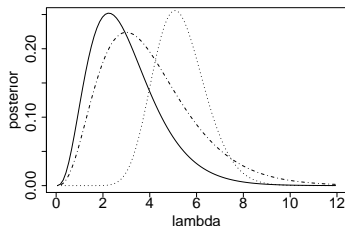
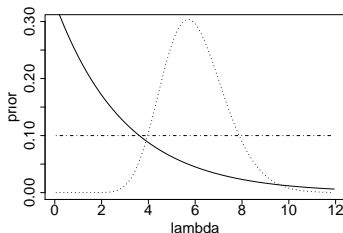
Bayesian Analyses: Prior and Posterior Dist'ns

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

Bayes Theorem and Posterior Distribution:

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

Combine past and current information:



Bayesian analyses rely on probability theory

Multi-Level Models

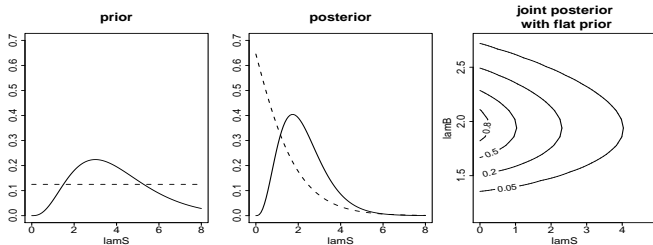
A Poisson Multi-Level Model:

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

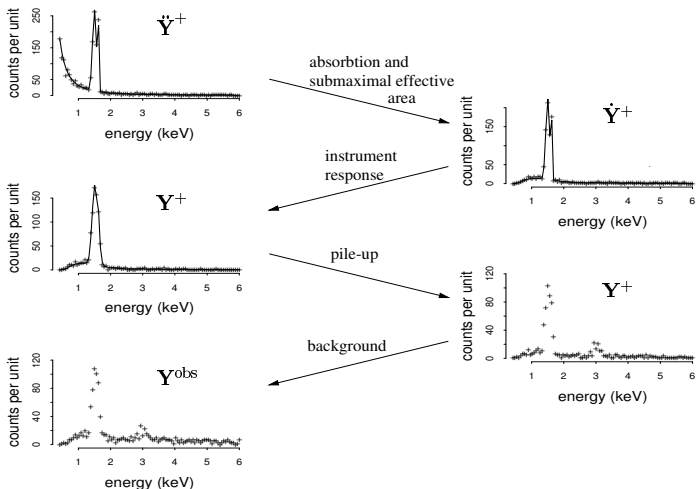
LEVEL 2: $Y_B|\lambda_B \stackrel{\text{dist}}{\sim} \text{Pois}(\lambda_B)$ and $X|\lambda_B \stackrel{\text{dist}}{\sim} \text{Pois}(\lambda_B \cdot 24)$,

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.

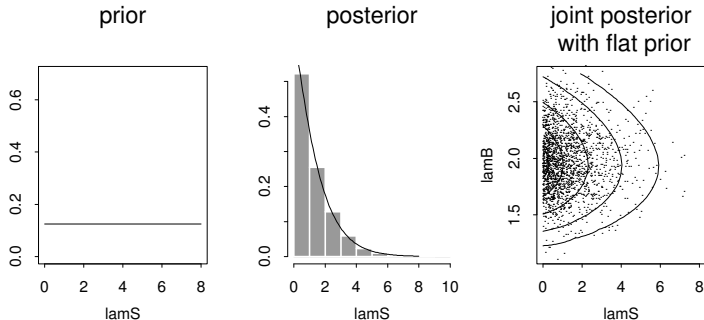
Build a multi-level model

- 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*.

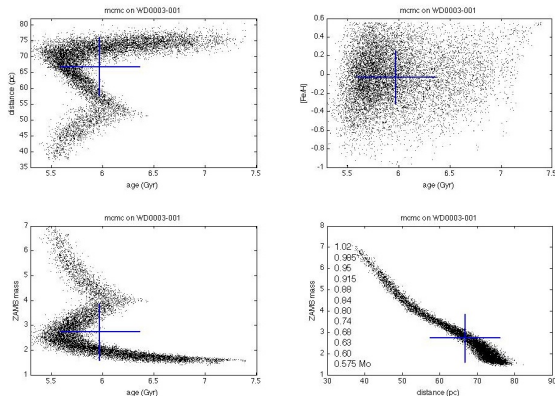
Computation becomes a real issue!

Markov Chain Monte Carlo

Exploring the posterior distribution via Monte Carlo.

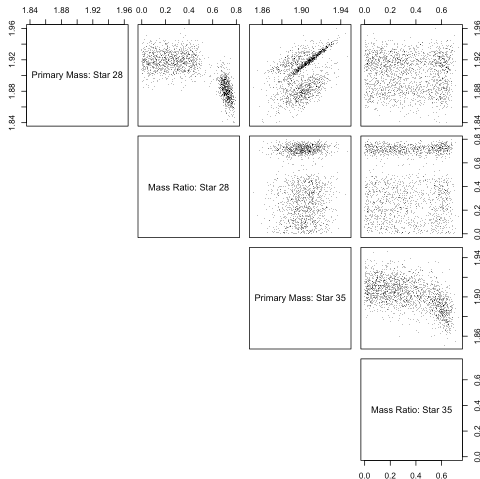


Model Fitting: Complex Posterior Distributions



Highly non-linear relationship among parameters.

Model Fitting: Complex Posterior Distributions

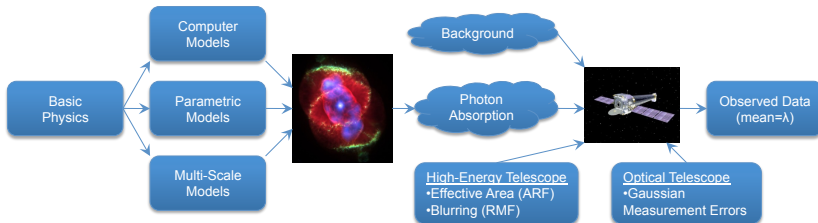


The classification of certain stars as field or cluster stars can cause multiple modes in the distributions of other parameters.

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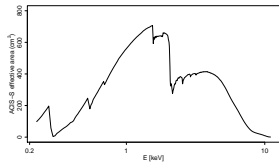
The Basic Statistical Model



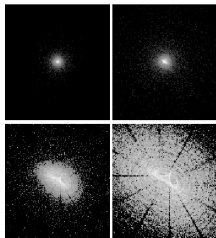
- Embed physical models into multi-level statistical models.
- Must account for complexities of data generation.
- State of the art computational techniques enable us to fit the resulting highly-structured model.

Calibration Products

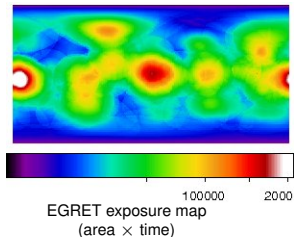
- Analysis is highly dependent on *Calibration Products*:
 - Effective Area Curves
 - Energy Redistribution Matrices
 - Exposure Maps
 - Point Spread Functions
- In this talk we focus on uncertainty in the effective area.



A Chandra effective area.



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

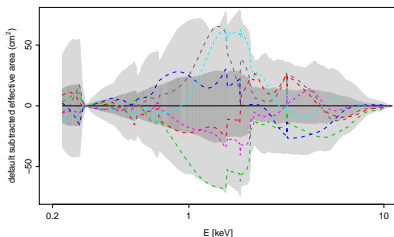
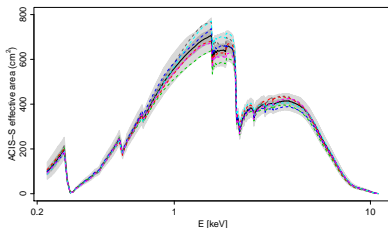


EGRET exposure map
(area \times time)

Calibration Sample

Calibration sample of 1000 representative curves¹

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



¹Thanks to Jeremy Drake and Pete Ratzlaff.

Generating Calibration Products on the Fly

We use Principal Component Analysis to represent uncertainty:

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

A_0 : default effective area,

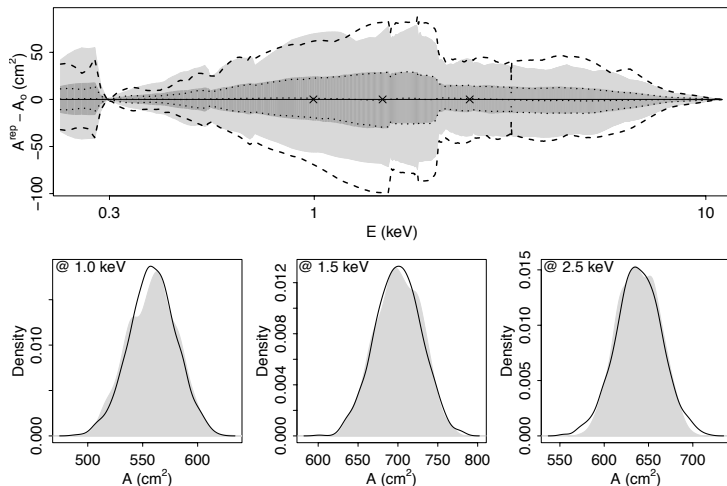
$\bar{\delta}$: mean deviation from A_0 ,

r_j and \mathbf{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 .

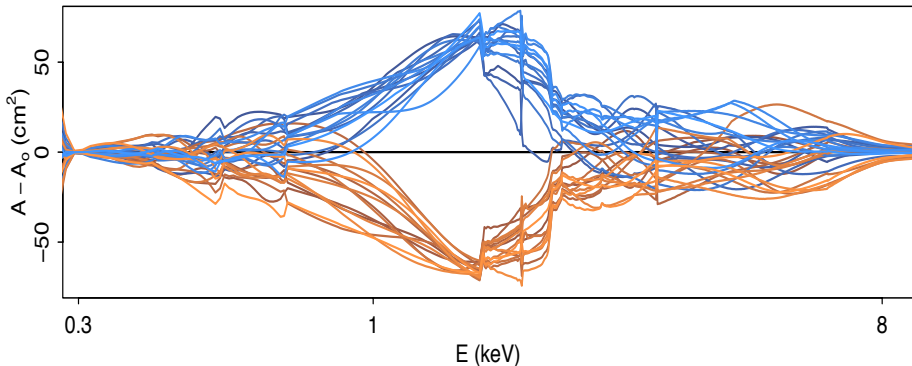
- Parameters (Γ and N_H) and sample size/exposure times:

	Effective Area		Nominal Counts		Spectral 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 $\Gamma = 2$, $N_H = 10^{23}/\text{cm}^2$

[‡]An absorbed powerlaw with $\Gamma = 1$, $N_H = 10^{21}/\text{cm}^2$

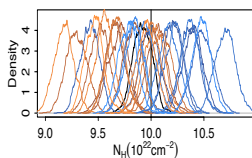
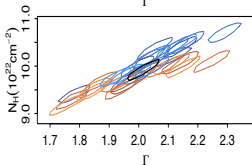
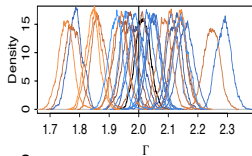
30 Most Extreme Effective Areas in Calibration Sample



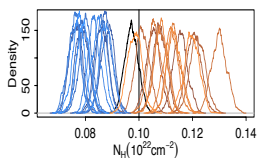
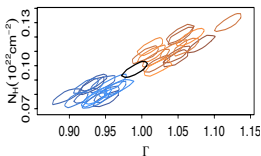
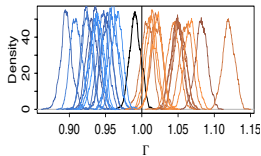
15 largest and 15 smallest determined by maximum value

The Effect of Calibration Uncertainty

SIMULATION 1

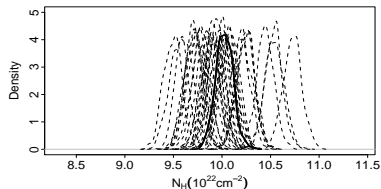
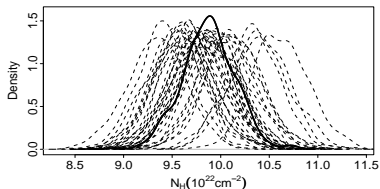
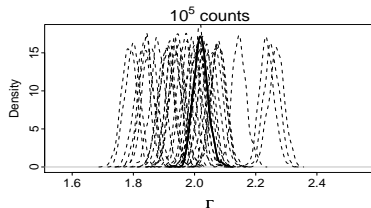
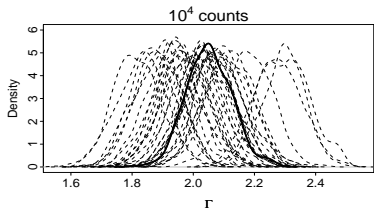


SIMULATION 2



- 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.

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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:

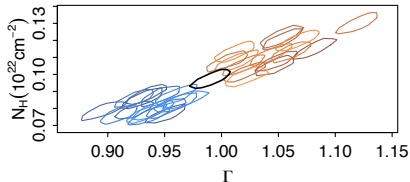
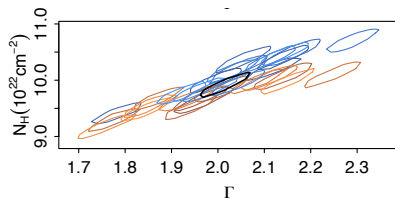
Statistical Fully Bayesian target is “correct”.

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 $p(A|Y)$?

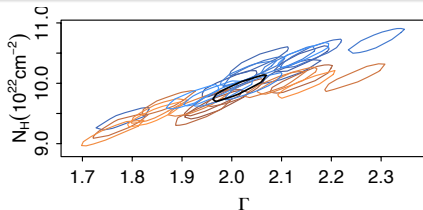
Using Multiple Imputation to Account for Uncertainty



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



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

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

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: $p(A|Y)$

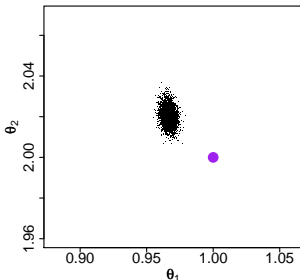
- Computational challenges arise in both cases.
- We focus on comparing the results of the two methods.

A Simulation.

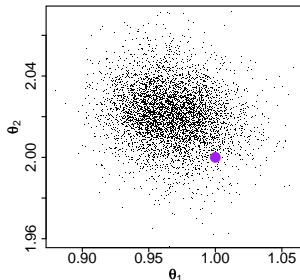
- Sampled 10^5 counts from a power law spectrum: E^{-2} .
- A_{true} is 1.5σ from the center of the calibration sample.

Sampling From the Full Posterior

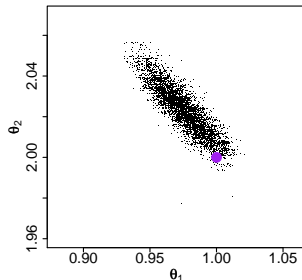
Default Effective Area



Pragmatic Bayes



Fully Bayes

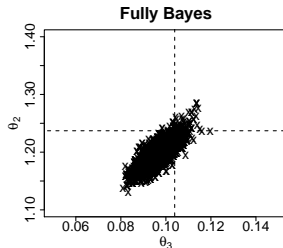
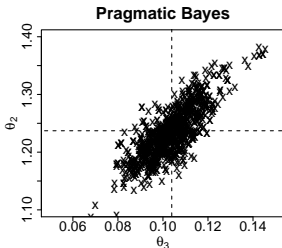
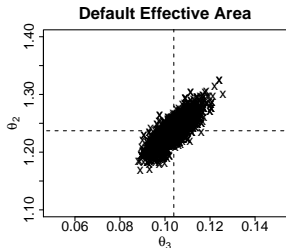
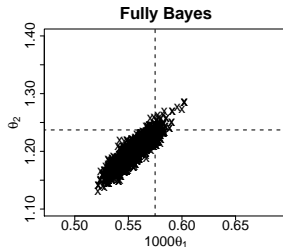
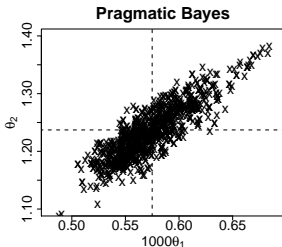
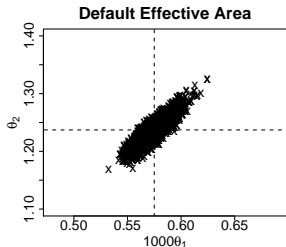


Spectral Model (purple bullet = truth):

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

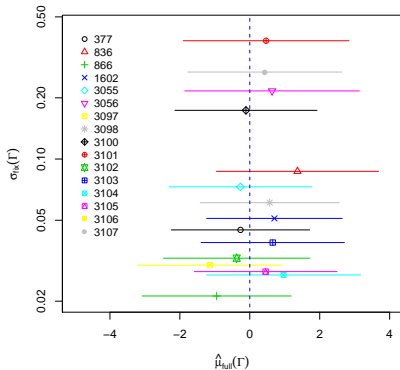
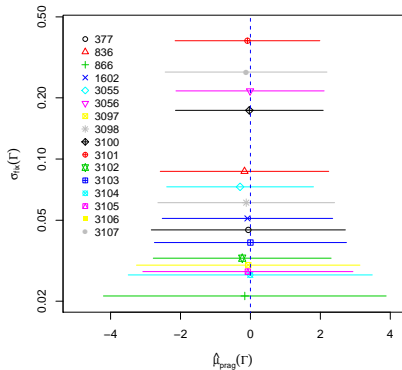
*Pragmatic Bayes is clearly better than current practice,
 but a Fully Bayesian Method is the ultimate goal.*

The Effect in an Analysis of a Quasar Spectrum



(obs ID = 866)

Results: 95% Intervals Standardized by Standard Fit



*For large spectra calibration uncertainty swamps statistical error.
 In large spectra 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., Park, T., Ratzlaff, P., Siemiginowska, A., and Zezas, A.

Accounting for Calibration Uncertainties in X-ray Analysis: Effective Area in Spectral Fitting. *The Astrophysical Journal*, **731**, 126–144, 2011.