Astrostatistics: The Intersection of Statistics and Outer Space

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Joint work with Y. Chen (Michigan), X. Wang (Two Sigma Inc.), D. van Dyk (Imperial College London), H. Marshall (MIT)

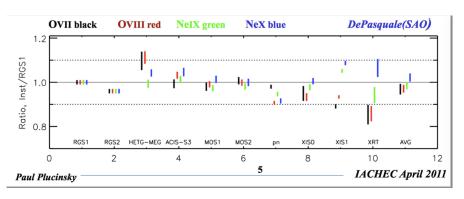
October 29, 2019

Calibration Concordance Problem (Example: E0102)



- Supernova remnant E0102
- Four sources correspond to four spectral lines in E0102

Calibration Concordance Problem (Example: E0102)



- Four spectral lines observed with 11 X-ray detectors
- Main challenge the data/instruments do not agree

Outline

- Introduction
- Scientific and Statistical Models
- Concordance Model
- Advantages of Our Approach
 - Multiplicative Shrinkages
 - Benefits of fitting the variances
 - Extentions to handle outliers
 - Results from Astronomy Data
- Summary

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- Lower cases: data / estimators.
- Upper cases: parameter / estimand.

Calibration Concordance Problem

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$$\frac{c_{ij}}{a_i} \neq \frac{c_{i'j}}{a_{i'}}$$
 for $i \neq i'$.

Different instruments give different estimated flux of the same object!

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- Scientific Question:
 - Are there systematic errors in 'known' effective areas?
 - Can we derive properly adjusted effective areas?
 - Can we unify estimates of the same flux with different instruments?

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Scientific and Statistical Models

Scientific Model

Multiplicative in original scale and additive on the log scale.

Counts = Exposure × Effective Area × Flux,

$$C_{ij} = T_{ij}A_iF_j$$
, \Leftrightarrow log $C_{ij} = B_i + G_j$,

where log area = $B_i = \log A_i$, log flux = $G_i = \log F_i$; let $T_{ij} = 1$.

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Statistical Model

log counts
$$y_{ij} = \log c_{ij} - \alpha_{ij} = B_i + G_j + e_{ij}$$
, $e_{ij} \stackrel{indep}{\sim} \mathcal{N}(0, \sigma_{ij}^2)$; where $\alpha_{ii} = -0.5\sigma_{ii}^2$ to ensure $E(c_{ii}) = C_{ii} = A_i F_i$.

- Known Variances: σ_{ij} known.
- Unknown Variances: $\sigma_{ii} = \sigma_i$ unknown.

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Log-Normal Hierarchical Model.

log counts | area & flux & variance
$$\stackrel{\text{indep}}{\sim}$$
 Gaussian distribution, $y_{ij} \mid B_i, G_j, \sigma_i^2 \stackrel{\text{indep}}{\sim} \mathcal{N}\left(B_i + G_j, \sigma_i^2\right),$

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$$G_j \stackrel{\text{indep}}{\sim} \ \text{Inv-Gamma}(df_g, \ \beta_g).$$

Setting the prior parameters.

• $b_i = \log a_i$, τ_i are given by astronomers.

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Setting the prior parameters.

- **1** $b_i = \log a_i$, τ_i are given by astronomers.
- ② df_g , β_g are given based on the variability in data.

Posterior Propriety. The posterior is proper if each source is measured by at least one instrument, i.e., $|I_i| \ge 1$ for all $1 \le j \le M$.

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$$\frac{\lambda_{\max}(\Omega(\sigma^2))}{\lambda_{\min}(\Omega(\sigma^2))} \ge \frac{u^{\top}\Omega(\sigma^2)}{v^{\top}\Omega(\sigma^2)} \frac{u}{v} = 1 + \frac{4\sum_{i=1}^{N}|J_i|\sigma_i^{-2}}{\sum_{i=1}^{N}\tau_i^{-2}}, \quad (1)$$

where $u = (\mathbf{1}_N, \mathbf{1}_M)^{\top}$ and $v = (\mathbf{1}_N, -\mathbf{1}_M)^{\top}$.

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Alternative: setting $B_1 = 0$ or $\tau_1 = 0$.

Markov Chain Monte Carlo (MCMC) algorithms.

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 - Highly correlated parameters, high-dim parameter space.

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Shrinkage Estimators: Known Fluxes and Errors

Hierarchical model \Rightarrow Shrinkage estimators (weighted averages of evidence from 'Prior' and evidence from 'Data').

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(1) When fluxes and variances are known,

Original Scale

$$\hat{A}_i = a_i^{W_i} \left[(\tilde{c}_i.\tilde{f}^{-1}) e^{\sigma_i^2/2} \right]^{1-W_i},$$

where

$$ilde{c}_{i\cdot} = \prod_j c_{ij}^{1/M}, \,\, ilde{f} = \prod_j f_j^{1/M}$$

Log-Scale

$$\hat{B}_i = W_i b_i + (1 - W_i)(\bar{y}_{i\cdot} - \bar{G}),$$

where

$$ar{G} = rac{\sum_{j} g_{j}}{M}, ar{y}_{i\cdot} = rac{\sum_{j} y_{ij}}{M}$$

are arithmatic means.

The 'weights', $W_i = \frac{\tau_i^{-2}}{\tau_i^{-2} + M\sigma_i^{-2}}$, represents the direct information in b_i relative to indirect information in fluxes.

are geometric means.

Shrinkage Estimators: Known Errors

(2) When fluxes are unknown and variances are known,

$$\hat{B}_i = W_i b_i + (1 - W_i)(\bar{y}_{i\cdot} - \bar{G}_i), \quad \hat{G}_j = \bar{y}_{\cdot j} - \bar{B},$$

where
$$\bar{G}_i = \frac{\sum_j \hat{G}_j}{M}$$
, $\bar{B} = \frac{\sum_i \hat{B}_i \sigma_i^{-2}}{\sum_i \sigma_i^{-2}}$, $\bar{y}_{i.} = \frac{\sum_j y_{ij}}{M}$, $\bar{y}_{.j} = \frac{\sum_i y_{ij} \sigma_i^{-2}}{\sum_i \sigma_i^{-2}}$.

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(3) When variances are unknown, shrinkage estimator of variance,

$$\hat{\sigma}_{i}^{2} = \frac{2}{1 + \sqrt{1 + S_{y,i}^{2}}} S_{y,i}^{2}, \quad S_{y,i}^{2} = \frac{1}{|J_{i}| + \alpha} \left[\sum_{j \in J_{i}} (y_{ij} - \hat{B}_{i} - \hat{G}_{j})^{2} + \beta \right]$$

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 - ⇒ possible false discoveries
 - 'known variances' ≥ true variability
 - ⇒ noninformative results

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Extentions: Log-t Model

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$$y_{ij} \mid B_i, G_j, \xi_{ij} = -\frac{\sigma^2}{2\xi_{ij}} + B_i + G_j + \frac{Z_{ij}}{\sqrt{\xi_{ij}}},$$
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If $\xi_{ij} \stackrel{\mathrm{indep}}{\sim} \chi^2_{\nu}$, i.e. independent chi-squared distributions, the error term

 $Z_{ij}/\sqrt{\xi_{ij}}$ follows independent student-t distributions, i.e. $\frac{Z_{ij}}{\sqrt{\xi_{ij}}} \stackrel{\mathrm{indep}}{\sim} \frac{\sigma}{\sqrt{\nu}} t_{\nu}$.

A Numerical Example with Outliers

Simulation: N = 10, M = 40, $G_1 = -1$ and $G_j = 3, j > 1$. Asymptotic variance of log-counts: $e^{-B_i - G_j} \Rightarrow$ outliers.

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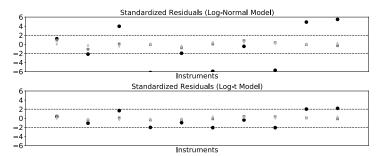
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$$\hat{\mathcal{R}}_{ij} = \frac{y_{ij} - \hat{\mathcal{B}}_i - \hat{\mathcal{G}}_j + 0.5 \times \hat{\sigma}_i^2}{\hat{\sigma}_i}, \hat{\mathcal{R}}_{ij} = \frac{y_{ij} - \hat{\mathcal{B}}_i - \hat{\mathcal{G}}_j + 0.5 \times \kappa^2 / \hat{\xi}_{ij}}{\kappa / \hat{\xi}_{ij}^{1/2}}$$

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Coverage Properties With Outliers, Misspecification

Poisson	Para.	Coverage Probability		Length of Interval		
Model	гага.	log-Normal	log-t	log-Normal	log-t	
N = 10	В	[0.941, 0.959]	[0.971, 0.975]	0.067 ± 0.005	0.073 ± 0.002	
N = 10	G_1	0.399	0.700	0.090± 0.015	0.182 ± 0.045	
N = 10	$G_{2:M}$	[0.967, 0.977]	[0.996, 0.999]	0.077±0.003	0.104±0.002	
N = 40	В	[0.953, 0.969]	[0.993, 0.998]	0.041 ± 0.007	$0.050 {\pm} 0.001$	
N = 40	G_1	0.398	0.686	0.045±0.003	0.093±0.013	
N = 40	$G_{2:M}$	[0.965,0.977]	[0.996,0.999]	0.038 ± 0.001	0.051 ± 0.001	

Table 1: M=40. Coverage of nominal 95% posterior intervals calculated from 2000 datasets simulated under a Poisson model. The intervals in columns 3 and 4 give the smallest and largest coverage observed for the corresponding parameter. The last two columns give the lengths of nominal 95% intervals in the format: mean \pm standard deviation.

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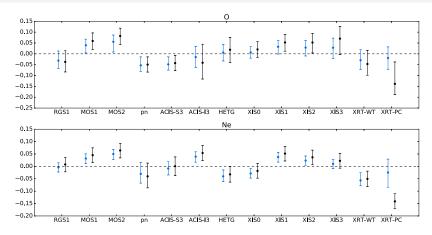
Numerical Results (E0102)

Recap: Supernova remnant E0102.

Four sources are four spectral lines in E0102.



Estimates of $B_i = \log A_i$ (M = 2 each panel)



- Adjusted so that default effective area, $b_i = \log a_i = 0$.
- 95% posterior intervals (black: $\tau = 0.05$; blue: $\tau = 0.025$).
- Some instruments systematically high, others low.

Prior Influence

Instrument	Oxy	gen	Neon		
	au=0.025	$\tau = 0.05$	au=0.025	$\tau = 0.05$	
RGS1	0.570	0.205	0.063	0.016	
MOS1	0.279	0.077	0.075	0.019	
MOS2	0.355	0.065	0.077	0.017	
pn	0.250	0.041	0.620	0.218	
ACIS-S3	0.218	0.040	0.270	0.088	
ACIS-I3	0.906	0.640	0.099	0.026	
HETG	0.648	0.341	0.129	0.034	
XIS0	0.180	0.051	0.069	0.018	
XIS1	0.298	0.078	0.071	0.019	
XIS2	0.463	0.140	0.063	0.016	
XIS3	0.772	0.364	0.062	0.018	
XRT-WT	0.726	0.278	0.154	0.026	
XRT-PC	0.934	0.235	0.906	0.017	

Table 2: Proportion of prior influence, as defined by $1 - W_i$, for E0102 data.

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- Three EPIC instruments: the EPIC-pn, and the two EPIC-MOS detectors (pn, MOS1, and MOS2).
- Three datasets: hard (2.5 10.0 keV), medium (1.5 2.5 keV) and soft (0.5 1.5 keV) energy bands. The three instruments (pn, MOS1 and MOS2) measured 41, 41, and 42 sources respectively in hard, medium, and soft bands. Faint sources.

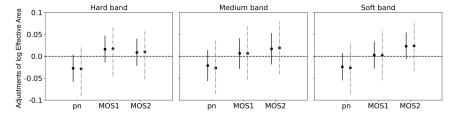


Figure 3: Adjustments of the log-scale Effective Areas for hard band (left), medium band (middle) and soft band (right) of the 2XMM datasets.

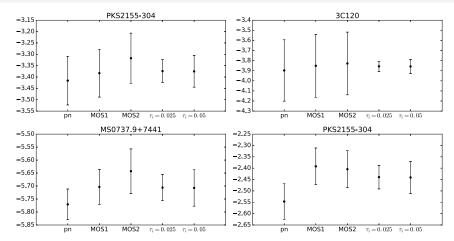
Numerical Results (XCAL)

- XCAL data: Bright active galactic nuclei from the XMM-Newton cross-calibration sample.
 - Observed in hard (n = 94), medium (n = 103), soft (n = 108) bands.
- Pileup: Image data are clipped to eliminate the regions affected by pileup, determined using epatplot.
- Three detectors: MOS1, MOS2 and pn.
- We fit our model and show results on

Sources: M=103 (in medium band).

The hard and soft bands data are fitted similarly – treating hard/medium/soft band as three different data sets.

Numerical Results (XCAL): Calibration Concordance



4 out of 103 Sources in medium band. y-axis: G (log flux); vertical bars (left 3 in each panel): mean \pm 2 s.d. based on observed fluxes, vertical bars (right 2 in each panel): 95% posterior intervals based on our model.

Prior Influence

Data Name	$ au_{i} = 0.025$			$ au_i = 0.05$		
	pn	mos1	mos2	pn	mos1	mos2
hard band 2XMM	0.093	0.075	0.082	0.025	0.020	0.022
medium band 2XMM	0.250	0.216	0.222	0.076	0.065	0.067
soft band 2XMM	0.093	0.075	0.069	0.025	0.020	0.018
hard band XCAL	0.010	0.019	0.031	0.003	0.005	0.008
medium band XCAL	0.023	0.016	0.028	0.006	0.004	0.007
soft band XCAL	0.021	0.011	0.007	0.005	0.003	0.002

Table 3: Proportion of prior influence.

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Astronomy

Adjustments of effective areas of each instrument.

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- Adjustments of effective areas of each instrument.
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- Correlations among instruments.
 - Estimated correlations based on theoretical simulations.
 - Prior? Extra data? Uncertainty?

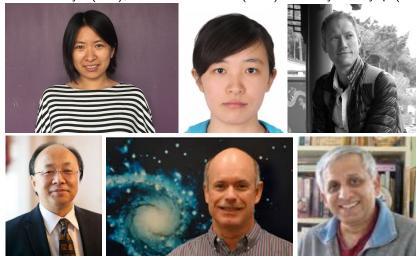
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- Robustness ⇒ Misspecified models.
- Better quantification of prior influence.
- Coverage properties when outliers exist.

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Future of Astrostatistics