## Astrostatistics: <br> 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)

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## 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

(1) Introduction
(2) Scientific and Statistical Models
(3) Concordance Model
(4) Advantages of Our Approach

- Multiplicative Shrinkages
- Benefits of fitting the variances
- Extentions to handle outliers
- Results from Astronomy Data
(5) Summary


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## Notation

- $N$ Instruments with true effective area $A_{i}, 1 \leq i \leq N$.
- For each instrument $i$, we know estimated $a_{i}\left(\approx A_{i}\right)$ but not $A_{i}$.


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- Photon counts $c_{i j}$ : from measuring flux $F_{j}$ with instrument $i$.


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- Photon counts $c_{i j}$ : from measuring flux $F_{j}$ with instrument $i$.
- Lower cases: data / estimators.
- Upper cases: parameter / estimand.


## Calibration Concordance Problem

(1) Astronomers' Dilemma:

$$
\frac{c_{i j}}{a_{i}} \neq \frac{c_{i^{\prime} j}}{a_{i^{\prime}}} \text { for } i \neq i^{\prime}
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Different instruments give different estimated flux of the same object!

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Different instruments give different estimated flux of the same object!
(2) 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 $\times$ Effective Area $\times$ Flux,

$$
C_{i j}=T_{i j} A_{i} F_{j}, \quad \Leftrightarrow \quad \log C_{i j}=B_{i}+G_{j},
$$

where $\log$ area $=B_{i}=\log A_{i}, \log$ flux $=G_{j}=\log F_{j} ;$ let $T_{i j}=1$.

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## Statistical Model

$$
\log \text { counts } y_{i j}=\log c_{i j}-\alpha_{i j}=B_{i}+G_{j}+e_{i j}, \quad e_{i j} \stackrel{i n d e p}{\sim} \mathcal{N}\left(0, \sigma_{i j}^{2}\right) ;
$$

where $\alpha_{i j}=-0.5 \sigma_{i j}^{2}$ to ensure $E\left(c_{i j}\right)=C_{i j}=A_{i} F_{j}$.

- Known Variances: $\sigma_{i j}$ known.
- Unknown Variances: $\sigma_{i j}=\sigma_{i}$ unknown.


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## Bayesian Hierarchical Model

## Log-Normal Hierarchical Model.

$$
\begin{aligned}
& \text { log counts |area \&flux \&variance } \stackrel{\text { indep }}{\sim} \\
& \text { Gaussian distributi } \\
& y_{i j} \mid B_{i}, G_{j}, \sigma_{i}^{2} \stackrel{\text { indep }}{\sim} \mathcal{N}\left(B_{i}+G_{j}, \sigma_{i}^{2}\right),
\end{aligned}
$$

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& \stackrel{\text { indep }}{\sim} \\
G_{j}\left(b_{i}, \tau_{i}^{2}\right), \\
& \underset{\sim}{\text { indep }}
\end{array} \text { flat prior, }, ~ l
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$B_{i} \stackrel{\text { index }}{\sim}$
$G_{j} \quad \stackrel{\text { index }}{\sim}$
If variance unknown: $\sigma_{i}^{2} \stackrel{\text { indep }}{\sim}$ Inv-Gamma $\left(d f_{g}, \beta_{g}\right)$.

Setting the prior parameters.
(1) $b_{i}=\log a_{i}, \tau_{i}$ are given by astronomers.

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Setting the prior parameters.
(1) $b_{i}=\log a_{i}, \tau_{i}$ are given by astronomers.
(2) $d f_{g}, \beta_{g}$ are given based on the variability in data.

## Posterior Propriety and Identifiability

Posterior Propriety. The posterior is proper if each source is measured by at least one instrument, i.e., $\left|l_{j}\right| \geq 1$ for all $1 \leq j \leq M$.

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## Identifiability

- $\tau_{i}^{2}=\infty$ : same posteriors with $\left\{B_{i}, G_{j}\right\}$ and $\left\{B_{i}+\delta, G_{j}-\delta\right\}$;


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- $\tau_{i}^{2}=\infty$ : same posteriors with $\left\{B_{i}, G_{j}\right\}$ and $\left\{B_{i}+\delta, G_{j}-\delta\right\}$;
- the condition number of $\Omega\left(\sigma^{2}\right)$ (conditional variance of $\left.\boldsymbol{B}, \boldsymbol{G}\right)$ is

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\begin{equation*}
\frac{\lambda_{\max }\left(\boldsymbol{\Omega}\left(\boldsymbol{\sigma}^{2}\right)\right)}{\lambda_{\min }\left(\boldsymbol{\Omega}\left(\boldsymbol{\sigma}^{2}\right)\right)} \geq \frac{u^{\top} \boldsymbol{\Omega}\left(\boldsymbol{\sigma}^{2}\right) u}{v^{\top} \boldsymbol{\Omega}\left(\boldsymbol{\sigma}^{2}\right) v}=1+\frac{4 \sum_{i=1}^{N}\left|J_{i}\right| \sigma_{i}^{-2}}{\sum_{i=1}^{N} \tau_{i}^{-2}}, \tag{1}
\end{equation*}
$$

where $u=\left(\mathbf{1}_{N}, \mathbf{1}_{M}\right)^{\top}$ and $v=\left(\mathbf{1}_{N},-\mathbf{1}_{M}\right)^{\top}$.

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Alternative: setting $B_{1}=0$ or $\tau_{1}=0$.

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- Hamiltonian Monte Carlo (HMC) - Stan package.
- 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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Hierarchical model $\Rightarrow$ Shrinkage estimators (weighted averages of evidence from 'Prior' and evidence from 'Data').
(1) When fluxes and variances are known,

## Original Scale

$$
\hat{A}_{i}=a_{i}^{W_{i}}\left[\left(\tilde{c}_{i} \cdot \tilde{f}^{-1}\right) e^{\sigma_{i}^{2} / 2}\right]^{1-W_{i}},
$$

where

$$
\tilde{c}_{i .}=\prod_{j} c_{i j}^{1 / M}, \tilde{f}=\prod_{j} f_{j}^{1 / M}
$$

$$
\begin{aligned}
& \text { Log-Scale } \\
& \qquad \hat{B}_{i}=W_{i} b_{i}+\left(1-W_{i}\right)\left(\bar{y}_{i}-\bar{G}\right),
\end{aligned}
$$

where

$$
\bar{G}=\frac{\sum_{j} g_{j}}{M}, \bar{y}_{i}=\frac{\sum_{j} y_{i j}}{M}
$$

are arithmatic means.
are geometric 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.

## Shrinkage Estimators: Known Errors

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

$$
\hat{B}_{i}=W_{i} b_{i}+\left(1-W_{i}\right)\left(\bar{y}_{i}-\bar{G}_{i}\right), \quad \hat{G}_{j}=\bar{y}_{\cdot j}-\bar{B},
$$

where $\bar{G}_{i}=\frac{\sum_{j} \hat{G}_{j}}{M}, \quad \bar{B}=\frac{\sum_{i} \hat{i}_{i} \sigma_{i}^{-2}}{\sum_{i} \sigma_{i}^{-2}}, \bar{y}_{i}=\frac{\sum_{j} y_{i j}}{M}, \quad \bar{y}_{\cdot j}=\frac{\sum_{i} y_{j} \sigma_{i}^{-2}}{\sum_{i} \sigma_{i}^{-2}}$.

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

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

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- Overly optimistic 'known variances'
$\Rightarrow$ overly narrow confidence intervals
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- Overly optimistic 'known variances'
$\Rightarrow$ overly narrow confidence intervals
$\Rightarrow$ possible false discoveries
- 'known variances' $\geq$ true variability
$\Rightarrow$ noninformative results
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## Extentions: Log-t Model

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$$
\begin{aligned}
y_{i j} \mid B_{i}, G_{j}, \xi_{i j} & =-\frac{\sigma^{2}}{2 \xi_{i j}}+B_{i}+G_{j}+\frac{z_{i j}}{\sqrt{\xi_{i j}}}, \\
Z_{i j} & \stackrel{\text { indep }}{\sim} N\left(0, \sigma^{2}\right), \\
B_{i} & \stackrel{\text { indep }}{\sim} N\left(b_{i}, \tau_{i}^{2}\right) .
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B_{i} \\
\stackrel{\text { indep }}{\sim} N\left(b_{i}, \tau_{i}^{2}\right) .
\end{gathered}
$$

If $\xi_{i j}{ }^{\text {indep }} \chi_{\nu}^{2}$, i.e. independent chi-squared distributions, the error term
$Z_{i j} / \sqrt{\xi_{i j}}$ follows independent student-t distributions, i.e. $\frac{Z_{i j}}{\sqrt{\xi_{i j}}} \stackrel{\text { indep }}{\sim} \frac{\sigma}{\sqrt{\nu}} \mathrm{t}_{\nu}$.

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



## Coverage Properties With Outliers, Misspecification

| Poisson <br> Model | Para. | Coverage Probability |  | Length of Interval |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | log-Normal | log- $t$ | log-Normal | log- $t$ |
| $N=10$ | $B$ | $[0.941,0.959]$ | $[0.971,0.975]$ | $0.067 \pm 0.005$ | $0.073 \pm 0.002$ |
| $N=10$ | $G_{1}$ | 0.399 | 0.700 | $0.090 \pm 0.015$ | $0.182 \pm 0.045$ |
| $N=10$ | $G_{2: M} M$ | $[0.967,0.977]$ | $[0.996,0.999]$ | $0.077 \pm 0.003$ | $0.104 \pm 0.002$ |
| $N=40$ | $B$ | $[0.953,0.969]$ | $[0.993,0.998]$ | $0.041 \pm 0.007$ | $0.050 \pm 0.001$ |
| $N=40$ | $G_{1}$ | 0.398 | 0.686 | $0.045 \pm 0.003$ | $0.093 \pm 0.013$ |
| $N=40$ | $G_{2: M}$ | $[0.965,0.977]$ | $[0.996,0.999]$ | $0.038 \pm 0.001$ | $0.051 \pm 0.001$ |

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 | Oxygen |  | Neon |  |
| :---: | :---: | :---: | :---: | :---: |
|  | $\tau=0.025$ | $\tau=0.05$ | $\tau=0.025$ | $\tau=0.05$ |
| 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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- 2XMM catalog: used to generate large, well-defined samples of various types of astrophysical objects; collected with the XMM-Newton European Photon Imaging Cameras (EPIC).


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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 ( $0.5-1.5 \mathrm{keV}$ ) energy bands. The three instruments (pn, MOS1 and MOS2) measured 41, 41, and 42 sources respectively in hard, medium, and soft bands. Faint sources.


## Numerical Results (2XMM)



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 | $\tau_{i}=0.025$ |  |  | $\tau_{i}=0.05$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | pn | mos1 | mos2 | pn | $\operatorname{mos} 1$ | $\operatorname{mos} 2$ |
| 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.

## (1) Introduction

## (2) Scientific and Statistical Models

(3) Concordance Model
(4) Advantages of Our Approach

- Multiplicative Shrinkages
- Benefits of fitting the variances
- Extentions to handle outliers
- Results from Astronomy Data
(5) Summary


## Summary

## Statistics

(1) Multiplicative mean modeling:
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