

Chandra X-ray Center

Aneta Siemiginowska

Images and videos courtesy of NASA/Chandra/HST unless otherwise noted

Adventures in Astrostatistics

CENTER FOR





Chandra X-ray Center

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Images and videos courtesy of NASA/Chandra/HST unless otherwise noted

Adventures in Astrostatistics

High Energy Astrophysics





Solar System



Hot gas $> 10^5$ K **Energetic particles**

Quasar Jets



X-ray Universe

RAB NEBULA

Supernova Remnants

Clusters of Galaxies



Radio Galaxies



CHANDRA FIRST LIGHT... AUGUST 12 1999









Beginning

- Adventures:
 - A1 Bayesian Framework:

 - A3 Hardness Ratio Upper limits, detection significance
 - A4 High resolution images reconstruction, source boundaries, significance
- Emerging Methodology and Future

Outine

likelihood, priors, marginalization, MCMC, calibration uncertainties Why?

A2 Model Selection - hypothesis testing, Protassov et al, Park et al - detecting spectral lines





Scientific Experiment



Beginning

 Astro-Statistics started in the ancient times with the statistical methodology developed and applied to astronomical data over thousands years.

Note: modern statistics is much more than calculating mean and std!

- X-ray astronomy started in the '60s
- Methodology based on techniques developed in the past is not directly applicable to X-ray data - several issues and potential approaches were noted in the early papers
- **Collaborations with Statisticians!**

Energy Spectra of X-ray Clusters of Galaxies Avni, Y. 1976, ApJ, 210, 642 Parameter Estimation in Astronomy through Application of the Likelihood Ratio Cash, W. 1979, ApJ, 228, 939 Generation of Confidence Intervals for Model Parameters in X-ray Astronomy Cash, W. 1976, A&A, 52, 307 Parameter Estimation in X-ray Astronomy Lampton, M.; Margon, B.; Bowyer, S. 1976, ApJ, 208, 177 Parameter Estimation in X-ray Astronomy using Maximum Likelihood Wachter, K.; Leach, R.; Kellogg, E. 1979, ApJ, 230, 274 Chi-squared and C Statistic Minimization for Low Count per Bin Data Nousek, John A.; Shue, David R. 1989, ApJ, 342, 1207 Determination of Confidence Limits for Experiments with Low Numbers of Counts Kraft, R.P.; Burrows, D.N. Nousek, John, A. 1991, ApJ, 374, 344





- SCIMA 1996 Chandra Data Challenges
- Collaboration with the Harvard Department of Statistics
- Workshops at the AAS HEAD meetings



CHASC web site: http://hea-www.harvard.edu/AstroStat/

International CHASC Astro-Statistics Collaboration

This page lists resources of specific interest to astronomers. For detailed descriptions and reports of C-BAS/ICHASC activities, see www2.imperial.ac.uk/~dvandyk/astrostat.php

Software Activities Bibliography Astro jargon Stat jargon Mailing-List Internal

astrostat-announce GoogleGroup | GoogleCalendar | AstroStat Slog Archive

Beginning



AXAF Data Analysis Challenges

Aneta Siemiginowska¹, Martin Elvis¹, Alanna Connors², Peter Freeman³, Vinay Kashyap³, and Eric Feigelson⁴

ABSTRACT The high quality of the AXAF X-ray data provides new challenges for the X-ray data analysis. It is clear that an "old" approach is not enough to fully exploit the capabilities of the AXAF instruments. We describe a few of the statistical and computational problems that we have so far identified. Some of them appear to be theoretically solvable but computationally challenging, while others state problems for theoretical statistics which, so far as we know, are unsolved. The problems divide, from an astronomical point of view, into: Modeling the Data (e.g. nonlinear parameter estimation, uncertainties in the model, weighting the data, correlated residuals), Source Detection (events in N-space, use of wavelets, significance of detected structures) and Instrument Related Issues (pile-up in AXAF ACIS, overlapping orders in grating spectra).



People

Faculty/Researchers/Postdocs

Statisticians

David van Dyk, Imperial College London Thomas Lee, University of California, Davis Xiao-Li Meng, Harvard Yaming Yu, University of California, Irvine David Jones, Texas A&M University Hyungsuk Tak, Penn State University David Stenning, Simon Fraser University Yang Chen, University of Michigan Raymond Wong, Texas A&M University Sara Algeri, University of Minnesota Alex Geringer-Sameth, Imperial College London Jianing Zhang, Imperial College London Bernhard Klingenberg, Williams College

Astronomers

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http://hea-www.harvard.edu/AstroStat/people.html

Former Faculty / Post Docs / Researchers / Associates

Adam Roy, ReVision Optics Alanna Connors Alex Young, NASA-GSFC Brandon Kelly, Goodyear Eric Kolaczyk, Boston University Hyunsook Lee, Lam Research James Chiang, Stanford Jason Kramer, UC Irvine Jeremy Drake, Center for Astrophysics | Harvard & Smithsonian Margarita Karovska, Center for Astrophysics | Harvard & Smithsonian Pavlos Protopapas, Harvard Peter Freeman, Carnegie Mellon Rima Izem Taeyoung Park, Yonsei Yue Wu, University of Washington

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International CHASC Astro-Statistics Collaboration

We briefly describe here a number of terms normally used by statisticians, with translations where appropriate into the terminology used in X-ray astrophysics; this information is taken from the CHASC jargon page at http://heawww.harvard.edu/AstroStat/statjargon.html.

CAMBRIDE | OTHER DESIGNATION | CONTRACTOR AND IN THE

Handbook of X-ray Astronomy

Edited by Keith Arnaud, Randall Smith and Aneta Siemiginowska



Astro-Stat Language

pecific interest to astronomers. For detailed descriptions and reports of C-BAS/ICHASC activities, see www.imperial.a

Software Activities Bibliography Astro jargon Stat jargon Meiling-List Internal

Background marginalization is integration of a background probability over uninteresting parameters.

Bias is a systematic difference between an estimated and a true value of a parameter.

Biased sample is a sample of objects selected from a population such that some objects are more likely to be included than others.

Bootstrap is a method for estimating parameter variance or other properties using an approximation to a distribution created by resampling the observed data themselves.

Cash statistic is a formulation of Poisson likelihood for a parametric model in X-ray astronomy.

Chi-square statistic is a statistic applied in X-ray astronomy which provides a measure of the goodness-of-fit. The name comes from the χ^2 distribution, however many of the "chi-square statistic" expressions do not follow the χ^2 distribution. Here are the most common expressions used:

model variance $\chi^2 = (D - M)^2/M$ data variance $\chi^2 = (D - M)^2/D$ iterative Primini approximation $\chi_i^2 = (D - M_i)^2 / M_{i-1}$, where *i* is the iteration fitting step.

Conditional distribution (or probability density) is the probability distri-



X-ray data

- Collecting X-ray data means counting arriving photons (Poisson counts) - different from optical data
- For each photon location on the sky, arrival time and energy are recorded (x,y,t,E) - events
- X-ray observations take a long time a short observation with Chandra last ~10 ksec (~3 hours) while typical observations take a day or more. Chandra Deep Field observations took about 23 days.

Chandra Deep Field North

https://chandra.harvard.edu/photo/2003/goods/

The faintest sources - one X-ray photon every 4 days!



Poisson Counts

Light curve of a steady source HZ 43 binned in 1 sec time bins Notice asymmetry scatter around the mean









Adventure 1 Issues in Modeling low counts X-ray Spectra

- Spectral fitting:
 - Includes instrument response directly -> calibration impact on the results Counts(i) = Int [arf (E) * rmf(E,i) * Model(p, E) dE]
 - Non-linear astrophysical models, computer generated models ightarrow
 - Appropriate fit statistics, no binning/grouping data, no background subtraction
 - Modification to the fit statistics (weighted chi2) still not good for ulletlow number of counts, e.g. Gehrels (1986)
 - Formulations for the Poisson likelihood Cash (1979), cstat, wstat
- Why important?
 - bias, negative data if subtracting background or false spectral features, loss of information with binning, optimization with high number of parameters (e.g. finding the best-fit)



channel





Aneta Siemiginowska CfA Colloquium Nov. 4, 2021

convert



Fit Statistics and Bias



Fig. 7.3 Distributions of a photon index parameter γ obtained by fitting simulated X-ray spectra with 60 000 counts and using the three different statistics: S_{Pearson}^2 , S^2 and C (i.e. the Poisson likelihood) statistics. The true value of the simulated photon index is marked with a dashed line and it was set at $\gamma = 1.28$

Chapter 7 on Statistics

Handbook of X-ray Astronomy (Arnaud, Smith, Siemiginowska): https://doi.org/10.1017/CBO9781139034234.008

Simulations:

Distribution of photon index parameter obtained by fitting simulated X-ray spectra using different fit statistics: Gaussian likelihood (χ^2 data, χ^2 model) and Poisson likelihood (Cash). The assumed photon index =1.28 is marked.

 X_i - data M_i - model





Adventure 1 **Bayesian Model for Low Counts X-ray Spectra**

Poisson likelihood and application of Markov Chain Monte Carlo (MCMC) and Gibbs Sampler

THE ASTROPHYSICAL JOURNAL, 548:224–243, 2001 February 10 © 2001. The American Astronomical Society. All rights reserved. Printed in U.S.A.

Van Dyk et al 2001

ANALYSIS OF ENERGY SPECTRA WITH LOW PHOTON COUNTS VIA BAYESIAN POSTERIOR SIMULATION

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$p_{\text{std}}(\theta \mid Y, A_0^*) \propto \mathcal{L}(Y \mid \theta, A_0^*) p(\theta).$

posterior distribution

likelihood

prior on model parameters

Bayesian framework:

- probability of the model given the data
- takes into account all information (data, instruments, model etc.)
- no binning of data
- background as part of the statistical model
- non-biased results
- full information on the posterior distribution (probability of the model given the observation)
- can take into account calibration uncertainties (see Lee et al 2011, Xu et al 2014, Marshall et al 2021)

pyBLoXCS

Note:

Included in Sherpa https://cxc.harvard.edu/sherpa/

Applied in processing of the Chandra Source Catalog (Evans et al 2010)









Adventure 1 **Bayesian Model for Low Counts X-ray Spectra**

Systematic (Calibration) Uncertainties non-linear uncertainties - non-additive

posterior likelihood model prior distribution Standard $p_{\text{std}}(\theta \mid Y, A_0^*) \propto \mathcal{L}(Y \mid \theta, A_0^*) p(\theta).$ **Fixed ARF**

 $p(\theta, A|Y) \propto \mathcal{L}(Y|\theta, A) \ p(\theta) \ p(A),$ Full Bayes ARF prior

Lee+ 2010, Xu+ 2014













Adventure 2 Hypothesis testing and Model Selection

- Spectral features line detections
- Additional model components



Siemiginowska+ 2016











Adventure 2

Hypothesis testing and Model Selection

The Astrophysical Journal, 571:545–559, 2002 May 20 © 2002. The American Astronomical Society. All rights reserved. Printed in U.S.A.

STATISTICS, HANDLE WITH CARE: DETECTING MULTIPLE MODEL COMPONENTS WITH THE LIKELIHOOD RATIO TEST

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ABSTRACT

The likelihood ratio test (LRT) and the related *F*-test, popularized in astrophysics by Eadie and coworkers in 1971, Bevington in 1969, Lampton, Margon, & Bowyer, in 1976, Cash in 1979, and Avni in 1978, do not (even asymptotically) adhere to their nominal χ^2 and F-distributions in many statistical tests common in astrophysics, thereby casting many marginal line or source detections and nondetections into doubt. Although the above authors illustrate the many legitimate uses of these statistics, in some important cases it can be impossible to compute the correct false positive rate. For example, it has become common practice to use the LRT or the F-test to detect a line in a spectral model or a source above background despite the lack of certain required regularity conditions. (These applications were not originally suggested by Cash or by Bevington.) In these and other settings that involve testing a hypothesis that is on the boundary of the parameter space, contrary to common practice, the nominal χ^2 distribution for the LRT or the F-distribution for the F-test should not be used. In this paper, we characterize an important class of problems in which the LRT and the Ftest fail and illustrate this nonstandard behavior. We briefly sketch several possible acceptable alternatives, focusing on Bayesian posterior predictive probability values. We present this method in some detail since it is a simple, robust, and intuitive approach. This alternative method is illustrated using the gamma-ray burst of

Protassov et. al.2002

- Testing for a presence of an emission line
- Standard LRT and F-test does not apply
- Simulations needed to calibrate test statistics
- Posterior Predictive p-values Protassov+2002 Park+2008



Adventure 2 Hypothesis testing and Model Selection

Bayesian Posterior Predictive P-values



Computing the p-value:

the proportion of simulated test statistics LRT values larger (more extreme) than the observed LRT

Note:

Included in Sherpa https://cxc.harvard.edu/sherpa/

Simulations:

Simulate L data sets under null model (H0) and compute the test statistic for each of the L data sets fit with null (H0) and the complex model (H1)

2 A histogram of the simulated test statistics approximates the sampling distribution of the test statistic.

3 Compute the p-value for the observed value of the test statistics



Adventure 2 Hypothesis testing and Model Selection

Searching for lines in low counts low resolution spectrum: - line locations and intensity

High Posterior Density (HPD) - most likely line locations



Park et al 2008



fixed line location at 2.84 keV

location unknown



Adventure 3 Analysis of Faint Sources

- Upper limits in the source detection? Kashyap et al 2010
- For faint sources not enough counts for spectral modeling
- Hardness Ratio calculations
- What are the errors on the hardness ratios? BEHR - Park et al 2006



Kuraszkiewicz et al 2021





Adventure 3 Hardness Ratios

YSICAL JOURNAL, 652:610–628, 2006 November 20 merican Astronomical Society. All rights reserved. Printed in U.S.A

Park et al 2006

BAYESIAN ESTIMATION OF HARDNESS RATIOS: MODELING AND COMPUTATIONS

TAEYOUNG PARK,¹ VINAY L. KASHYAP,² ANETA SIEMIGINOWSKA,² DAVID A. VAN DYK,³ ANDREAS ZEZAS,² CRAIG HEINKE,⁴ AND BRADFORD J. WARGELIN² Received 2005 December 24; accepted 2006 June 14 **BEHR**

simple ratio,
$$\mathcal{R} \equiv \frac{S}{H}$$
,
color, $C \equiv \log_{10} \left(\frac{S}{H} \right)$,
al difference, $\mathcal{HR} \equiv \frac{H-S}{H+S}$,

fractiona

$$\mathcal{R} = rac{S-B_S/r}{H-B_H/r},$$
 $\mathrm{C} = \log_{10}igg(rac{S-B_S/r}{H-B_H/r}igg),$
 $\mathcal{HR} = rac{(H-B_H/r)-(S-B_S/r)}{(H-B_H/r)+(S-B_S/r)}.$

Classical Approach

$$\begin{split} \sigma_{\mathcal{R}} &= \frac{S - B_S/r}{H - B_H/r} \sqrt{\frac{\sigma_S^2 + \sigma_{B_S}^2/r^2}{(S - B_S/r)^2} + \frac{\sigma_H^2 + \sigma_{B_H}^2/r^2}{(H - B_H/r)^2}},\\ \sigma_{\mathrm{C}} &= \frac{1}{\ln\left(10\right)} \sqrt{\frac{\sigma_S^2 + \sigma_{B_S}^2/r^2}{(S - B_S/r)^2} + \frac{\sigma_H^2 + \sigma_{B_H}^2/r^2}{(H - B_H/r)^2}},\\ \sigma_{\mathcal{HR}} &= 2 \left[(H - B_H/r)^2 (\sigma_S^2 + \sigma_{B_S}^2/r^2) \right. \\ &\quad + (S - B_S/r)^2 (\sigma_H^2 + \sigma_{B_H}^2/r^2) \right]^{1/2} \\ &\quad \times \left[(H - B_H/r) + (S - B_S/r) \right]^{-2}, \end{split}$$

with Gehrels errors on measured counts

$$\sigma_X \approx \sqrt{X + 0.75} + 1$$

Note:

C-code available https://hea-www.harvard.edu/AstroStat/BEHR/ Applied in processing of the Chandra Source Catalog (Evans et al 2010, Primini et al. 2011) **Issues with Classical Method:**

Background subtraction

R is positive - probability distribution skewed

- HR is within [-1,+1]
- C asymmetric errors





- Chandra takes the highest resolution X-ray images of the Universe
- Poisson counts sparse images, with many empty pixels
- PSF variable across the images cannot be described in an analytical form, the PSF image is a simulation from the computer model of the Chandra mirrors with calibration measurements
- Some issues:
 - detection of features and upper limits
 - detecting and identifying low surface brightness structures
 - resolving source in crowded fields overlapping sources, diffuse emission
 - finding source boundaries
 - PSF uncertainties



structures



Chandra Image of the Galactic Center









LIRA - Low-Counts Image Reconstruction and Analysis Bayesian Hierarchical Model





Posterior Draws with MCMC Expected photon counts in each pixel given the observed counts

Point Source + Bkg **Baseline Model**





McKeough et al 2016



McKeough et al 2016

Posterior Mean

Note: Code available: https://github.com/astrostat/LIRA Esch et al 2004, Connors & Van Dyk 2007, Stein et al. 2015



0.004 0.003 0.002 0.001

Finding the source boundary



Posterior Draws with MCMC probability distribution of pixel assignments



ISING Prior Correlation between neighboring pixels **Optimal Boundary**

Boundary with maximum probability given LIRA-Ising posterior

McKeough et al (in prep)



Finding the source boundary

Posterior Draws with MCMC probability distribution of pixel assignments



ISING Prior Correlation between neighboring pixels



Optimal Boundary

Boundary with maximum probability given LIRA-Ising posterior

McKeough et al (in prep)



0.003 0.002

0.004

0.001

Evaluate Significance of feature over pre-specified region







Stein et al. 2015, McKeough et al. 2016

Adventures so far...

Low Counts Spectra

- fitting complex spectral models
- line detection
- hardness ratio

Sparse Poisson Images

- source detection and upper limits
- structures in high resolution Poisson images
- source boundaries
- significance



X-ray Analysis Standard Domains

 X-ray image is made by binning events into images, e.g. accumulating photons in a selected energy band and fixed exposure time:

- no spectral or temporal information

- analysis require a point spread function

• Spectra for selected regions are generated by binning the events in energy:

- no spatial or temporal information

- require additional calibration files

 Lightcurves for selected region and energy band binning the events in time:

- no spatial or energy information



Cassiopeia A Supernova Remnant













Emerging Multi-Domain Analysis

Analysis	Description	Current Method	Challenges	Emerging M
Spectral-Image	loss of time	source detection (VTP), spectral- image model, project, deproject in clusters, SNR	multi-spectra, averaging over image, overlapping sources, transients	BASC
Spectral-Time	loss of location	multi-spectra, inter- band correlation	low counts spectra, non-even sampling, different apertures, multi-components	cross-spec ABC, JAV Auto-M
Image-Time	loss of energy	image difference, source detection	spectral information, evolving boundaries, PSF, averaging	eBASC 4D-autor



Examples:

Probabilistic separation of photons from two close sources with eBASCS using location, spectrum and time (Meyer+ 2021)

Change-points and Image Segmentation for Time series of Images - 4D_Automark (Xu+ 2021)



Chandra X-ray Image of Orion Nebula

Credit: NASA/CXC/Penn State/E.Feigelson & K.Getman et al.



Example:

Probabilistic separation of photons from two close sources with eBASCS using location, spectrum and time



locations of the events posterior mean of the locations of Aa and Bb with BASCS

spectra for each star with eBASCS

Meyer et al 2021







light curves of each component eBASCS









Counts

Soft: 0.3 - 0.9 keV Medium: 0.9 - 2 keV Time 25 30

eBASCS:

Bayesian model to separate events from each star using energy, timing and location to mark X-ray photons assigned to each star to calculate intensity and hardness ratio variation in time.

Meyer et al 2021



XMM data Proxima Centauri







Change-points and Image Segmentation for Time Series Images - 4D-Automark

Xu+ 2021



Future Full Multi-Domain Analysis



Description	Current Methods	Challenges	Emergir Methodol
use energy, location, time	multi-band images in several time bins	non-binned events instrument response, background	eBASCS 4D-autom
new domain	simultaneous 3D spectral modeling	no energy information, correlation between Stokes vectors	





Adventures Summary

Past

Low Counts X-ray Spectra

- fitting complex spectral models
- line detection
- hardness ratio

Sparse X-ray Images

- source detection and upper limits
- structures in high resolution Poisson images
- source boundaries
- significance

Future

- full multi-domain analysis
- rising interest in methodology
- likelihood free simulation based methods





Astro2020 White Papers

Siemiginowska et al (2019) AAS WGAA The Next Decade of Astroinformatics and Astrostatistics https://ui.adsabs.harvard.edu/abs/2019BAAS...51c.355S/abstract

Eadie et al (2019) AAS WGAA Realizing the potential of astrostatistics and astroinformatics https://ui.adsabs.harvard.edu/abs/2019BAAS...51g.233E/abstract

Peek et al (2019) Robust Archives Maximize Scientific Accessibility https://ui.adsabs.harvard.edu/abs/2019BAAS...51g.105P/abstract

Fabbiano et al (2019) Increasing the Discovery Space in Astrophysics - A Collation of Six Submitted White Papers https://ui.adsabs.harvard.edu/abs/2019arXiv190306634F/abstract

Kurtz et al (2020) Enabling Synergy: Improving the Information Infrastructure for Planetary Science https://ui.adsabs.harvard.edu/abs/2020arXiv200914323K/abstract





Future

- Steady growth of the field
- Collaboration with statisticians and computer scientists necessary
- Funding to support research in astrostatistics
- Education and curriculum
- Faculty jobs in Astrostatistics •

Note: 3 job postings on the AAS Job register

1957 refereed research papers in ApJ, MNRAS, A&A with words "Bayesian & X-rays"





Astrostatistics Organizations

- AAS Working Group on Astroinformatics and Astrostatistics (WGAA) 2012
- ASA Astrostatistics Interest Group 2014 <u>https://astrostat.org/join.html</u>
- IAU Commision B3 on Astroinformatics and Astrostatistics 2015 https://www.iau.org/science/scientific_bodies/commissions/B3/
- IAA International Astrostatistics Association 2012 http://iaa.mi.oa-brera.inaf.it/IAA/home.html
- ISI International Statistical Institute 2010 Astrostatistics Network

Activities:

Newsletters Seminars

IAU-IAA <u>https://sites.google.com/view/iau-iaa-seminar/home</u> CHASC http://hea-www.harvard.edu/AstroStat/CHASC 2122/

https://aas.org/comms/working-group-astroinformatics-and-astrostatistics-wgaa

AIG Student Paper Competition 2022 deadline Dec.13, 2021 https://astrostat.org/competition/





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Thank you CHASC!

David Van Dyk Imperial College London Harvard Statistics Xiao-Li Meng Vinay Kashyap CfA

- Chandra X-ray Center NAS8-03060
- 18-11083 18-11661
- NASA APRA 80-NSSC21-K0285

International CHASC Astro-Statistics Collaboration

est to astronomers. For detailed descriptions and reports of C-BAS/ICHASC activities, see <u>www2.imperial.ac.uk/~dvandyk/astrostat.ph</u>

<u>Software | Activities | Bibliography | Astro jargon | Stat jargon | People | Mailing-List | Intern</u>

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