Report:
CalStats Working Group

IACHEC XVII Osaka

Vinay Kashyap (CXC/CfA) : 2025-may-15

About the CalStats WG

Vinay Kashyap (CfA; Chair) & Ivan Valtchanov (ESA; co-Chair)

A forum for the discussion of statistical, methodological, and algorithmic issues that affect the calibration of astronomical instruments, of how calibration data are used in data analysis, and how the analysis results are interpreted.

- Membership: 47 members
  - to join, send email to join the mailing list at the iachec-calstat google group iachec-calstat+subscribe@cfa.harvard.edu
  - To unsubscribe, send email to iachec-calstat+unsubscribe@cfa.harvard.edu
- WWW
  - Webpage: https://iachec.org/calibration-statistics/
  - Library: https://iachec.org/calibration-statistics/#library
  - Wiki: https://wikis.mit.edu/confluence/display/iachec/Calibration+Statistics
    - τ matrix for Concordance, Background models and scripts
  - Slack: iachec.slack.com #calstats

iachec-calstat@cfa.harvard.edu

I. Main WG Session

Pileup, Methods, Cal uncertainties (MCCal, Athena)

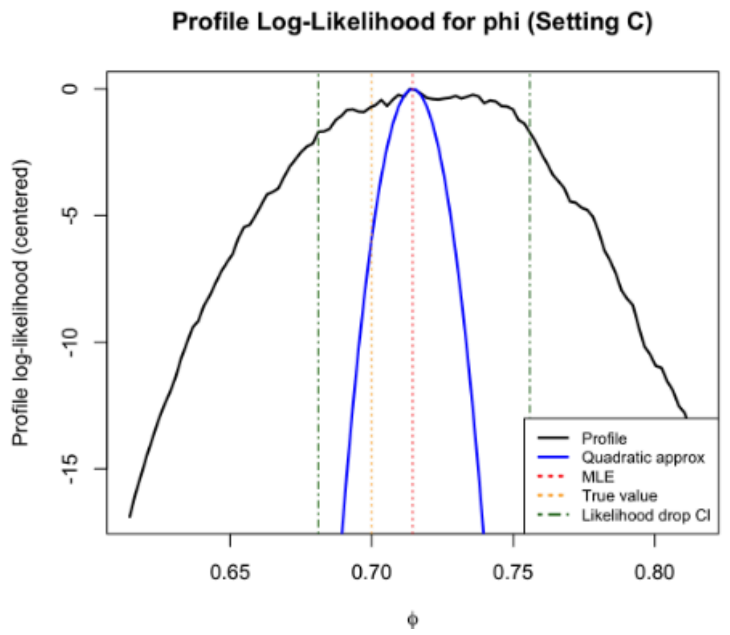
1. Pileup — Robert Zimmerman (Imperial)

ACIS Pileup via direct probability modeling

Account for grade migration, PSF, to fit spectral model shape

Key Modelling Idea

- Model the number of piled-up photons P_r in region r in one time frame as having a Poisson distribution
- Within a given region r and time frame, let (g, c) be the observed grade-channel pair
- We marginalize over all possible photon configurations and energies:



$$\mathbb{P}_{\boldsymbol{\theta}}(G_r = g, C_r = c)$$
$$= \sum_{p=1}^{\infty} \mathbb{P}_{\boldsymbol{\theta}}(G = g, C = c \mid P_r = p) \cdot \mathbb{P}_{\boldsymbol{\theta}}(P_r = p)$$
$$= \sum_{p=1}^{\infty} \int \mathbb{P}_{\boldsymbol{\theta}}(G_r = g, C_r = c \mid P_r = p, \boldsymbol{E}_{1:p} = \boldsymbol{e}_{1:p}) \cdot q_{p,\boldsymbol{\theta}}(\boldsymbol{e}_{1:p}) \, \mathrm{d}\boldsymbol{e}_{1:p} \cdot \mathbb{P}_{\boldsymbol{\theta}}(P_r = p)$$

- ...where $q_{p,\boldsymbol{\theta}}(\boldsymbol{e}_{1:p}) = \prod_{k=1}^{p} q_{\boldsymbol{\theta}}(e_k)$ is the joint density of the vector of p energies $\boldsymbol{E}_{1:p} = (E_1, \ldots, E_p)$

Setting	α	$\widehat{\alpha} \pm$ SE
A	0.70	0.71 $\pm$ 0.048
B	0.70	0.70 $\pm$ 0.025
C	0.70	0.77 $\pm$ 0.030
D	0.70	0.68 $\pm$ 0.022

Setting	θ	$\widehat{\theta} \pm$ SE
A	0.70	0.67 $\pm$ 0.005
B	1.50	1.63 $\pm$ 0.013
C	0.70	0.68 $\pm$ 0.006
D	1.50	1.63 $\pm$ 0.017

Setting	ϕ	$\widehat{\phi} \pm$ SE
A	1.00	(fixed)
B	1.00	(fixed)
C	0.70	0.69 $\pm$ 0.004
D	0.30	0.28 $\pm$ 0.008

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Book chapter

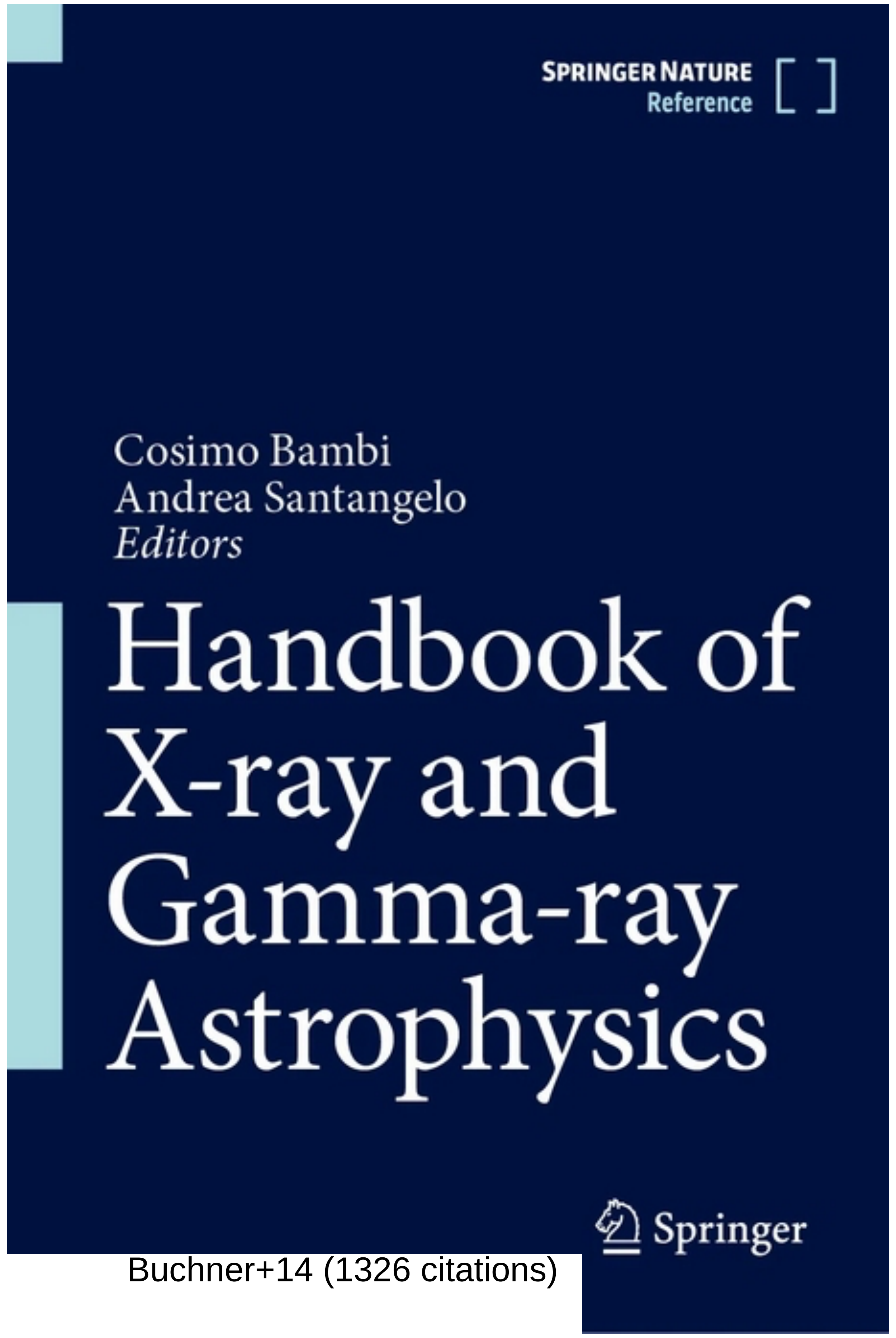
Statistical Aspects of X-ray Spectral Analysis

Johannes Buchner & Peter Boorman

freely available at:

https://arxiv.org/abs/2309.05705

includes hands-on exercises
for both sherpa & xspec



Buchner+14 (1326 citations)

Idea: make
physical parameter inference &
model comparison
easy & practical

XMM2Athena
319,565 X-ray sources
processed (Webb+23)

parallelisation,
resuming
sophisticated, robust

inference engine

based on nested sampling

MultiNest
UltraNest

BXA

community models
fully-fledged
data formats

fitting
environment

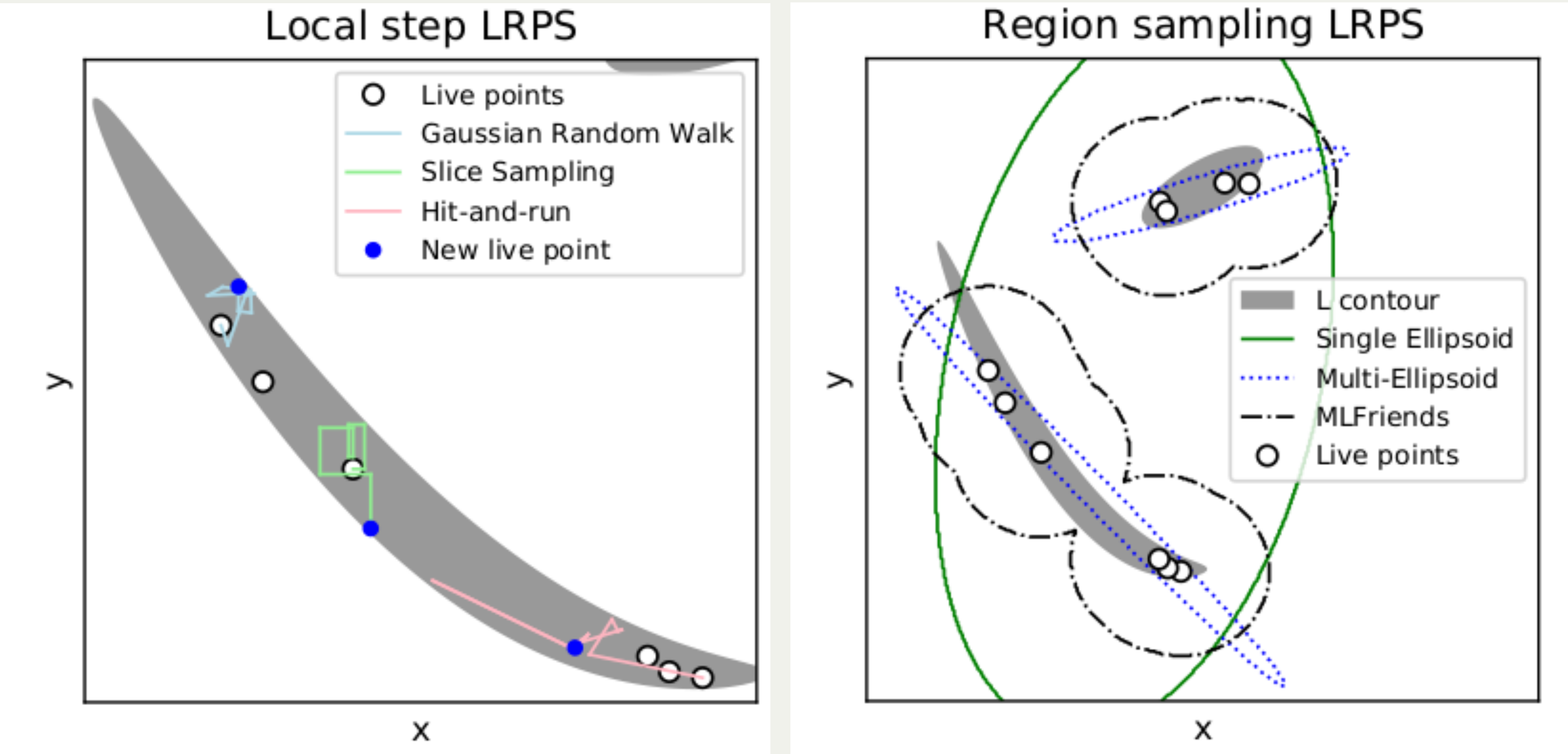
sherpa
pyxspec
(threeml)
(spex)

- Nested sampling &
  model comparison

Buchner (2022), Statistics Surveys

Missing ingredients

- MCMC: Insert tuned transition kernel
- NS: Likelihood restricted prior sampling (LRPS)
  - General solutions: MultiNest, MCMC, HMCMC, Galilean, RadFriends (UltraNest), PolyChord



Animation:
https://johannesbuchner.github.io/mcmc-demo/app.html#RadFriends-NS,standard
(via chi-feng.github.io)

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3. Calibration uncertainties
    a. MC Cal — Pete Ratzlaff, Jeremy Drake, Vinay Kashyap (CfA/CXC)

MC Cal — "a la Drake"

- What we have now is a github repository of the code to generate the samples at **https://github.com/pratzlaff/mccal**

- Easy to implement: just make a plain ascii file with edges and maximum allowed deviations

```
COMP1
emin1 eminsigma1 emax1 emaxsigma1 maxdiff1 edgemax1
emin2 eminsigma2 emax2 emaxsigma2 maxdiff2 ...
```

- Some mission-specific contacts to implement this: AstroSat (Gulab Dewangan), *New*Athena (Matteo Guainazzi), eROSITA (Konrad Dennerl), XMM (Anon 2021), NuSTAR (Kristin Madsen 2016), IXPE (Herman Marshall?), XRISM/Xtend (Shun Inoue & Hiroyuki Uchida), SVOM/ECLAIR (Laurent Bouchet), SVOM/GRM (Shijie Zheng), XRISM/Resolve, HXMT, NICER, Einstein Probe, NinjaSat, ...

- SOXS (John ZuHone?), SIXTE?

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    b. Science implications for Athena — Matteo Guinazzi (ESA/ESTEC)

Science implications for Athena — Matteo Guinazzi

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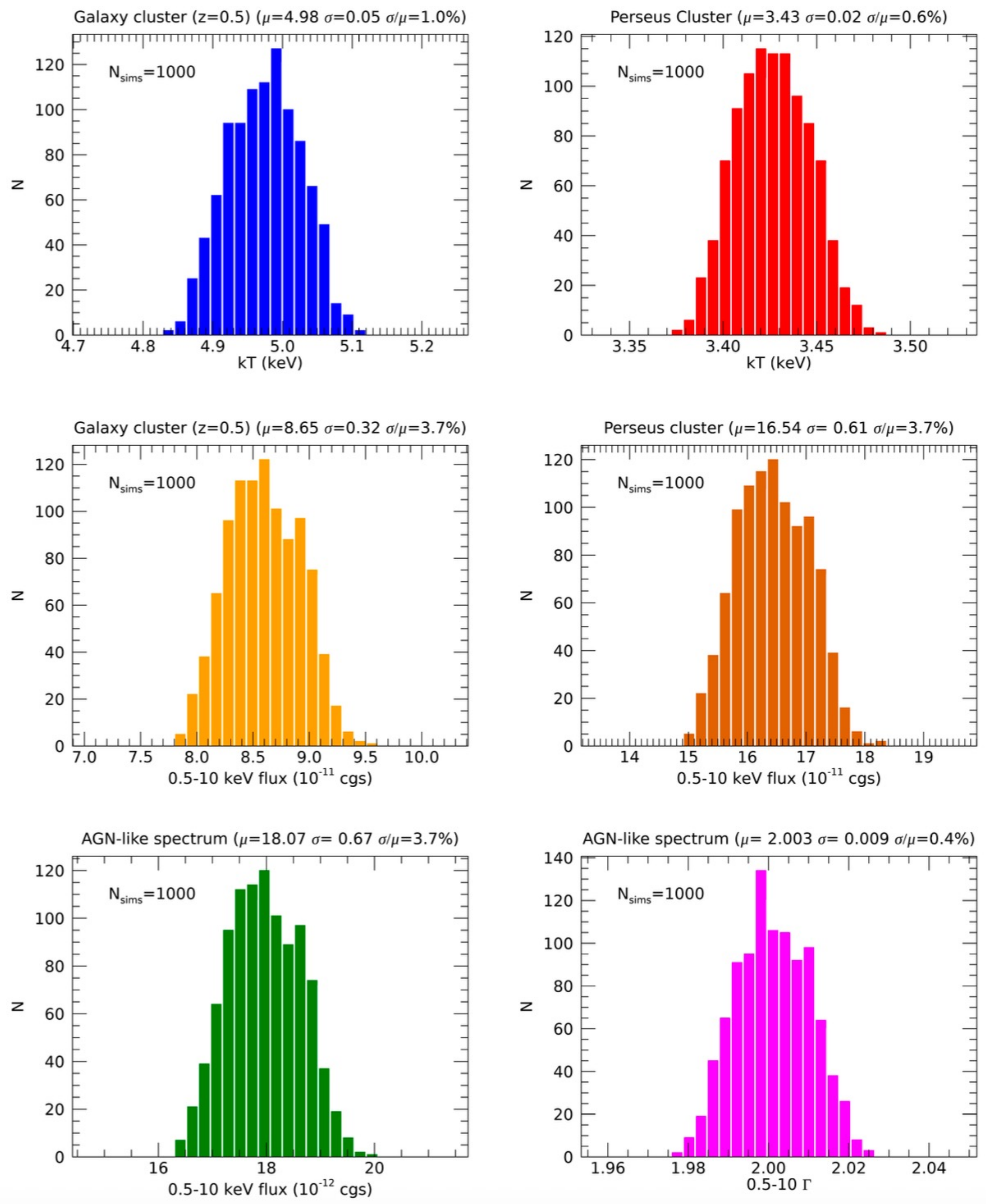
On the scientific impact of the uncertainties in the *Athena* mirror effective area

Matteo Guainazzi,[a,*] Richard Willingale,[b] Laura Brenneman,[c] Esra Bulbul,[d] Jan-Willem den Herder,[e] Erik Kuulkers,[a] Jan-Uwe Ness,[f] and Lorenzo Natalucci[g]

RESULTS: GALAXY CLUSTERS AND AGN SPECTRAL SHAPE

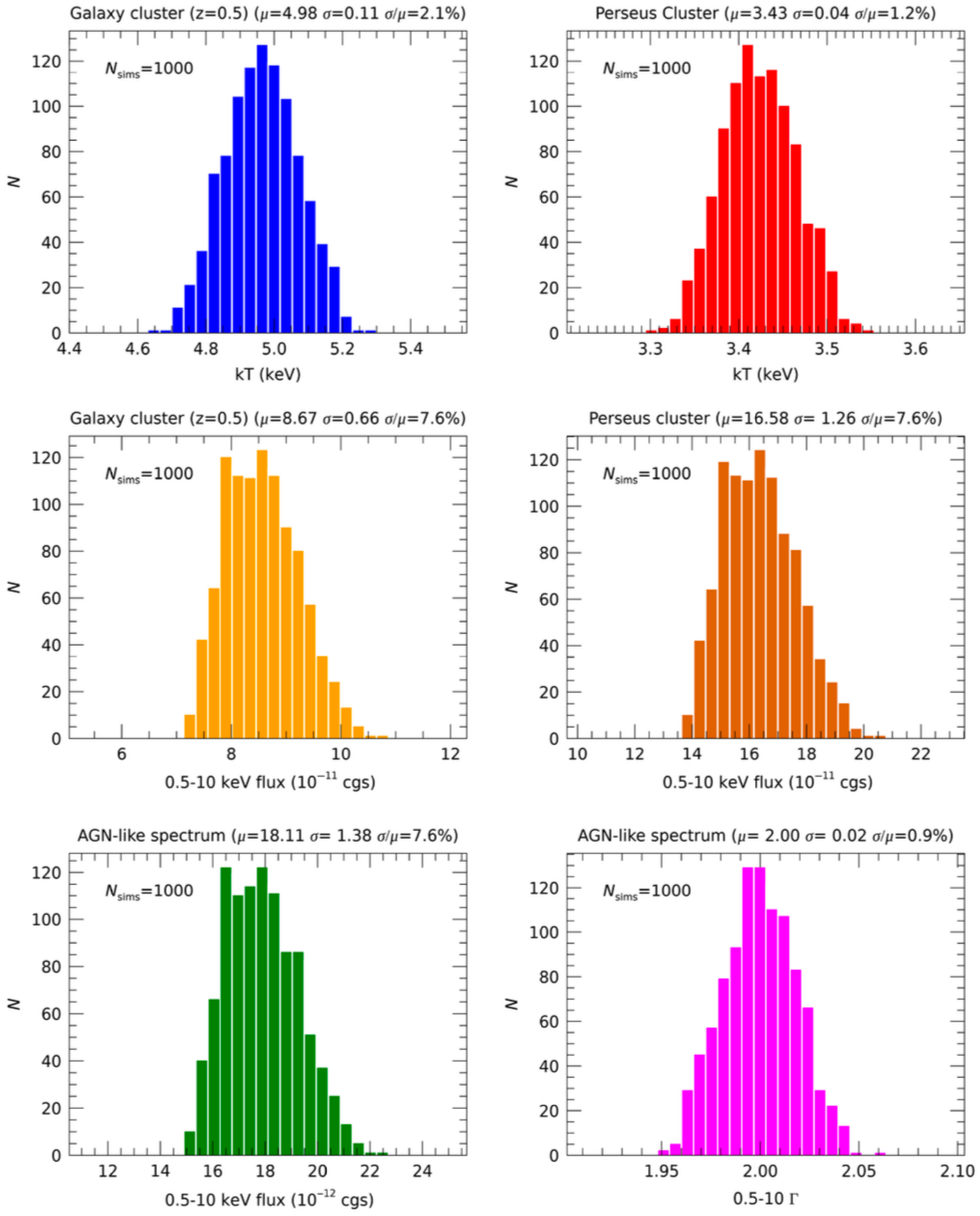


- Use the perturbed ARFs to simulate driving science objectives
- Calculate distributions of critical observables
- Compare to science requirements (critical observable accuracies)

Table 3 Standard deviations for the distribution of the critical observables.

Critical observable	σ	Verification criterion
σ_{kT}/kT (high-redshift cluster)	1.0%	$\leq$ 2%
σ_{kT}/kT (Perseus cluster)	0.6%	$\leq$ 2%
σ_F/F (high-redshift clusters)	3.7%	$\leq$ 6%
σ_F/F (Perseus cluster)	3.7%	$\leq$ 6%
σ_F/F (AGN)	3.7%	$\leq$ 6%
σ_Γ (AGN)	0.009	$\leq$ 0.008

WHAT IF WE OFFSHOOT THE CALIBRATION REQUIREMENTS?



The accuracy of (these) astrophysical observables scales ~linearly with the effective area calibration requirements

Critical observable	σ
σ_{kT}/kT (high-redshift cluster)	2.1%
σ_{kT}/kT (Perseus cluster)	1.2%
σ_F/F (high-redshift clusters)	7.6%
σ_F/F (Perseus cluster)	7.6%
σ_F/F (AGN)	7.6%
σ_Γ (AGN)	0.020

Violation!

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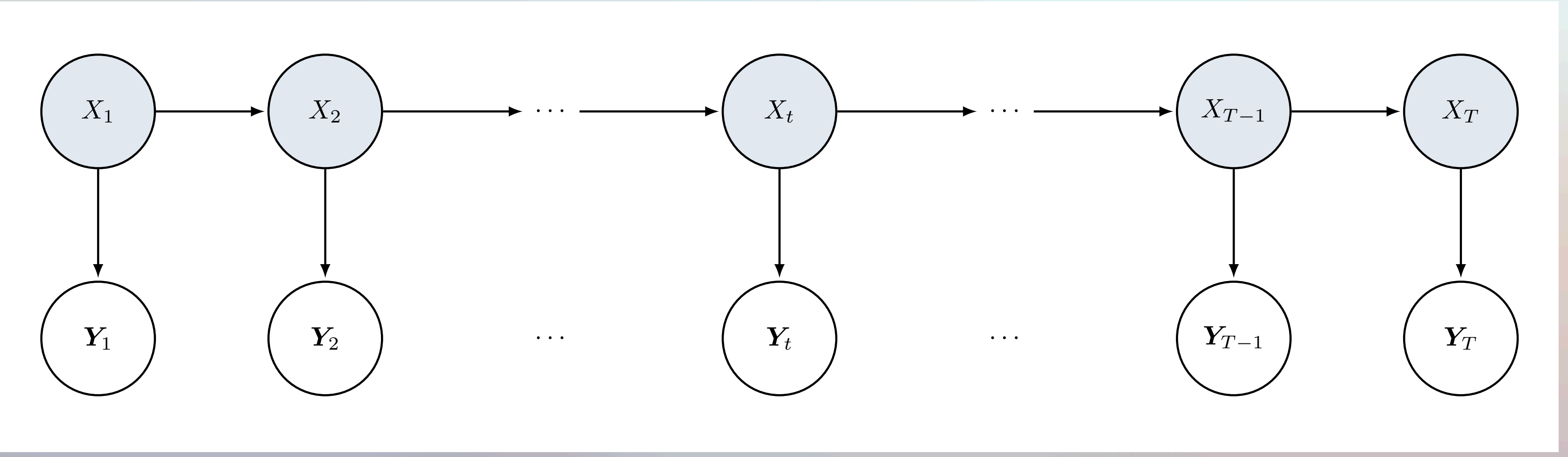
4. Future Directions (later!)

II. Hidden Markov Models

Tutorial by Robert Zimmerman Wed May 14 7:45pm-8:45pm

- HMMs are a way to incorporate changes in state that are manifested indirectly
- If you tie an observable to an underlying Markov state (e.g., could be as simple as intensity during a high or low accretion state, or plasma temperature during flaring or quiescence), you can model variations in the data as arising from changes in the hidden state, which greatly reduces the dimensionality of the problem and makes it more tractable
- Well suited to calibration problems because things constantly shift underfoot, and HMMs can provide a useful framework to handle changes
  - varying background (over time, over orbit)
  - drifts in detector characteristics (whether due to temperature or non-linearity of detector response)
  - ??



Hidden Processes in Real Data

- Real-world time series often exhibit abrupt or gradual changes in behavior that are driven by unobserved states (i.e., latent variables)

Astronomy: Flaring and quiescence in stellar X-ray light curves
- Latent variable: flare intensity or state

Ecology: Animal movement switching between foraging and resting
- Latent variable: behavioral mode

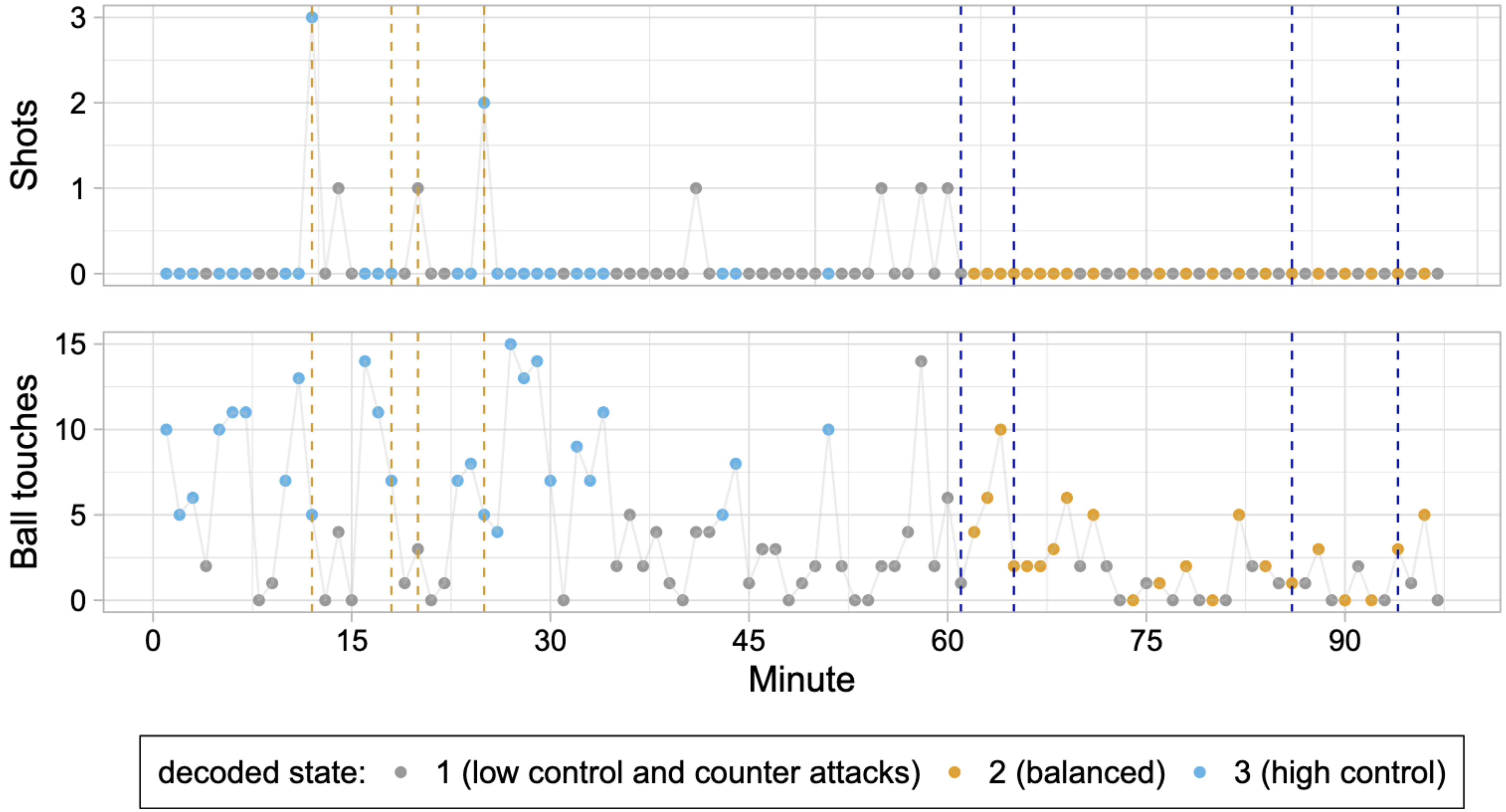
Finance: Stock returns alternating between volatility regimes
- Latent variable: market state

Bioinformatics: Coding vs. non-coding DNA regions
- Latent variable: genomic structure

Speech: Recognizing spoken units from acoustic signals
- Latent variable: spoken unit

- [Ötting et al., 2023] fit a 3-state HMM to the data, with state classifications shown below

- The vertical dashed lines show goals scored by Borussia (yellow lines) and Schalke 04 (blue lines)



Example: Flaring Behaviour on EV Lac

- [Zimmerman et al., 2024] use a univariate Poisson state-space model to the capture flaring behaviour

- The latent Markov chain $\{X_t\}$ evolves as an AR(1) process:

$$X_t = \phi X_{t-1} + \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2)$$

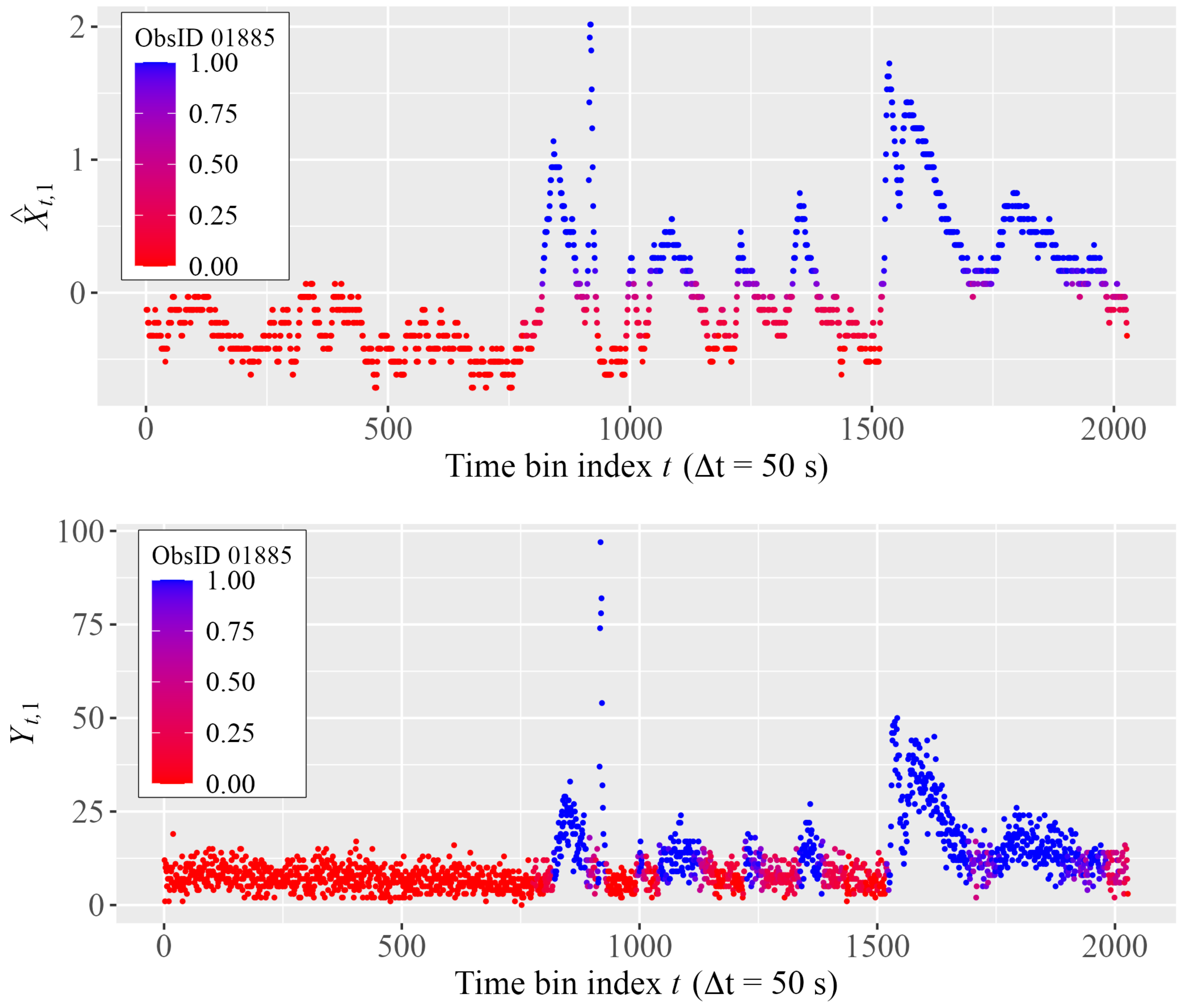
- The observed process $\{\boldsymbol{Y}_t = (Y_{t,1}, Y_{t,2})\}$ is a 2-tuple of soft and hard band X-ray photon counts:

$$Y_{t,h} \mid X_t = x_t \sim \text{Poisson}(w \cdot \beta_h \cdot e^{x_t}), \quad h = 1, 2$$

- Smooth transitions in $\{X_t\}$ capture variability in flaring activity as manifested in $\{\boldsymbol{Y}_t\}$

EV Lac: Flaring and Quiescence

- The fitted mixture model above allows us to estimate the "probability" of flaring for each observation:



III. Concordance

Thursday May 15 3:00-3:20pm — Herman Marshall

- Updates since IACHEC 16
  - Dealing with outliers
  - The τ's need fine tuning
- Send updated τ_{EA} and τ_{gain} to Herman (hermanm@mit.edu) or me (vkashyap@cfa.harvard.edu)

#finally Future Directions

- Difficulties with high spectral resolution (large RMFs)
- Codifying sampling of systematic calibration errors (J.Drake+)
- Concordance (S.Das+, H.Marshall+)
- Cstat (M.Bonamente, Y.Chen+)
- Pileup (R.Zimmerman+, J.Yang+)
- Machine Learning tools and techniques for calibration — if you have projects and/or ideas, contact Ivan at ivan.valtchanov@ext.esa.int
- RMF rescaling? HMM? Atomic data uncertainties? Background modeling?