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ASTROPHYSICS

HARVARD & SMITHSONIAN

ASTROAI

The Chandra Source Catalog as Legacy Product for Machine Learning Discovery in High Energy Astrophysics

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CfA/AstroAI

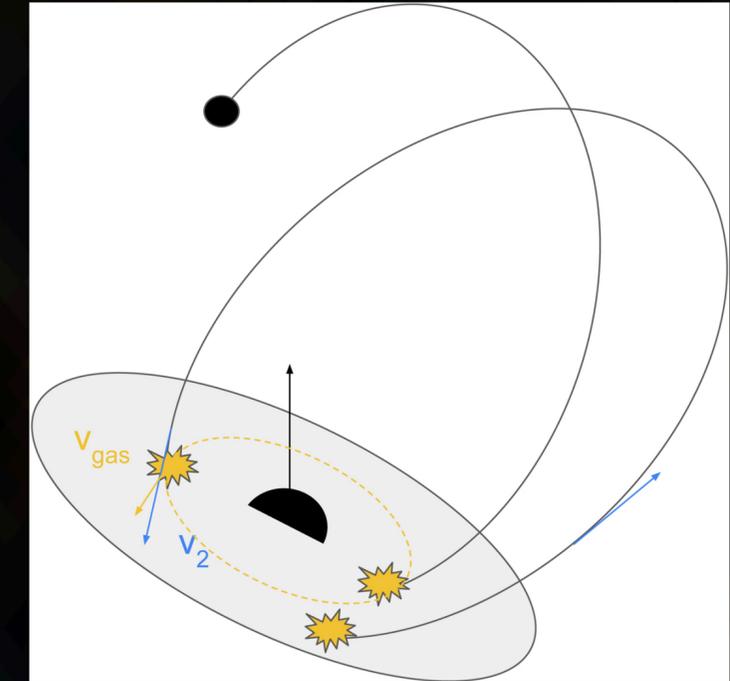
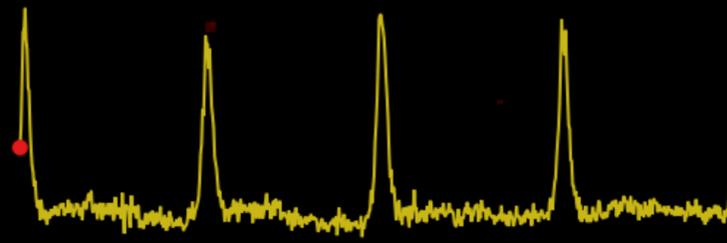
CfAO Workshop, U. Mass Lowell, May 2025



Quasi-Periodic Eruptions

Miniutti et al. 2019, Arcodia et al. 2021, Chakraborty et al. 2021

GSN 069



Franchini et al. 2023

- X-ray QPEs are puzzling eruptions associated to the nuclei of nearby galaxies. Their soft (thermal), repeating bursts appear associated with Tidal Disruption Events.
- The ones above happen every 9 hours. The host is a Seyfert 2 galaxy at $z=0.018$
- Possible explanations: Mass transfer? Gravitational Lensing? Collisions between orbiting compact object and accretion disk?

These findings have been serendipitous and have started whole new lines of research

X-ray datasets are a fertile ground for the discovery of astrophysical objects that inform models of gravitational wave emission, extrasolar planet, and the most violent explosions of the Universe.

How do we efficiently harvest X-ray catalogs to enable new science?

A fundamental transformation

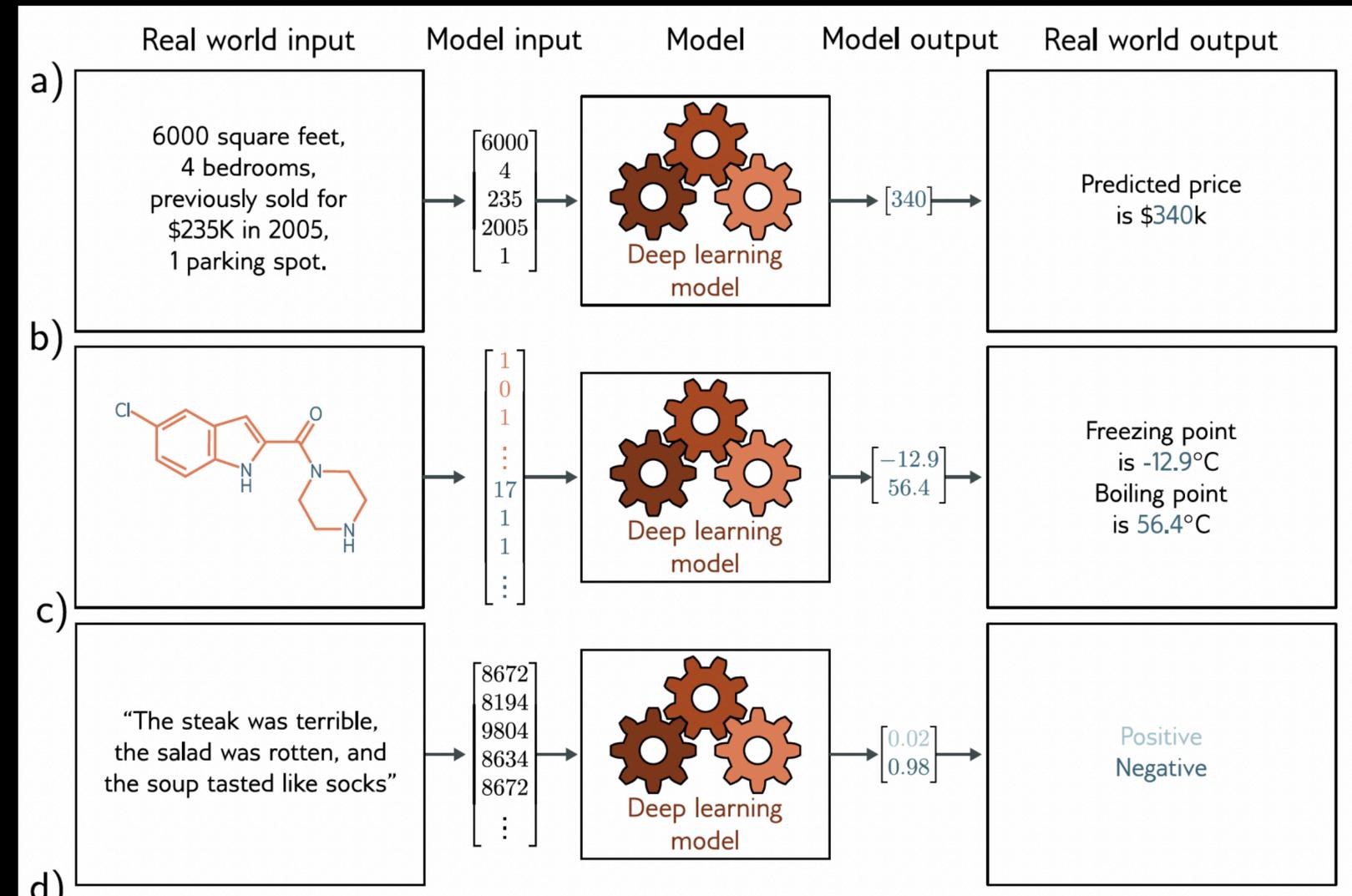
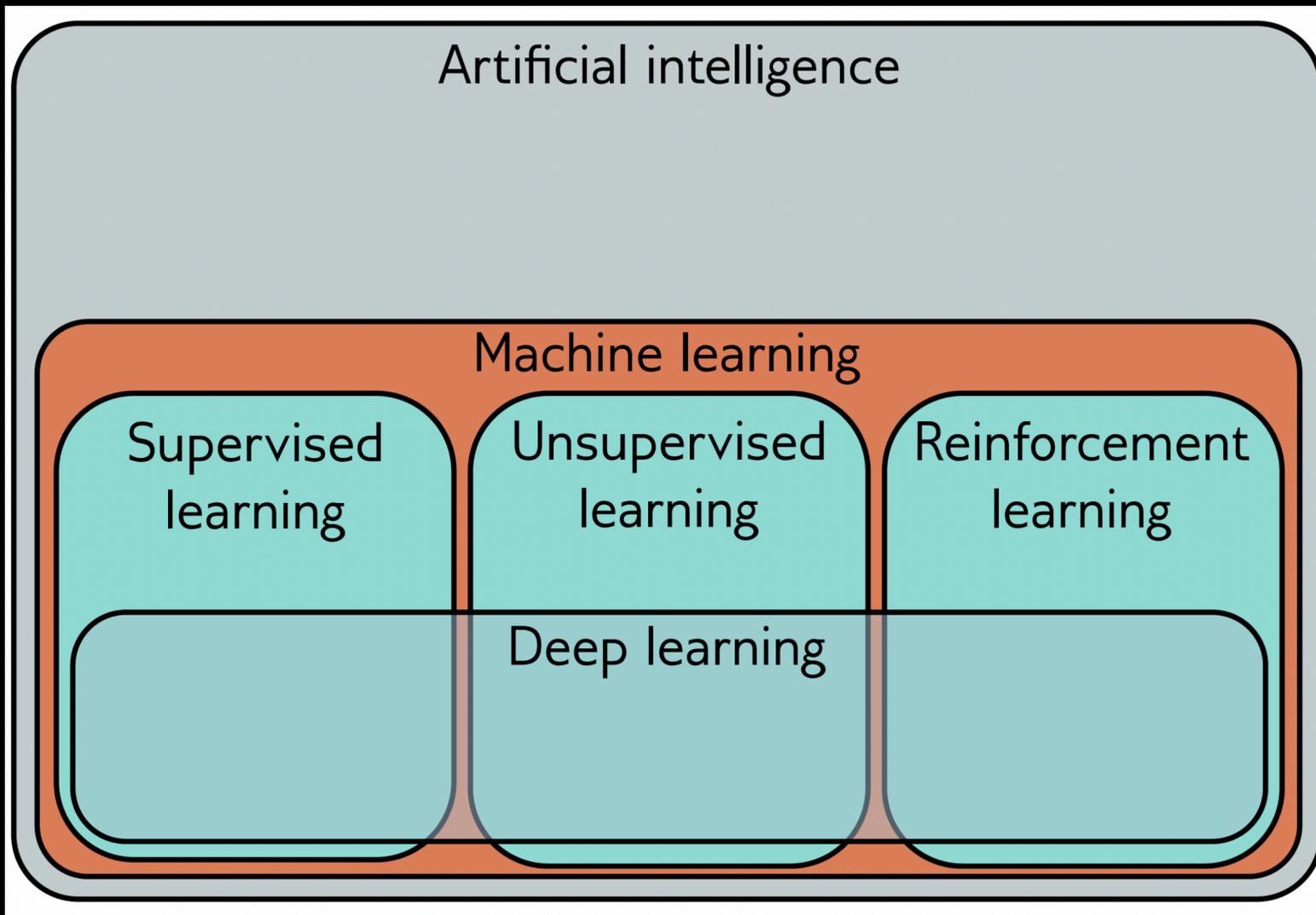
Over the last ~10 years, machine learning has transformed astrophysics research in at least two ways:

1. By improving the efficiency at which astrophysical objects can be found and classified in large surveys, including in X-ray datasets.
2. By speeding up the inference of model parameters, for example when performing X-ray spectral fitting. [Bayesian treatment](#).

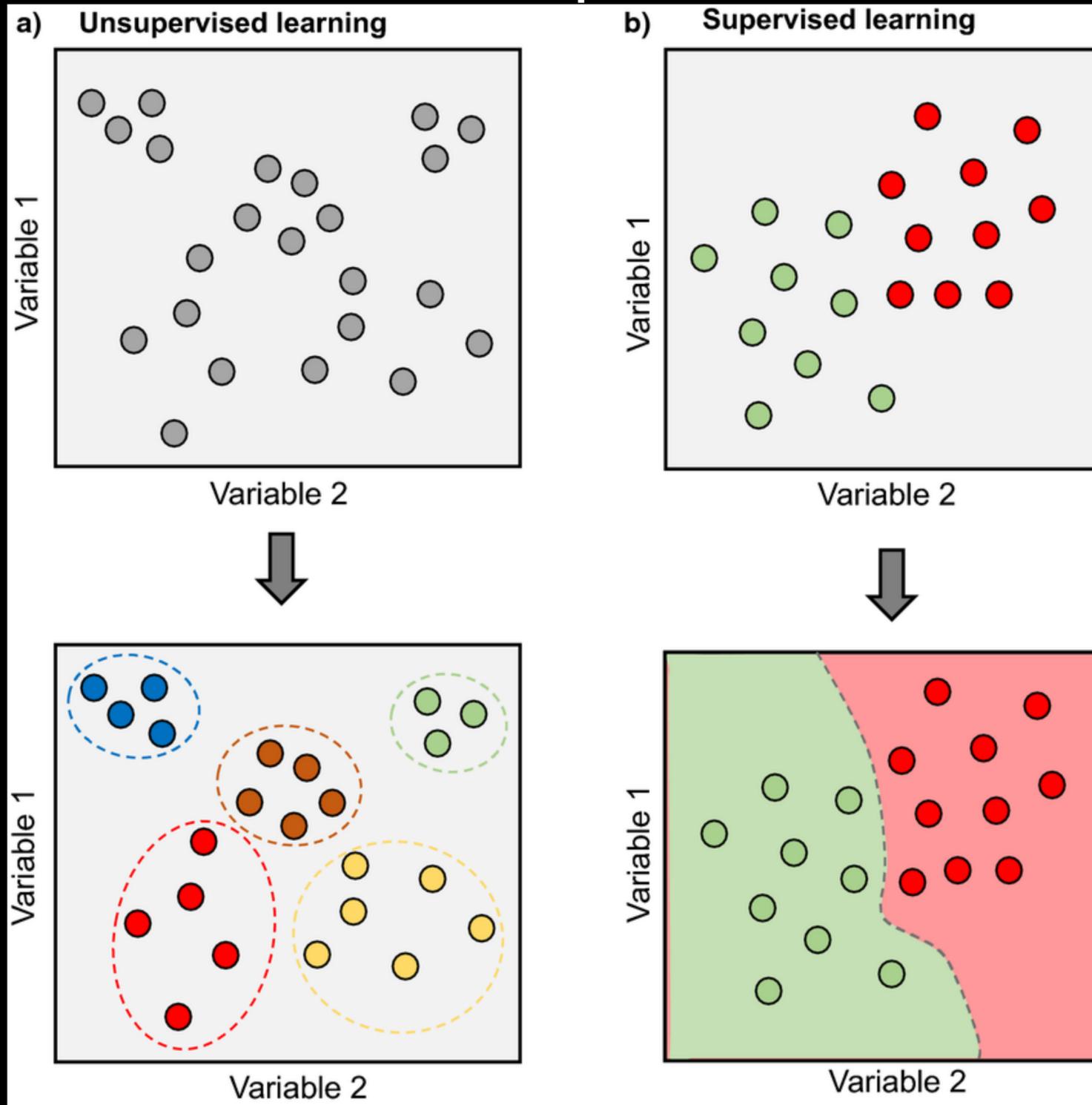
Are the simulations on which we train ML algorithm realistic enough?

Can we effectively use neural networks to recover full posteriors for relevant parameters?

What is machine learning anyway?



Supervised vs. Unsupervised

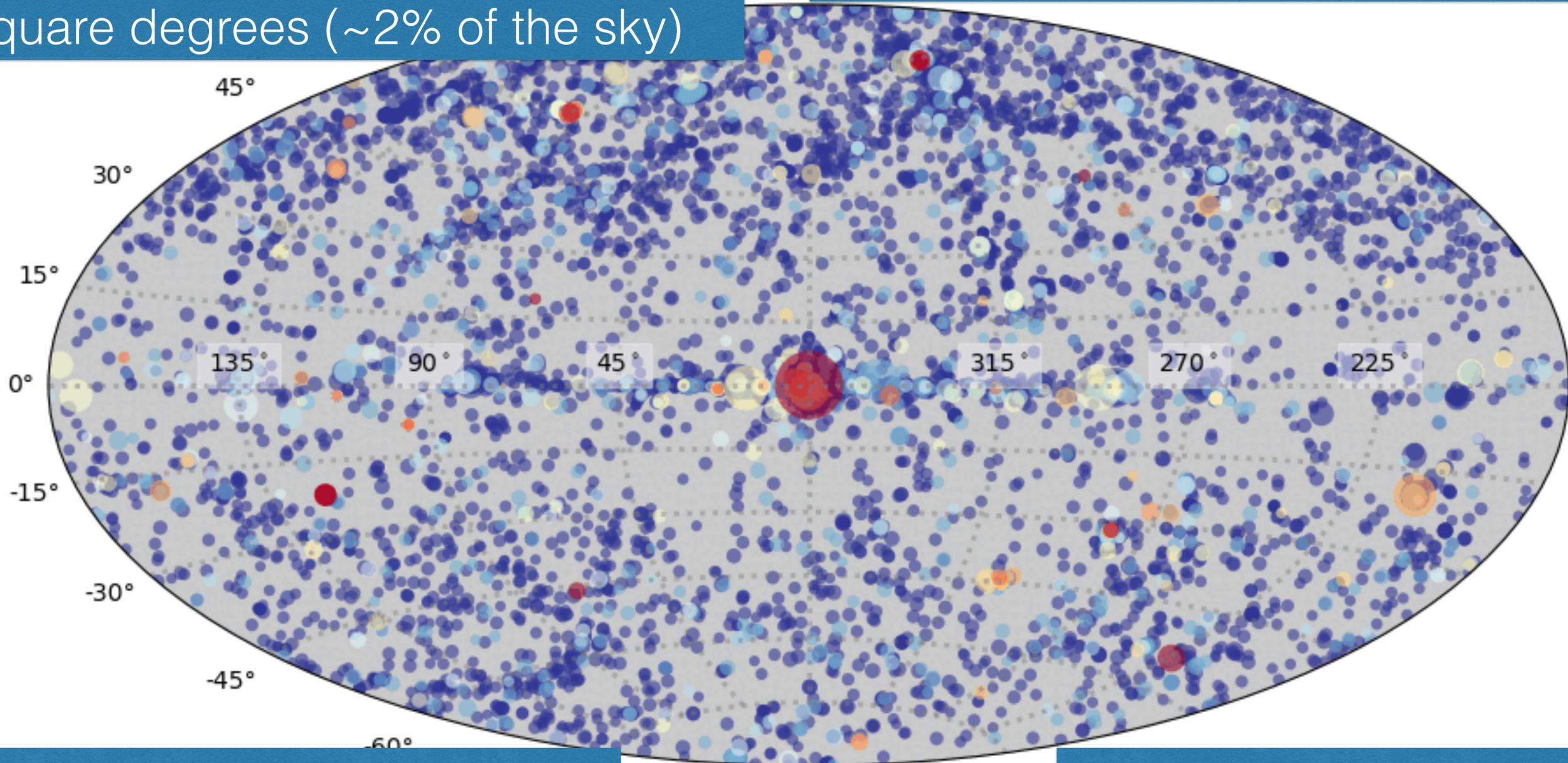


1. In unsupervised learning, we try to learn the function that describes the probability of the data, we do not have a GROUND TRUTH.
2. In supervised learning, we try to learn the probability of a label, given the data, the function that maps inputs to labels. We do have a GROUND TRUTH.

The Chandra Source Catalog Version 2.1

~408k (~93k+) individual sources in the sky
~1.3 million individual detections
~730 square degrees (~2% of the sky)

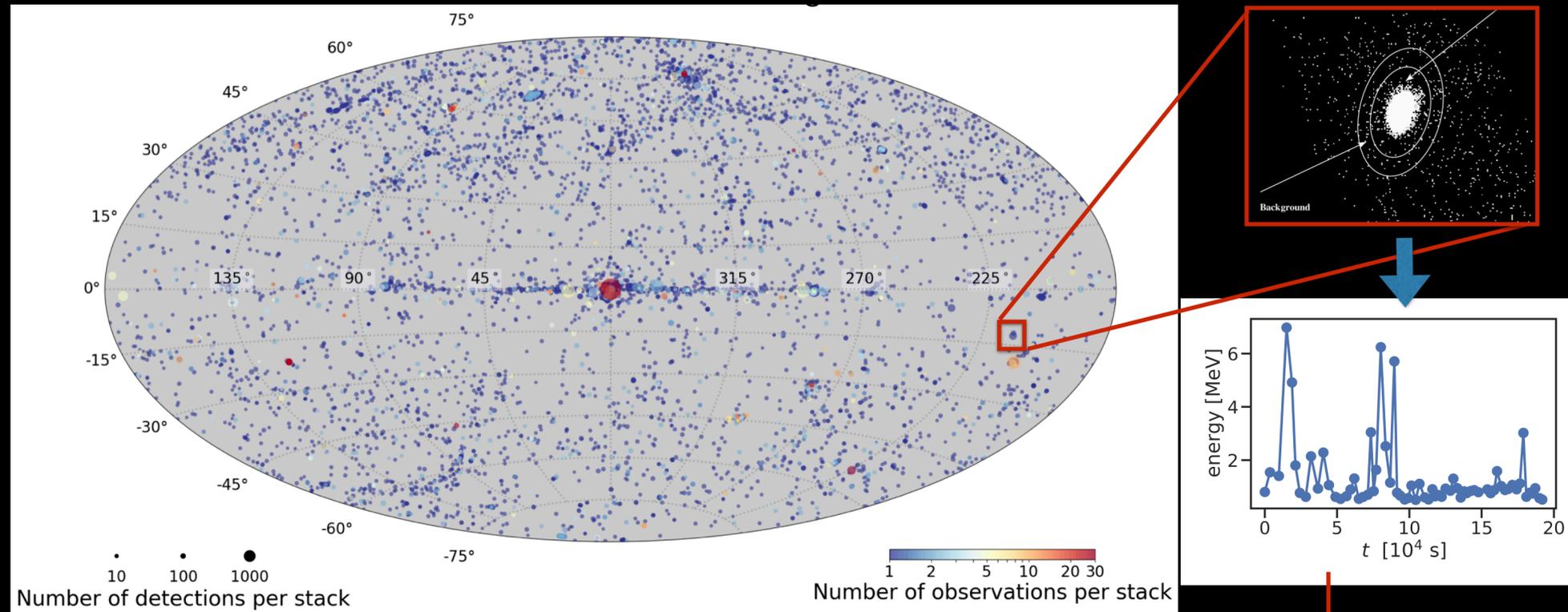
~15.5k individual Chandra Observations
Detection performed on stacked observations



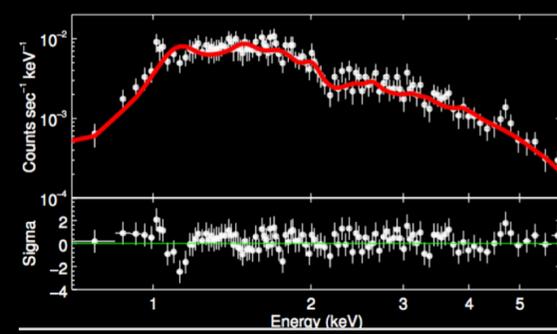
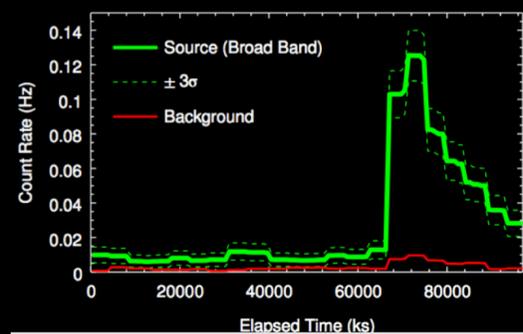
Astrometry tied to the GAIA reference frame. $\epsilon = 0.29''$ (95% conf.)

~36k SDSS counterparts provided
+ ~17k with SDSS spectra

The building block of any X-ray survey are lists of individual photon detections



- Unlike optical data, X-ray detections are a collection of individual photon recordings of different length.
- These events effectively constitute a time series of photon energies, from which light curves and spectra are obtained.
- All relevant physical information is ultimately contained in the event list.
- No automatic alert system exists for serendipitous transients in Chandra, XMM exists.

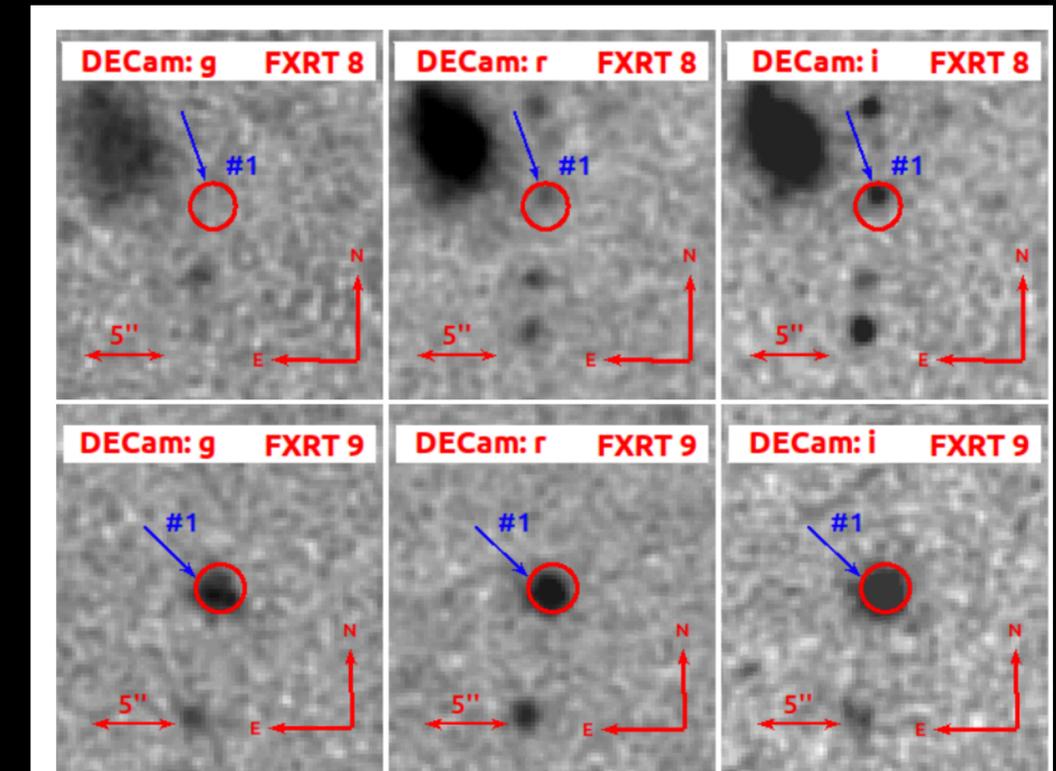
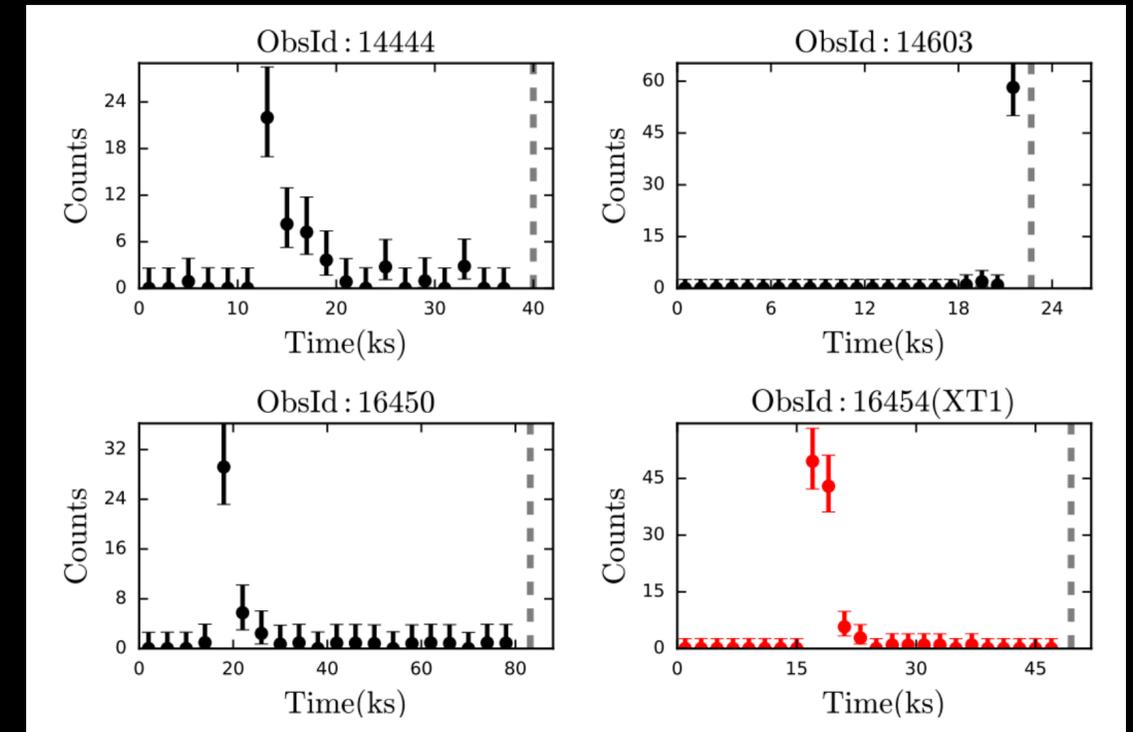




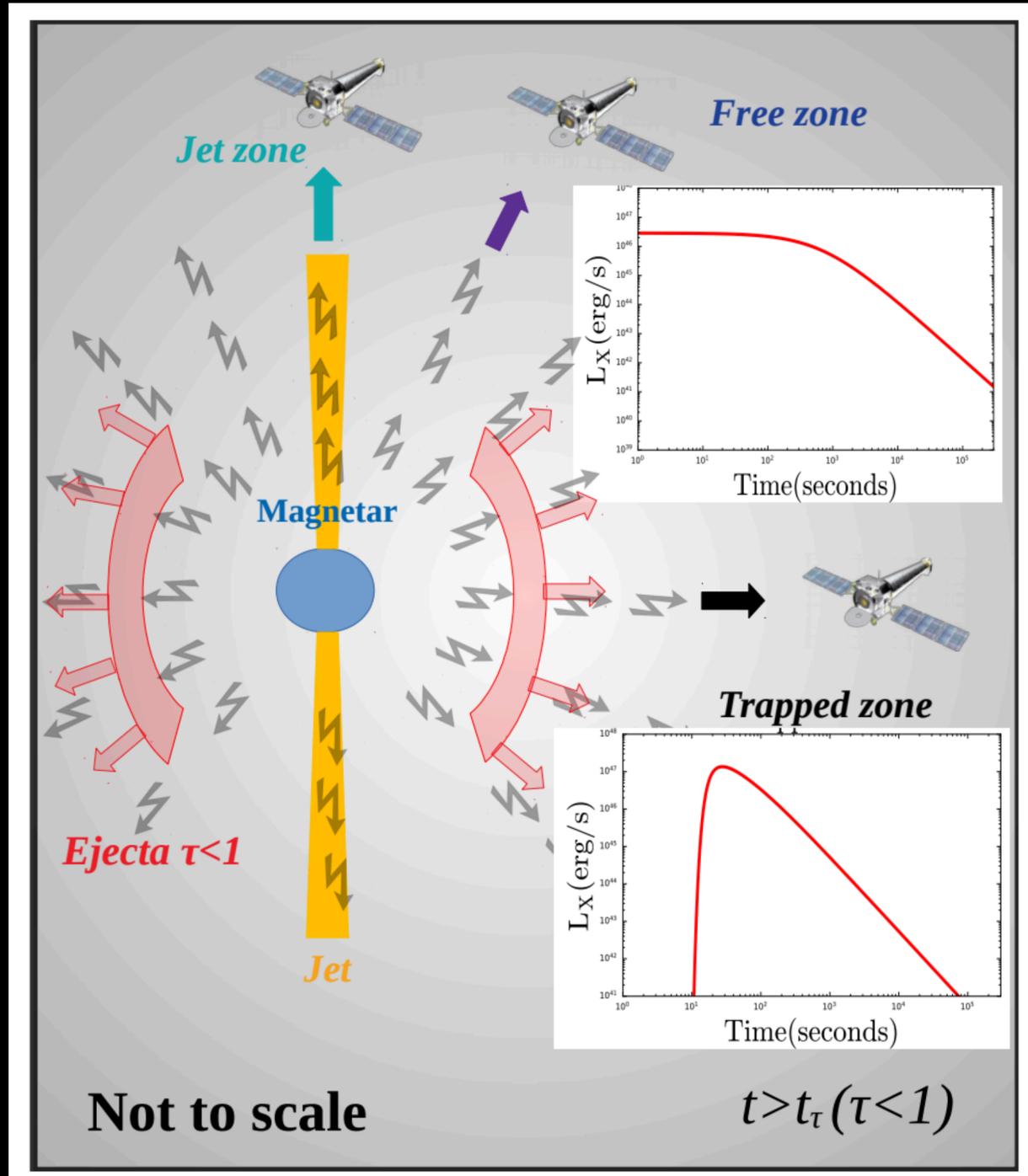
Time-Domain and Multi-Messenger Science

Fast X-ray Transients (FXTs)

- Fast X-ray transients are rapid bursts of X-ray emission typically located in extragalactic environments.
- Spectrally soft, lasting between a few minutes to hours. Typically discovered serendipitously, days to years after the bursts. Optical counterpart are rare, but a third of the ~35 known cases are associated with host galaxies.
- What is their origin?
 - Shock breakout emission in core-collapse supernovae
 - TDE: Accretion of part of a white dwarf into an IMBH.
 - BNS mergers: fallback accretion, magnetar related?
- Dedicated search in CSC using unbind light curves. Methods are limited in time resolution.

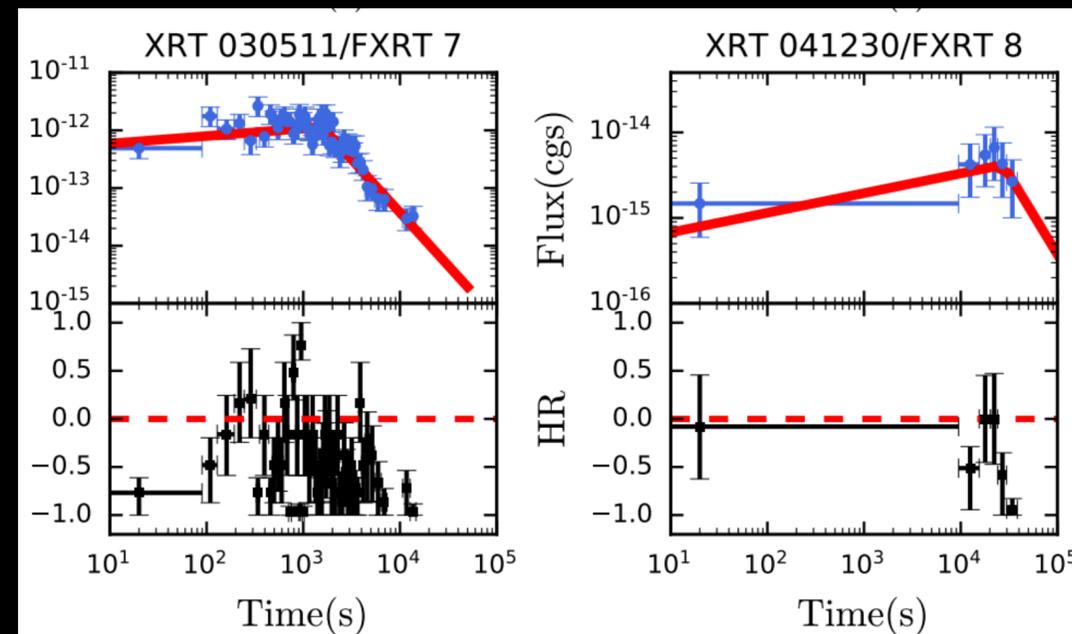


A possible magnetar origin for FXTs

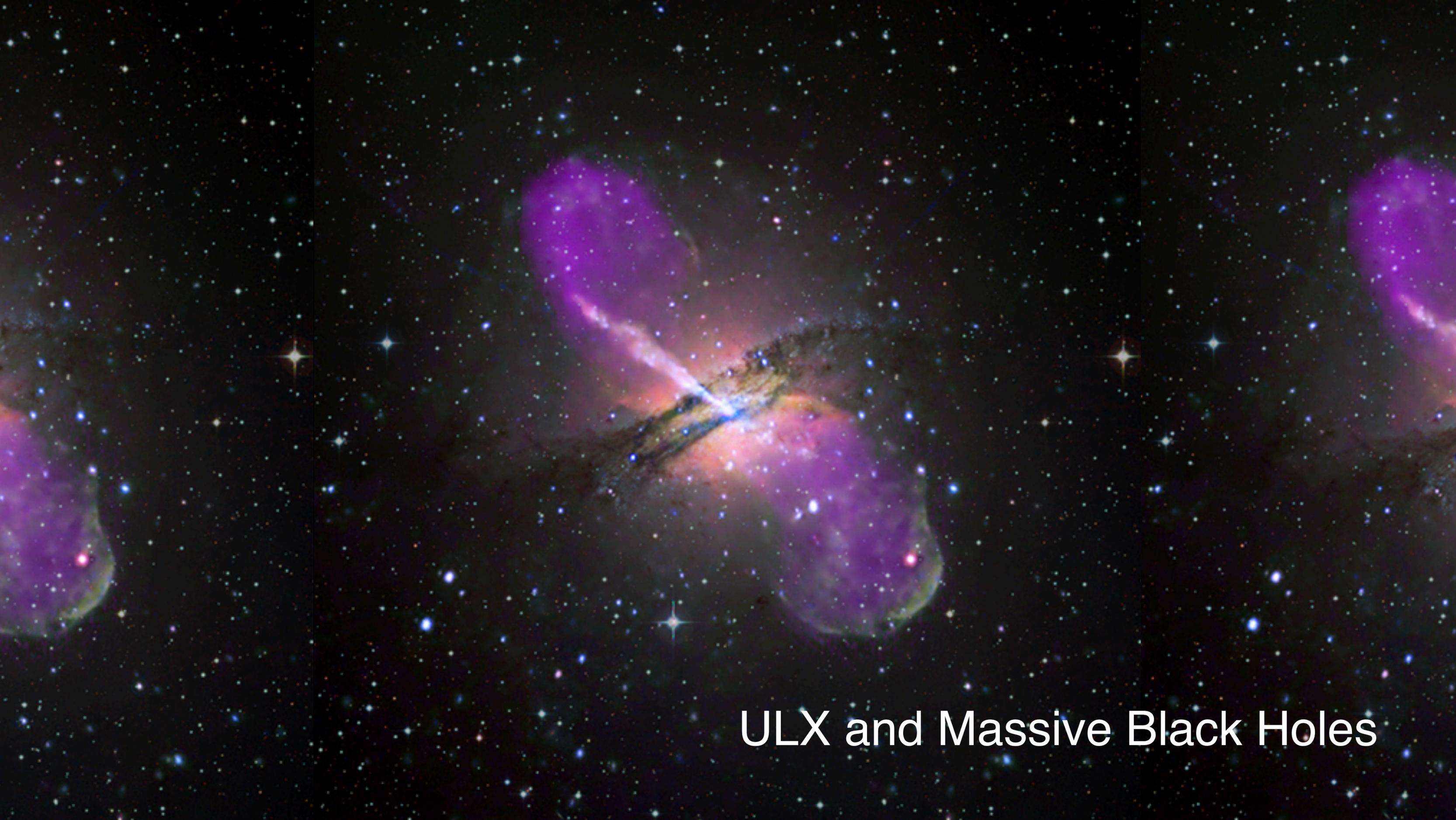


Quirola-Vásquez et al.

- BNS mergers resulting in a massive rapidly spinning magnetar produce X-ray afterglows with higher solid angles compared to the sGRB (Zhang 2013).
- Such afterglows can be used to probe EM counterparts to GW events that lack a γ -ray counterpart, and to search for massive millisecond magnetars.
- Light curve profile consistent with spin down luminosity of a rapidly spinning magnetar (e.g. Xue et al. 2019).



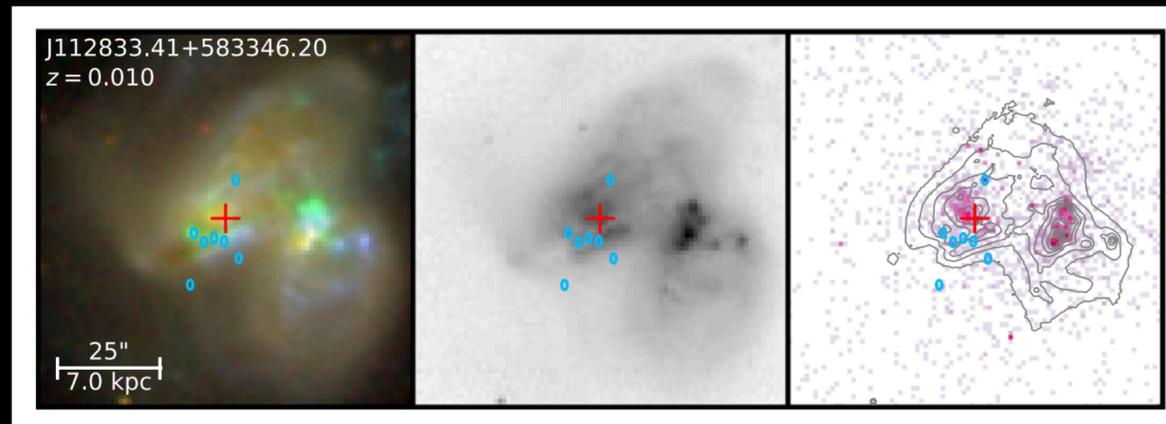
Several candidates identified in CSC dedicated searches.



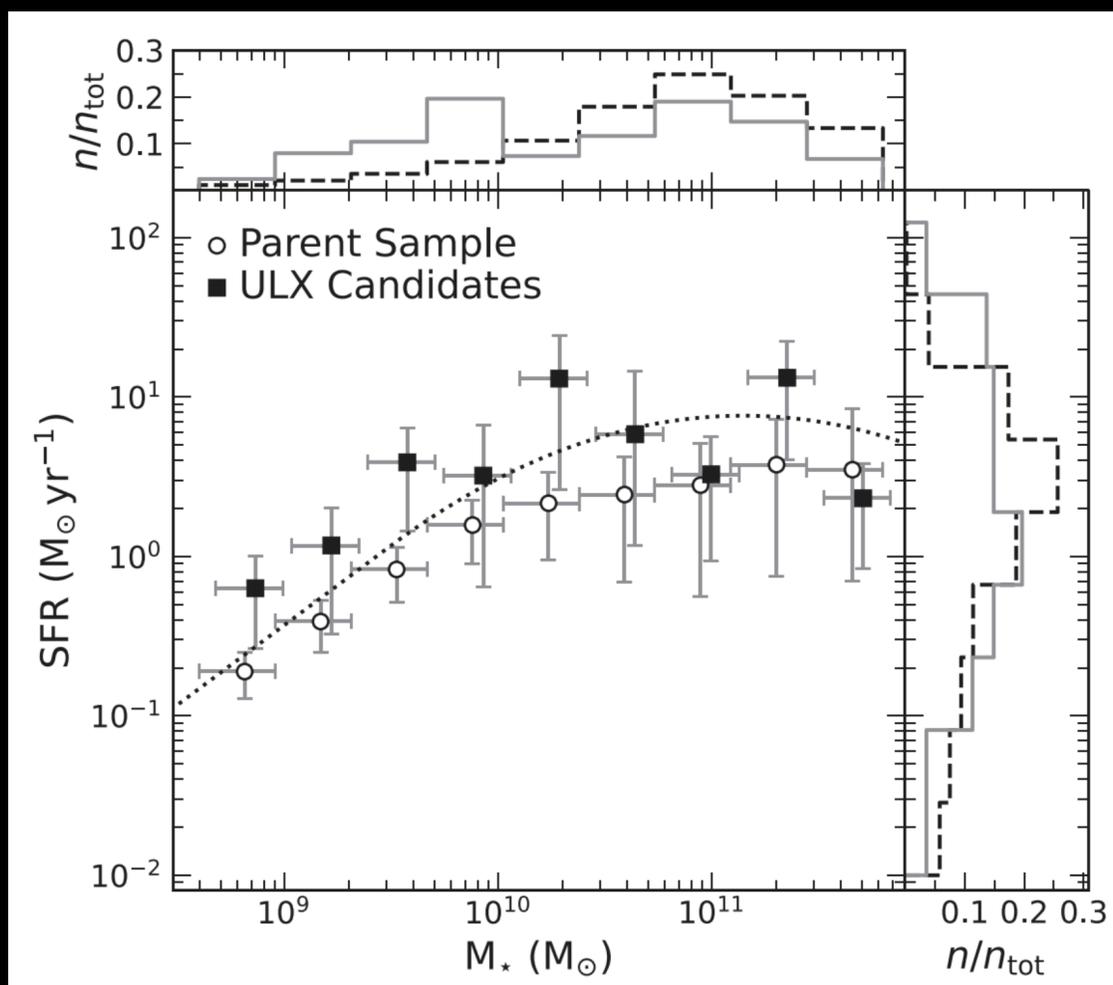
ULX and Massive Black Holes

The redshift evolution of ULXs out to $z \sim 0.5$

(Barrows et al. 2019, 2022)



- ULXs ($L_x > 10^{39}$ ergs/s) and HLXs ($L_x > 10^{41}$ ergs/s) appear to accrete above the Eddington limit.
- Uniform sample of ~ 260 off-nuclear ULXs with redshifts $z < 0.5$

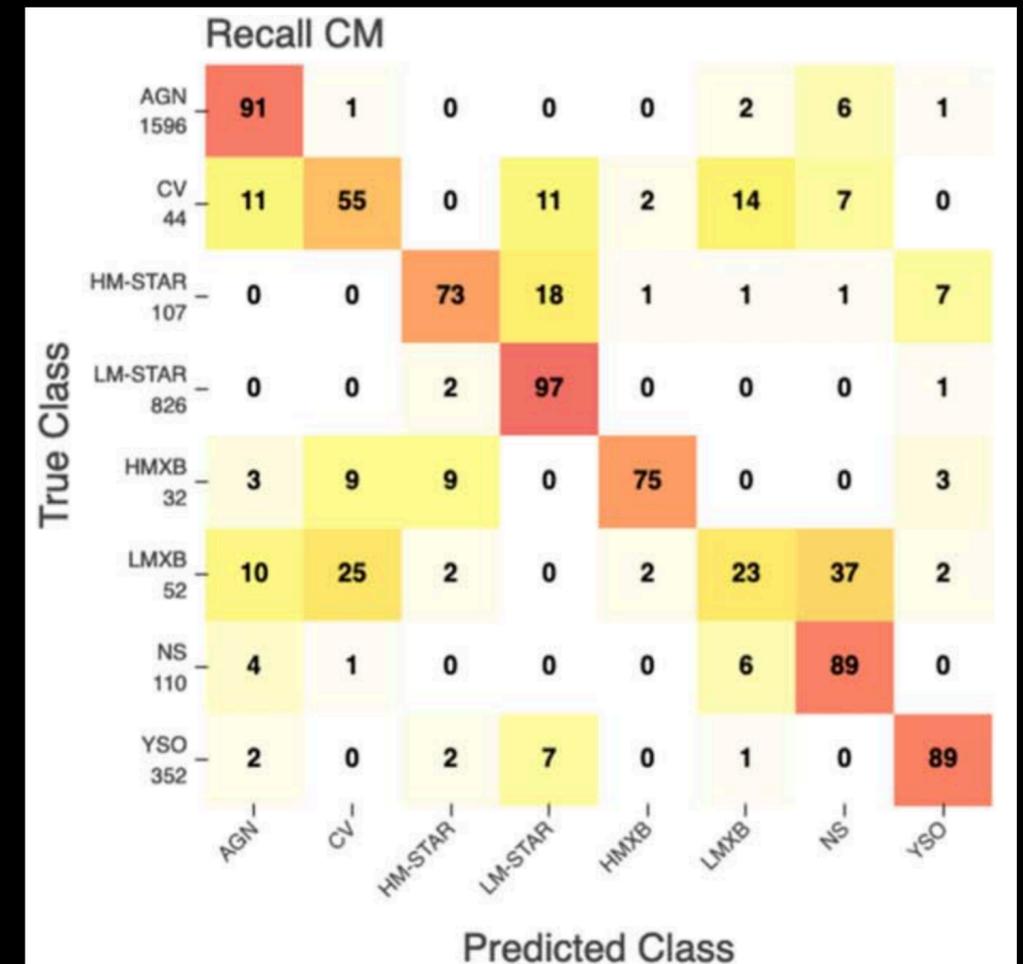


- Largest sample of intermediate redshift ULXs, extends to higher redshifts with respect to other catalogs.
- Systematically enhanced sSFR in ULX host galaxies compared with the parent population, suggesting an X-ray binary nature for the ULXs.
- Similar study of HLXs finds that fraction of them are consistent with IMBHs injected into galaxies through mergers (not in GCs).

CSC enables spatially resolved studies of ULX and HLX hosts!

Why machine learning in high energy astrophysics

- X-ray datasets are becoming larger and richer, but they remain unlabeled and unannotated. The vast majority of sources remain unclassified.
- Astrophysical anomalies of relevance for gravitational wave science, binary evolution, and galaxy assembly continue being identified in archival datasets, mostly serendipitously.
- Parameter inference in the presence of instrumental effects, such as pileup, remain challenges. Data-driven approach offer a way forward.



See research by the Kargaltsev group at GWU:
Yang et al. 2022, 2024, Chen et al. 2023, 2024,
See talk by Jeremy Hare

Unsupervised Classification using Gaussian Mixtures

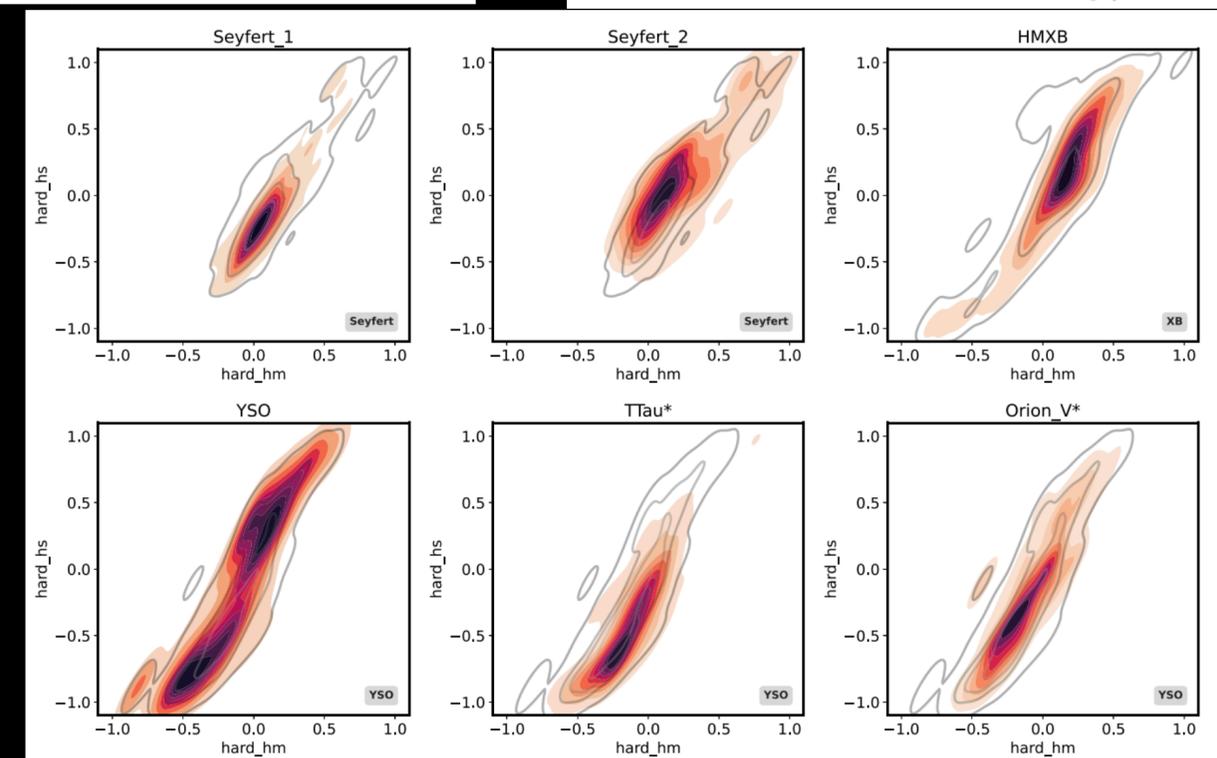
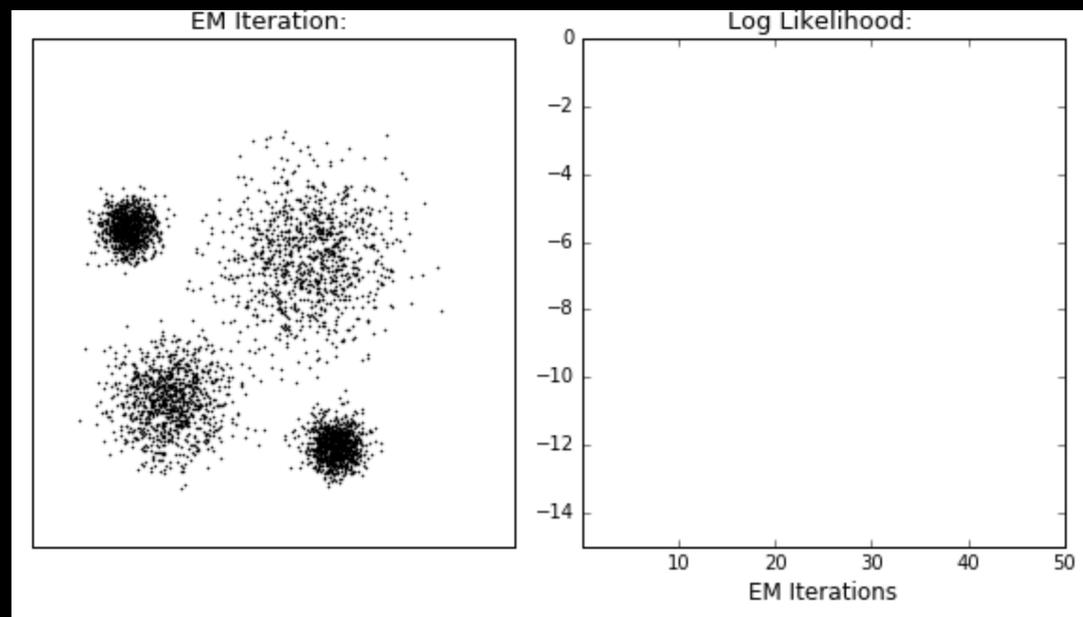
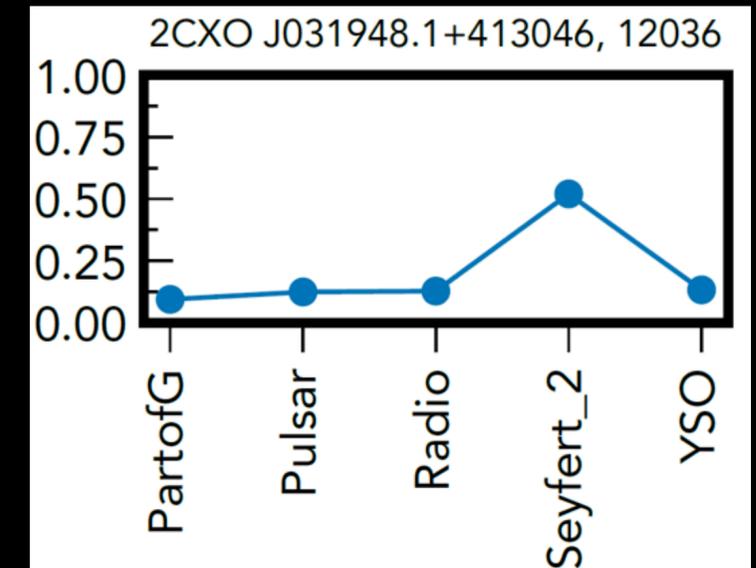
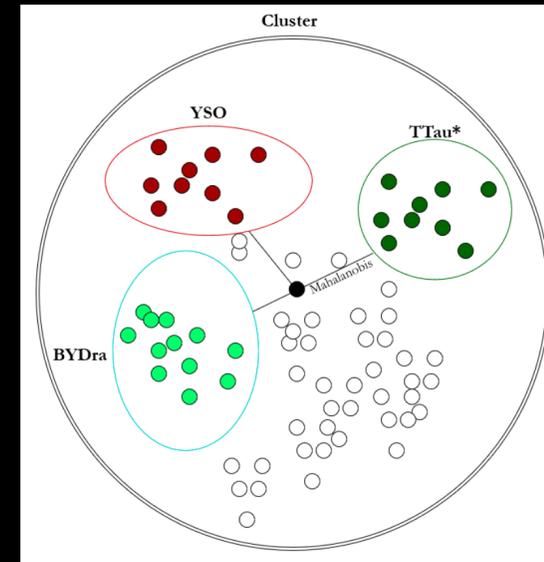
Pérez-Díaz et al.
2024MNRAS.528.4852P

By crossmatching the clusters with existing catalogs of independent classifications, we assign probabilistic classes based on distance

CSC Properties:

- Hardness ratios
- Variability
- Fluxes

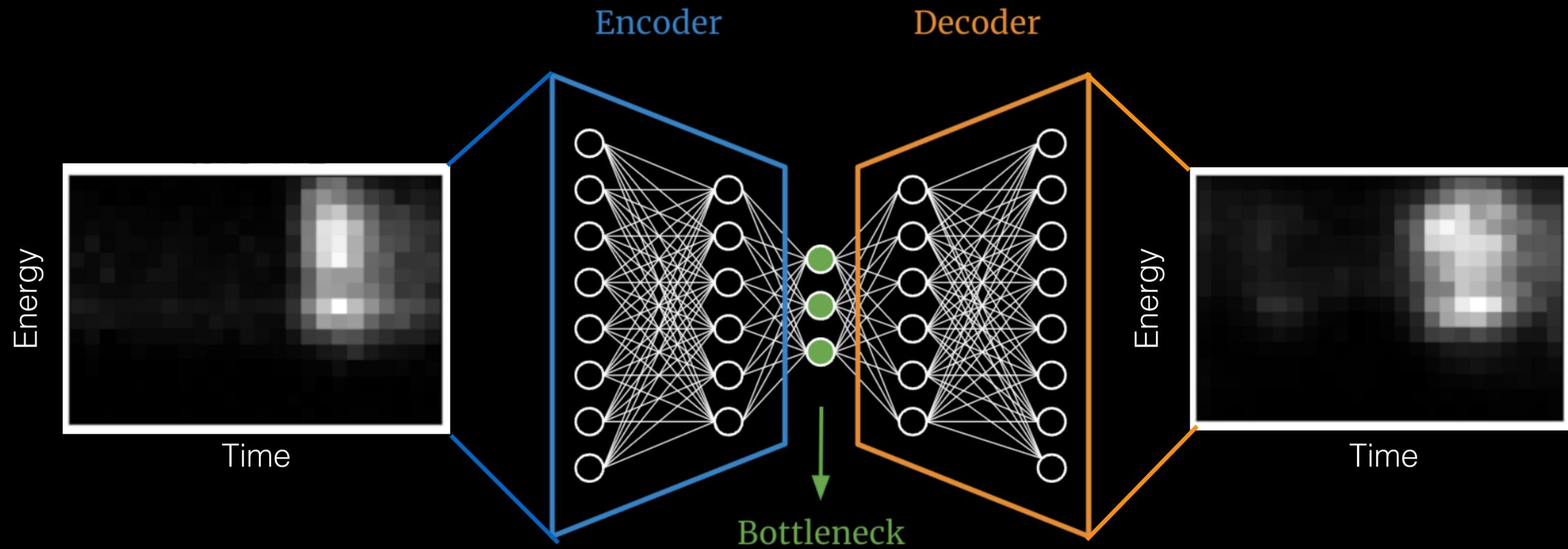
Published Catalog
of >15k probabilistic
Classifications



CLUSTERS

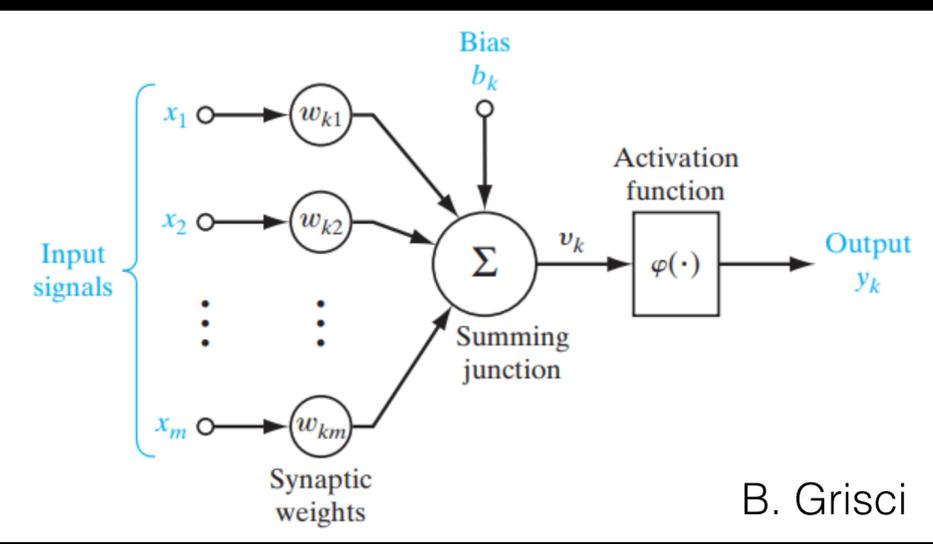
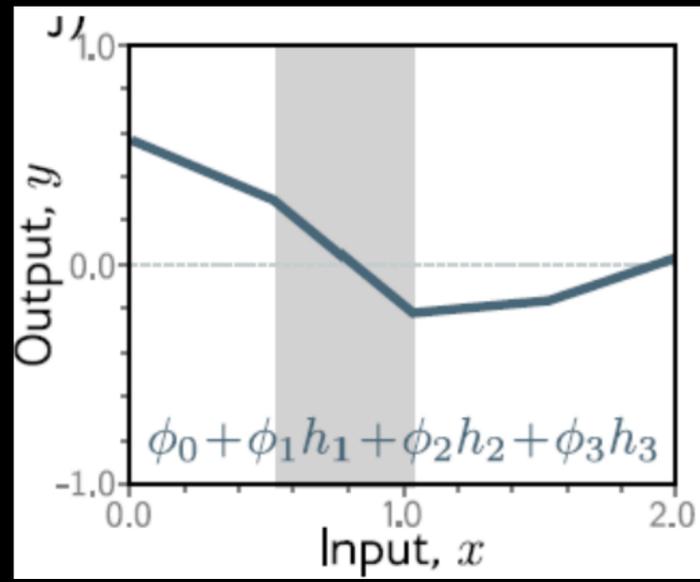
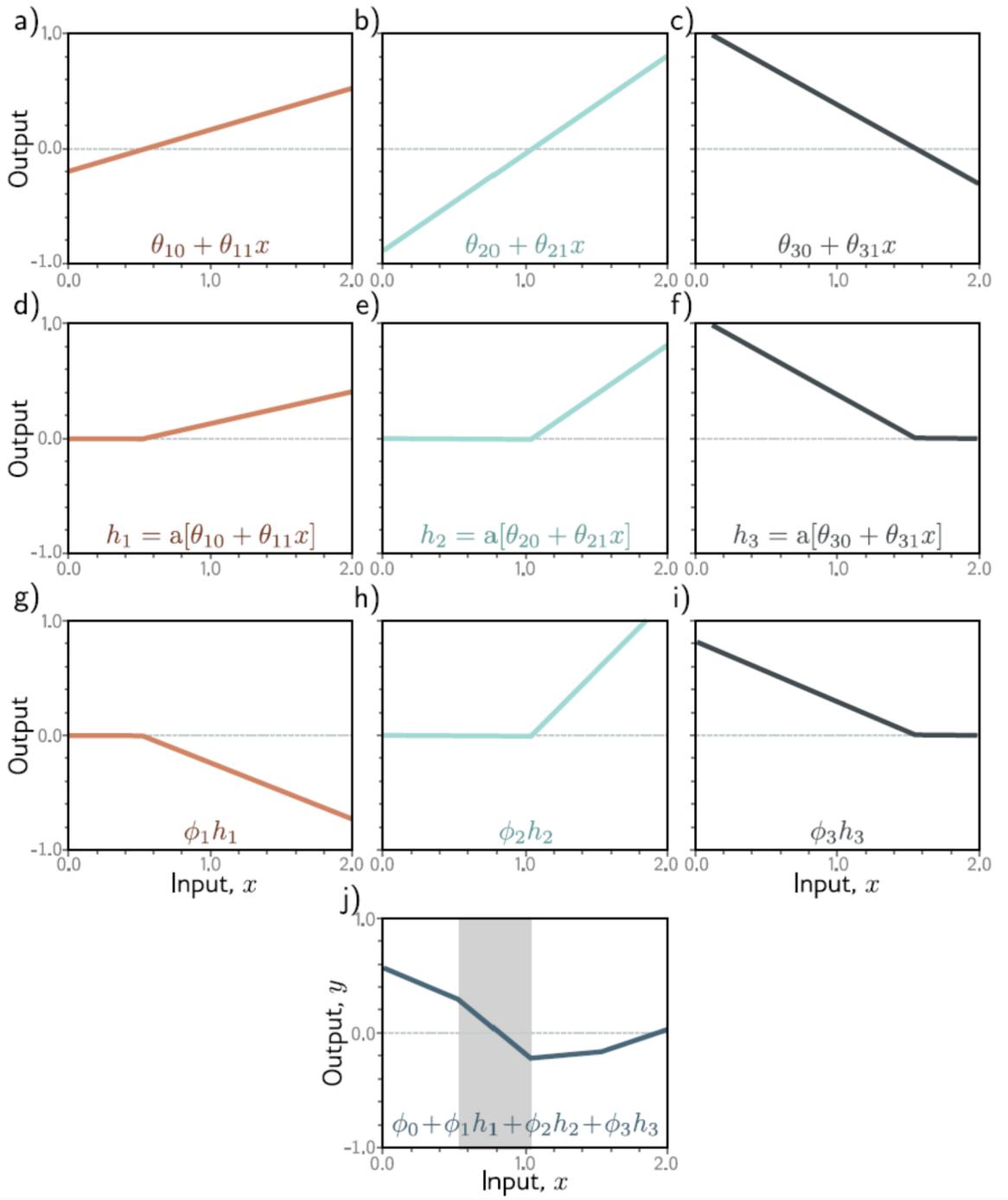
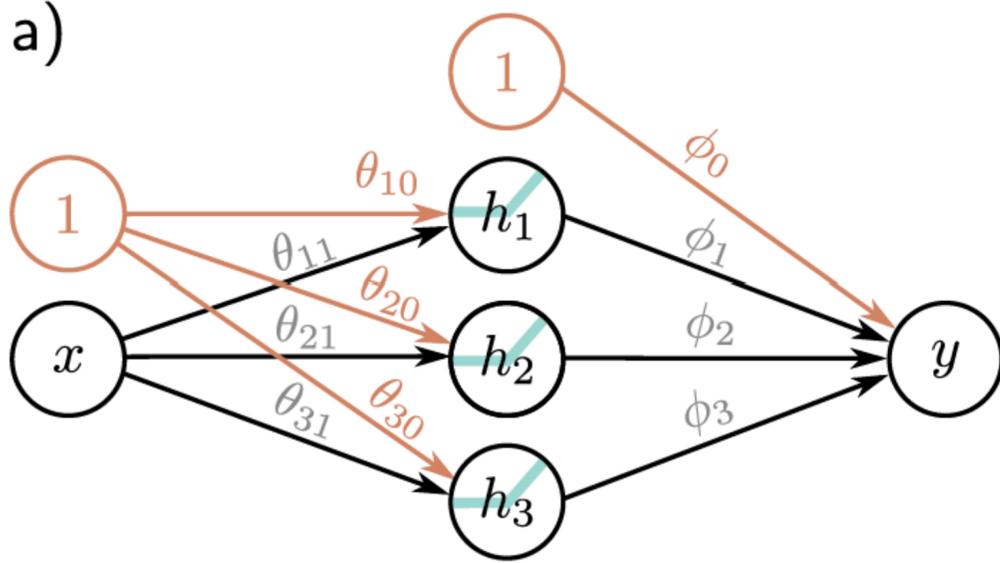
<https://umlcaxs-playground.streamlit.app/>

See also Yang et al. 2023

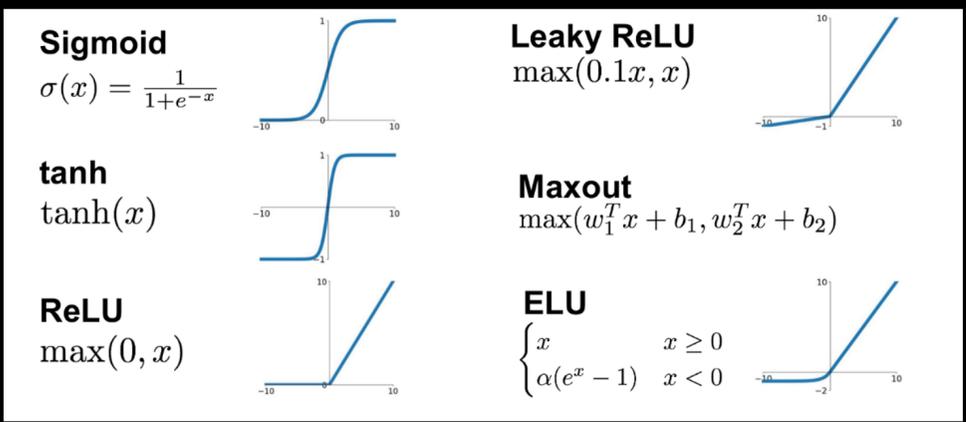
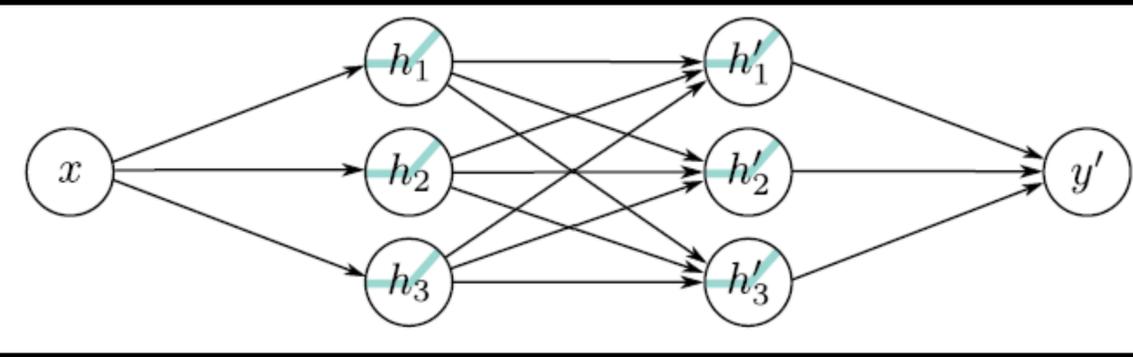


X-ray Datasets in the Era of Artificial Intelligence

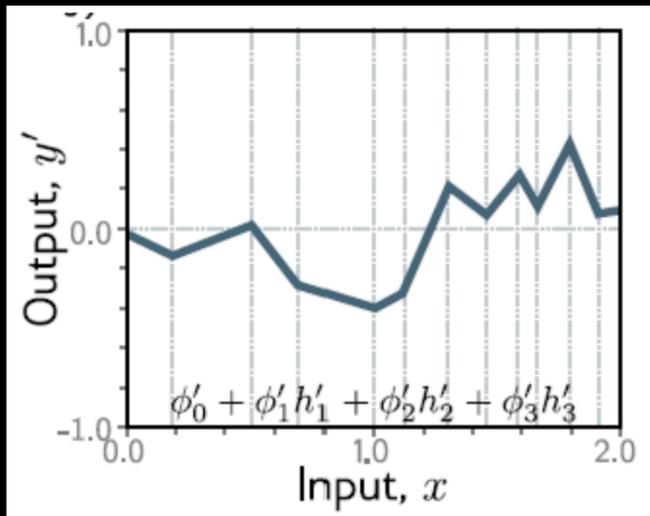
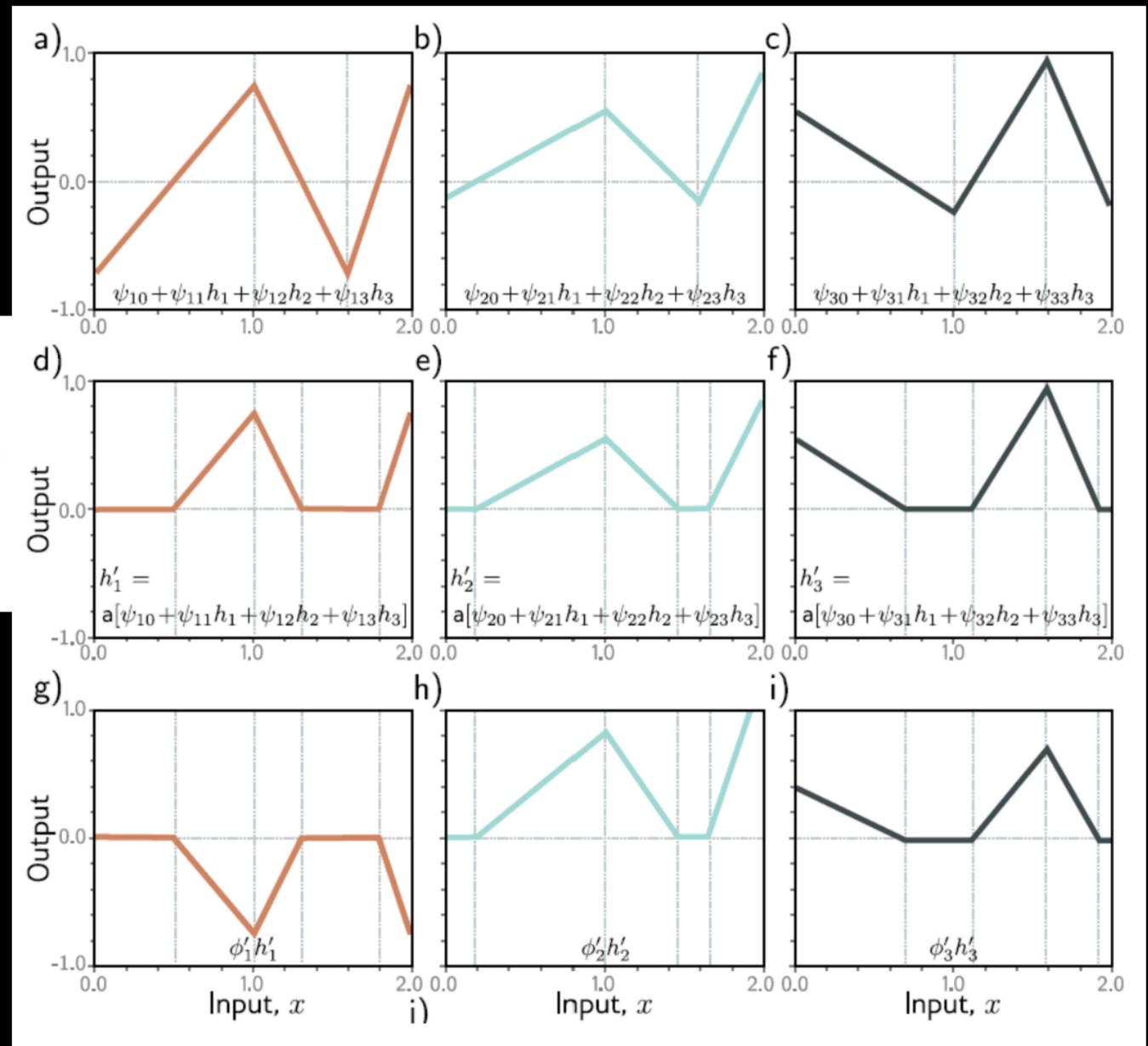
Neural networks are universal function approximators



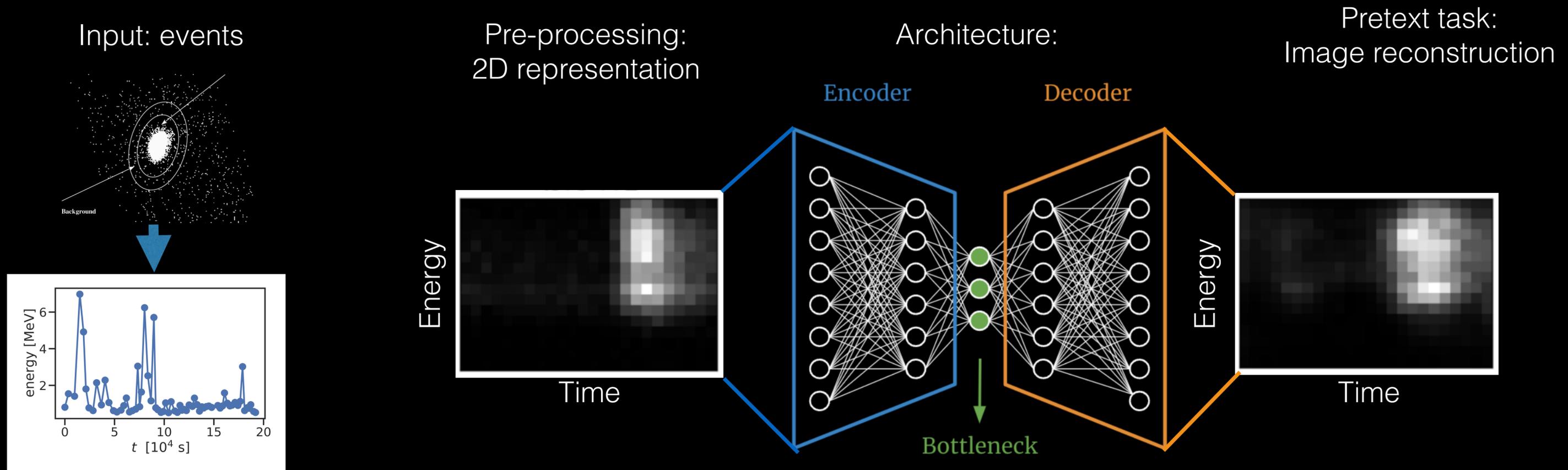
Neural networks are universal function approximators



Medium

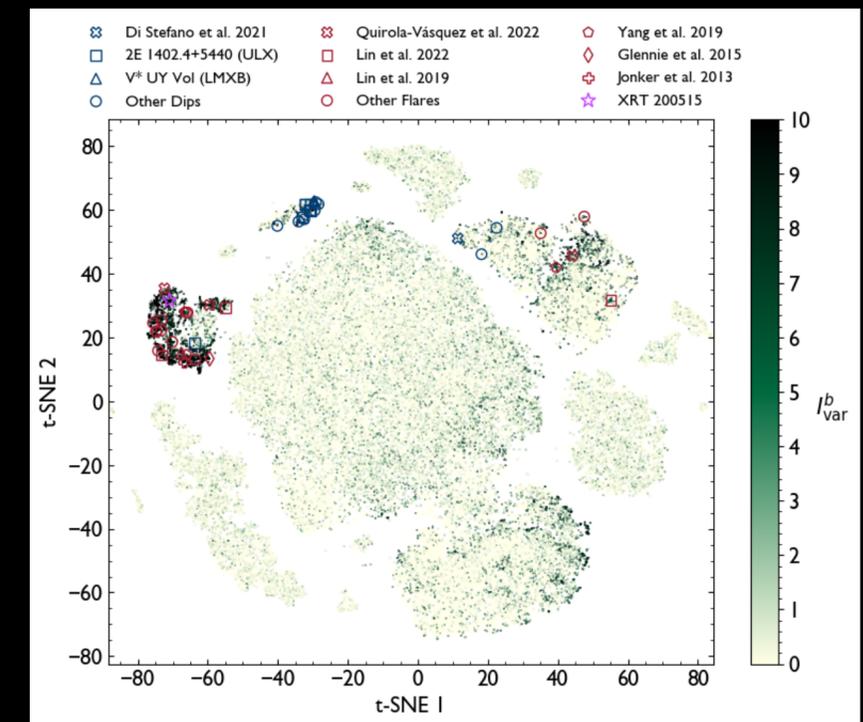
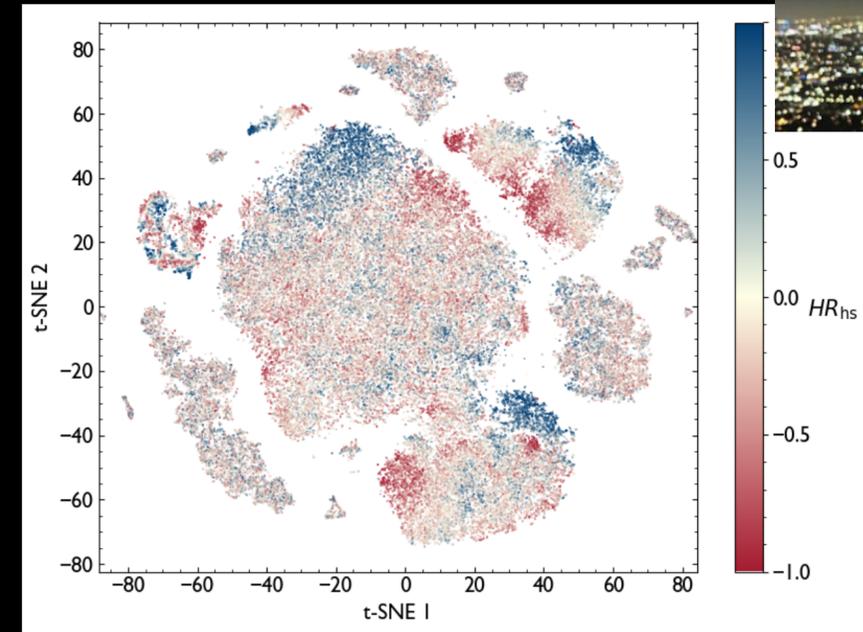
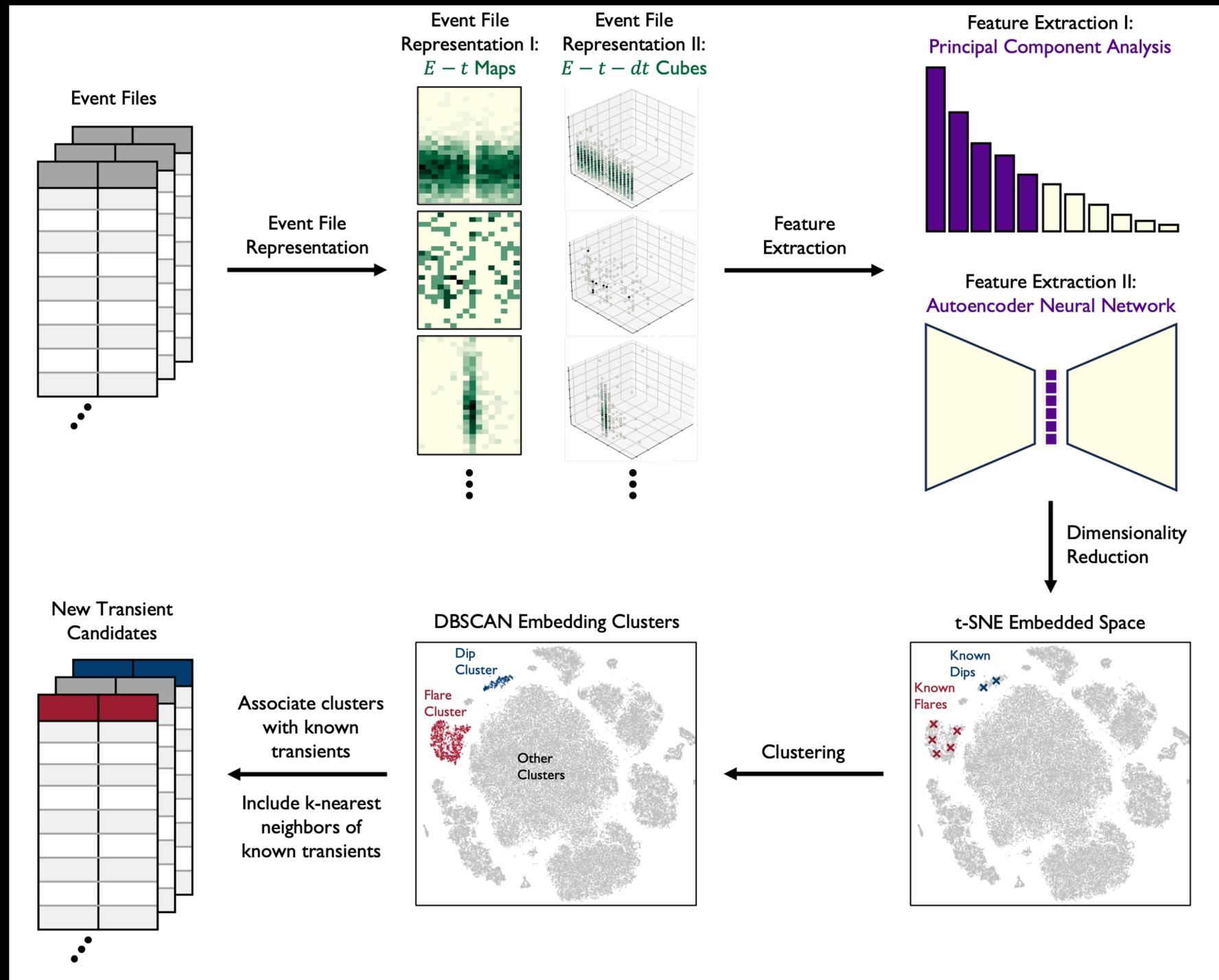


Representation Learning in X-ray Datasets



- Trained with all CSC detections with S/N ratio larger than 5.
- Size of the latent space: 24
- Spectral/spatial resolution optimized over all examples, but same for all examples

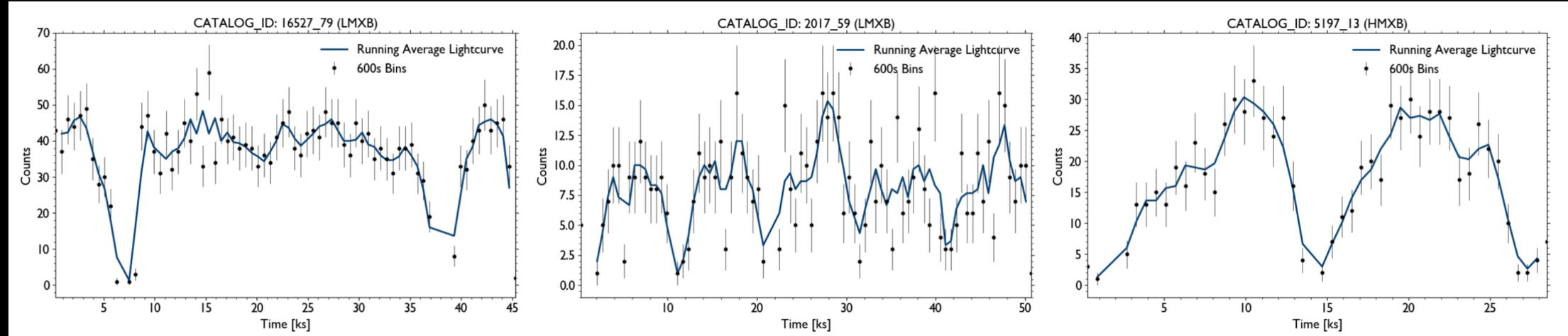
Representation Learning in X-ray Datasets



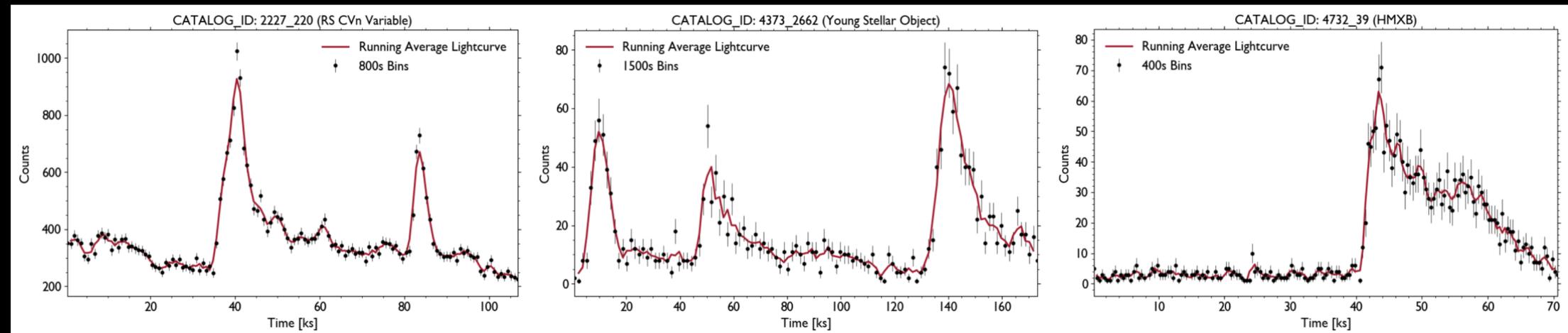
- Catalog of ~3000 dip and flare candidates in CSC

Examples of catalog objects

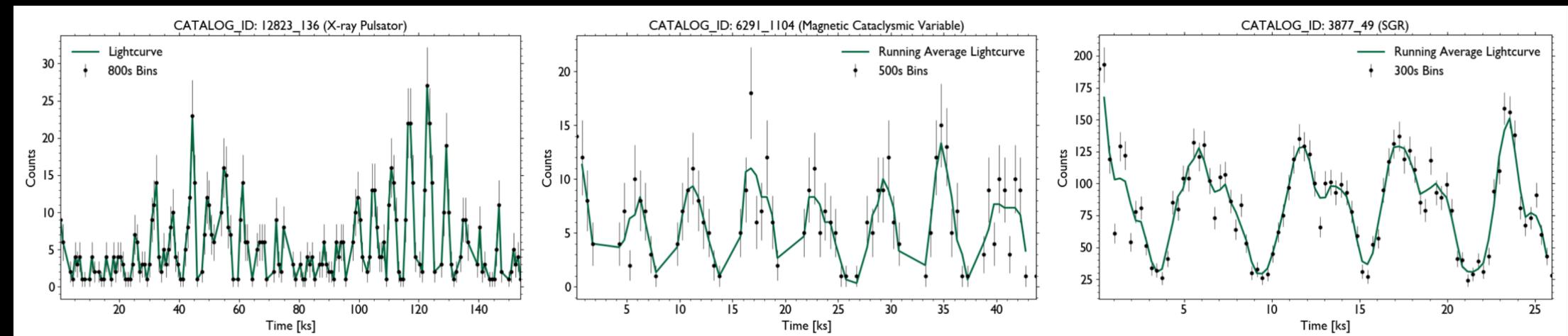
Dips



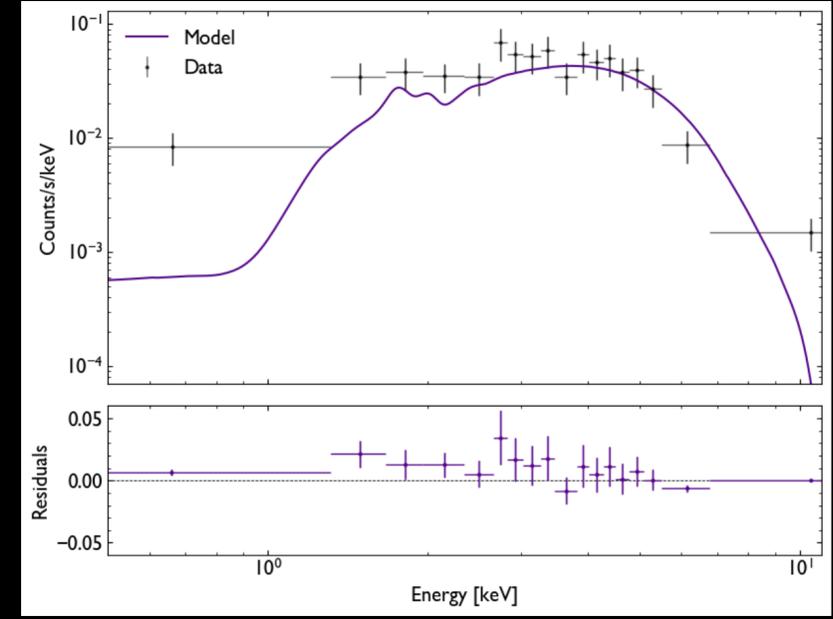
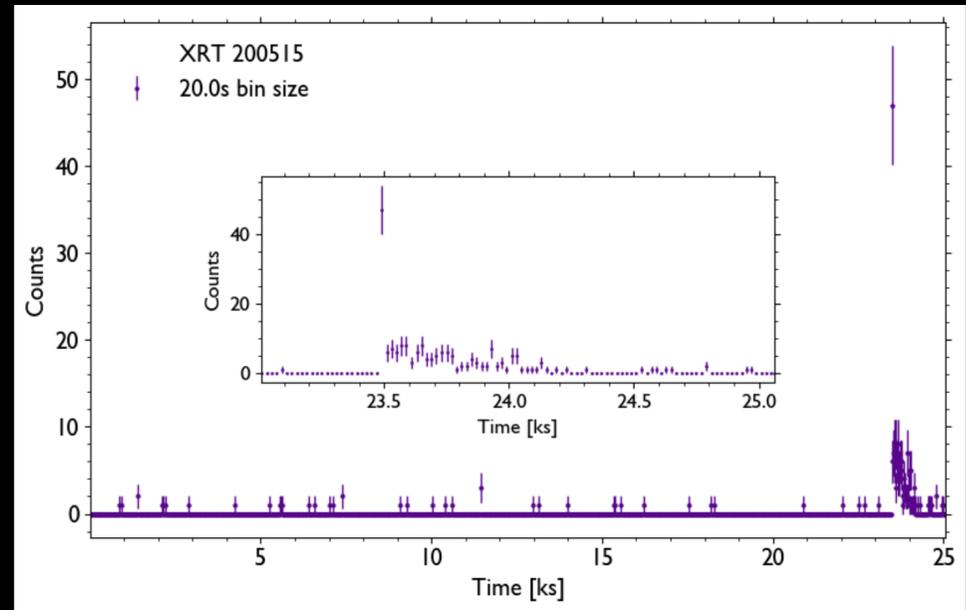
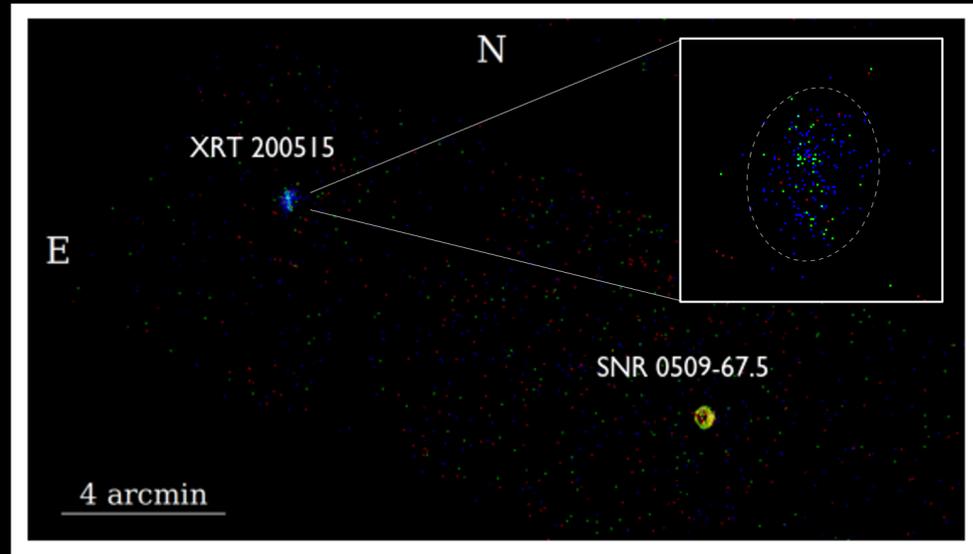
Flares



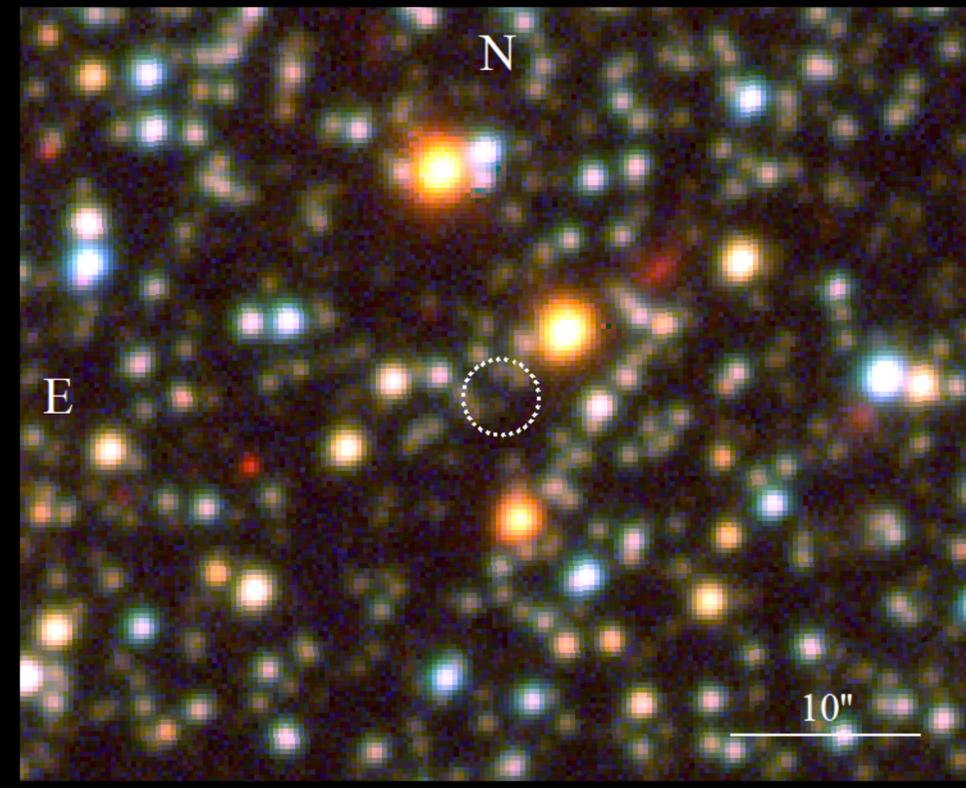
Periodic



X200515: A Fast X-ray Transient in the LMC



- Fast (~ 10 s) rise of the flux, followed by long tail with spectral softening after the burst.
- Peak luminosity: $L_x \sim 2 \times 10^{38}$ erg/s
- Potential counterparts are consistent with the old stellar population in this region of the LMC.
- Harder than other FXT reported, no plateau.



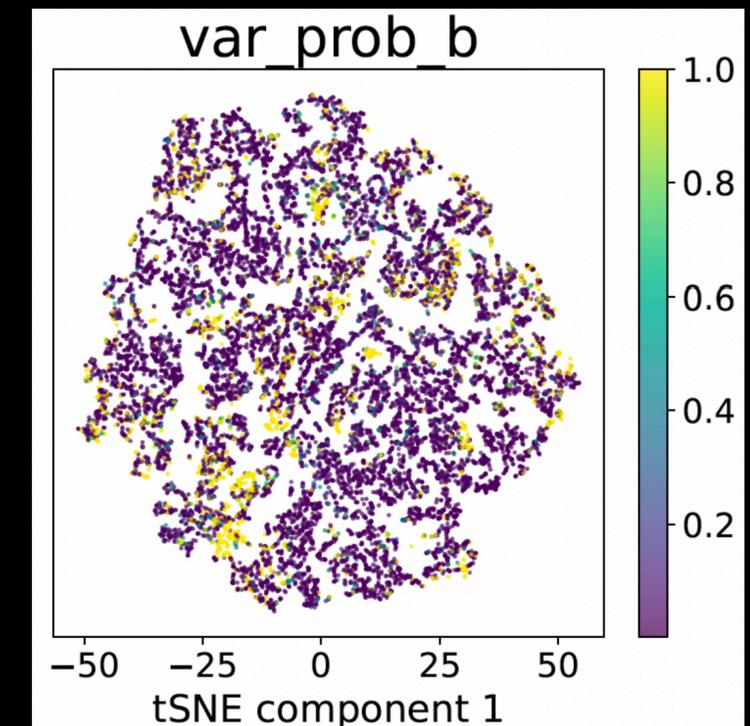
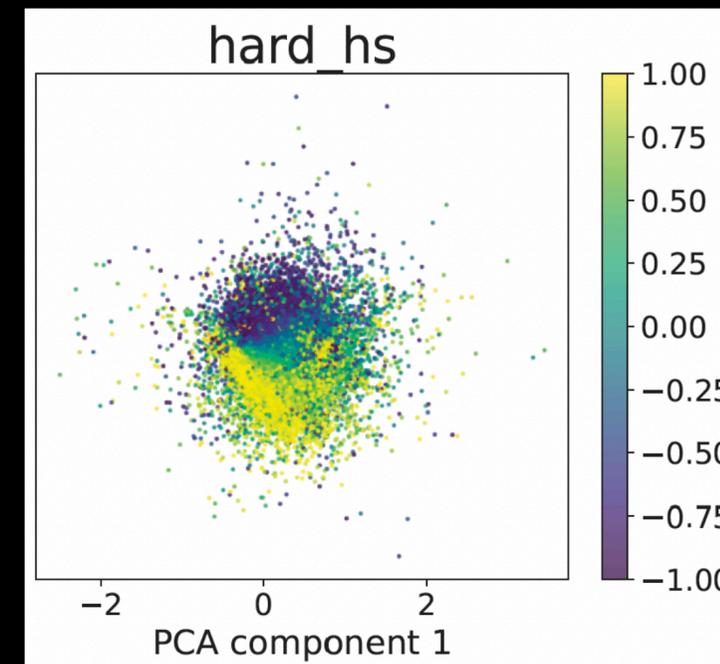
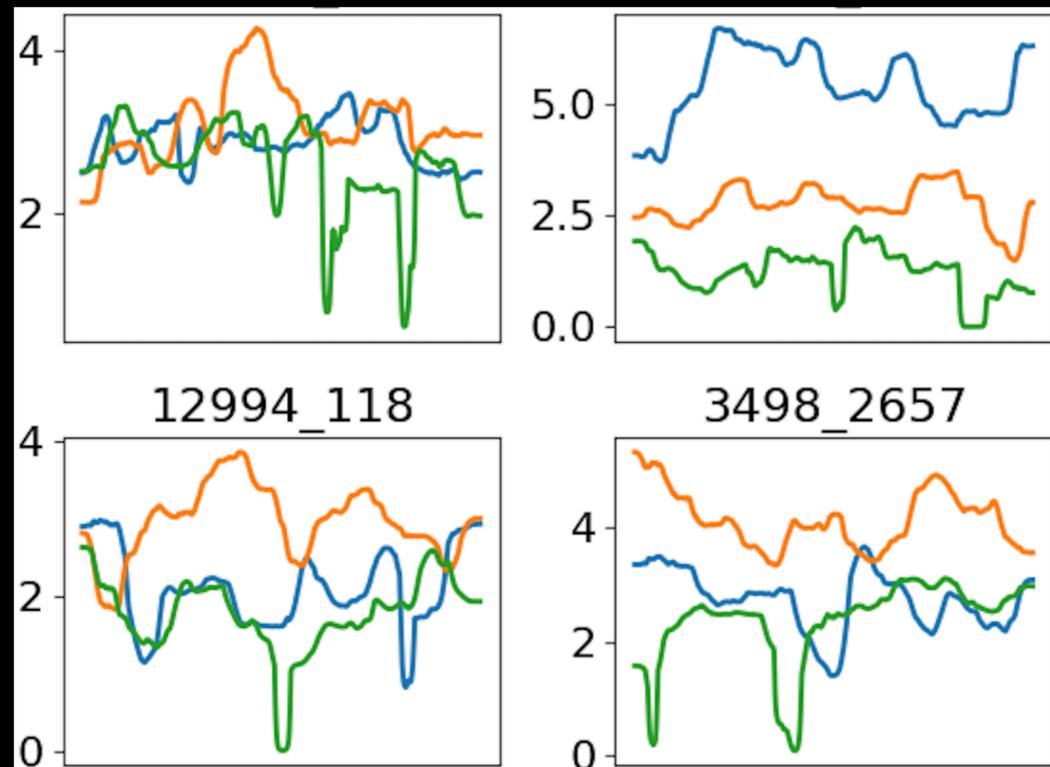
- Too fast to be consistent with a stellar flare.
- No known flares in the Milky Way halo, that resemble XRT 200515.
- Observed time scale and hard spectrum suggest connection to magnetic fields or relativistic jets.
- Oscillating tail. Type 1 burst in a NS? GRB from more distant merger?

Testing on unrelated downstream tasks



- We test the representation power of our self-learned latent features by using them as the input for regression and classification.
- Performance in classification is comparable with multi-wavelength supervised approaches.
- Nearest neighbor anomaly search:

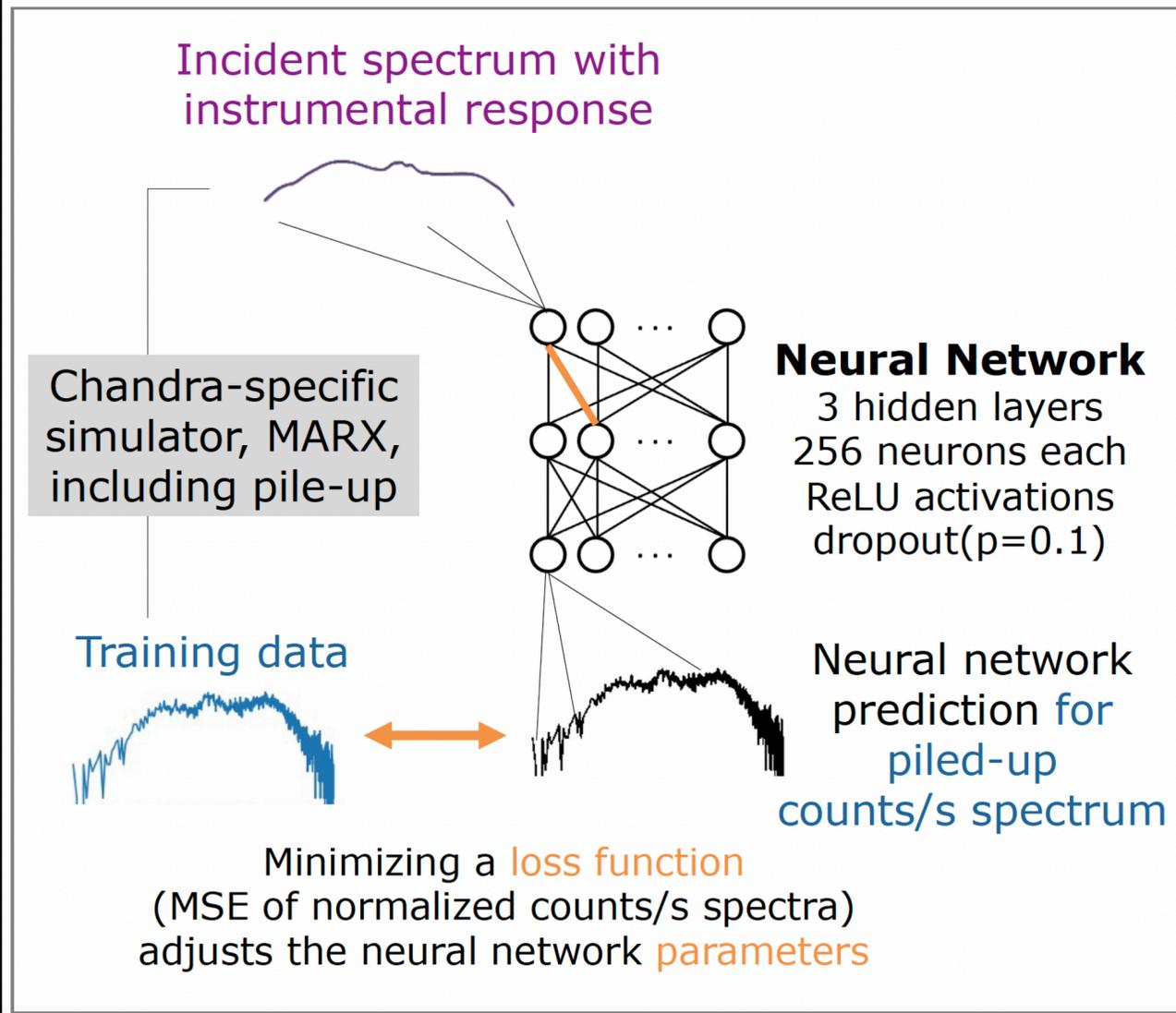
Regression Target	MSE	R^2
hard_ms	0.02	0.87
hard_hm	0.01	0.88
hard_hs	0.02	0.93
Classification Target	Accuracy	F1 Score
var_index_b > 0.5?	0.92	0.63
source type	0.62	0.25
YSO vs AGN	0.75	0.70



Inferring physical parameters while accounting for instrumental effects

J. Yang et al., in prep

A neural network can emulate simulated pile-up in relativistic reflection spectra



Trained
On ~22,000
simulations of
reflexion models



García & Dauser's relxill model (2014)

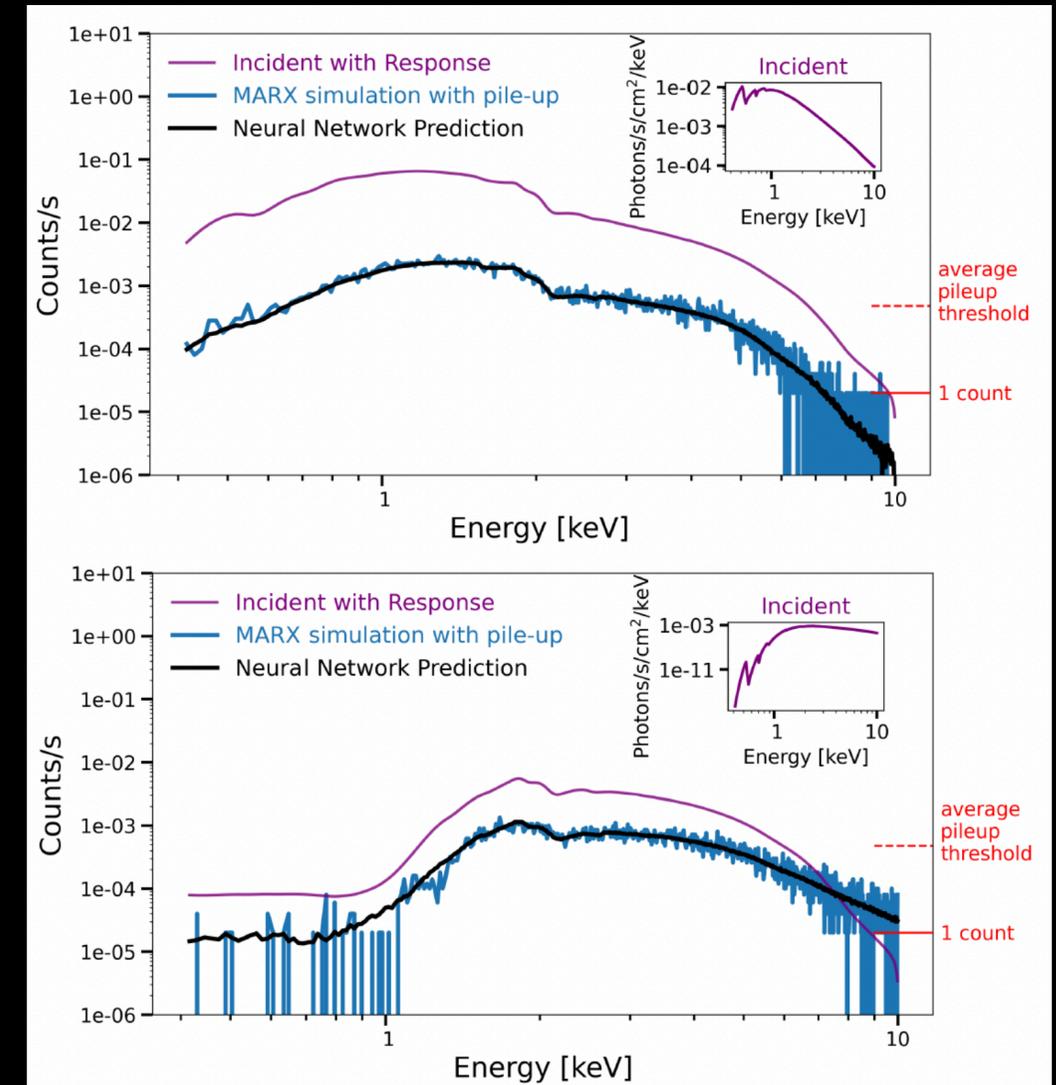
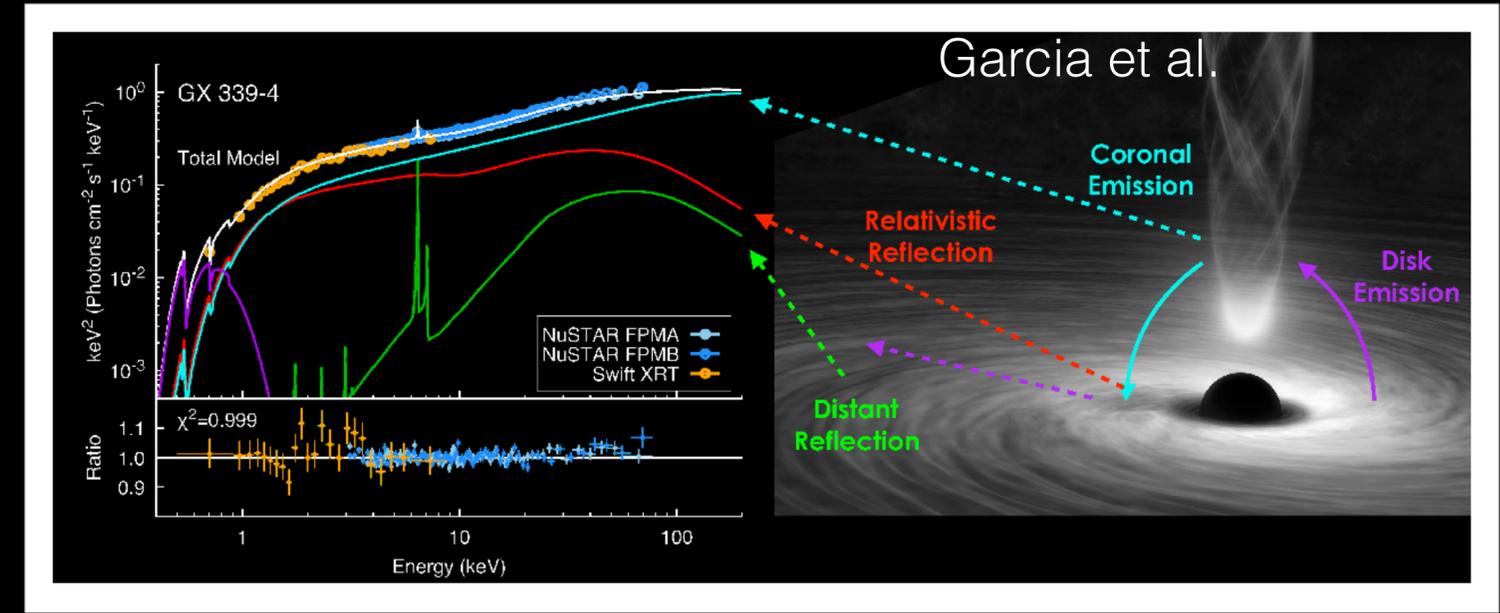
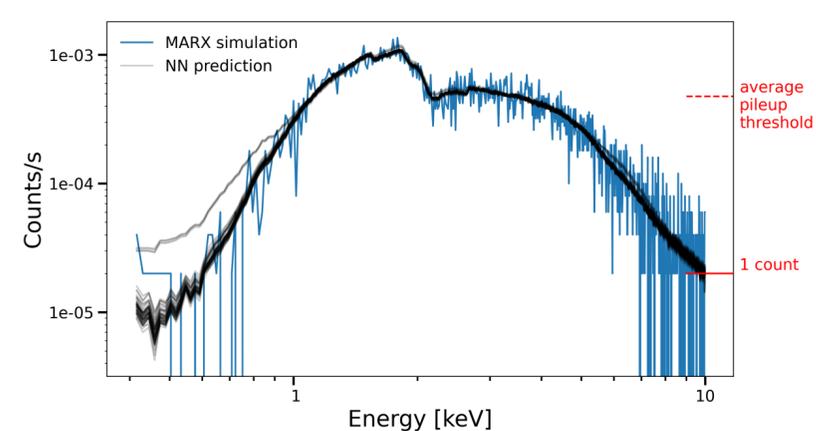
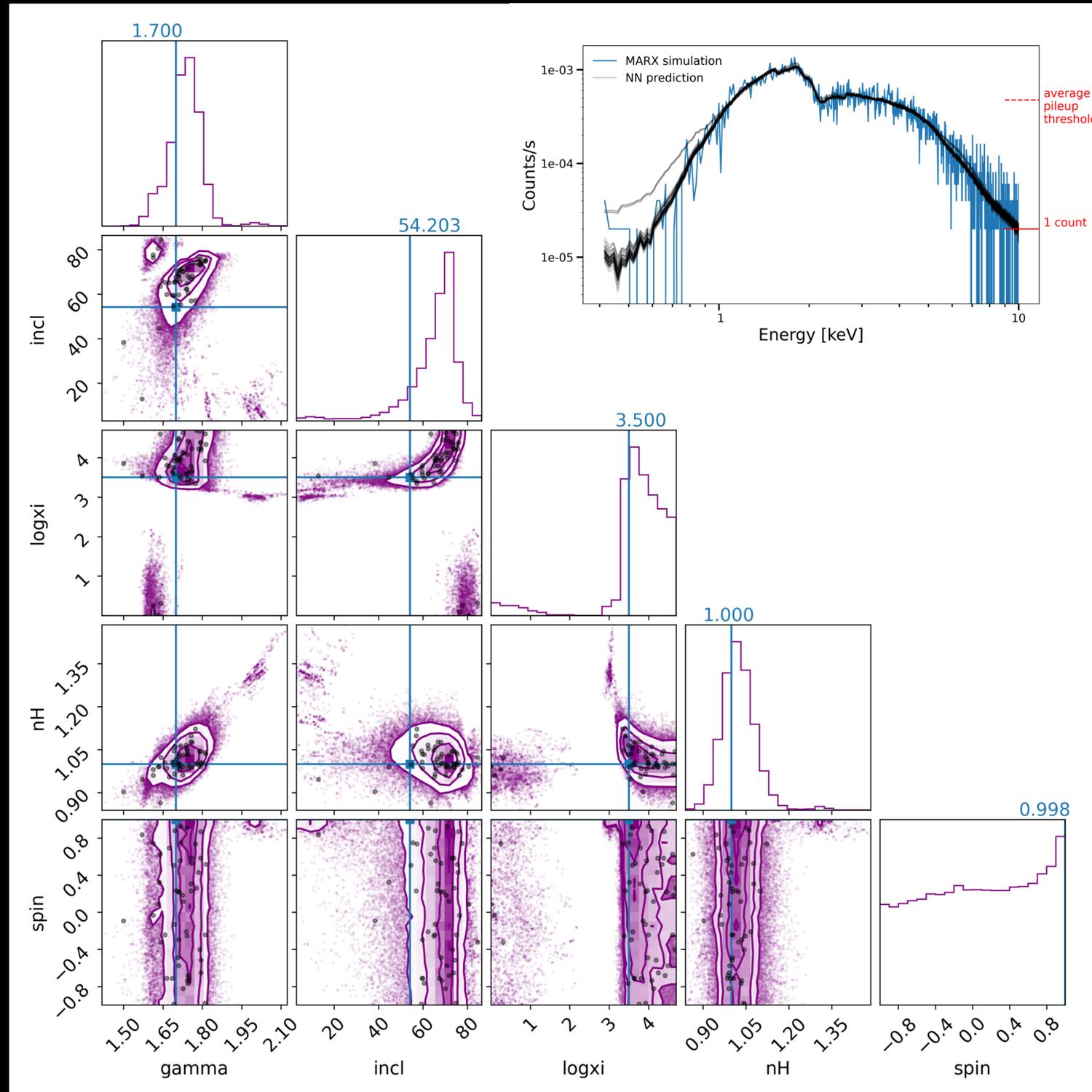
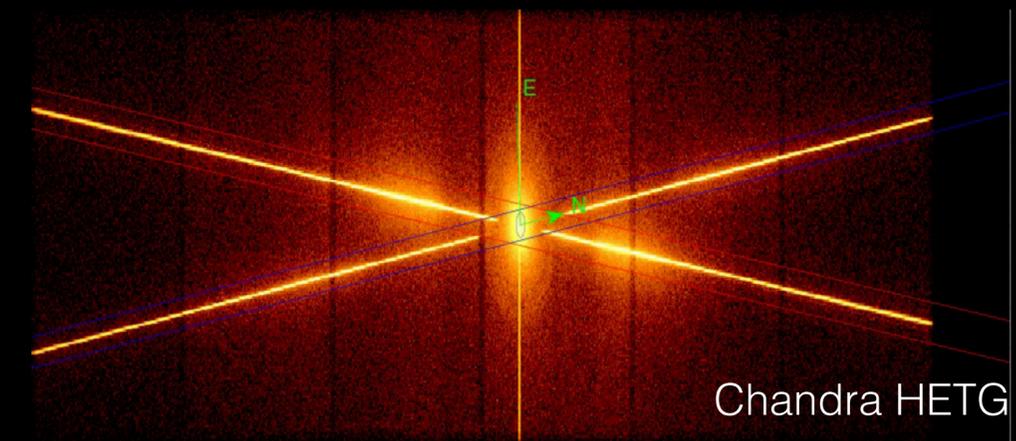


Fig. 2: examples of the neural network successfully predicting a piled-up spectrum that is consistent with a MARX simulation. Each incident spectrum is generated from relxill and each MARX simulation assumes an exposure of 5e4 s.

Inferring physical parameters while accounting for instrumental effects



- The Bayesian MCMC emulator has been incorporated in the fitting process for parameter inference.
- But, we don't want to learn the simulation prescription of pile-up. We want to learn from the data.
- Domain adaptation using spectral grating data.



The Multimodal Universe

Overview

The Multimodal Universe is a massive multimodal dataset of astronomical observations designed to enable large-scale machine learning research in scientific domains

225M Spectra

- Impact:**
- Bridges gap between ML research and scientific applications
 - Enables development of multimodal approaches
 - Standardizes data access for astronomy ML research



Auxiliary Data Products:

- Labels for classification, regression and image translation from auxiliary data
- Millions of samples across multiple modalities, instruments, and surveys
- Scientific metadata including instrument properties

Format: 1D signals with varying resolution.

Key Properties:

- Variable wavelength sampling
- Detailed features
- Complex noise patterns
- Instrument-specific artifacts

ML Challenges:

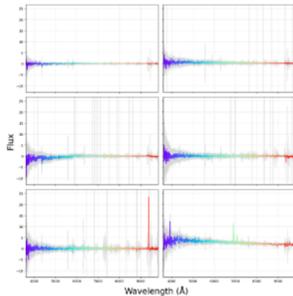
- Variable-length sequences
- Handling missing/masked data
- Cross-matching with other modalities
- Emission line predictions
- Redshift estimation

Data format:

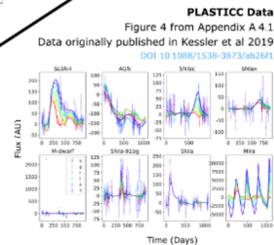
- 'flux': Measured flux as a function of wavelength
- 'ivar': Inverse variance of noise on the measured flux
- 'sf_sigma': The size of the instrumental response (Line Spread Function, LSF)
- 'lambda': Wavelength of each flux measurement

DESI Data

DESI spectra with gaussian smoothing applied show characteristic structures with standard deviation bounds. See Appendix A 5.3 for dataset details. Data published in DESI Collaboration et al 2024 DOI 10.3847/1538-3881/ac3217



4.5M Lightcurves



PLASTICC Data

Figure 4 from Appendix A 4.1 Data originally published in Kessler et al 2019 DOI 10.1088/1538-3873/ab2691

Format: Irregular temporal sequences. Usually measurements of variable stars, including supernovae.

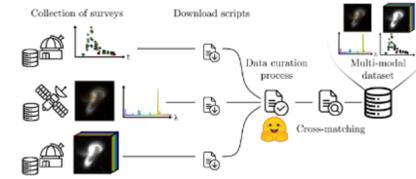
Key Properties:

- Irregular sampling
- Multiple wavelenghts
- Heterogeneous coverage
- Variable time scales

ML Challenges:

- Irregular time intervals
- Missing observations
- Multi-band alignment
- Real-time classification

Hosting and Infrastructure



- Open-source** with clear contribution guidelines and support for non-developers
- Utilities** for cross-matching (finding matching data across modalities)
- Community** driven development with an active team of maintainers
- Huggingface** hosted data samples for development
- Globus** endpoint for safe TB scale data download
- Extendable** - new data are already pending!
- Expert selected** science ready data

140M Images

Format: Multi-channel arrays (3-7 channels)

Key Properties:

- High dynamic range spanning several orders of magnitude
- Complex noise characteristics
- Instrument-specific distortions

ML Challenges:

- Handling measurement uncertainties
- Multi-channel processing
- Dealing with varying PSF
- Distribution shifts between instruments
- Finegrained classification
- Redshift estimation

Data format:

- 'flux': An array of flux measurements of the image
- 'ivar': An array of the inverse variance of noise in the image
- 'band': A string indicating the wavelength range of the image
- 'psf_fwhm': A value indicating the size of the instrumental response (point spread function, PSF)
- 'scale': A value describing the scale of the image's pixels on the sky

GZ10 Benchmark

Galaxy morphology classification task results - see the paper for more details. This dataset was produced in Leung & Bovy 2018 https://astron.readthedocs.io/en/v1.0/galaxy10.html based on Lintott et al 2008 DOI 10.1111/j.1365-2966.2008.13689.x. The Galaxy Zoo team maintains the original, expanded, and full fidelity records of classifications

Pretraining	Model	Top-1 Accuracy
No pretraining	EfficientNetB0	80.9 ± 0.1 %
	*ConvNext-nano	75.6 ± 1.8 %
	ResNet18	73.9 ± 0.9 %
Galaxy Zoo	DenseNet121	73.5 ± 2.4 %
	*ConvNext-nano	89.3 ± 0.1 %
ImageNet-12k	*ConvNext-nano	83.9 ± 0.3 %



*Trained in Walmsley et al 2024 arXiv:2404.02973

12k Spectral Cubes

Format: 3D datacubes providing detailed spectral information across spatial regions of galaxies tracing chemistry and kinematics

Key Properties:

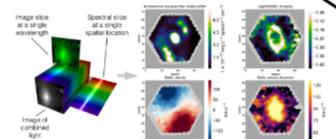
- Combines imaging and spectroscopy
- High-dimensional data structure
- Rich physical information

ML Challenges:

- High memory requirements
- 3D data processing
- Joint spatial-spectral learning
- Translation between modalities

MaNGA Data

Described in Appendix A 6.1 Data originally published in Bundy et al 2015 DOI 10.1088/1538-3873/ab26f1

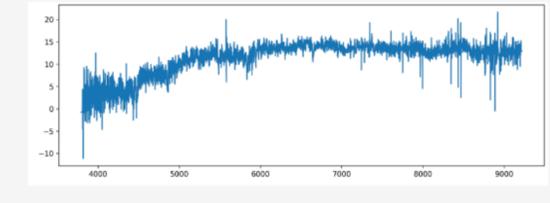


This figure is adapted from Cherinka et al 2019 DOI 10.3847/1538-3881/ab2634

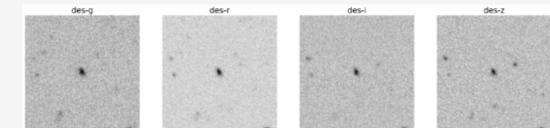
Getting Started



```
dset_sdss = load_dataset("MultimodalUniverse/sdss",
                        streaming=True,
                        split='train')
```



```
dset_ls = load_dataset("MultimodalUniverse/legacysurvey",
                      streaming=True,
                      split='train')
```

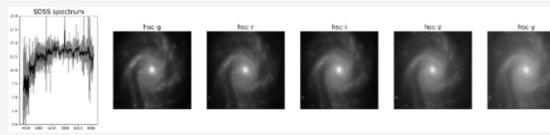


```
from datasets import load_dataset_builder
from mmu.utils import cross_match_datasets
```

```
sdss = load_dataset_builder(
    "data/MultimodalUniverse/v1/sdss",
    trust_remote_code=True
)
```

```
hsc = load_dataset_builder(
    "data/MultimodalUniverse/v1/hsc",
    trust_remote_code=True
)
```

```
dset = cross_match_datasets(
    sdss, # Left dataset
    hsc, # Right dataset
    matching_radius=1.0, # Distance in arcsec
)
```



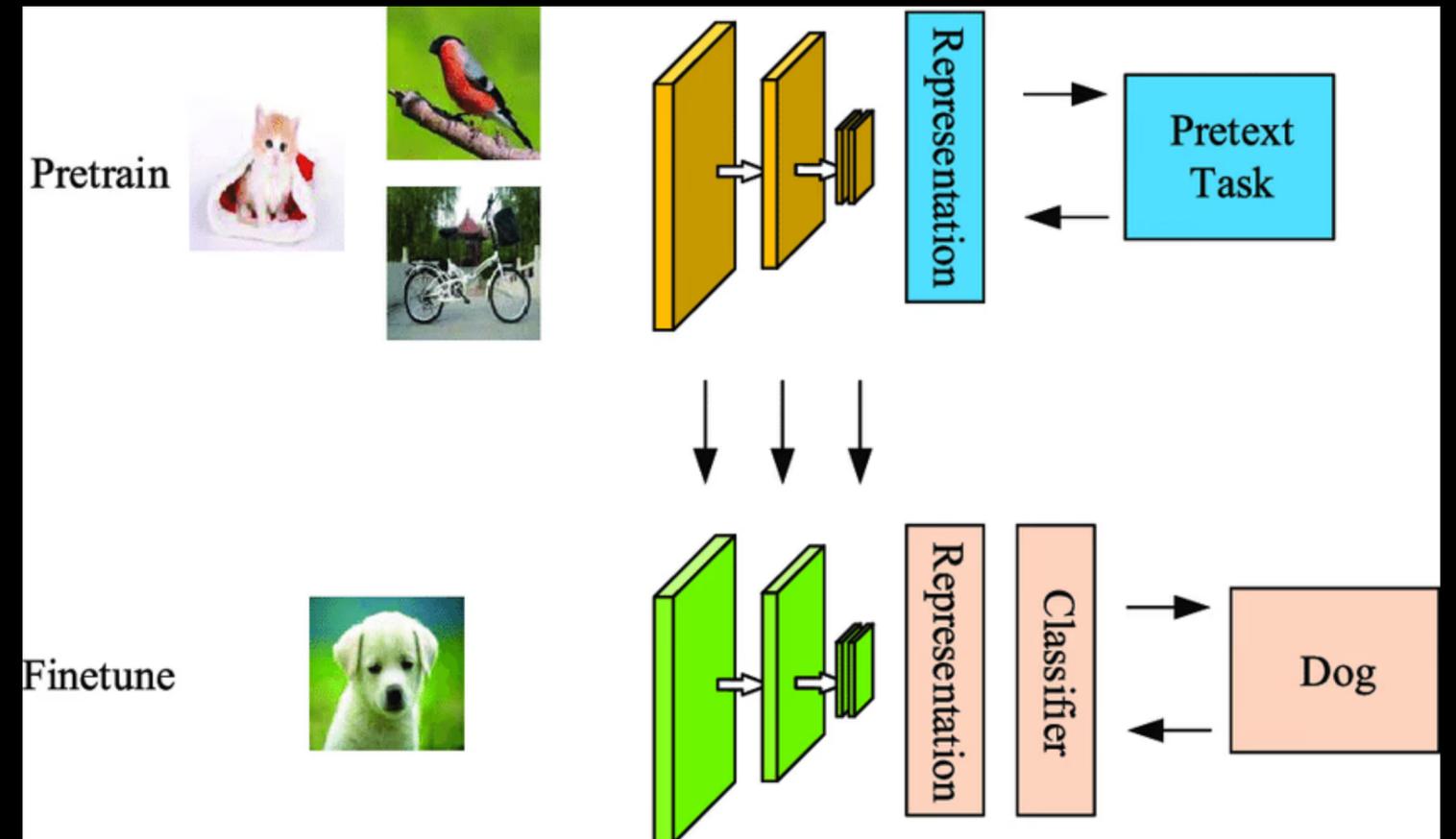
The Multimodal Universe Collaboration

Eirini Angeloudi, Jeroen Audenaert, Micah Bowles, Benjamin M. Boyd, David Chemaly, Brian Cherinka, Ioana Ciucă, Miles Cranmer, Aaron Do, Matthew Grayling, Erin E. Hayes, Tom Hehr, Shirley Ho, Marc Huertas-Company, Kartheik G. Iyer, Maja Jablonska, Francois Lanasus, Henry W. Leung, Kaisey Mandel, Juan Rafael Martínez-Galarza, Peter Melchior, Lucas Meyer, Liam H. Parker, Helen Qu, Jeff Shen, Michael J. Smith, Connor Stone, Mike Walmsley, John F. Wu



Self-supervised (representation) learning

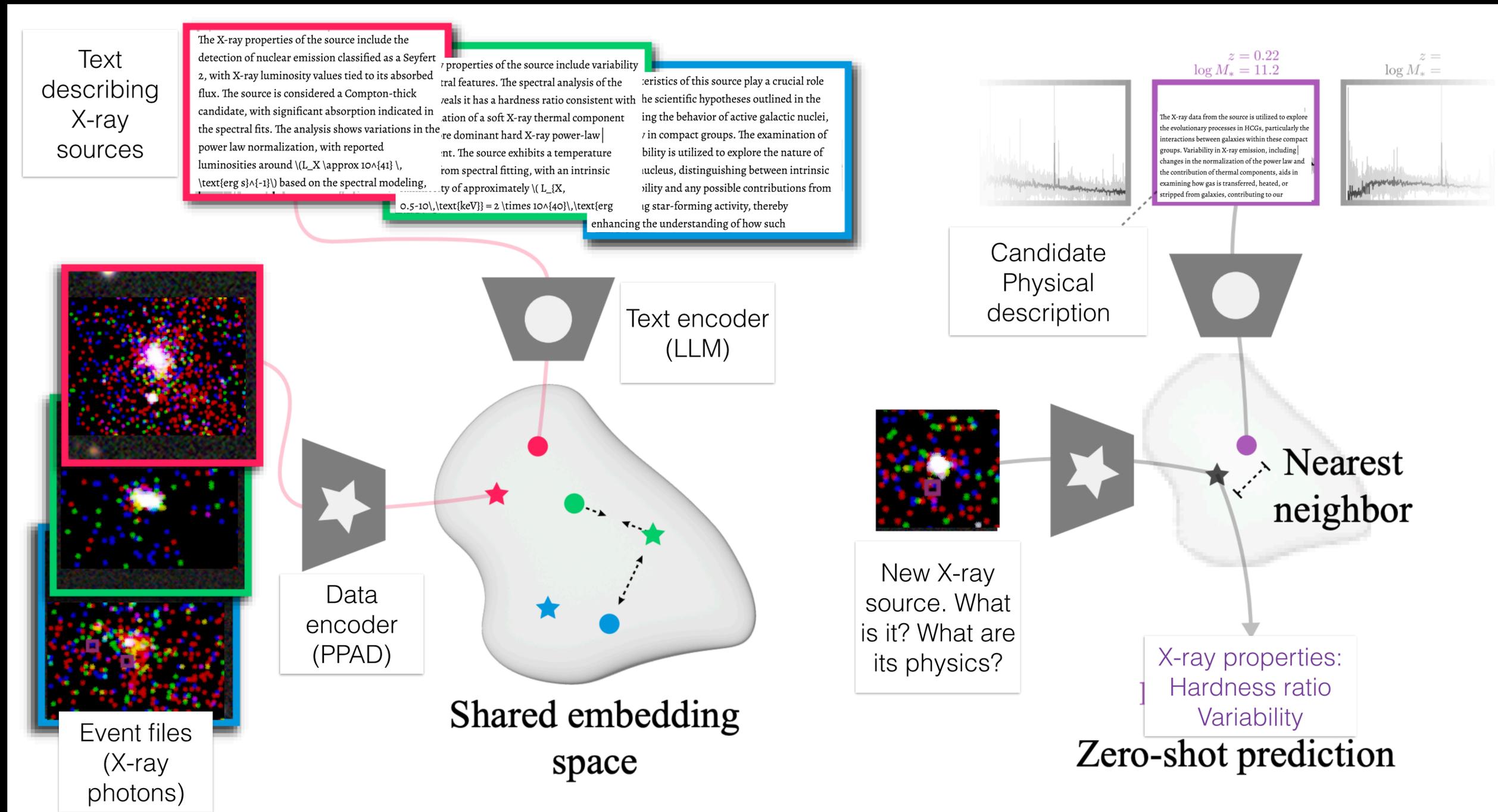
- Self-supervised learning is a type of machine learning where the system learns representations of data without the need for explicit human-provided labels.
- Instead, labels are generated by the system to solve a “pretext” task.
- If trained on lots of data, the representations can be used for downstream tasks in which they were not trained (e.g. Classification)



Rohit Kundu

I grew up in France, I speak fluent...French

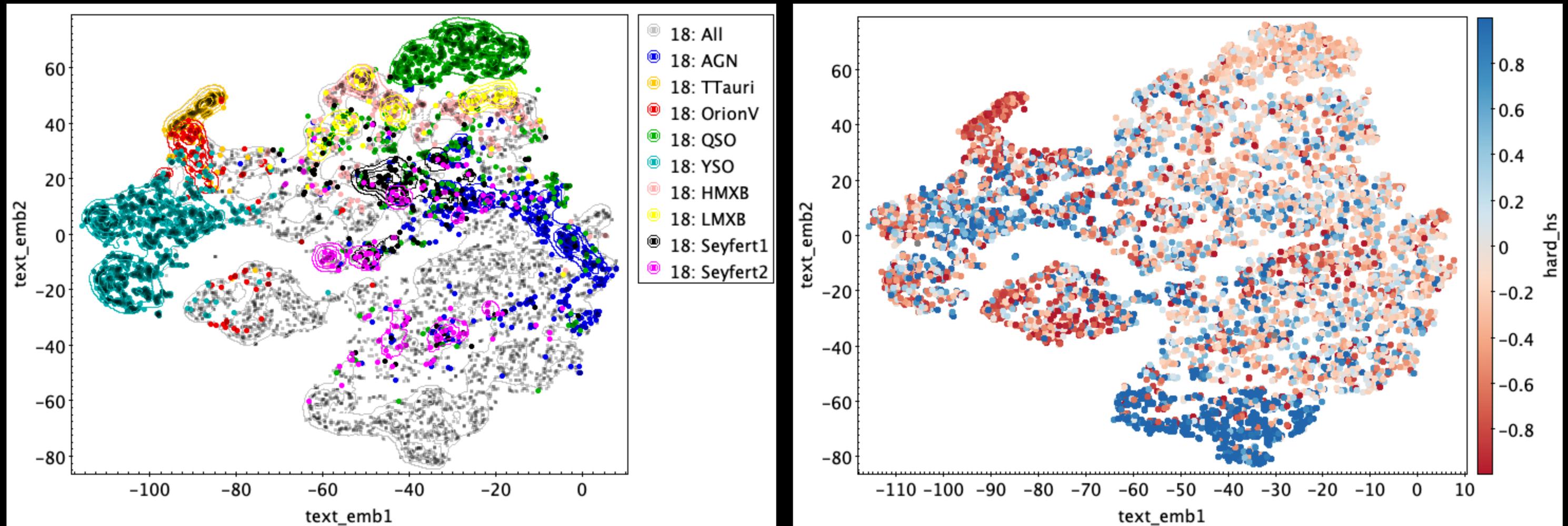
Contrastive Learning Astro+Natural Language



$$\mathcal{L}_{InfoNCE}(\mathbf{X}, \mathbf{Y}) = -\frac{1}{K} \sum_{i=1}^K \log \frac{\exp(S_C(\mathbf{x}_i, \mathbf{y}_i)/\tau)}{\sum_j^K \exp(S_C(\mathbf{x}_i, \mathbf{y}_j)/\tau)}$$

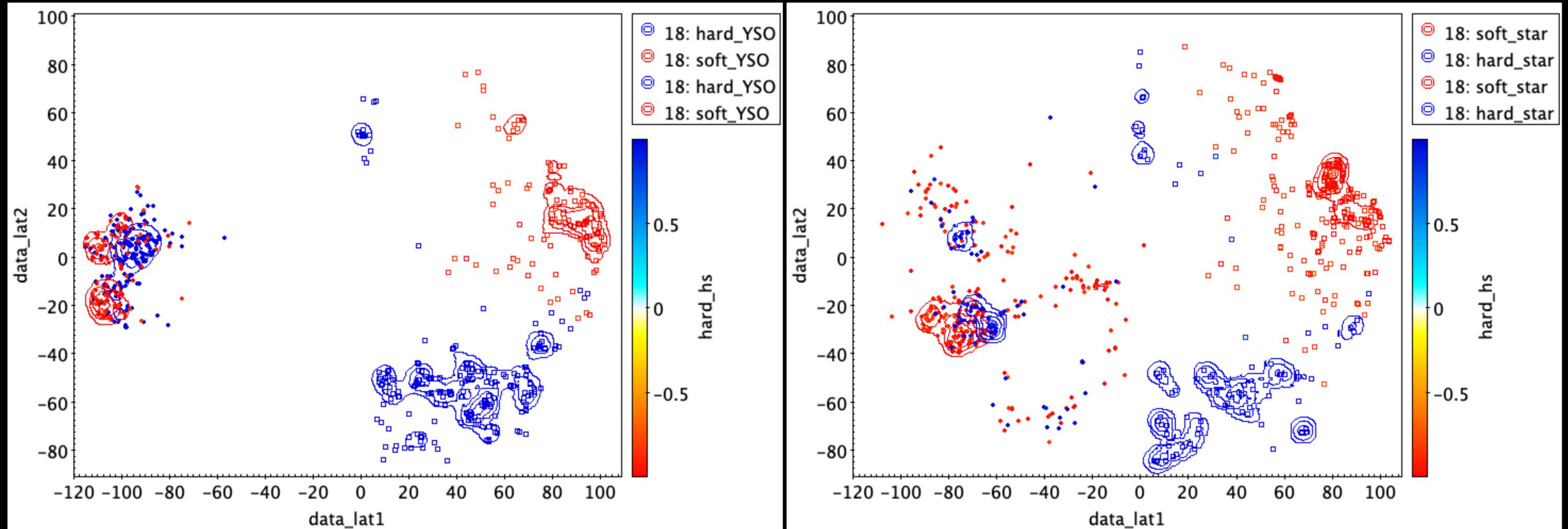
Adapted from Parker, Lanusse, et al. 2024

Text embeddings contain physical information



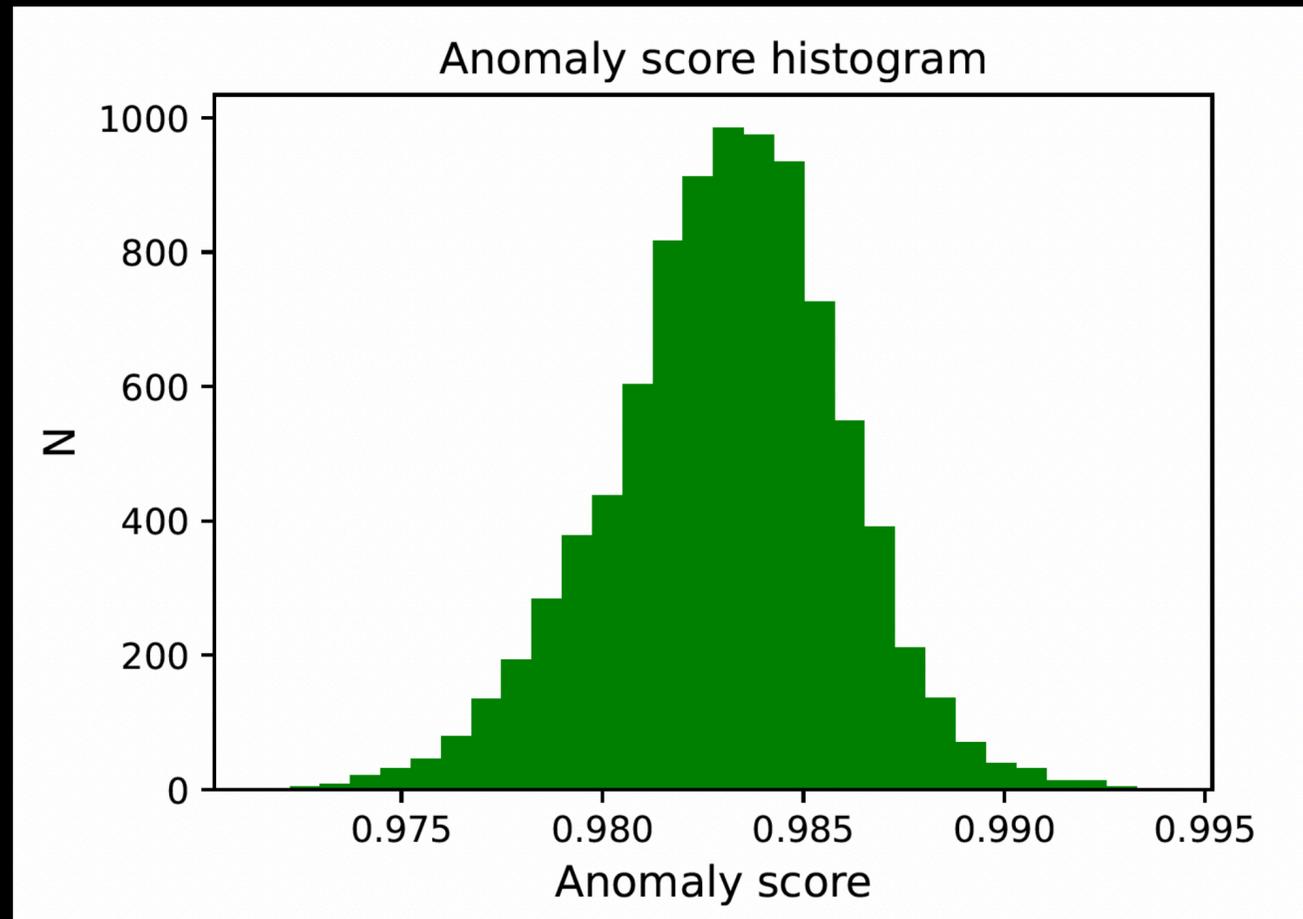
Here are some *LLM embeddings* from a GPT-like model for text summaries extracted from astronomical papers about different types of X-ray sources. You can see how they encode both the class of the object, and also some information about the physics.

Pre-alignment embeddings



Specific regions of the embedding space of each morality corresponds to X-ray sources of a given class and specific spectral properties. There is a correspondence between the data embeddings and the text embeddings

An LLM summary of an anomalous source



'The source identified with "[WSG84] 2" is mentioned in the text provided. I summarize the X-ray properties and their implications: A) X-ray Properties

- Variability**: The source has transient behavior with significant luminosity fluctuations. Specifically, periodicities have been highlighted. The periodic signals were found at approximately 55 d, although the stability of this modulation was questioned, implying that the source does not maintain consistent brightness levels over time.
- Spectral Features**:
 - The source was fitted using models that include power-law and thermal components. The photon index for the power-law fit was constrained to be around $\Gamma = 1.33 \pm 0.15$ in the energy range of 0.5–8 keV.
 - For the thermal model component, the temperatures were estimated at around 0.6 keV, suggesting an emission predominantly from hot plasma.
 - The absorption column density (N_H) was determined to be around $3 \times 10^{22} \text{ cm}^{-2}$, which suggests a significant amount of interstellar material obscuring the X-ray emissions from the source.
- Luminosity**: The source's observed X-ray luminosity was reported to exceed $10^{39} \text{ erg s}^{-1}$ during various observations, indicating that the source operates above the Eddington limit, which is characteristic of sources of type X.

B) Scientific Hypotheses Testing

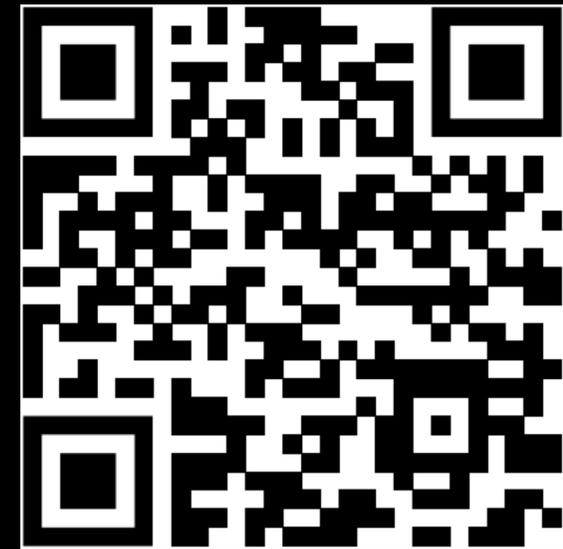
The properties of the source are critical in evaluating hypotheses regarding the nature of ultraluminous X-ray sources. The variability observed in the light curves across the different temporal analyses suggested that the source operates under the "propeller regime" of accretion. This regime indicates the presence of a strong magnetic field and can be key for understanding the behavior of neutron stars in binary systems.

The spectral features, including the determined N_H and photon index, help to classify the source's emission mechanism. They also provide insight into the environmental conditions surrounding the source, including the level of obscuration by interstellar matter. The correlation of the measured luminosity and the spectral characteristics with other known sources – particularly how they fit within the expected theoretical frameworks for ultraluminous X-ray sources – serves to validate or challenge prevailing models. The emission patterns can assist in distinguishing whether the source behaves more like an intermediate-mass black hole or if it is instead a neutron star system undergoing unusual accretion dynamics. In summary, the X-ray properties of the source serve to reinforce the arguments made regarding the diversity of ULXs and their potential to test existing astrophysical models related to black hole (or neutron star) formation and evolution through observations of their variability and spectral characteristics.'

A few final remarks

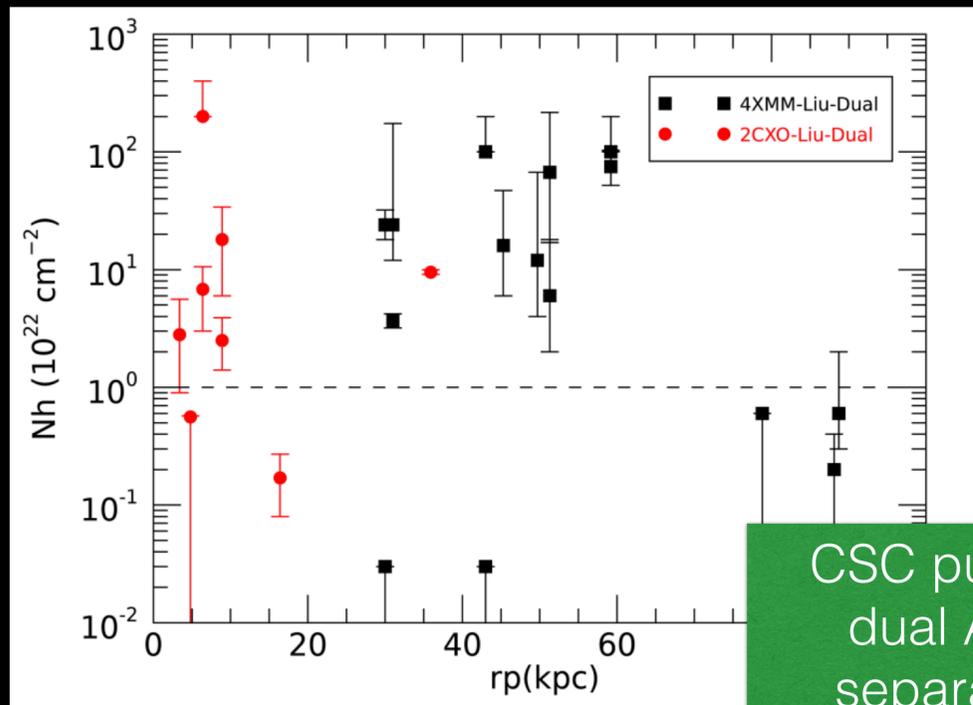
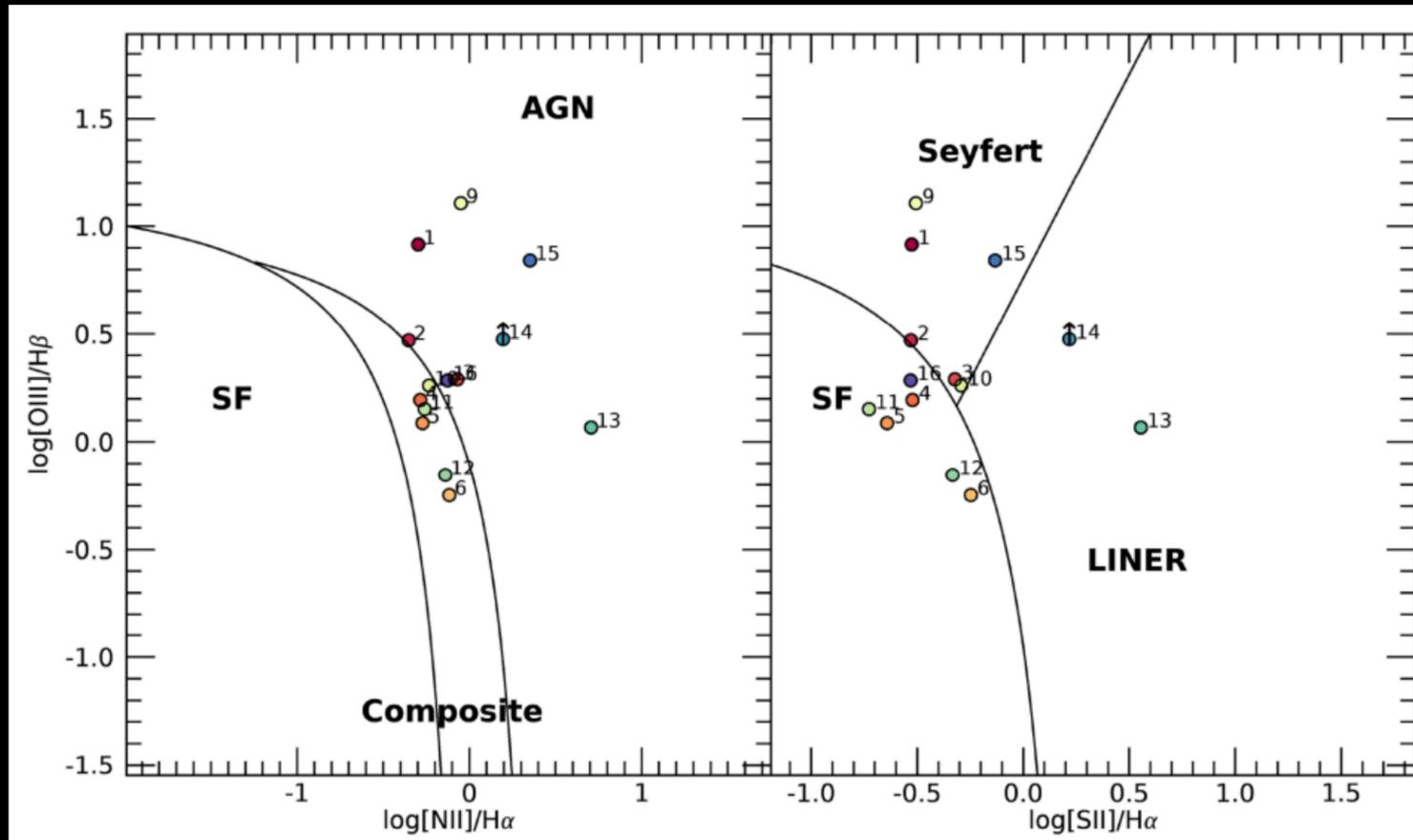
- X-ray astronomy was always the science of “a few photons”. We now have enough photons to learn relevant patterns from them that inform physical models.
- X-ray catalogs and archival research have enabled an era of data-driven discovery in high energy astrophysics, in particular transient science and multi-messenger themes. The moment is ripe for profiting from cutting-edge machine learning methods.
- Self-supervised learning can result in meaningful representations of X-ray event data that can be effectively used for downstream tasks such as classification, regression, and anomaly detection, without having to rely on features or labels created by humans.
- As we move to the next generation of X-ray facilities, data complexity will continue growing, but the non-linear instrumental effects such as pileup will also be there. ML emulation offers an opportunity to learn those effects from data.

Your Science Here!



<https://cxc.cfa.harvard.edu/csc/>

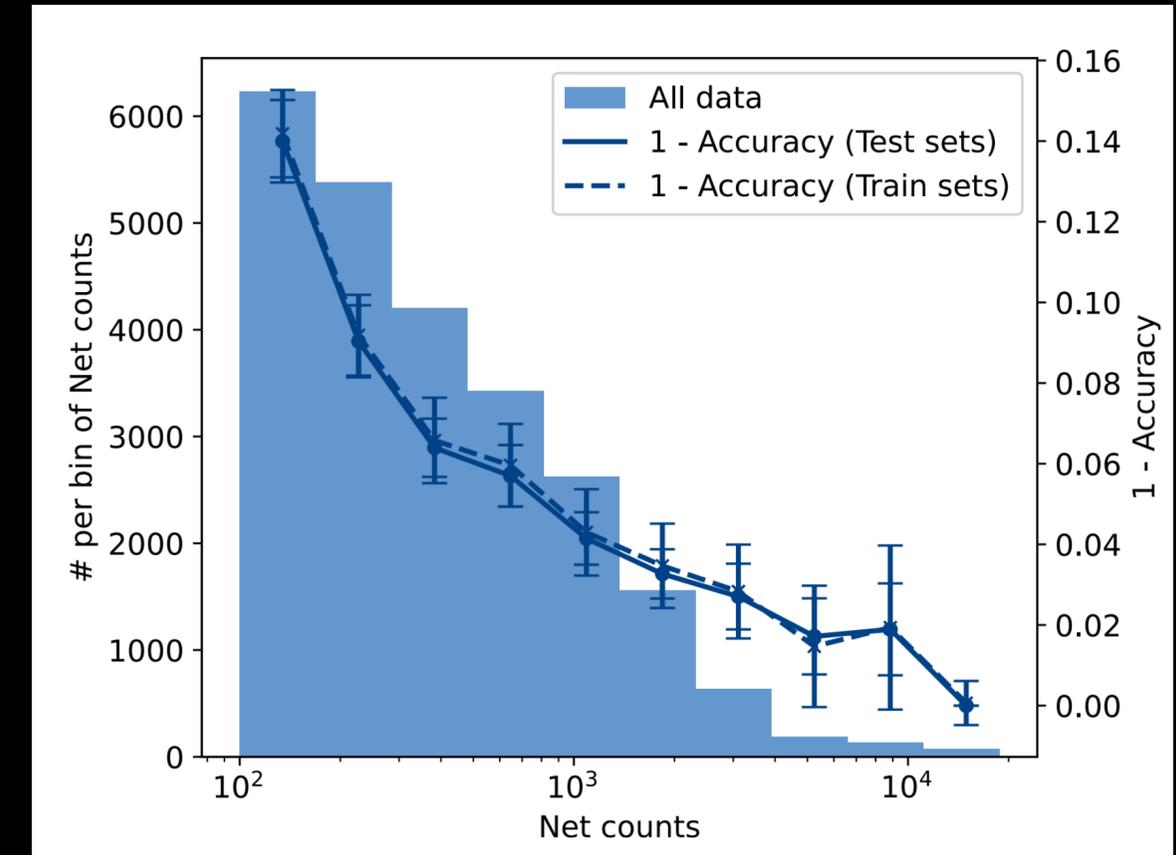
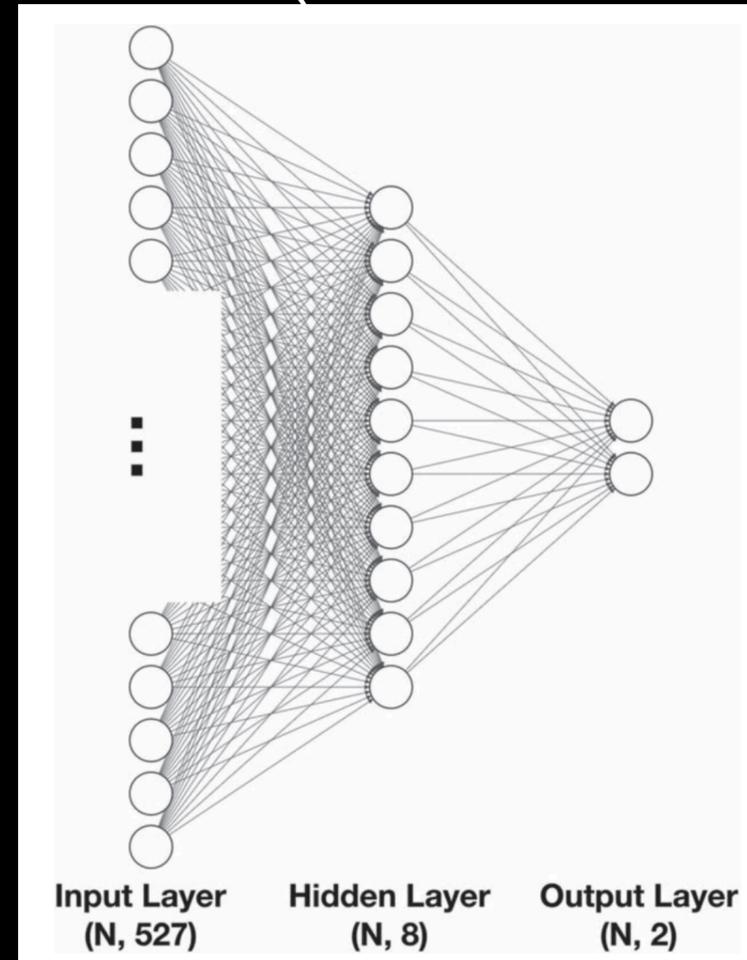
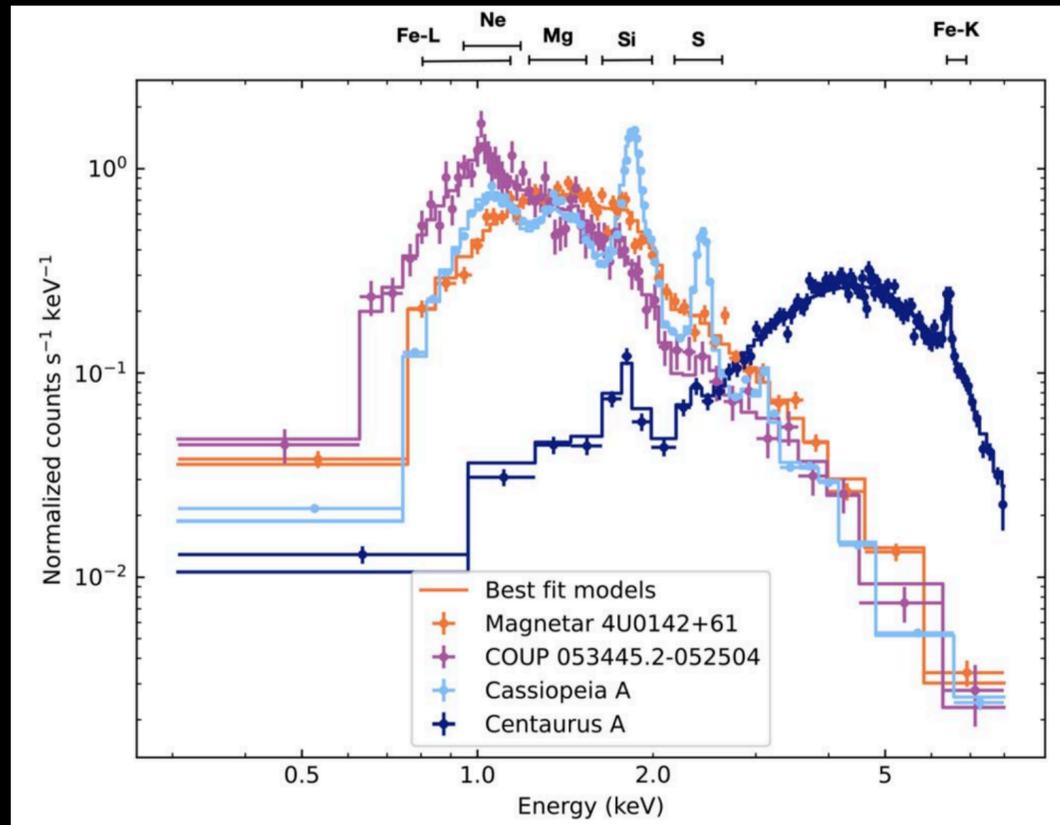
X-ray view of optically selected dual AGNs



CSC pushes the limit of dual AGN studies to separations of <5kpc

- Cross-matching of CSC sources with optical and IR catalogs allows for multi-wavelength identification and classification of dual AGNs.
- >80% of the targets identified in pairs have confirmed AGN emission.
- X-ray luminosity increases with decreasing pair separation, suggesting that mergers contribute to more luminous AGNs.
- From X/mid-IR ratio vs. HR, evidence that dual AGNs are more obscured than isolated ones, and less obscured than more evolved mergers.

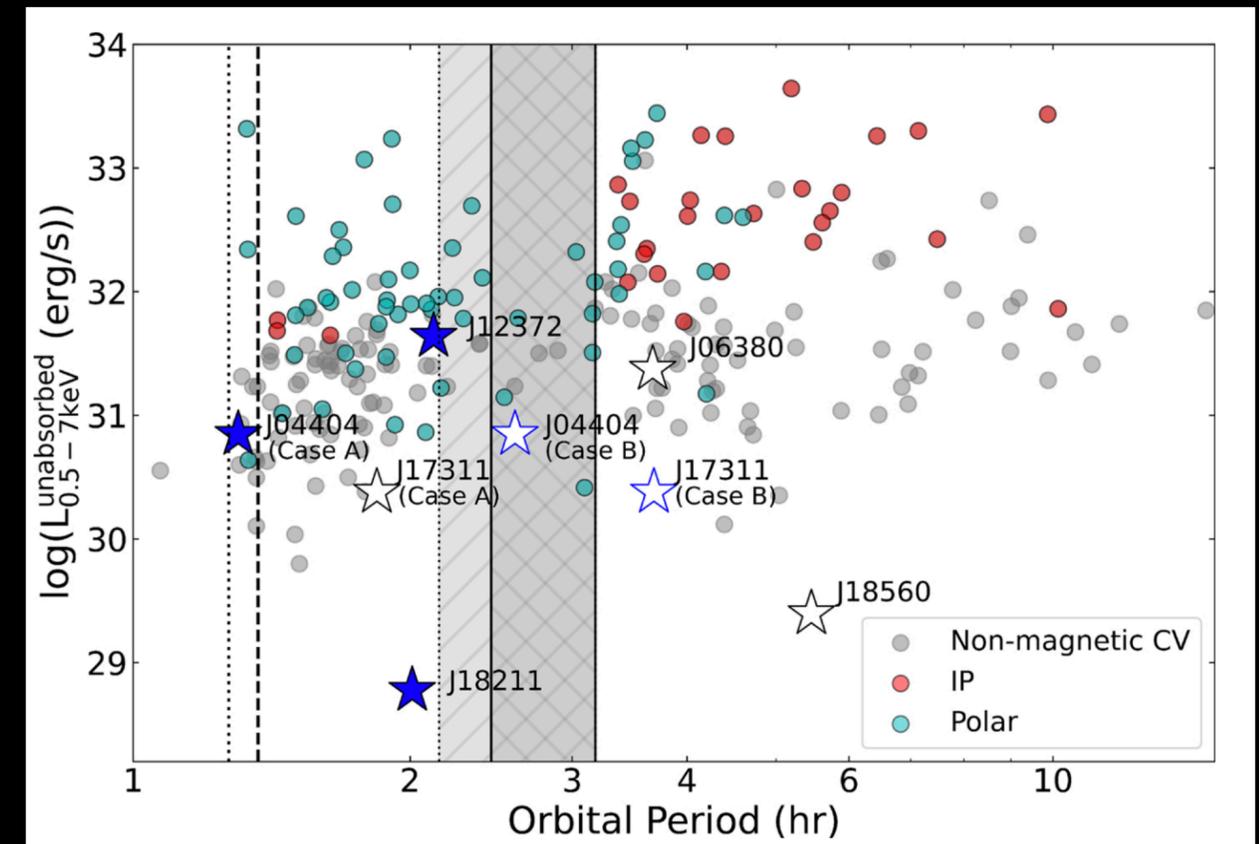
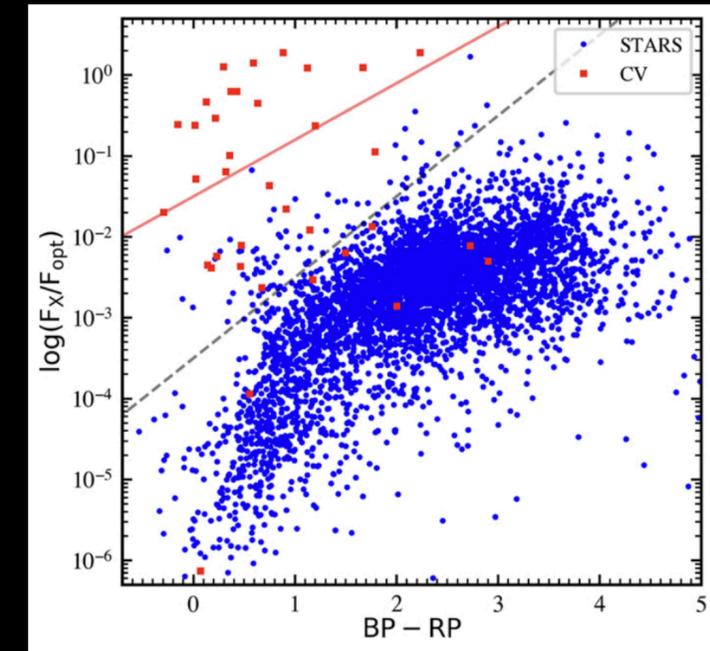
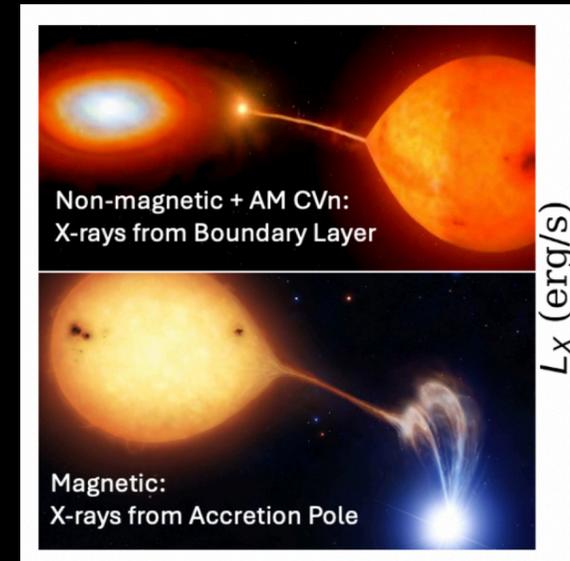
Classification of CSC spectra using Neural Nets (Hebbar et al. 2023)



- A Neural Network trained to classify stars and AGNs, using the simulated spectra computed using priors derived from CSC spectra.
- Trained model applied to both the simulated and observed CSC spectra, and achieve accuracies over 90%
- See also Yang et al. 2022, Chen et al. 2023, Kumaran et al. 2023, Perez et al 2023

Nearby Cataclysmic variables and Accreting WD

- Accreting WDs are the more abundant interacting compact binaries. 14 newly identified using the CSC+ Gaia
- Ultra-compact versions of WD in binaries are probes of general relativity and are expected to emit GWs in the LISA band.
- The study of their formation channels is relevant for binary evolution and subsequent multi-messenger science.
- Joint X-ray and optical searches efficiently find CVs. Chandra: magnetic and low accretion rate CVs, which could be missed by purely optical surveys.

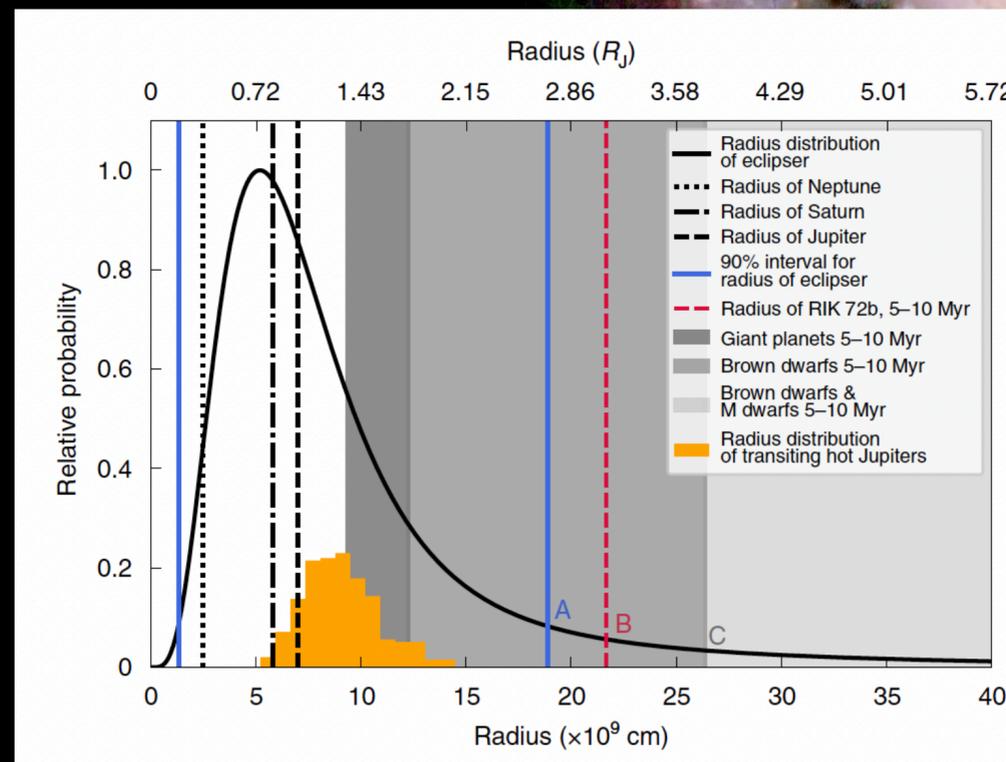
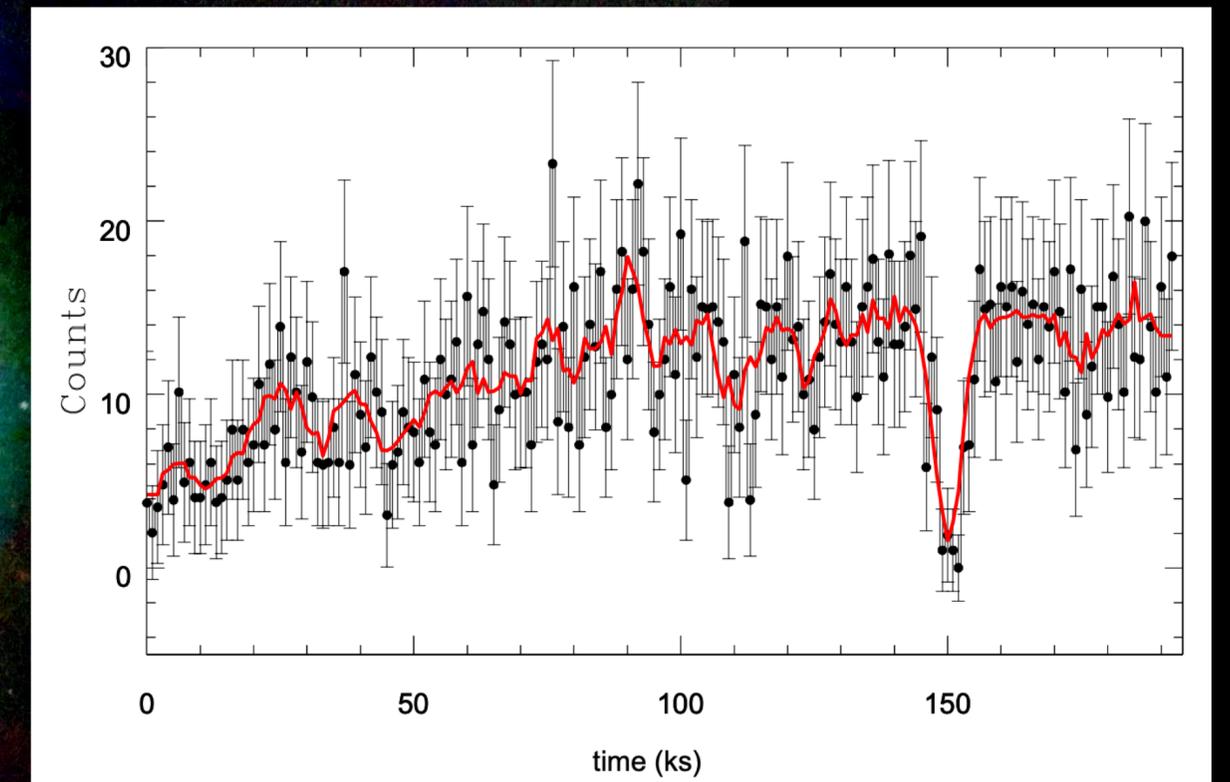


A planet candidate in M51

Di Stefano et al. 2021



M51-ULS-1b



Inferring physical parameters while accounting for instrumental effects

J. Yang et al., in prep

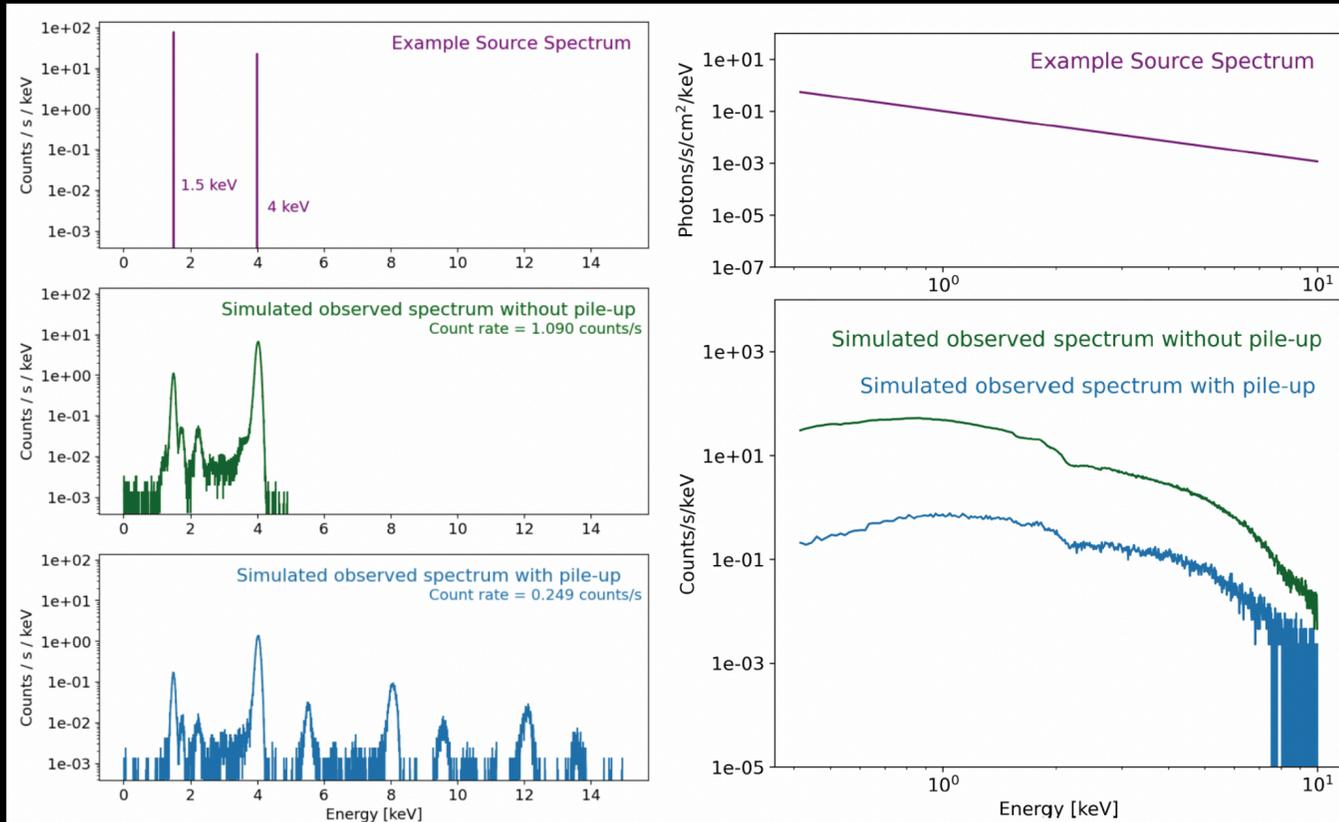
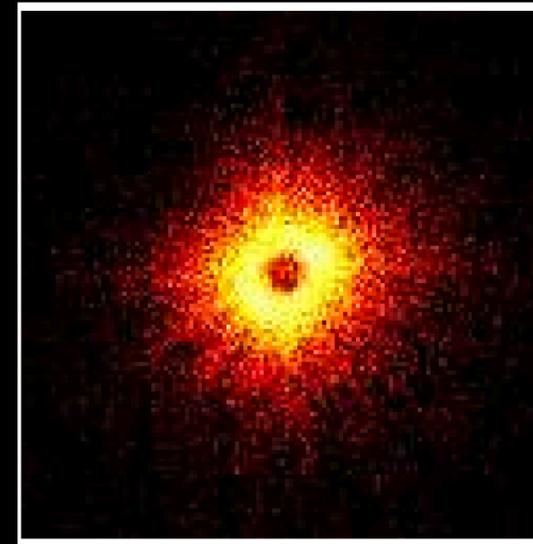


Fig. 1: simulations of how *Chandra*/ACIS-S would observe different source spectra with no pile-up vs. with a large amount of pile-up. Photons of low energies are observed as events at higher energy.

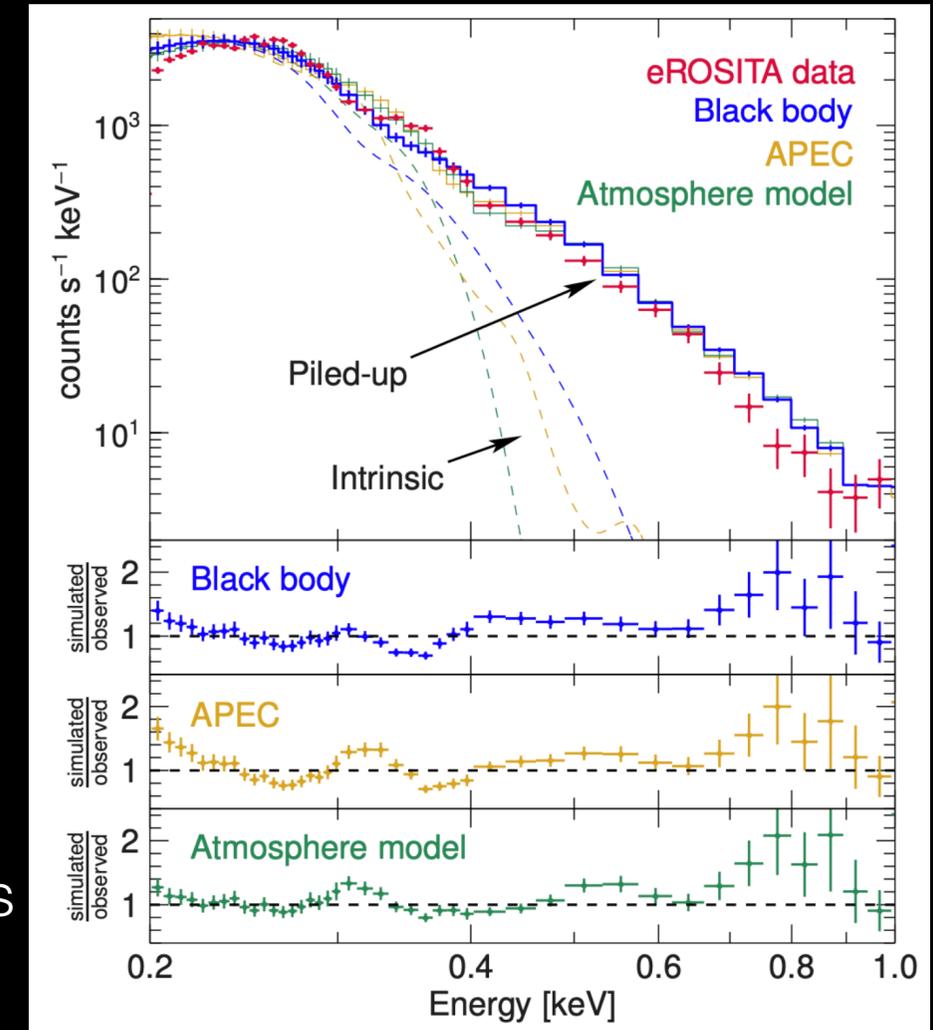
When 2 or more photons strike a detector in nearby pixels and within a single readout time, they are interpreted as a single “piled-up” event with aggregated properties

YZ Reticuli - eROSITA



- 1000 counts per second. Severely piled-up.
- Pile-up correction depends on instrument simulation.
- Pile-up itself strongly depends on the actual spectra shape and charge cloud. Systematic error is 10%-20%/

König et al.2022, Nature



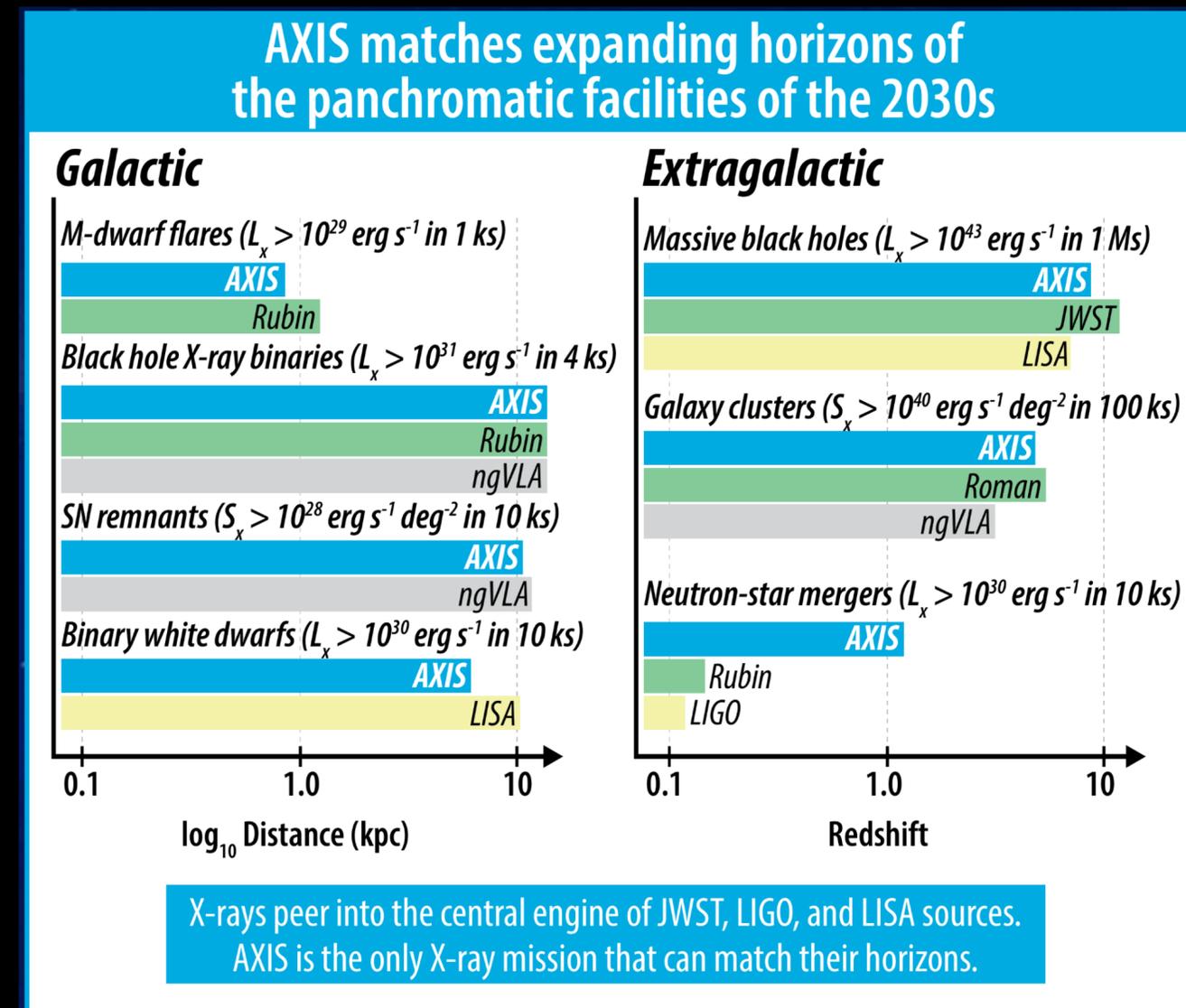
Non-linear detector effects will remain an issue in the AXIS and Athena era



ATHENA

- Compared with Chandra, AXIS will have 5 to 10 times the effective area, and better PSF performance across the field. AXIS will have fast response alert capabilities for TOOs and other transients, including BNS mergers at $z \sim > 1$.
- The ESA-led Athena mission will operate at energies between 0.2-1.2 keV, with a resolution similar to XMM-Newton, but with a wide field imager, better collecting area, and high resolution spectroscopy capabilities.

Future facilities



AXIS Team

A Family of X-ray Catalogs

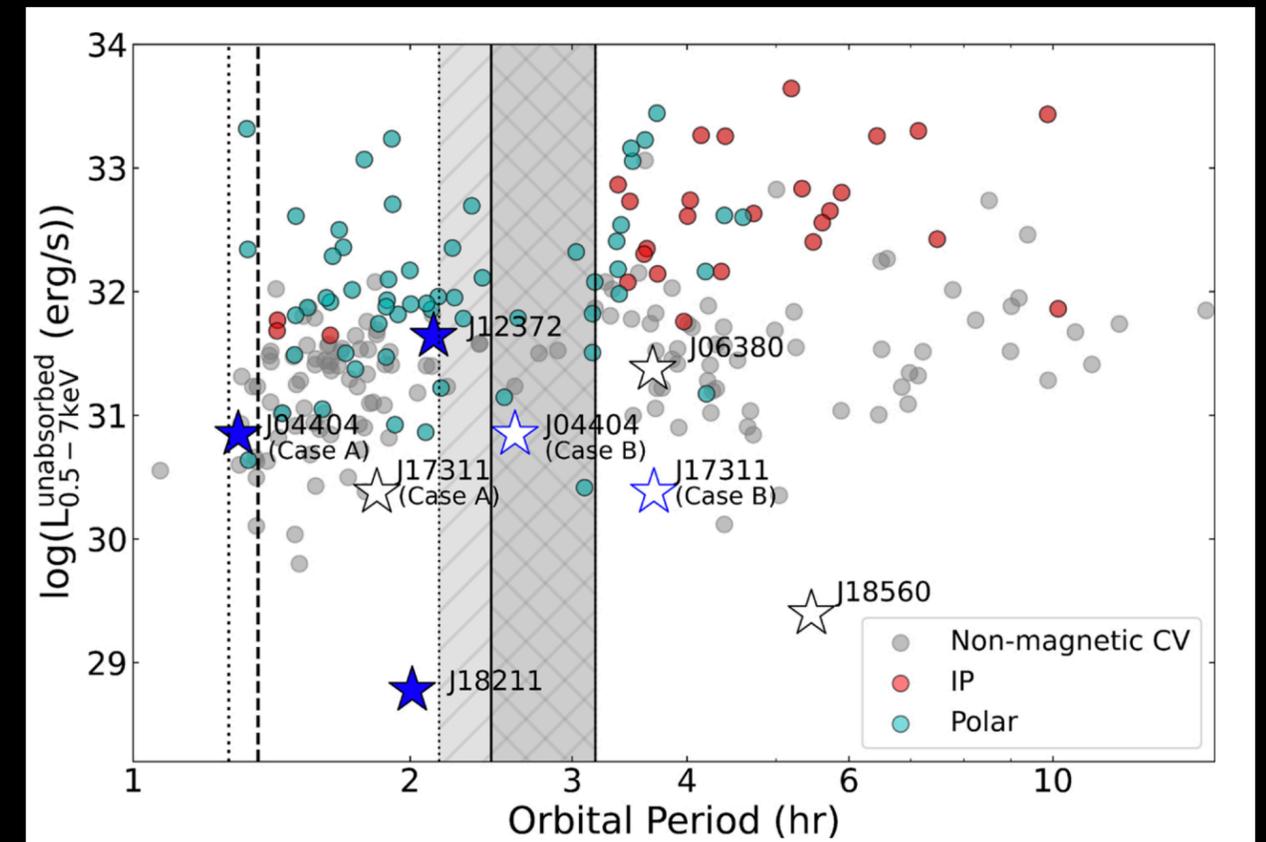
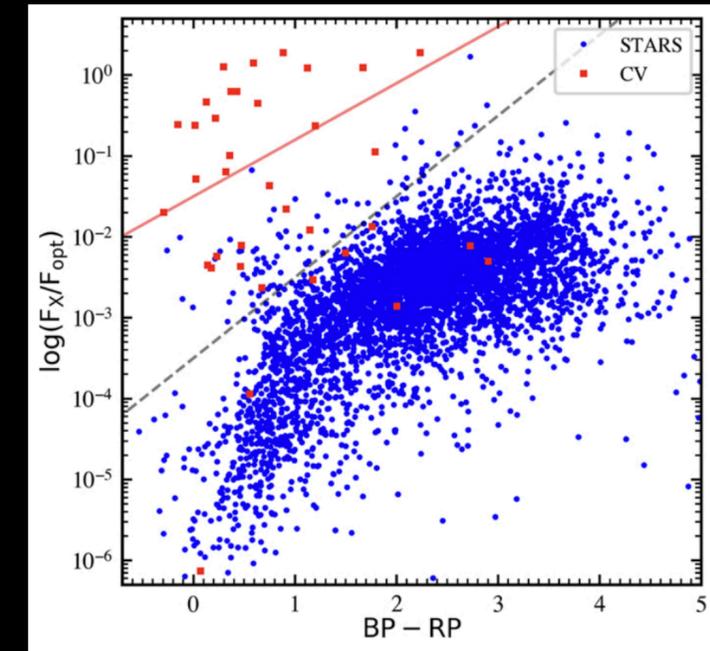
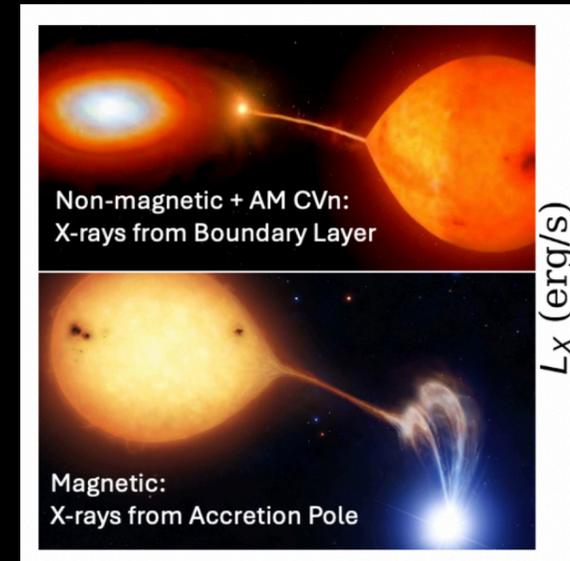
- The Chandra Source Catalog v. 2.1 contains ~408k unique sources and over 1.3 million X-ray detections at high resolution and low background, together with a **very** rich set of data products. Median flux 8.0×10^{-15} erg/cm/s. Spatial resolution 0.5".
- The XMM-Newton Source Catalog v. 4XMM-DR13 contains ~657k sources, half of which have spectra and light curves. Median flux 2.2×10^{-14} erg/cm/s. Spatial resolution ~5".
- The eROSITA eRASS catalog contains ~930k sources over a large portion over the entire sky, light curves, and spectra. Median flux 4.3×10^{-14} erg/cm/s. Spatial resolution ~10".



Watch for the future: Athena, AXIS, Lynx!

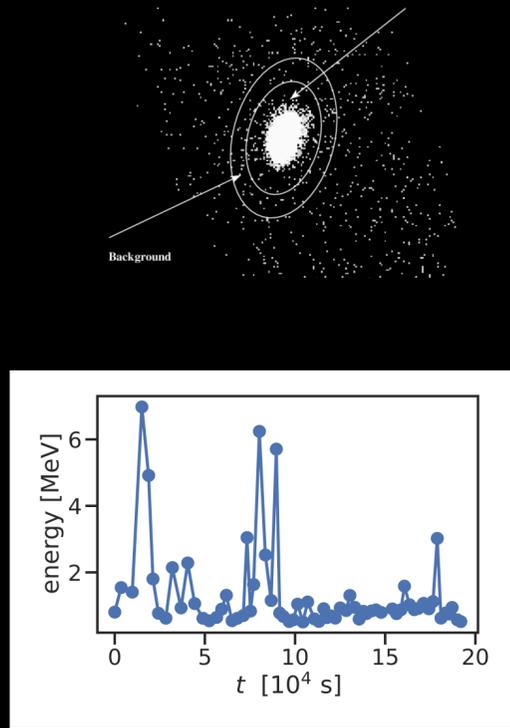
Nearby Cataclysmic variables and Accreting WD

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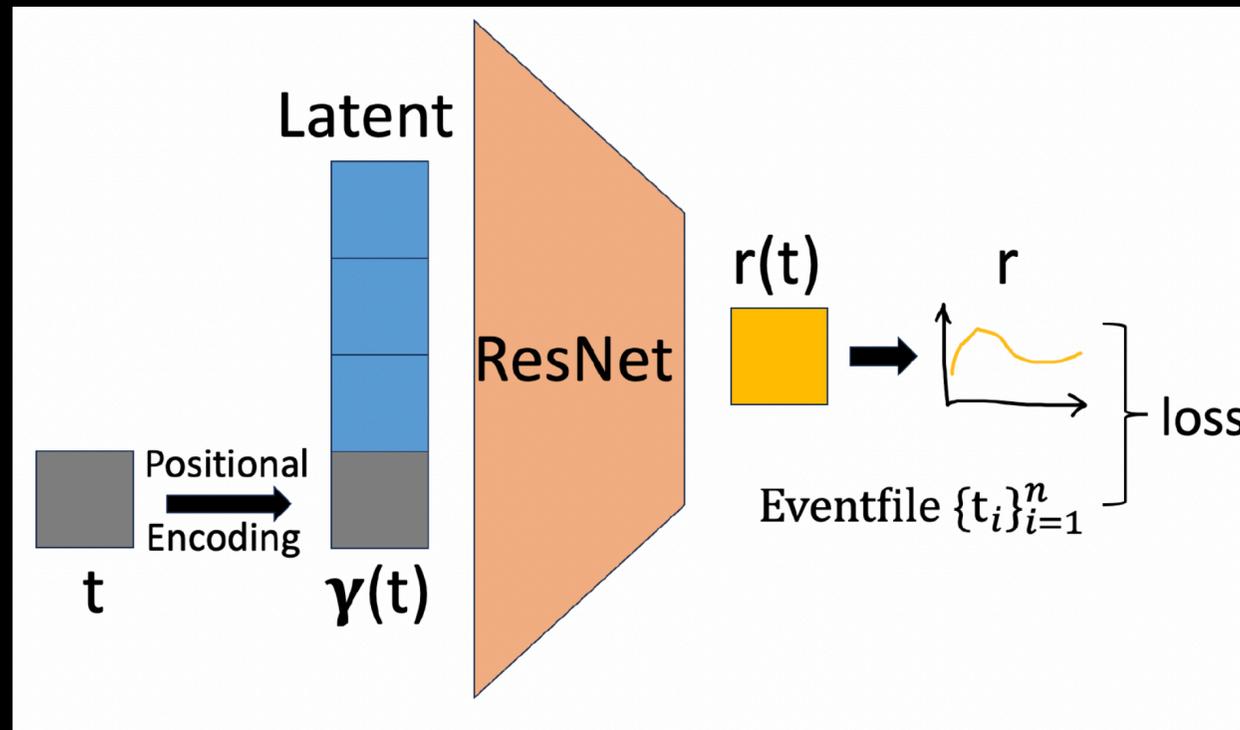


Accounting for every photon: a Poisson Process Autodecoder

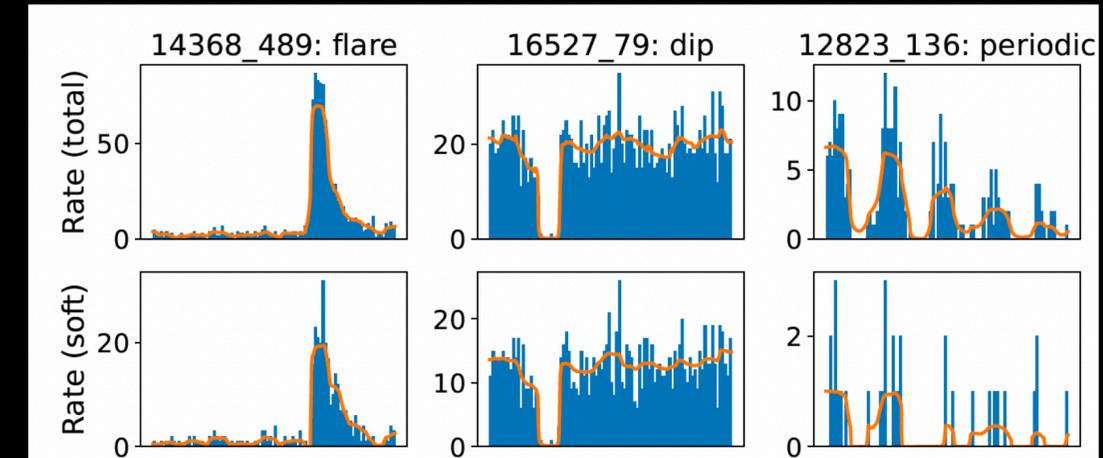
Input: events



Architecture: PPAD



Pretext task:
Poisson $r(t)$ reconstruction



- We train to maximize the likelihood of a set of events, given the Poisson rate $r(t)$
- Positional encoding helps for faster convergence
- At training, both ResNet weights and latent vectors are optimized. At inference, ResNet is frozen.
- Light curve can be reconstructed at any resolution, for given energy bands.

Loss function

Given the output neural field r and an eventfile $\{t_i\}_{i=1}^n$,

$$L(r_e; \{t_{e,i}\}_{i=1}^{n_e}) := \underbrace{-\sum_{i=1}^{n_e} \log r(t_{e,i}) + \int_0^T r_e(t) dt}_{\text{negative log likelihood}} + \underbrace{\lambda_{TV} \cdot \sum_{i=1}^{n-1} |r_e(t_{e,i}) - r_e(t_{e,i-1})|}_{\text{smoothness penalty}}$$