XGA: A module for the large-scale scientific exploitation of archival X-ray astronomy data

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Summary

The XMM Cluster Survey (XCS, Romer et al., 2001) have developed a new Python module, X-ray: Generate and Analyse (hereafter referred to as XGA) to provide interactive and automated analyses of X-ray emitting sources observed by the XMM-Newton space telescope. XGA only requires that a set of cleaned, processed, event lists has been created, and (optionally) that a source detector has generated region lists for the observations. XGA is centered around the concept of making all available data easily accessible and analysable. The user provides information (e.g. RA, Dec, redshift) on the source they wish to investigate, and XGA will locate all relevant observations and generate all required data products. This approach means that the user can quickly and easily complete common analyses without manually searching through large amounts of archival data for relevant observations, thus being left free to focus on extracting the maximum scientific gain. In the future, we will add support for X-ray telescopes other than XMM (e.g. Chandra, eROSITA), as well as the ability to perform multi-mission joint analyses. With the advent of new X-ray observatories such as eROSITA (Predehl et al., 2021), XRISM (XRISM Science Team, 2020), ATHENA (Nandra et al., 2013), and Lynx (Gaskin et al., 2019), it is the perfect time for a new, open-source, software package that is open for anyone to use and scrutinise.

Statement of need

X-ray telescopes allow for the investigation of some of the most extreme objects and processes in the Universe; this includes galaxy clusters, active galactic nuclei (AGN), and X-ray emitting stars. This makes the analysis of X-ray observations useful for a variety of fields in astrophysics and cosmology. Galaxy clusters, for instance, are useful as astrophysical laboratories, and provide insight into how the Universe has evolved during its lifetime.

Current generation X-ray telescopes have large archives of publicly available observations; XMM-Newton has been observing for over two decades, for instance. This allows for analysis of large amounts of archival data, but also introduces issues with respect to accessing and analysing all the relevant data for a particular source. XGA solves this problem by automatically identifying the relevant XMM observations then generating whatever data products the user requires; from images to sets of annular spectra. Once the user has supplied cleaned event lists (and optionally region files) an analysis region can be specified and spectra (along with any auxiliary files that are required) can be created.

Software to generate X-ray data products is supplied by the telescope teams, and most commands require significant setup and configuration. The complexity only increases when analysing multiple observations of a single source, as is often the case due to the large archive of data available. XGA provides the user with an easy way to generate XMM data products.

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for large samples of objects (which will scale across multiple cores), while taking into account complex factors (such as removing interloper sources) that vary from source to source.

Figure 1: Demonstration of the view methods of the RateMap and Spectrum classes, when applied to the Abell 907 galaxy cluster. Data from the XMM EPIC-PN instrument of 0404910601 is used. **Left**: A count-rate map with a mask that removes contaminant sources (using XCS region information) and applies an $R_{500}$ aperture. **Right**: A spectrum generated for the $R_{500}$ region with contaminants removed, and fit with an absorbed plasma emission model using XSPEC.

Features

XGA is centered around source and sample classes. Different source classes, which represent different types of X-ray emitting astrophysical objects, all have different properties and methods. Some properties and methods are common to all sources, but some store quantities or perform measurements that are only relevant to a particular type of astronomical source.

XGA also contains product classes, which provide interfaces to X-ray data products, with built-in methods for analysis, manipulation, and visualisation. The RateMap (a count rate map of a particular observation) class for instance includes view methods (left hand side of Figure 1), methods for coordinate conversion, and for measuring the peak of the X-ray emission. We also provide classes for interacting with, analysing, and viewing spectra (see right hand side of Figure 1), both global and annular; as such we can use XGA to investigate both average properties and, in the case of extended sources, how these properties vary radially. Similar procedures for image based analysis are also available, where images (and merged images from all available data for a given source) can be easily generated en masse, then combined with masks automatically generated from supplied region files to perform photometric analyses.

We also include a set of profile classes, with built-in viewing methods, and a fitting method based around the emcee ensemble MCMC sampler (Foreman-Mackey et al., 2013). Profiles also support storing and interacting with fitted models; including integration and differentiation methods, inverse abel transforms, and predictions from the model. An example of the utility of these profiles is the galaxy cluster hydrostatic mass measurement feature; this requires the measurement of 3D gas density profiles, 3D temperature profiles, gas mass, and total mass profiles.

To extract useful information from the generated spectra, we implemented a method for fitting models, creating an interface with XSPEC (Arnaud, 1996), a popular X-ray spectral fitting language. This interface includes the ability to fit XSPEC models (e.g. plasma emission and blackbody) and simplifies interaction with the underlying software and data by automatically performing simultaneous fits with all available data.
Figure 2: A flowchart giving a brief overview of the XGA workflow.
Figure 3: A demonstration of the application of XGA to an artificial observation of a simulated Illustris-TNG cluster created by another XCS tool (XCSim; Turner et al. in prep). The simulated cluster was injected into the 0302351301 XMM observation. Cross-hair is the peak position of the simulated cluster in the middle image, dashed circle is the simulation-defined $R_{500}$ of the cluster. Red and green regions indicate XCS detected sources from the original observation. Left-hand-side: Zoomed view of the original combined PN+MOS1+MOS2 image. Middle: Zoomed view of the combined PN+MOS1+MOS2 image after the simulated cluster was added at $z = 0.35$. Right-hand-side: An view of an XGA AnnularSpectra object generated from the simulated cluster.

Existing software packages

To the knowledge of the authors, no software package exists that provides features completely equivalent to XGA, particularly in the open source domain. That is not to say that there are no software tools similar to the module that we have constructed; several research groups including XCS (Lloyd-Davies et al., 2011), XXL (Giles et al., 2016), LoCuSS (Martino et al., 2014), and the cluster group at UC Santa Cruz (Hollowood et al., 2019) have developed pipelines to measure the luminosity and temperature of X-ray emitting galaxy clusters, though these have not been made public. It is also important to note that these pipelines are normally designed to measure a particular aspect of a particular type of X-ray source (galaxy clusters in these cases), and as such they lack the generality and flexibility of XGA. Our new software is also designed to be used interactively, as well as a basis for building pipelines such as these.

Some specific analyses built into XGA have comparable open source software packages available; for instance pyproffit (Eckert et al., 2020) is a recently released Python module that was designed for the measurement of gas density from X-ray surface brightness profiles of galaxy clusters. We do not believe that any existing X-ray analysis module has an equivalent to the source and sample based structure which XGA is built around, or to the product classes that have been written to interact with X-ray data products.

The XSPEC (Arnaud, 1996) interface we have developed for XGA is far less comprehensive than the full Python wrapping implemented in the PyXspec module, but scales with multiple cores for the analysis of multiple sources simultaneously much more easily.

Research projects using XGA

XGA is stable and appropriate for scientific use, and as such it has been used in several recent pieces of work; this has included an XMM analysis of the eFEDS cluster candidate catalogue (Turner et al., 2021), where we produced the first temperature calibration between XMM and eROSITA, a multi-wavelength analysis of an ACT selected galaxy cluster (Pillay et al., 2021), and XMM follow-up of Dark Energy Survey (DES) variability selected low-mass AGN candidates (Burke et al., 2021).

There are also several projects that use XGA nearing publication. The first of these is a
hydrostatic and gas mass analysis of the redMaPPer (Rykoff et al., 2014) SDSS selected XCS galaxy cluster sample (Giles et al., 2022) and well as the ACTDR5 (Hilton et al., 2021) Sunyaev-Zel’dovich (SZ) selected XCS sample of galaxy clusters. This work also compares commonly measured X-ray properties of clusters (the X-ray luminosity $L_X$, and the temperature $T_X$ both to results from the existing XCS pipeline and from literature, confirming that XGA measurements are consistent with previous work. This process is repeated with XGA’s galaxy cluster gas and hydrostatic mass measurements, again showing they are consistent with previous work. XGA’s ability to stack and combine X-ray surface brightness profiles is currently being used, in combination with weak lensing information from DES, to look for signs of modified gravity in galaxy clusters. Finally, we intend to use XGA to analyse artificial XMM observations of simulated galaxy clusters (see Figure 3) produced by another XCS tool (XCSim; Turner et al. in prep). This will allow us to perform measurements of simulated cluster properties for various simulation suites (e.g. Illustris-TNG, the 300 project) in an identical manner to our standard analyses. As such we shall be able to probe the realism of hydrodynamical simulations, as well as explore sources of measurement bias in X-ray observables.

Future Work

In the future we intend to introduce support for the analysis of X-ray telescopes other than XMM-Newton, first focusing on Chandra and eROSITA, and then possibly considering the addition of other X-ray instruments. This will include the same ability to find relevant data and generate data products as is already implemented for XMM, and will also involve the introduction of powerful multi-mission joint analyses to fully exploit the X-ray archives. We have already begun work that pairs XGA with XCS’ simulated XMM observations (see Figure 3), and planned support for other telescopes will also extend to the analysis of simulated observations from future telescopes (e.g. ATHENA and Lynx).

We are also happy to work with others to introduce specific analysis features that aren’t already included in the module.

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