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

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Summary

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 (where a supermassive black hole at the centre of the galaxy is actively accreting matter), and supernovae remnants. This makes the analysis of X-ray observations very useful for a wide variety of fields in astrophysics and cosmology. Galaxy clusters, for instance, can act as laboratories for the exploration of many astrophysical processes, as well as providing insight into how the Universe has evolved during its lifetime, as they are excellent tracers of the formation of large scale structure.

Figure 1: The logo of the XGA module.

We 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. XGA is centered around `source` and `sample` classes, and the concept of making all available data and simple analyses easily accessible . These `source` classes all have different properties and methods, which either relate to relevant properties of or perform measurements which are only relevant to that type of astronomical source, with some properties/methods being common to all sources.

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 (demonstrated in Figure 2), methods for coordinate conversion, and for measuring the peak of the X-ray emission. We also provide classes for interacting with spectra (both global and annular), PSFs, and a base class for XGA profile objects, which allow for the storage, fitting, and viewing of radial profiles generated through XGA processes.

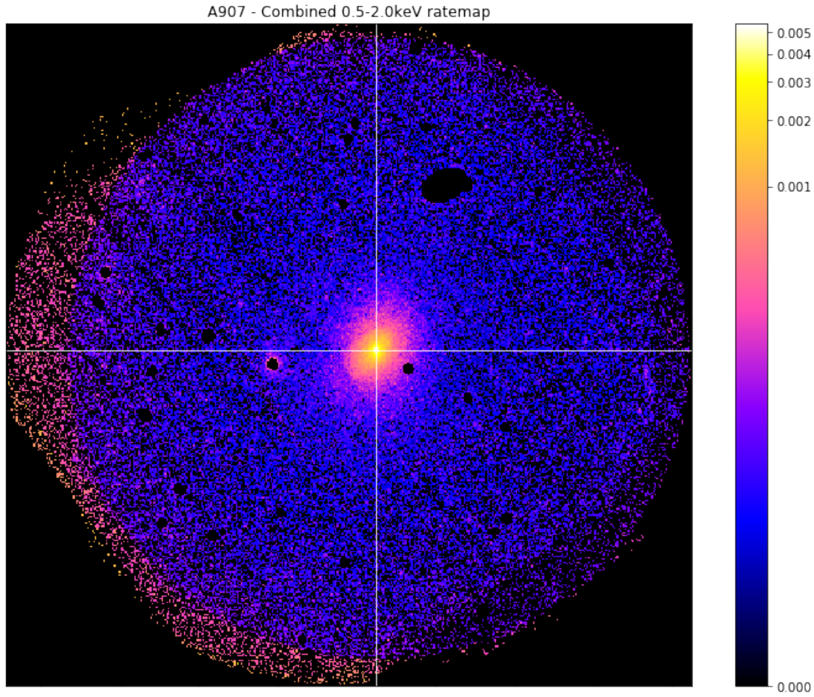

Figure 2: The output of the view method of a RateMap instance where a mask to remove interloper sources has been applied, with an added crosshair to indicate coordinates of interest.

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. 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

This module was developed by the XMM Cluster Survey (XCS, Romer et al. (2001)) to enable simple, interactive, analyses of X-ray sources, from galaxy clusters to AGN, for the whole astronomy community.

One of the chief advantages of this module is that it simplifies the process of generating the data products which are required for most work involving X-ray analysis; once the user has supplied cleaned event lists (and optionally region files), and a source object has decided which observations should be associated with it, an analysis region can be specified and spectra (along with any auxiliary files that are required) can be created. We can use XGA to investigate both average properties and, in the case of extended sources, how these properties vary spatially. 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.

Software to generate X-ray data products is supplied by the telescope teams, but in the case of XMM-Newton it can only be used on the command line, and most commands require significant setup and configuration. XGA wraps the most useful commands and provides the user with an easy way to generate these products 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. To extract useful information from the generated spectra, we implemented a method for fitting models, creating an interface with XSPEC (Arnaud (1996)), the popular X-ray spectral fitting language. This interface again provides simplified interaction with the underlying software that can be run simultaneously when multiple sources are being analysed at the same time.

Many more features are built into XGA, enabled by the source based structure, as well as the product generation and XSPEC interface. One of these features is the ability to measure hydrostatic galaxy cluster masses; this includes the measurement of 3D gas density profiles, 3D temperature profiles, gas mass, and total mass profiles. New methods for the measurement of central cluster coordinates and PSF correction of XMM images were also created to enable this, as well as Python classes for various data products (with many useful built in methods). This includes a radial profile class, with built-in viewing methods, and a fitting method based around the `emcee` ensemble MCMC sampler (Foreman-Mackey et al. (2013)). The profile fitting capability also motivated the creation of model class, with methods for storing and interacting with fitted models; including integration and differentiation methods, inverse abel transforms, and predictions from the model.

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. 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. (in prep)).

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. (in prep.)) 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. Similar work is being done on a Dark Energy Survey Year 3 (DESY3) optically selected XCS sample of clusters, though this will also include analysis from other XCS tools, and will not be focussed only on mass measurements. `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 an exploration of the X-ray properties of a new sample of Pea galaxies is being performed using the point source class, the `XSPEC` interface, and the upper limit luminosity functionality.

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