SURF 2024 Report 1:
Emulating X-Ray Reflection Spectroscopy with Machine Learning

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Background

Astronomers utilize X-ray spectroscopy to study compact objects such as neutron stars and stellar mass or supermassive black holes. In these extreme environments, X-ray photons are emitted around the compact object with a fraction of them reflecting off the accretion disk, with most emission in the X-ray portion of the electromagnetic spectrum. The observed X-ray spectroscopy data depends upon the state of the accreting compact object. So by analyzing the X-ray spectra of these neutron stars or black holes, we can understand the thermodynamic state of the object's accretion disk, such as its density, temperature, chemical composition, ionization, and geometry. Additionally, we can also learn about the compact object itself, such as its mass and angular momentum. Prior literature demonstrated how spectroscopic analysis of radiation emitted by compact objects allows us to derive information regarding the compact object's system (García et al., 2016).

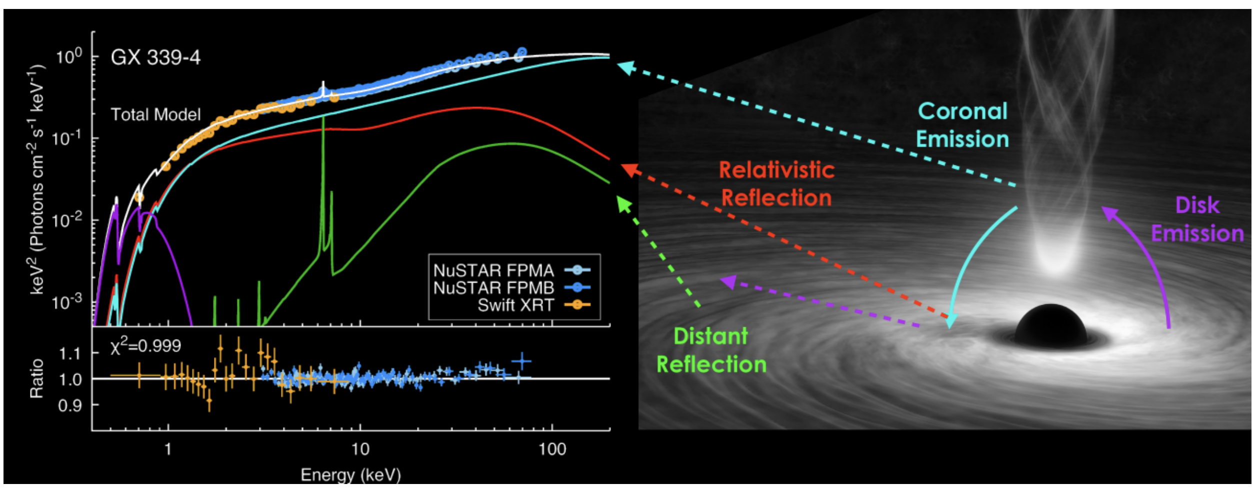

Figure 1: Figure adapted from García et al. (2019). The dotted lines represent X-rays that are reflected by the accretion disk or emitted by the black hole's corona that result in the observed spectroscopy. The solid lines are X-rays that are emitted from the black hole's corona to the accretion disk or vice versa.

As shown in Figure 1, photons are emitted around compact objects and reflected by their accretion disks, creating the X-ray spectrum shown. Astronomers have created models to simulate X-ray emission and reflection to produce X-ray spectra based upon some input parameters. This process involves simulating the radiation reprocessed within an accretion disk around the compact object and re-emitted towards the observer (García et al., 2019). This interaction between X-rays and the plasma within the disk creates distinct features in the spectra such as atomic emission lines and absorption edges, resulting from the presence of elements such as oxygen and iron. Using this spectra, we can better understand the physical conditions within the disk like its ionization state, density, and temperature. Additionally, X-rays originating close to the compact object itself are subject to general-relativistic effects of strong gravitational fields, modifying the X-ray's paths and energy, which allows us to learn about the compact object's mass and angular momentum. Currently, there are various models developed by the astronomical community that could be used to analyze X-ray reflection. The primary model we will focus on emulating will be the XILLVER model developed by García and Kallman (2010). XILLVER is a state-of-the-art framework, taking into account all atomic physics processes relevant to radiation reprocessing in astrophysical plasmas, and has now become an industry-standard in X-ray spectroscopic analysis.

The way that astronomers derive the physical parameters of a compact object's system is by finding the closest modeled X-ray spectra to the X-ray spectra observed. For this, a precomputed table of modeled X-ray spectra is required. This is because in modeling just one X-ray spectrum, various assumptions have to be made about the accretion disk such as its size, geometry, temperature, density, ionization, and chemical composition. Modeling multiple X-ray spectra will take a significant amount of time, which is why we use precomputed tables instead. These precomputed tables do not contain every possible set of parameters and their corresponding X-ray spectrum, due to limited computational resources. Consequently, the observed X-ray spectra will probably not exactly match one of the precomputed X-ray spectra. So instead, we collect the closest precomputed X-ray spectra and perform a linear interpolation, averaging out the physical parameters of those closest X-ray spectra. Here, the problem lies in the non-linear and complex nature of modeling X-ray spectra—the linear interpolation may result in inaccurate results. Additionally, the size of these precomputed X-ray spectra tables are quite large, taking up many gigabytes and potentially up to a terabyte.

Current Progress

This is where applying machine learning may solve the issues faced with current techniques. Utilizing a neural network's capability to capture the non-linear relationships between input and output, we are interested in using a neural network to emulate X-ray spectra based upon the physical parameters imputed. This would solve the issue of X-ray spectra modeling taking additional computational time, the inaccuracies with linear interpolation, and the large file sizes of precomputed X-ray spectra tables.

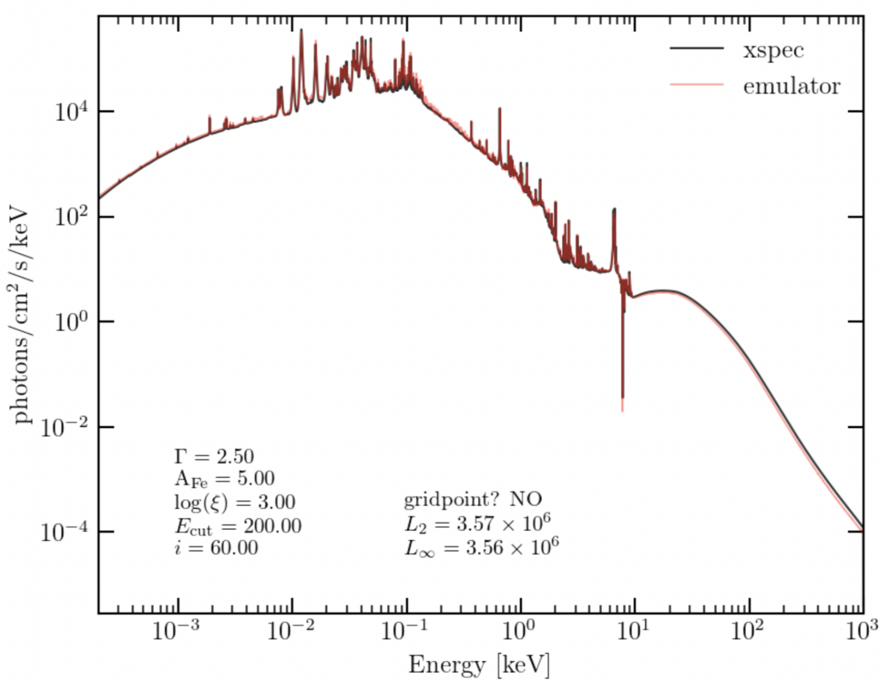

Figure 2: Output spectra for the emulator vs XILLVER model for an example moderate ionization state of the gas. Model input parameters are listed in the panel.

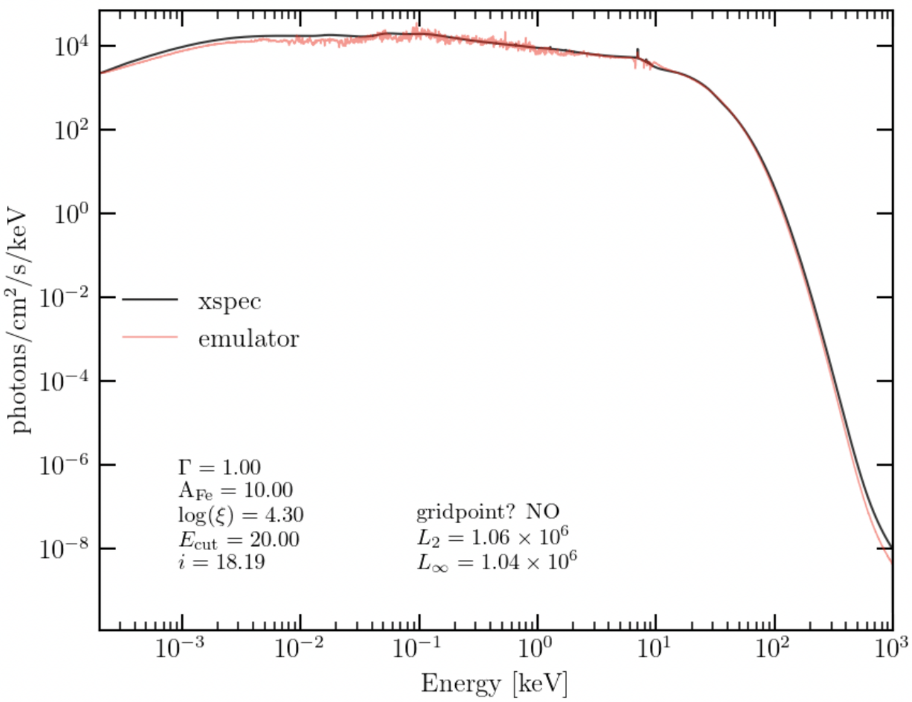

Figure 3: Output spectra for the emulator vs XILLVER model for an example high ionization state of the gas. Model input parameters are listed in the panel.

Matzeu et al. (2022) is the paper that serves as motivation for this SURF. Matzeu et al. (2022) developed a neural network to emulate X-ray spectra produced by a Monte Carlo radiative transfer model. This paper showed promising results demonstrating that neural networks can offer improved accuray over interpolation of a precomputed X-ray spectra table when it came to generating X-ray spectra off a set of input parameters. The neural network in the paper consists of 6 input nodes, then 3 densely connected layers of 1000 nodes each, and then 1000 output nodes. For this SURF, we were able to receive this model, retrained on precomputed XILLVER tables, and see how it well it is able to emulate spectra by the XILLVER model. This provided model seemed to perform well in some parameter ranges, as seen in Figure 2, but bad in other parameter ranges, as seen in Figure 3. I have explored the emulator's capabilities and characterized its performance with respect to the input parameters.

For this SURF, we plan to create our own neural network emulator with its own unique architecture to best emulate the XILLVER model. We are interested in creating a deeper neural network to capture more the complex non-linearity across X-ray spectra, as well as use convolutional layers due to the spatial relationship of points in X-ray spectra. We would also like to try using mean squared logarithmic error instead of mean squared error and use Pytorch instead of Tensorflow. We will also have to finetune parameters such as the number of layers, using dropoff, number of nodes, which optimizer to use, learning rate, etc.

My main issues for this SURF has been with properly installing the required software. Installing or compiling certain tools or packages have resulted in lots of errors, requiring me to complete a lot of trial and error to figure out how to fix it. Having prior computer science experience with debugging code and troubleshooting error messages has been very beneficial for me so far, as I create my own piece of software in the form of a sophisticated neural network. I expect to see some more issues with software installation and issues with debugging code, but I expect to see good progress.

References

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