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Relativistic reflection modeling in AGN and related variability from PCA: a brief review

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X-ray observations of active galactic nuclei (AGNs) reveal relativistic reflections from the innermost regions of accretion disks, which contain general-relativistic footprints caused by spinning supermassive black holes (SMBH). We anticipate the spin of a SMBH to be stable over the human timeframe, so brightness changes in the high-energy corona above the SMBH should slightly alter relativistic reflection. In this brief review, we discuss the latest developments in modeling relativistic reflection, as well as the rapid small variation in relativistic emission disclosed by the principal component analysis (PCA) of X-ray variability in AGN. PCA studies of X-ray spectra from AGNs have shown that relativistically blurred reflection has negligible fluctuations over the course of observations, which could originate from rapid (intra-hour) intrinsic variations in near-horizon accretion flows and photon rings. The PCA technique is an effective way to disclose relativistic reflection from X-ray observations of AGNs, simplifying the complexity of largely variable X-ray data for automated spectral analysis with machine learning algorithms.

KEYWORDS

active galactic nuclei, relativistic disks, black hole spin, reflection, X-ray sources, principal component analysis

1 Introduction

The center of the Milky Way is characterized by a supermassive black hole (SMBH), which is supported by indirect but compelling observational evidence such as stellar orbits in the vicinity of Sagittarius A* (Sgr A*; [Ghez et al., 1998](#); [Ghez et al., 2005](#)) and the near-infrared luminosity of Sgr A* being consistent with the presence of an event horizon ([Broderick and Narayan, 2006](#); [Broderick et al., 2009](#)). Similarly, we expect that active galactic nuclei (AGNs) in other galaxies host SMBHs at their centers ([Kormendy, 1988](#); [Kormendy and Richstone, 1992](#); [Kormendy et al., 1997](#); [Cretton and van den Bosch, 1999](#)), which are essential to explaining the X-ray features of quasars and AGNs (see review by [Mushotzky et al., 1993](#)). Several techniques, such as the reverberation mapping ([Blandford and McKee, 1982](#)), spectral energy distribution (SED) fitting ([Shields, 1978](#); [Malkan, 1983](#)), and broad-line region size–luminosity correlation ([Vestergaard, 2002](#)), have been developed to validate the presence of SMBHs and estimate their masses (e.g., [Kormendy and Richstone, 1995](#); [Miyoshi et al., 1995](#); [Wandel et al., 1999](#); [Peterson et al., 2004](#); [Calderone et al., 2013](#); [Capellupo et al., 2015](#); [Bentz and Katz, 2015](#); [Mejía-Restrepo et al., 2016](#)). Our constraints on SMBH masses have allowed us to establish the connections between SMBHs and the evolution of their host galaxies (e.g.,

Magorrian et al., 1998; Ferrarese and Merritt, 2000; Häring and Rix, 2004; Heckman and Best, 2014).

Some solutions of standard general relativity simply characterize black holes using two parameters, mass and spin (Kerr, 1963), which can fully describe the properties of SMBHs. In this regard, spins of SMBHs, along with masses, could produce some of the fundamental mechanisms for powering relativistic jets (e.g., Garofalo et al., 2010; Tchekhovskoy and McKinney, 2012), as well as describing the discrepancy between radio-loud and radio-quiet AGNs (Wilson and Colbert, 1995; Moderski et al., 1998), galaxy evolution (Di Matteo et al., 2005; Volonteri et al., 2013; Sesana et al., 2014), and galaxy mergers (Hughes and Blandford, 2003; Volonteri et al., 2005; Berti and Volonteri, 2008). In particular, ultra-fast outflows (UFOs) have been detected in X-ray observations of several radio-quiet AGNs (e.g., Tombesi et al., 2010; 2011; 2012; Danehkar et al., 2018; Boissay-Malaquin et al., 2019), while extended relativistic jets have been seen in radio observations of radio-loud AGNs (see review by Blandford et al., 2019). The spins of SMBHs could have a potential role in the formation of UFOs and jets seen in AGNs and quasars (MacDonald et al., 1986; Thorne et al., 1986). These phenomena can be explained by spinning SMBHs according to the Blandford–Znajek (Blandford and Znajek, 1977) and Penrose mechanism (Penrose, 1969; 2002; Penrose and Floyd, 1971), as well as frame-dragging vortexes (e.g., Owen et al., 2011; Nichols et al., 2011; Danehkar, 2020). Alternatively, they could originate magnetically from the innermost accretion disk in the vicinity of a spinning SMBH according to the Blandford–Payne mechanism (Blandford and Payne, 1982).

In the Boyer–Lindquist coordinates, the Kerr metric (Kerr, 1963) of a spinning black hole is expressed using the set of oblate spheroidal coordinates (r, θ, ϕ) as follows (Boyer and Lindquist, 1967):

$$ds^2 = -\left(1 - \frac{r_s r}{\Sigma}\right) c^2 dt^2 - \frac{2\bar{a} r_s r \sin^2 \theta}{\Sigma} c dt d\phi + \frac{\Sigma}{\Delta} dr^2 + \Sigma d\theta^2 + \left(r^2 + \bar{a}^2 + \frac{\bar{a}^2 r_s r \sin^2 \theta}{\Sigma}\right) \sin^2 \theta d\phi^2, \quad (1)$$

where $\Sigma = r^2 + \bar{a}^2 \cos^2 \theta$, $\Delta = r^2 - r_s r + \bar{a}^2$, $r_s = 2GM/c^2$ is the Schwarzschild radius, $\bar{a} = J/Mc$ is called the Kerr spin parameter describing angular momentum per unit mass having the length dimension, J the black hole angular momentum, M the black hole mass, G the Newtonian constant of gravitation, and c the speed of light. The *dimensionless spin parameter*, which is frequently used in the astrophysical community, is defined as $a \equiv 2\bar{a}/r_s = Jc/(GM^2)$, while $-1 \leq a \leq 1$; negative values describe retrograde rotation, in which the black hole rotates in the opposite direction of the accretion disk, whereas positive values are associated with prograde rotation, and zero implies non-rotating black holes. The outer and inner event horizons are determined by the roots of $\Delta = 0$, which are $r_{\pm} = r_s(1 \pm \sqrt{1 - a^2})/2$. In the case of $a = 0$, Equation 1 reduces to the Schwarzschild metric (Schwarzschild, 1916) with the event horizon at $r = r_s$. Unlike the Schwarzschild metric, which has a singularity at $r = 0$, the Kerr metric has one at $\Sigma = 0$. The innermost stable circular orbit (ISCO) of the accretion disk is located at a radius of marginal stability, r_{ms} , which is given by (Bardeen et al., 1972):

$$r_{\text{ms}}(a) = \frac{GM}{c^2} \left(3 + Z_2 - \text{sgn}(a) \sqrt{(3 - Z_1)(3 + Z_1 + 2Z_2)}\right), \quad (2)$$

where $\text{sgn}(a)$ is the signum function having the value -1 , 1 or 0 according to the sign of a , while Z_1 and Z_2 are defined as,

$$Z_1 = 1 + (1 - a^2)^{1/3} \left[(1 + a)^{1/3} + (1 - a)^{1/3} \right],$$

$$Z_2 = \sqrt{3a^2 + Z_1^2}.$$

This implies that the accretion disk has a limited extent at the marginal stability radius (r_{ms}), also called the ISCO radius. The value of this radius depends upon the dimensionless spin parameter, e.g.,

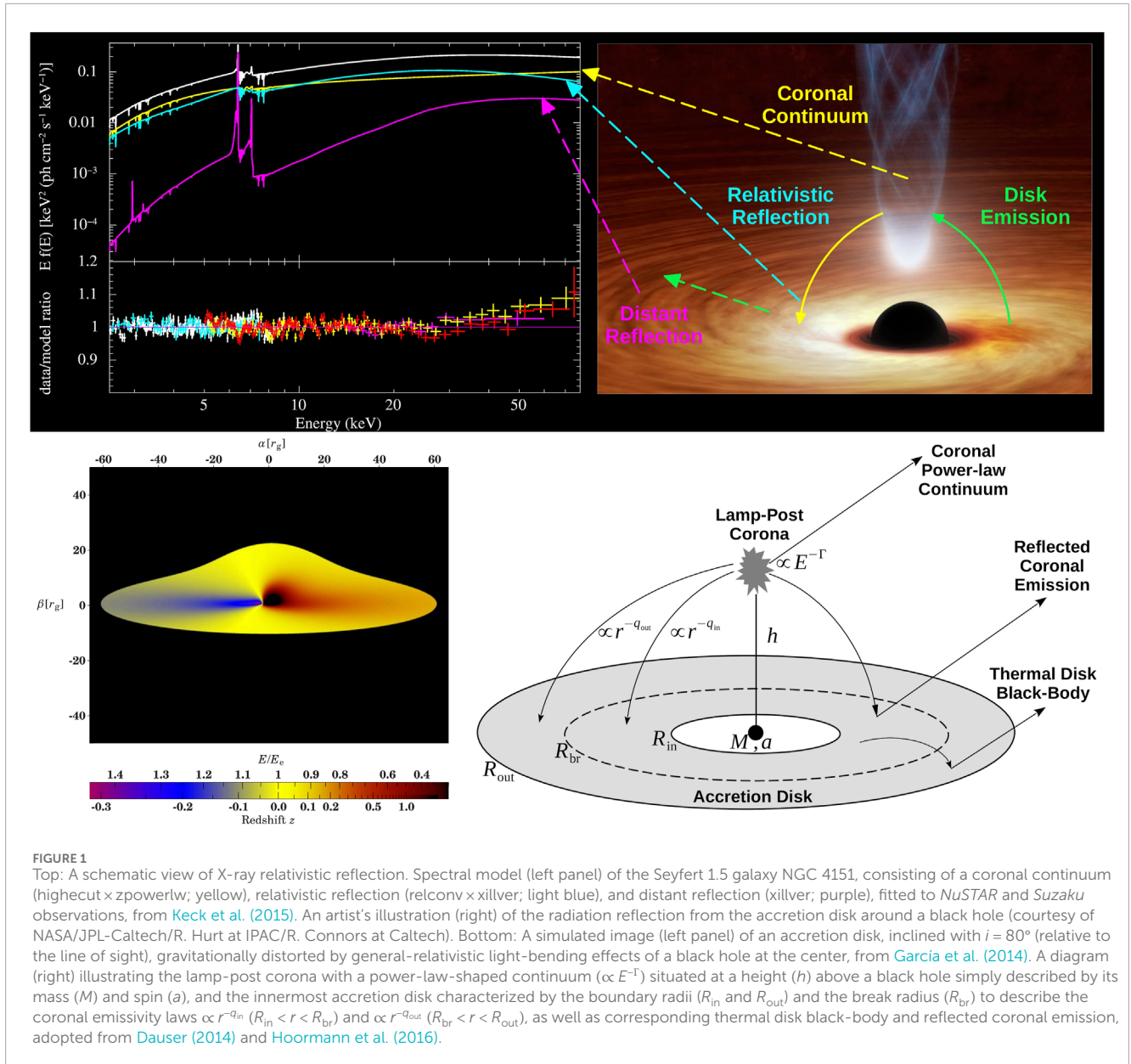
$$r_{\text{ms}} = \begin{cases} 0.5r_s & \text{for } a = 1 \\ 3r_s & \text{for } a = 0 \\ 4.5r_s & \text{for } a = -1 \end{cases}.$$

In prograde rotation, the ISCO radius shrinks to nearly half of the Schwarzschild radius as it approaches a near-maximal spin ($a \approx 1$), while it expands in retrograde rotation ($-1 < a < 0$). For a non-spinning black hole, the ISCO radius is precisely three times the Schwarzschild radius.

There are different methods available to measure the spin of a single SMBH (see review by Brenneman, 2013). All of them are based on general relativity solutions of the Kerr spacetime in the vicinity of the black hole. They use the aforementioned fact that the ISCO radius (r_{ms}) of the accretion disk depends on the spin, as seen in Equation 2, and assume a geometrically thin disk that is capable of irradiating the corona radiation with light-bending in the innermost regions (see Figure 1 bottom-left). Below are the techniques that have been used to constrain the spins of SMBHs:

1.1 X-ray reflection spectroscopy

High-energy radiation from a corona or the base of a jet illuminates the accretion disk, reflecting scattered photons, which forms the basis of this method. Multiple Compton scatterings (Comptonization) of soft thermal photons lead to the cooling of the hot electrons in the corona (Haardt and Maraschi, 1991; 1993). A portion of the comptonized radiation undergoes scattering outside of the ionizing source, resulting in the formation of a power-law-shaped continuum that is typically observed in X-rays from AGN (Haardt and Maraschi, 1991). However, a fraction of the scattered photons will undergo reflection on the surface of the disk (Haardt and Maraschi, 1993), as seen in Figure 1 (top). If the disk is not fully ionized, the continuum includes the emission of various fluorescent emission lines at energies below 7 keV, in addition to the Compton hump with a peak at around 20–30 keV caused by downscattering, as seen in Figure 1 (top panel). The most notable line is Fe K α , with a rest-frame energy of 6.4 keV, which is produced due to the significant iron abundance and fluorescence process. This line is the most important tool for describing the relativistic reflection from the innermost disk, as it becomes broadened and skewed due to Doppler and general-relativistic effects (see reviews by Reynolds and Nowak, 2003; Miller, 2007; Reynolds, 2013; 2014; 2019; Bambi et al., 2021). The truncation of its low-energy tail directly corresponds to the ISCO radius, i.e., the spin. This feature, independent of mass or distance from the black hole, enables the measurement of black



hole spins. One of the drawbacks of this method for AGN is the complex absorption from line-of-sight material, typically found at lower energies in the red tail. Moreover, exceptionally high counts are required to properly constrain the spin; 2×10^5 (Guinazzi et al., 2006) or 1.5×10^5 counts (de La Calle Pérez et al., 2010) in the energy range of 2–10 keV. Furthermore, this approach is actually model-dependent, as demonstrated by a list of reflection models in Table 1. However, the advancements in X-ray spectroscopy above 10 keV with the *Nuclear Spectroscopic Telescope Array* (*NuSTAR*; Harrison et al., 2013), which has no pile-up effects, have significantly improved the reliability of this approach by including the Compton hump reflection at high energies (> 10 keV, peaking within 20–30 keV; see, e.g., Parker et al., 2014c; Keck et al., 2015; Victoria-Ceballos et al., 2023). Most of the spectral models developed for X-ray relativistic reflection are briefly reviewed in Section 2.

1.2 Broad-band SED fitting

This method was initially began to be deployed for X-ray binaries by Zhang et al. (1997) and Gierliński et al. (2001). This approach depends on the distance, mass, and disk inclination angle of the accretion disk (see review by Remillard and McClintock, 2006), so it has mostly been used for the spin measurement of stellar-mass black holes (e.g., Shafee et al., 2006; McClintock et al., 2006). This method was first exploited by Done et al. (2013) to put constraints on the spins of SMBHs with the *optxconv* model (based on *optxagnf*; Done et al., 2012), which contains the SED spectrum made by a (color-temperature-corrected) blackbody, an optically thick warm Comptonisation (soft excess; < 2 keV) component, and an optically thin, hot Comptonisation (power-law; > 2 keV) component. Later, the same technique was employed to measure the spins of AGNs at $z \sim 1.5$ that evolved just after cosmic noon (Capellupo et al.,

TABLE 1 A list of spectral models developed for relativistically broadened emission of the accretion disk.

Relativistic broad line			
Model	Parameters ^a	Convolution	References
diskline	$a = 0, i, \Gamma, R_{in}, R_{out}$	rdblur	Fabian et al. (1989)
laor	$a = 0.998, i, q, R_{in}, R_{out}$	kdblur	Laor (1991)
kerrspec	$a = 0.001, 0.9981, i, \Gamma, R_{in}, R_{out}, h$	—	Martocchia et al. (2000)
kyrline/ky	$a (\geq 0), i, R_{in}, R_{out}, R_{br}, q_{in}, q_{out}, limb$	kyconv	Dovčiak et al. (2004, 2022)
kerrdisk	$a (\geq 0), i, R_{in}, R_{out}, R_{br}, q_{in}, q_{out}$	kerrconv	Brenneman and Reynolds (2006)
relline	$a, i, R_{in}, R_{out}, R_{br}, q_{in}, q_{out}, limb$	relconv	Dauser et al. (2010)
relline_lp	$a, i, \Gamma, R_{in}, R_{out}, R_{br}, h, limb$	relconv_lp	Dauser et al. (2013)
relxill ^b	$a, i, \Gamma, R_{in}, R_{out}, R_{br}, q_{in}, q_{out}, \log \xi, A_{Fe}, f_{refl,rel}, E_{cut}$	—	García et al. (2014), Dauser et al. (2014, 2016)
relxillp ^b	$a, i, \Gamma, R_{in}, R_{out}, h, \beta, \log \xi, A_{Fe}, f_{refl,rel}, E_{cut}$	—	García et al. (2014), Dauser et al. (2014, 2016)
relxillCp ^c	$a, i, \Gamma, R_{in}, R_{out}, R_{br}, q_{in}, q_{out}, \log \xi, A_{Fe}, f_{refl,rel}, kT_e, \log n$	—	García et al. (2014), Dauser et al. (2014, 2016)
relxillpCp ^c	$a, i, \Gamma, R_{in}, R_{out}, h, \beta, \log \xi, A_{Fe}, f_{refl,rel}, kT_e, \log n$	—	García et al. (2014), Dauser et al. (2014, 2016)
relline_nk ^d	$a, i, R_{in}, R_{out}, R_{br1}, R_{br2}, q_1, q_2, q_3, limb, \dot{m}, \alpha_{13}/\alpha_{22}/\epsilon_3$	relconv_nk	Bambi et al. (2017), Abdikamalov et al. (2019, 2020)
rellinelp_nk ^d	$a, i, \Gamma, R_{in}, R_{out}, R_{br}, h, limb, \dot{m}, \alpha_{13}/\alpha_{22}/\epsilon_3$	relconvlp_nk	Bambi et al. (2017), Abdikamalov et al. (2019, 2020)
relxill_nk ^d	$a, i, \Gamma, R_{in}, R_{out}, R_{br}, R_{br}, q_1, q_2, q_3, \log \xi, A_{Fe}, f_{refl,rel}, E_{cut}, \dot{m}, \alpha_{13}/\alpha_{22}/\epsilon_3$	—	Bambi et al. (2017), Abdikamalov et al. (2019, 2020)
relxillp_nk ^d	$a, i, \Gamma, R_{in}, R_{out}, h, \log \xi, A_{Fe}, f_{refl,rel}, E_{cut}, \dot{m}, \alpha_{13}/\alpha_{22}/\epsilon_3$	—	Bambi et al. (2017), Abdikamalov et al. (2019, 2020)
relxillCp_nk ^d	$a, i, \Gamma, R_{in}, R_{out}, R_{br1}, R_{br2}, q_1, q_2, q_3, \log \xi, A_{Fe}, f_{refl,rel}, kT_e, \dot{m}, \alpha_{13}/\alpha_{22}/\epsilon_3$	—	Bambi et al. (2017), Abdikamalov et al. (2019, 2020)
relxillpCp_nk ^d	$a, i, \Gamma, R_{in}, R_{out}, h, \log \xi, A_{Fe}, f_{refl,rel}, kT_e, \dot{m}, \alpha_{13}/\alpha_{22}/\epsilon_3$	—	Bambi et al. (2017), Abdikamalov et al. (2019, 2020)
reflkerr	$a, i, \tau/\Gamma, R_{in}, R_{out}, R_{br}, q_{in}, q_{out}, \log \xi, A_{Fe}, f_{refl,rel}, kT_e, kT_{bb}, geom$	—	Niedźwiecki and Życki (2008), Niedźwiecki et al. (2016, 2019)
reflkerr_lp	$a, i, \tau/\Gamma, R_{in}, R_{out}, h, \delta, \log \xi, A_{Fe}, f_{refl,rel}, kT_e, kT_{bb}, geom$	—	Niedźwiecki and Życki (2008), Niedźwiecki et al. (2016, 2019)
reltrans	$a, i, \Gamma, R_{in}, R_{out}, h, \log \xi, A_{Fe}, E_{cut}, N_H, 1/\mathcal{B}, M_{BH}, v_{min}, v_{max}, \phi_A, ReIm$	—	Ingram et al. (2019), Mastroserio et al. (2021)

(Continued on the following page)

TABLE 1 (Continued) A list of spectral models developed for relativistically broadened emission of the accretion disk.

Relativistic broad line			
Model	Parameters ^a	Convolution	References
reltransCp	$a, i, \Gamma, R_{\text{in}}, R_{\text{out}}, h, \log \xi, A_{\text{Fe}}, kT_e, N_{\text{H}}, 1/\mathcal{B}, M_{\text{BH}}, v_{\text{min}}, v_{\text{max}}, \phi_A, \text{ReIm}$	—	Ingram et al. (2019), Mastroserio et al. (2021)

^aParameters of relativistic broad line models are as follows: dimensionless black-hole spin parameter (a), disk inclination angle relative to the line of sight (i), power-law index (Γ), inner radius (R_{in}), outer radius (R_{out}), break radius (R_{br}), coronal emissivity law indexes (q as r^{-q} between R_{in} and R_{out} ; q_{in} as $r^{-q_{\text{in}}}$ between R_{in} and R_{br} ; and q_{out} as $r^{-q_{\text{out}}}$ between R_{br} and R_{out}), height of the primary source above the black hole (h), velocity of the primary source relative to the speed of light (β), limb describes limb-darkening/-brightening law (0: isotropic emission, 1: Laor's limb-darkening $1 + 2.06\mu$, and 2: Haardt's limb-brightening $\ln[1 + 1/\mu]$), ionization parameter of the accretion disk ($\log \xi$), iron abundance relative to solar (A_{Fe}), reflection fraction parameter ($f_{\text{refl,rel}}$), high energy cutoff (E_{cut}) of the primary source described by cutoffpl, the electron temperature (kT_e) in the corona described by nthcomp, logarithmic number density of the innermost accretion disk ($\log n$), break radii ($R_{\text{br}1}$ and $R_{\text{br}2}$) for non-Kerr spacetimes, coronal emissivity law indexes in non-Kerr spacetimes (q_1 between R_{in} and $R_{\text{br}1}$; q_2 between $R_{\text{br}1}$ and $R_{\text{br}2}$; and q_3 between $R_{\text{br}2}$ and R_{out}), hydrogen column density of the line-of-sight material (N_{H}), boosting factor of the reflection spectrum ($1/\mathcal{B}$), black hole mass (M_{BH}), frequency range of the transfer function (v_{min} and v_{max}), phase normalization (ϕ_A), cross-spectrum modes ($\text{ReIm} = 1, 2, 3, 4, 5, \text{ or } 6$), blackbody soft-excess temperature (kT_{bb}), Thomson optical depth $\tau(\Gamma, kT_e)$ yielding Γ , bottom-lamp attenuation ($0 < \delta < 1$), and geometry ($\text{geom} = -5, -4, 0, 4, \text{ or } 5$) defined similar to the same parameter in compPS (Poutanen and Svensson, 1996).

^bThe model relxill is a combination of relconv, xillver, and cutoffpl. The model relxillp is a mixture of relconv_lp, xillver, and cutoffpl. The number density is fixed ($\log n = 15$) in the models relxill and relxillp.

^cThe models relxillCp and relxillpCp are, respectively, similar to relxill and relxillp, but they use nthcomp instead of cutoffattenuation of the pl, as well as a free parameter for the number density ($\log n = 15-20$).

^d"nk" at the end of the spectral models stands for non-Kerr spacetimes, which are describe by the deformation parameters α_{13} , α_{22} , or ϵ_3 in the Johannsen metric (Johannsen, 2013), as well as the thickness of the accretion disk described by m (0: infinitesimally-thin, 1: 5%, 2: 10%, 3: 20%, 4: 30% of the Eddington accretion rate).

2015; Capellupo et al., 2016), and was benchmarked against X-ray reflection measurements for NGC 3783, an AGN known for its relativistically broadened Fe K α line (Capellupo et al., 2017). This method was employed to constrain the masses and spins of SMBSH in four blazars at high redshifts (Campitiello et al., 2018), which was implemented using the kerrbb model (Li et al., 2005) of multi-temperature blackbody spectrum of a thin accretion disk around a spinning black hole. The optxconv SED model (Done et al., 2012; Done et al., 2013) was also used by Porquet et al. (2019) to derive a well-measured spin rate of the SMBH in Ark 120, a well-known bare AGN with no intrinsic absorption along the line-of-sight. Subsequently, new SED models of the broad-band continuum of AGN, called agnsed and qsosed (Kubota and Done, 2018; Petrucci et al., 2018), have been developed, followed by a super-Eddington accretion model of the slim disk (agnslim; Kubota and Done, 2019), which provide better constraints on the masses and spins of SMBHs. More recently, Hagen and Done (2023) made a fully general-relativistic implementation of agnsed, referred to as the relagn model that includes general-relativistic ray tracing and the relativistic Novikov–Thorne disk model (Novikov and Thorne, 1973), leading to a complex disk spectrum in the soft excess instead of a simple blackbody, and was utilized to determine the SMBH spin in Fairall 9 from the broad-band spectrum, extending from Optical/UV to the X-ray.

1.3 Radio event horizon imaging

This method employs sub-mm data collected by several very long baseline interferometry (VLBI) stations over different locations (e.g., JCMT, SMT, SPT, IRAM, APEX, and ALMA) to achieve micro-arcsecond spatial resolution images of an SMBH event horizon (Event Horizon Telescope Collaboration et al., 2019a; Event Horizon Telescope Collaboration et al., 2022a). This has enabled the first-ever images of the accretion flow in the vicinity of nearby SMBHs to be produced, namely M87 and

Sgr A* (Event Horizon Telescope Collaboration et al., 2019b; Event Horizon Telescope Collaboration et al., 2022b). We can determine the SMBH spin by accurately modeling the appearance of accretion flows in VLBI images, accounting for general-relativistic light bending (see Figure 1 bottom-left) based on various characteristics such as the ISCO radius (r_{ms}). The VLBI imaging techniques have recently been used to deduce the spin values according to high-spatial-resolution images in Sgr A* and M87 (Event Horizon Telescope Collaboration et al., 2019c; Event Horizon Telescope Collaboration et al., 2021b; Event Horizon Telescope Collaboration et al., 2022c; Event Horizon Telescope Collaboration et al., 2022d). This method has the disadvantage of only being suitable for nearby SMBHs.

2 Relativistic reflection modeling

Various spectral models have been constructed to reproduce the general-relativistic effects of the Kerr metric on the iron K α line profile. Table 1 summarizes most of the well-known spectral models made for X-ray data analysis of relativistically blurred emission, along with their key parameters. The basic parameters in these models are the dimensionless spin parameter ($a = Jc/GM^2$), the line-of-sight inclination angle (i) of the accretion disk, the spectral photon index (Γ) of the primary source – the corona or the base of a jet above the black hole –, as well as the boundary radii (R_{in} and R_{out}) of the innermost accretion disk. Most of these models can be loaded into tools for X-ray spectral analysis, particularly the X-ray spectral fitting package XSPEC¹ (Arnaud, 1996; Arnaud et al., 1999) of HEASoft's data analysis package for X-ray astronomy XANADU (NASA HEASARC, 2014), MIT's Interactive Spectral Interpretation System² (ISIS; Houck and

1 <https://heasarc.gsfc.nasa.gov/xanadu/xspec/>

2 <https://space.mit.edu/cxc/isis/>

Denicola, 2000), CXC³'s Modeling and Fitting Package Sherpa⁴ (Freeman et al., 2001; Doe et al., 2007) of the Chandra Interactive Analysis of Observation (CIAO; Fruscione et al., 2006), and SRON⁵'s X-ray high-resolution spectral modeling and fitting package SPEX⁶ (Kaastra et al., 1996; de Plaa et al., 2020). These models are often applied to integrated spectra of AGNs without accounting for the variability of the X-ray sources.

The early models, developed to analyze relativistic reflection, featured fiducial values for the spin parameter. Black hole spin measurement began with the diskline (Fabian et al., 1989) and laor (Laor, 1991) fixed-spin models, which were run with fiducial spin values of $a = 0$ and 0.998, respectively. The diskline model was based on analytic, time-consuming calculations, whereas the laor model relied on extensive pre-calculated tabulated Flexible Image Transport System (FITS) data created for different combinations of the model parameters: inclination angle, spectral photon index (Γ), inner radius (R_{in}), and outer radius (R_{out}). The laor model recreates the relativistic line shape by interpolating data from the extensive FITS table. Later, Martocchia and Matt (1996) examined how the “lamp post” geometry affected the broad iron $K\alpha$ lines, in which the ionizing source is located on the polar axis at a height (h) above the black hole, as illustrated in Figure 1 (bottom-right). This investigation was followed by a comprehensive analysis for $a = 0.001$ and 0.9981 leading to the kerrspec model (Martocchia et al., 2000; Martocchia et al., 2002). We should note that the reflection continuum was not included in these models and needed to be handled by a separate model such as reflionx (Ross et al., 1999; Ross and Fabian, 2005; Ross and Fabian, 2007), which should be convolved with the corresponding convolution models to make a smoothed spectrum of relativistic smearing in an accretion disk. The convolution models rdblur and kdblur were prepared using diskline and laor, respectively, which can be used with a reflection model (e.g., reflionx). Nandra et al. (2007) used a modified version of the kdblur model to characterize the broad iron $K\alpha$ line in *XMM-Newton* observations of a sample of Seyfert galaxies. However, the spectral models with fixed spin rates obviously prevented us from straightforwardly measuring the black hole spin.

The next-generation of relativistic reflection models has a free parameter for the positive spin rates, which allows for the determination of the black hole spin in prograde rotation ($0 \leq a < 1$). The kyrline (or ky) model (Dovčiak, 2004; Dovčiak et al., 2004; Dovčiak et al., 2022) was developed to incorporate extensive tables calculated for transfer functions. This model rapidly computes the shape of relativistically broadened line emission using transfer function tables without relying heavily on interpolation, yielding a significantly greater level of spectral resolution compared to the laor model. Furthermore, the black hole spin was a free parameter, ranging from $a = 0$ to 1. The model can therefore reproduce the relativistic blurred emission more accurately than the laor model for all positive spin rates and inclination degrees. In addition,

the kyrline model features coronal emissivity law indexes (q_{in} as $r^{-q_{in}}$ between R_{in} and R_{br} ; and q_{out} as $r^{-q_{out}}$ between R_{br} and R_{out}) for precisely creating the emitted radiation (see Figure 1 bottom-right), describing the emissivity characteristics on both sides of the break radius (R_{br}), as well as including the limb prescriptions for limb-darkening/-brightening laws (Chandrasekhar, 1960), namely isotropic emission ($I \propto 1$), Laor's limb-darkening ($I \propto 1 + 2.06\mu$; Laor, 1991), and Haardt's limb-brightening ($I \propto \ln(1 + 1/\mu)$; Haardt, 1993), where $\mu = \cos(\theta_e)$ and θ_e is the inclination angle of the emitted radiation with respect to the disk. These features were accomplished by computing them for inclusion in the comprehensive FITS table. In order to address the problems with the excessive table size and lack of smoothness in the kyrline model, Brenneman and Reynolds (2006) created an alternative model for relativistic reflection known as kerrdisk (Brenneman, 2007). Their model has a relatively smaller FITS table and a robust interpolation approach. Using a high level of smoothness in the transfer function allows for effective interpolation in kerrdisk. Furthermore, this model employs a distinct methodology, approximating the narrow line of the distant reflection from the accretion disk using a δ -function instead of a Gaussian function. Their model computes a larger portion of the integration using analytic approaches, thereby excluding the emissivity law from the calculated table. However, fitting methods can handle the modeling of the emissivity law. This model effectively reduces the table size to a fraction of the kyrline FITS table. Nevertheless, the relativistic emission produced by kerrdisk appears less smooth than those made by kyrline, with some noticeable spikes in the red wing of the relativistic line. However, data accumulated with the spectral resolutions of detectors aboard the *XMM-Newton* and *Suzaku* telescopes could not distinguish these spikes. The kyrline model has been used to conduct an *XMM-Newton* survey on a sample of radio-quiet Type 1 AGNs (de La Calle Pérez et al., 2010). Unlike the fixed-spin models (laor and diskline), kyrline and kerrdisk, which can relativistically be convolved with a reflection model (e.g., reflionx) using the kyconv and kerrconv models, respectively, are more accurate in producing the shape of relativistic emission for any positive spin rates. However, a black hole spinning in retrograde relative to the accretion disk ($-1 < a < 0$) could not have its spin constrained by the kyrline and kerrdisk models.

Since 2010, several spectral models have been developed for relativistic blurred emission (see Table 1) that incorporate both positive and negative spin values, enabling the measurement of the black hole's spin in both the prograde and retrograde directions with respect to the accretion disk. To accommodate the full spin range ($-0.998 \leq a \leq +0.998$), Dauser et al. (2010) has created the relline model, together with relline_lp, featuring the “lamp post” geometry (for detail see Dauser, 2010), using FITS tables for Cunningham's photon transfer function (Cunningham, 1975) pre-calculated with a customized version of the F77 program photon_transferfct⁷ (also called spx; Speith, 1993; Speith et al., 1995) (a gravitationally-distorted appearance of an accretion disk made with a modified version of this program is shown in the bottom-left panel of Figure 1). The relline model employs Green's functions to calculate the radiated radiation for arbitrary angular and radial

3 The Chandra X-Ray Center (CXC) is operated for NASA by the Smithsonian Astrophysical Observatory (SAO).

4 <https://cxc.cfa.harvard.edu/sherpa/>

5 Netherlands Institute for Space Research (Stichting Ruimteonderzoek Nederland; SRON) is a Dutch institute for astrophysical research.

6 <https://www.sron.nl/astrophysics-spx/>

7 <https://pisrv1.am14.uni-tuebingen.de/~speith/misc.html>

variations, as well as robust interpolation techniques that lead to a decrease in pre-calculated tabulated data. Moreover, relativistic line profiles calculated for a hard X-ray source located on the rotational axis at a height (h) above the black hole, i.e., the “lamp post” geometry, are provided in the `relline_lp` model (Dauser et al., 2013). Both the models includes prescriptions for the limb-darkening/-brightening laws. Their corresponding convolution models, `relconv` and `relconv_lp`, are able to convolve the reflection continuum created by a reflection model such as `reflionx` (Ross et al., 1999; Ross and Fabian, 2005; Ross and Fabian, 2007) and `xillver` (García, 2010; García and Kallman, 2010; García et al., 2011; García et al., 2013). As this simple combination of the relativistic convolution model (`relconv`) and the reflection model (`xillver`) can lead to inconsistent results, García et al. (2014) made a self-consistent implementation of the spectrum reflected from the disk irradiated by an ionizing source and relativistically blurred emission in a new model called `relxill`, as well as an additional new model called `relxill_lp` for a lamp-post geometry.⁸ These models incorporated angle-dependent reflection tables of `xillver`⁹ into the relativistic blurring calculations, which exhibits like behavior to a convolution of `xillver` and `relconv` (or `relconv_lp`), albeit with self-consistently calculated X-ray reflection (Dauser, 2014). Subsequently, Dauser et al. (2014) and Dauser et al. (2016), further extended them to include the reflection fraction parameter ($f_{\text{refl,rel}}$), a flux ratio between the direct and reflected radiation that depends on the geometry and location of the radiation source. In the updated model `relxillCp` (Dauser et al., 2016), the primary source is made by a thermally Comptonized continuum model (`nthcomp`; Zdziarski et al., 1996; Życki et al., 1999) and offers a free parameter for the disk density ranging from 10^{15} to 10^{20} cm^{-3} , whereas the previous model `relxill` uses a power law with a high-energy exponential cutoff (`zcutoffpl`) and assumes a disk density of 10^{15} cm^{-3} . Recently, the inclusion of returning radiation is implemented in the latest model of `relxillCp` by Dauser et al. (2022), featuring the “lamp post” geometry with a thermally comptonized continuum as the primary source and an unrestricted density parameter (10^{15} – 10^{20} cm^{-3}). Additionally, García et al. (2022) also present the model `relxillNS` featuring a black body spectrum, specifically tailored to accommodate the reflection from the disk around an accreting neutron star. The relativistic X-ray reflection models provided by the `relxill` package were also extended to describe the reflection spectrum in the Johannsen metric (Johannsen, 2013), referred to as `relline_nk` (Bambi et al., 2017; Abdikamalov et al., 2019; Abdikamalov et al., 2020; Abdikamalov et al., 2021b; Abdikamalov et al., 2021a),^{10, 11} whose model names contain “nk” at the end (e.g., `relxill_nk` and `relxillCp_nk` stand for non-Kerr spacetimes) to distinguish them from those in the Kerr metric (see Table 1). These models allow to validate the Kerr metric through the deformation parameters α_{13} , α_{22} , or ϵ_3 in the Johannsen metric, where $\alpha_{13} = \alpha_{22} = \epsilon_3 = 0$ restores the Kerr metric (for non-Kerr metrics, see review by Bambi, 2017).

8 <https://www.sternwarte.uni-erlangen.de/~dauser/research/relxill/>

9 <https://sites.srl.caltech.edu/~javier/xillver/>

10 https://www.tat.physik.uni-tuebingen.de/~nampalliwar/relxill_nk/

11 https://github.com/ABHModels/relxill_nk, doi:10.5281/zenodo.13906295

X-ray time-resolved observations of AGNs have shown *variability* in the relativistically blurred reflection (e.g., MCG–6–30–15; Fabian and Vaughan, 2003; Vaughan and Fabian, 2004; Larsson et al., 2007; Miller et al., 2008) that could be caused by general relativistic effects, particularly light bending near the black hole event horizon. Niedźwiecki and Życki (2008) and Niedźwiecki and Miyakawa (2010) investigated variability patterns of the red wing in X-ray reflection of the AGN in the Seyfert 1 galaxy MCG–6–30–15 using a detailed light-bending model (Miniutti and Fabian, 2004), which led to the development of the spectral model `reflkerr` and its corresponding lamp-post model `reflkerr_lp` (Niedźwiecki et al., 2016; Niedźwiecki et al., 2019).¹² In particular, Niedźwiecki et al. (2016) identified some inconsistencies between `reflkerr` and `relxilllp` owing to the neglect of the general-relativistic redshift of the direct coronal radiation in `relxilllp`, though they found that the `relxilllp` model still produces acceptable results in weak-gravity in the energies below 80 keV. Moreover, the lamp-post model `reflkerr_lp` developed by Niedźwiecki et al. (2019) demonstrated a departure from `relxilllp` in the energies above 30 keV. Another model-family for spectral and timing variability in accreting black holes has been developed (Ingram et al., 2019; Mastroserio et al., 2021; 2022), named `reltrans` and `reltransCp`,¹³ which calculated the emergent reflection spectrum using `xillver` (or `xillverCp` in the case of `reltransCp`). The `reltrans` model considers all the general-relativistic effects to calculate the time delays and energy changes that occur when X-ray photons from the corona reflect from the accretion disk and scatter towards the observer. The calculations of `reltrans` incorporate both continuum lags and reverberation lags in a self-consistent manner to produce most of the practical X-ray variability time scales.

3 Variability in relativistic reflection from PCA

Principal component analysis (PCA; Hotelling, 1933),¹⁴ also referred to as the “Hotelling transform,” is a well-known method in multivariate statistics relying on eigenvalues and eigenvectors (see review by Jolliffe and Cadima, 2016) that has been extensively discussed in detail in the literature (e.g., Mardia et al., 1979; Jolliffe, 2002; Izenman, 2008; Rencher and Christensen, 2012). It bears a close relation to the “Kosambi–Karhunen–Loève transform” (Kosambi, 1943; Karhunen, 1947; Loève, 1948) in probability theory, and is among three classical techniques in multivariate analysis to determine the principal dimensions of large data, along with independent component analysis (ICA; Héroult and Ans, 1984; Héroult et al., 1985; Héroult and Jutten, 1986) and non-negative matrix factorization (NMF; Lee and Seung, 1999; Lee and Seung, 2000). PCA can be employed to separate various characteristics

12 <https://users.camk.edu.pl/mitsza/reflkerr/>

13 <https://adingram.bitbucket.io/reltrans.html>

14 It was first innovated by Pearson (1901) in the context of principal axes of ellipsoids in geometry, but it was independently developed and called *the method of principal components* by Hotelling (1933) for statistical analysis.

that are mostly responsible for complex variations in large data in astronomy (e.g., Wall and Jenkins, 2012; Ivezić et al., 2020) as well as to simplify complex data for machine learning approaches (e.g., Bishop, 2006; Müller and Guido, 2016; Witten et al., 2017; Géron, 2019). This is implemented by reducing the number of available data into a group of independent PCA components, which then provide information about the different levels of their contributions to the complexity of the entire data. Astronomers have extensively employed it as a practical multivariate method. The early application of this technique in astronomy (see review by Francis and Wills, 1999) can be traced back to some studies on spectral analyses of stars (Deeming, 1964; Whitney, 1983), galaxies (Faber, 1973; Bujarrabal et al., 1981; Efstathiou and Fall, 1984), and quasars (Mittaz et al., 1990; Francis et al., 1992; Boroson and Green, 1992). This approach was also employed for imaging analysis of the interstellar medium (Heyer and Schloerb, 1997; Brunt et al., 2009). It was later used for X-ray binaries (e.g., Malzac et al., 2006; Koljonen et al., 2013; Koljonen, 2015) and blazars (Gallant et al., 2018), and more recently for X-ray variability in symbiotic stars (Danehkar et al., 2024a) and starburst regions (Danehkar et al., 2024b). Especially, it has extensively been leveraged for X-ray data analysis of AGNs in Seyfert 1 galaxies (e.g., Vaughan and Fabian, 2004; Miller et al., 2008; Parker et al., 2014b; Gallo et al., 2015).

PCA can decompose time-resolved spectroscopic data into groups of PCA components and eigenvectors, yielding eigenvalues in the process. Normalized eigenvalues can yield the contribution of each eigenvector to the temporal evolution of the whole data over time. Each decomposed PCA component and eigenvector can be referred to as a principal spectrum with its corresponding light curve. The process of conducting PCA requires performing the decomposition of a matrix into its eigenvectors and eigenvalues. To analyze variability of a source in astronomy, this data matrix for PCA contains a set of spectroscopic data collected at n time intervals, each binned into m spectral channels. Let consider a rectangular ($m \times n$) matrix \mathbf{X} consisting of n rows by m columns, one can determine the principal components of \mathbf{X} through the following three methods:

3.1 Singular value decomposition

The most common approach to obtaining the PCA components is the singular value decomposition (SVD; Beltrami, 1873; Jordan, 1874a; Jordan, 1874b; Sylvester, 1889a; Sylvester, 1889b; Sylvester, 1889c). The SVD of \mathbf{X} is performed as follows:

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T, \quad (3)$$

where \mathbf{U} is a square matrix of order m containing *principal components* (spectra in time-resolved spectroscopic data), $\mathbf{\Sigma}$ is a rectangular diagonal matrix ($m \times n$) containing square roots of *eigenvalues* in its diagonal, i.e., $\mathbf{\Lambda} = \mathbf{\Sigma}^T\mathbf{\Sigma} = \text{diag}(\lambda_1, \dots, \lambda_n)$ (contribution fractions in spectral variability), \mathbf{V} is a square matrix of order n containing *eigenvectors* (light curves in astronomical data).

3.2 Eigendecomposition

A classical way to determine the PCA components is through the eigenvalue decomposition (EVD; Cauchy, 1829a; Cauchy, 1829b)¹⁵ of the covariance matrix expressed as $\mathbf{C}_{XX} = \mathbf{X}^T\mathbf{X}$, which is a square matrix of order m . The eigendecomposition of \mathbf{C}_{XX} is as follows:

$$\mathbf{C}_{XX} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T,$$

which yields eigenvectors (\mathbf{V}) and eigenvalues ($\mathbf{\Lambda}$). The principal components (\mathbf{U}) are obtained from the decomposed eigenvectors and eigenvalues by considering Equation 6, which leads to the following solution:¹⁶

$$\mathbf{XV} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T\mathbf{V} = \mathbf{U}\mathbf{\Sigma}.$$

Constructing the diagonal matrix $\mathbf{\Sigma} = \mathbf{\Lambda}^{\frac{1}{2}}$ from the eigenvalues ($\mathbf{\Lambda}$) and obtaining the least-squares solution to $\mathbf{XV} = \mathbf{U}\mathbf{\Sigma}$ lead to the principal components (\mathbf{U}) of \mathbf{X} .

3.3 QR decomposition

Another faster method suitable for high-performance computing, which was proposed by Sharma et al. (2013) to conduct PCA, is performed using QR decomposition (Golub, 1965), also known as QR factorization (Golub and van Loan, 1996; Trefethen and Bau, 1997). In this approach, \mathbf{X} is first factorized into an orthogonal matrix \mathbf{R} of $n \times m$ dimensions and an upper triangular square matrix \mathbf{Q} of order m :

$$\mathbf{X} = \mathbf{QR}.$$

Then, the SVD of \mathbf{R}^T is obtained:

$$\mathbf{R}^T = \mathbf{\tilde{U}}\mathbf{\tilde{\Sigma}}\mathbf{\tilde{V}}^T.$$

As demonstrated by Sharma et al. (2013), this leads to the same diagonal matrix and eigenvectors of Equation 3, $\mathbf{\Sigma} = \mathbf{\tilde{\Sigma}}$ and $\mathbf{V} = \mathbf{\tilde{U}}$, while the equivalent principal components are obtained via $\mathbf{U} = \mathbf{Q}\mathbf{\tilde{V}}$.

For a set of timing spectroscopic data stored in a data matrix, the PCA components (\mathbf{U}), the eigenvectors (\mathbf{V}), and the eigenvalues ($\mathbf{\Lambda} = \mathbf{\Sigma}^2$) decomposed from the data matrix via either SVD, EVD, or QR are the principal spectra, the corresponding light curves, and their contribution fractions, respectively. As shown in Supplementary Material, these PCA methods can simply implemented with the linear algebra functions of NumPy in Python, albeit with neither CPU parallelization nor GPU acceleration. Currently, there are two publicly available packages made for PCA in the astronomical community: (1) the SVD-based Python package PCA¹⁷ (Parker et al., 2015) based on the SVD function (Press et al., 1997) from NumPy (Harris et al., 2020), and (2) the QR-based

¹⁵ For a historical review, see Hawkins (1975).

¹⁶ Based on the fact that $\mathbf{V}^T\mathbf{V} = \mathbf{I}$, where $\mathbf{I} = \text{diag}(1, \dots, 1)$ is the identity matrix of order n , so $\mathbf{\Sigma}\mathbf{I} = \mathbf{\Sigma}$ and $\mathbf{\Lambda}\mathbf{I} = \mathbf{\Sigma}$.

¹⁷ <https://www.michaelparker.space/pca-code>

library `qrpc` in Python¹⁸ and R¹⁹ (de Souza et al., 2022a; de Souza et al., 2022b) implemented with `pyTorch` (Paszke et al., 2019) and `Scikit-learn` (Pedregosa et al., 2011) in Python, and with `torch` (Falbel and Luraschi, 2022) and the built-in `prcomp` function in R, allowing for seamless GPU acceleration. In particular, the package `PCA` distributed by Parker et al. (2015) is capable of conducting PCA on X-ray *XMM-Newton* EPIC-pn observations. To perform PCA with this package, it is necessary to generate a set of X-ray spectra sliced at fixed time intervals (e.g., 10 ks) from event data via custom reduction methods (for details, see Danehkar et al., 2024a).

Vaughan and Fabian (2004) made initial attempts to conduct PCA on X-ray variability in AGN using low-spectral resolution data, suggesting that the X-ray variations in MCG–6–30–15 reported by Fabian and Vaughan (2003) are primarily due to a variable power-law component, with a small partial fraction likely originating from a reflection-dominated component. Later, Miller et al. (2007) employed SVD for PCA, resulting in the generation of exhaustive principal spectra of Mrk 766, which Turner et al. (2007) confirmed these spectral variations through time-resolved spectroscopy. Moreover, Miller et al. (2008) investigated the X-ray variability of MCG–6–30–15 using PCA, resulting in similar spectral components (absorbed, varying power-law) in MCG–6–30–15 and Mrk 766, with a less variable, heavily absorbed component characterizing the relativistically broadened red wing. PCA conducted by Parker et al. (2014a) and Parker et al. (2014b) demonstrated that SVD can successfully separate different spectral components responsible for the X-ray variability in AGNs by exploiting large archival data. In particular, Parker et al. (2014a) discovered that the X-ray variations in MCG–6–30–15 are mostly caused by only three spectral components (see Figure 2): the normalization factor of the power-law continuum (variability fraction of ~96%), the power-law spectral index (~2.1%), and the normalization factor of a relativistically broadened reflection emission (~0.5%). Similarly, PCA by Parker et al. (2015) provided evidence for the slight variability ($\leq 0.5\%$) of relativistic reflection in other AGNs hosted by other Seyfert 1 galaxies (NGC 4051, NGC 3516, Mrk 766, and 1H 0707-495), as seen in Figure 2. Various spectral analysis approaches, including PCA, performed by Gallo et al. (2015) also indicated that the variability in the narrow-line Seyfert 1 galaxy, Mrk 335, is mostly caused by changes in the power-law flux and photon index, although small variations in the ionization state of the reflection were found to be necessary. The PCA study of the extreme narrow-line Seyfert 1 galaxy IRAS 13224–3,809 by Parker et al. (2017a) also showed three principal spectra: a varying power-law continuum, a slightly variable soft excess, and a less variable broad soft excess being linked to strong reflection (see Figure 2 bottom). In addition, the PCA component associated with a variable power-law continuum contain absorption footprints caused by the relativistic UFO detected by Parker et al. (2017b).

As seen in Figure 2, the third or/and fourth PCA components obtained by Parker et al. from X-ray observations of five AGNs (MCG –6–30–15, NGC 4051, NGC 3516, Mrk 766, and 1H 0707-495) resemble the relativistically broadened iron emission features shown in Figure 1 (top). Their normalized eigenvalues of $\leq 0.5\%$

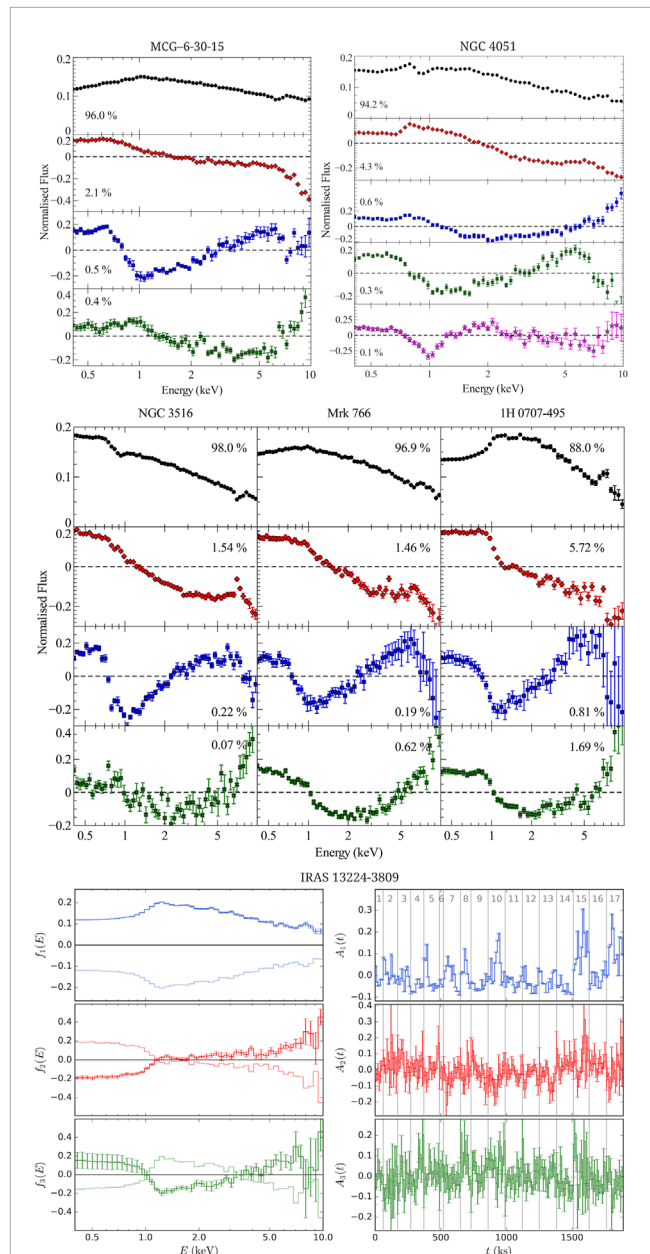


FIGURE 2 PCA spectra found in different AGNs hosted by nearby Seyfert 1 galaxies: MCG –6–30–15 (Parker et al., 2014a), NGC 4051, NGC 3516, Mrk 766, and 1H 0707-495 (Parker et al., 2015), with percentages of variability fractions, as well as PCA spectra $f_{1-3}(E)$ and related light curves $A_{1-3}(t)$ found in IRAS 13224–3,809 (Parker et al., 2017a). The PCA components from the first to the third or/and fourth order, respectively, correspond to variations in the power-law normalization, the power-law spectral index, and the relativistic reflection.

imply that they have negligible variations compared to the X-ray variability in the power-low source continuum. This insignificant variability in the relativistic emission is consistent with the fact that the SMBH spin remains constant over the course of the human timescale. Magnetohydrodynamic (MHD) simulations of an black hole accretion disk by Schnittman et al. (2006) revealed that the light curves indeed contain very low levels of variability (see animations by Schnittman, 2019). Further MHD simulations

¹⁸ <https://github.com/xuquanfeng/qrpc>

¹⁹ <https://github.com/RafaelSdeSouza/qrpc>

by [Schnittman et al. \(2013\)](#) suggested that the noticeable X-ray variability mostly originates from the corona and not the disk. This is in agreement with the results found by [Parker et al.](#), which show $\geq 90\%$ of X-ray variations are due to changes in the power-law continuum, i.e., the corona. General-relativistic magnetohydrodynamic (GRMHD) simulations by [Shiokawa et al. \(2017\)](#) also indicated the presence of some flux fluctuations in the emission from the innermost accretion disk due to the fast-moving turbulent formations, as well as some variations in the photon ring with spin-dependent frequencies (see animations by [Shiokawa, 2017](#)). Interestingly, the polarimetric light-curve observations of Sgr A* have also shown intraday variability in circular polarization ([Bower et al., 2002](#)) and linear polarization ([Marrone et al., 2006](#)), as well as Faraday rotation variability on timescales from hours to months ([Marrone et al., 2007](#); [Bower et al., 2018](#)). Similarly, the near-infrared GRAVITY-Very Large Telescope Interferometer (VLTI) observations exhibited that the polarization loop in Sgr A* is regularly changing clockwise over ~ 30 min, indicating a closed, loop motion with the speed of $0.3c$ ([GRAVITY Collaboration et al., 2018](#)). The observed polarization variations in Sgr A* were in line with predictions from general-relativistic ray-tracing models of slightly tilted accretion flows in the presence of powerful magnetic fields ([GRAVITY Collaboration et al., 2020](#)). More recently, the polarimetric Event Horizon Telescope (EHT) imaging observations of the SMBHs in M87 and Sgr A* confirmed rapid (intra-hour) intrinsic variations in near-horizon accretion flows and polarized rings, which were attributed to spiraling polarization structures based on the results from GRMHD simulations ([Event Horizon Telescope Collaboration et al., 2021a](#); [Event Horizon Telescope Collaboration et al., 2021b](#); [Event Horizon Telescope Collaboration et al., 2023](#); [Event Horizon Telescope Collaboration et al., 2024a](#); [Event Horizon Telescope Collaboration et al., 2024b](#)). Therefore, the recent polarization GRAVITY-VLTI and EHT imaging observations of two nearby SMBHs (Sgr A* and M87), together with numerical simulations, imply that small variations in the relativistically broadened iron emission revealed by PCA could be associated with intrahour intrinsic variations and varying spiraling polarization features in near-horizon accretion flows and photon rings.

4 Future perspective: machine learning

SVD and PCA decomposition closely relate to the optimal solution for neural networks in auto-association mode ([Bourlard and Kamp, 1988](#); [Baldi and Hornik, 1989](#)). As discussed by [Hertz et al. \(1991\)](#) in the context of unsupervised Hebbian learning, PCA can be used for dimensionality reduction of large data before proceeding with machine learning algorithms, such as artificial neural networks (ANNs). PCA can indeed alleviate the “curse of dimensionality” (coined by [Bellman, 1957](#); [Bellman, 1961](#)), also known as the “Hughes phenomenon” ([Hughes, 1968](#)) or “peaking phenomenon” ([Trunk, 1979](#)), which often arises when searching for patterns in unknown large data. It has been extensively demonstrated in the literature that PCA can be utilized as a pre-processing step to simplify complex data prior to machine learning (e.g., [Bishop, 2006](#)), data mining ([Witten et al., 2017](#)), and deep

learning ([Goodfellow et al., 2017](#)). Recently, [Ivezić et al. \(2020\)](#) also discussed in detail the applications of PCA, ICA, and NMF in dimensionality reduction for data mining and machine learning in astronomy.

Using PCA for the pre-processing of astronomical data enables a significant reduction in dimensionality and complexity of data, leading to an improvement in machine learning performance. The use of PCA to reduce the dimensionality of the data for training ANNs can be traced back to earlier efforts on the classification of galaxy spectra ([Folkes et al., 1996](#); [Lahav et al., 1996](#)) and stellar spectra ([Bailer-Jones et al., 1998](#); [Singh et al., 1998](#)). Later, [Zhang and Zhao \(2003\)](#) applied PCA to the multiwavelength data of AGNs, stars, and normal galaxies in order to reduce the dimensionality of the parameter space for support vector machines (SVM) and learning vector quantization (LVQ), two supervised classification algorithms in machine learning, resulting in the classification of stars, AGNs, and normal galaxies. PCA also reduced the complexity of image data for the morphological classification of galaxies with an ANN ([de la Calleja and Fuentes, 2004](#)). Moreover, [Bu and Pan \(2015\)](#) deployed PCA to pre-assemble stellar atmospheric parameters from spectra for Gaussian process regression (GPR) and then compared the results of GPR with those from ANNs, kernel regression (KR), and support-vector regression (SVR). [Kuntzer et al. \(2016\)](#) also conducted stellar classification from single-band images using pre-processed data from PCA to train ANNs to determine the spectral type. More recently, we see the application of PCA to construct input data for ANNs in stellar population synthesis modeling ([Alsing et al., 2020](#)), finding thermal components in X-ray spectra of the Perseus cluster ([Rhea et al., 2020](#)), and finally X-ray spectral analysis of AGN ([Parker et al., 2022](#)).

The avenue of automated spectral analysis with machine learning algorithms has not yet been fully explored for constraining the relativistically broadened iron emission in AGN, mostly because of the complicated variability seen in the X-rays over the course of observations. X-ray observations of AGNs have shown some X-ray changes in power-law continua, which were ascribed to so-called transient obscuration events caused by eclipsing material near the primary source, such as NGC 3783 ([Mehdipour et al., 2017](#)), NGC 3227 ([Turner et al., 2018](#)), and Mrk 335 ([Longinotti et al., 2019](#); [Parker et al., 2019](#)), or flaring variations in the corona in the innermost central regions, e.g., PDS 456 ([Matzeu et al., 2017](#); [Reeves et al., 2021](#)) and NGC 3516 ([Mehdipour et al., 2022](#)). This kind of change in X-rays over time, along with a relatively large number of parameters in relativistic reflection models (see [Table 1](#)), makes it much more complicated for machine learning algorithms to automatically determine the spins of SMBHs from the archival X-ray data. Nevertheless, as seen in [Figure 2](#), the dimensionality reduction offered by PCA can avoid the curse of dimensionality in the X-ray data of AGNs. In the future, we will be able to use machine learning to automatically conduct the spin analysis of SMBHs in AGNs thanks to the principal spectra of relativistic reflection disentangled by PCA from X-ray observations.

Author contributions

AD: Writing—original draft, Writing—review and editing.

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Supplementary material

The Supplementary Material for this article can be found online at: <https://www.frontiersin.org/articles/10.3389/fspas.2024.1479301/full#supplementary-material>

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