Unveiling the black hole black box – what determines the black hole mass? (SDS 384: Scientific Machine Learning Final Project)

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Abstract

The physical properties of the black hole are an ongoing research topic that remains poorly understood. In this study, we want to explore factors that affect the mass of a black hole, with the public simulations dataset from the IllustrisTNG project. We examine the correlation between the black hole mass and the properties of the dark matter halo that the black hole resides in using XGBoost. Interestingly, we find that the "stellar mass" has shown the greatest influence on predicting the black hole mass at low redshift (z = 0.0, 0.5), and at higher redshift (z = 1.0, 1.5, 2.0), "stellar metallicity" becomes the most dominant feature in the prediction results. Machine learning offers a new channel to study such correlations between astrophysical properties, and further investigations can be done on exploring the efficiency of other algorithms and the time evolution of the correlations.

1 Introduction

The study of the early universe stands as a captivating frontier in astrophysics, inviting exploration into the origins and evolution of astrophysical objects in the universe. There are two primary avenues in unfolding the history of the universe: observational data and computational simulations, each offering unique perspectives on the formative epochs of the universe. On the observational front, the launch of the James Webb Space Telescope (JWST) greatly strengthens our ability to look into the past, discovering early galaxies and black holes emerging in the aftermath of the Big Bang. These observational data offer invaluable empirical evidence complementing theoretical frameworks. In parallel, computational simulations, particularly N-body simulations, are employed to mimic the dynamics and interactions of matter. They help to formulate theoretical frameworks that depict how everything in the universe evolves over time, from small particles to entire galaxies, across different scales. One of the most well-known cosmological simulation suites designed for such studies is *The Next Generation Illustris Simulations* (IllustrisTNG project).

The IllustrisTNG suite has greatly promoted the study of a broad range of topics surrounding how the universe and its contents evolved with time. We find this simulation set a good approach to studying the properties of black holes and dark matter, as opposed to visible ordinary matters, it is challenging to directly observe them in the universe. Previous works have shown such methods successful [He20, IMY+21, MAB+21, vCN+22, WNT+23].

While simulations have proven effective in modeling and explaining cosmic evolution, their computational demands pose significant challenges due to high time complexity. In light of this, the emergence of machine learning algorithms presents an opportunity to expedite inference regarding properties such as the formation of black holes, cosmic histories, and large-scale structures without the need for extensive computational simulations.

Numerous studies utilizing IllustrisTNG data have incorporated machine-learning techniques to enhance their findings. Additionally, other research has developed and validated the algorithms and models using the accessible and rich datasets provided by IllustrisTNG, including but not limited to XGBoost, regression, and neutral network [WVHP20, MAB+21, MK22, WNT+23, MWL+24]. For example, [DHZ+19] developed an unsupervised machine-learning algorithm, named auto-GMM, to isolate intrinsic structures in simulated galaxies based on their kinematic phase space, and they have shown it successful in identifying different kinds of intrinsic structures of the simulated galaxies in IllustrisTNG. Similarly, [SZL+20] employed a convolutional neural network, ResNet-18, to classify clusters drawn from the IllustrisTNG simulations.

In this study, our objective is to investigate how dark matter halo properties influence the mass of black holes within, using the IllustrisTNG simulation suite with machine learning algorithms. Previous works have investigated the correlation between black holes and their host galaxies ([LHG+20, HLS+21, HOB+22]). As black holes and host galaxies both reside in a dark matter halo, we want to test whether similar correlations exist between black hole mass and dark matter halo properties.

Given the inherent complexity of black hole formation and evolution, which remains incompletely understood, it is plausible that numerous parameters are correlated with black hole mass. By employing machine learning algorithms, we aim to comprehensively evaluate the impact of various halo parameters on black hole mass, thereby offering a robust approach to understanding this intricate phenomenon. In Section 2, we describe the IllustrisTNG data and our data reduction method. The exploratory analysis is presented in Section 3. We introduce the models used in this work in Section 4 and the results are shown and discussed in Section 5 and Section 6, respectively. Lastly, we summarize and conclude in Section 7.

2 IllustrisTNG and Data Reduction

Hydrodynamical simulations of galaxy formation have now reached sufficient volume to reveal when and how galaxies evolve into the structures that are observed today. In this work, we employ the data from an ongoing cosmological hydrodynamical simulation suite of galaxy formation, namely *The Next Generation Illustris Simulations* (IllustrisTNG project[1]), to study the black hole mass's correlation with its host dark matter halo properties. Each simulation evolves a large swath of a mock Universe from its early epoch until the present day, including a wide range of physical processes that drive galaxy formation.

The original IllustrisTNG project involves simulations with three different physical sizes of a cube in the mock universe, roughly 50, 100, and 300 Mpc side length, which we refer to as TNG50, TNG100, and TNG300, respectively. TNG300 has the largest physical column, enabling the analysis of rare objects such as galaxy clusters and providing the largest galaxy sample. In contrast, TNG50 is limited in sampling rare objects, but in turn, it provides a channel to look into the details such as the structural properties of galaxies and gas around galaxies, due to its high mass resolution which is a few hundred times higher than the larger volume TNG300 simulation. In this study, since we do not have a preference for details structures or rare objects, we choose TNG100 with an intermediate simulation volume. The simulation series TNG100 has a box side length of $L \sim 100$ Mpc and uses a particle number of $N = 2 \times 1820^3$ at its highest resolution. The redshift range of the simulation spans from $z = 20 - 0$, which corresponds to the cosmic age of ~ 180Myr all the way to ~ 13.8Gyr as the age of the present day. The halo information is extracted from each snapshot of the simulation, and in total we have 100 snapshots labeled as snapshot 0 (z = 20) to snapshot 100 (z = 0).

In this work, we want to investigate if we can predict the black hole masses from dark halo mass properties. First, we took the available simulation data from TNG100 as our parent data, by looking at the information extracted from all the snapshots. In the data reduction process, we constructed a set of data with dark matter halo properties and the mass of black holes residing in those dark matter halos. To achieve this, we removed the dark halos containing no black holes and further restricted our data to those with reasonable black hole masses. After data reduction, there are $\sim 200,000$ qualified black hole − host dark matter halo pairs. On top of this, we also want to track the evolution of the black holes and their host halos throughout the cosmic evolution. Therefore, we use the halo merger tree data catalogue to trace the progenitor of a halo at an earlier snapshot and connect to this halo at the current snapshot.

To simplify our model and expedite training, we first carefully filter out the features that are stochastic in nature, such as the position and velocity of the halos. Then, we reduce some features that are physically correlated with other features, such as the half mass radius of different particles (Radius for which half mass of certain particles are contained within) and the total mass of the black hole type particles (SubhaloMassType5). For the remaining features, we take a log scale of all the data points following the convention in astronomy, and this would also help us to reveal the non-linear relationship between variables and predictors. After data reduction and feature selection, there are 8 dark matter halo parameters and 1 black hole mass data in our reduced data. The parameters are as follows:

1. **Redshift/Age**: Redshift and cosmic ages are two properties that are used to characterize the evolution stage of the universe. In the simulation, the redshift range of the snapshots spans from 0 to 20.

2. **(Log)SubhaloMass**: Total mass of all member particles/cells which are bound to this Subhalo, of all types.

[1] https://www.tng-project.org/.

3. **(Log)SubhaloMassType** (0, 1, 4): Total mass of all member particles/cells which are bound to this Subhalo, separated by type. 0 for halo gas mass, 1 for dark matter mass, 4 for stellar mass.

4. **(Log)SubhaloSpin** (in x-, y-, z- directions): Total spin per axis, computed for each as the mass-weighted sum of the relative coordinate times the relative velocity of all member particles/cells.

5. **(Log)SubhaloVmax**: Maximum value of the spherically-averaged rotation curve. All available particle types (e.g. gas, stars, DM, and SMBHs) are included in this calculation.

6. **(Log)SubhaloVmaxRad**: Comoving radius of rotation curve maximum (where Vmax is achieved). As above, all available particle types are used in this calculation.

7. **(Log)SubhaloStarMetallicity**: Mass-weighted average metallicity ($\sum M_Z/M_\star$, where Z represents any element above He) of the star particles bound to this Subhalo, but restricted to stars within twice the stellar half mass radius.

8. **(Log)SubhaloSFR**: Sum of the individual star formation rates of all gas cells in this subhalo.

In addition, we are also interested in testing whether the relation between black hole masses and host dark matter halo properties change over time, meaning if prediction results and the dominating factors of the prediction vary at different redshifts. To achieve this, we further truncated our reduced data set into different 5 redshift bins, with z = 0.0, 0.5, 1.0, 1.5, and 2.0.

3 Exploratory Analysis and Hypothesis

We make a correlation map of the dark matter halo parameters as shown in Figure. 1. The color bar reflects how strong the correction is between the variables. The redder the stronger the positive correlation, and the bluer the stronger the negative correlation. Along the diagonal, since the correlation between the same quantity must be positively correlated, the values are 1.00. By checking the last column, we can tell the linear correlation between black hole mass and other features. The highest values of ~ 0.7 come from *(Log)SubhaloMass* and *(Log)SubhaloMassType1*, inferring that the black hole mass is more positively related to the total stellar mass, which has a perfect linear relationship with the halo mass. Also, we find that black hole mass is most negatively correlated with the redshift whereas it is highly positively correlated with the cosmic age. Therefore, the cosmic age significantly influences the black hole mass since it is related to the growth of the black hole, as the later universe tends to have more massive black holes as compared to the early universe. On the other hand, we find that black hole mass is much less correlated with the *SubhaloStarMetallicity*, indicating that the supporting physical process of the two variables is not closely related.

Naturally, we employ multi-linear regression model as the simplest model in finding the correlations between different quantities. However, it is a good fit if the relations between the independent and dependent variables are linear. To determine if such a machine learning algorithm is suitable for our research proposal, we first investigate the relations between the variables and black hole mass. In Figure 2 where we examine the *SubhaloVmax*– and *SubhaaloMassType4* (stellar mass)–*SubhaloBHMass* relations, we see that the parameters considered in our reduced data are not linearly related, due to the long tails in small *SubhaloBHMass* regions.

Based on the previous works done, we hypothesize that black hole masses can be predicted accurately given their host halo properties. We also predict that the feature significances will vary for data in different redshift bins.

4 Model and comparisons

We have considered several ML models for processing such data. Multi-linear regression, XGBoost, Random forest, and a simple case of neural network for regression. Among these models, XGBoost is shown to have the least MSE in actual vs. prediction (Figure 3). The XGBoost classifier fits our research goals and the trained regressor is capable of predicting black hole masses given the host halo properties. We split out reduced data into training and testing sets. We feed the properties of the host dark matter halo and the true black hole masses into the classifier in the training process; after the trained XGBoost classifier is trained, we input the host halo parameters into the classifier, obtaining the predicted black hole masses as the output.

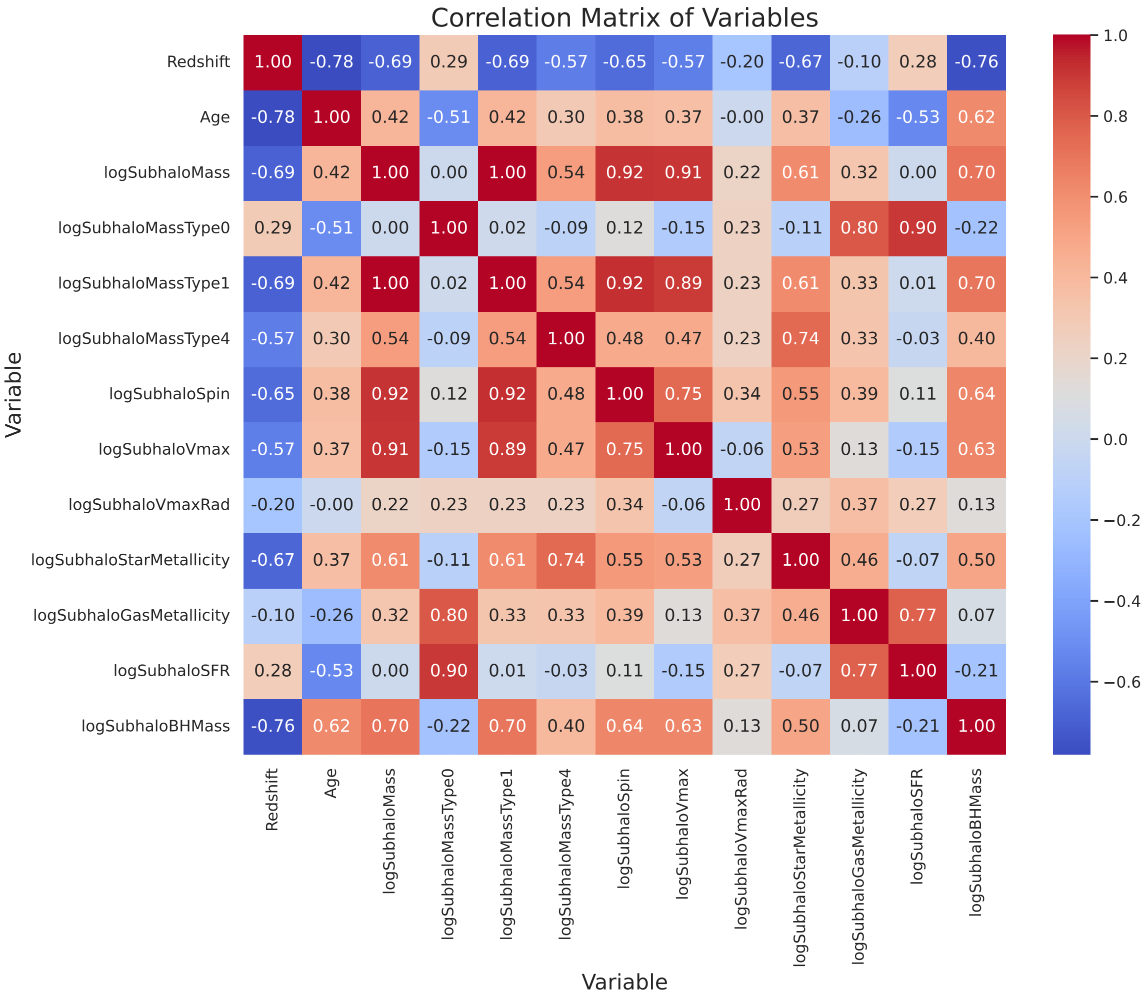


Figure 1: The correlation matrix of the dark halo described in Section 2. The color bar reflects how strong the correction is between the variables, ranging between 0 and 1. The redder the stronger the positive correlation, and the bluer the stronger the negative correlation.

In the assembly of the classifier, to determine an optimal value for "max_depth" which needs to be specified by the user, we examined the mean square error (MSE) between the predicted vs. true black hole mass. MSE thus served as an indicator for the performance of the classifier under different "max_depth" values. According to Figure 4, where we examined MSE values for z=0 data with varies "max_depth", MSE is minimized at "max_depth" = 4. Therefore, we adopted this value and conducted the following analysis with it. The results are shown in Section 5.

5 Results

In this section, we present our results on how well we can predict the black hole masses based on their host galaxy properties. Figure 5 shows the predicted black hole mass returned from the trained XGBoost classifier vs. actual black hole mass. If the classifier perfectly predicts the mass, then all data points lie along the diagonal. From Figure 5, we see that most of our data does lie along the diagonal (marked using the red dashed line). We notice that towards smaller "Actual BH Mass regions" ($\sim 6 - 7 M_{\odot}$), the predicted masses start to deviate from the actual values, indicating that the XGBoost classifier does not perform well on predicting small mass black holes.

To evaluate the quality of the predicted mass given by the trained XGBosst classifier, we computed the mean square error (MSE), accessing the difference between the predicted black hole masses and the actual

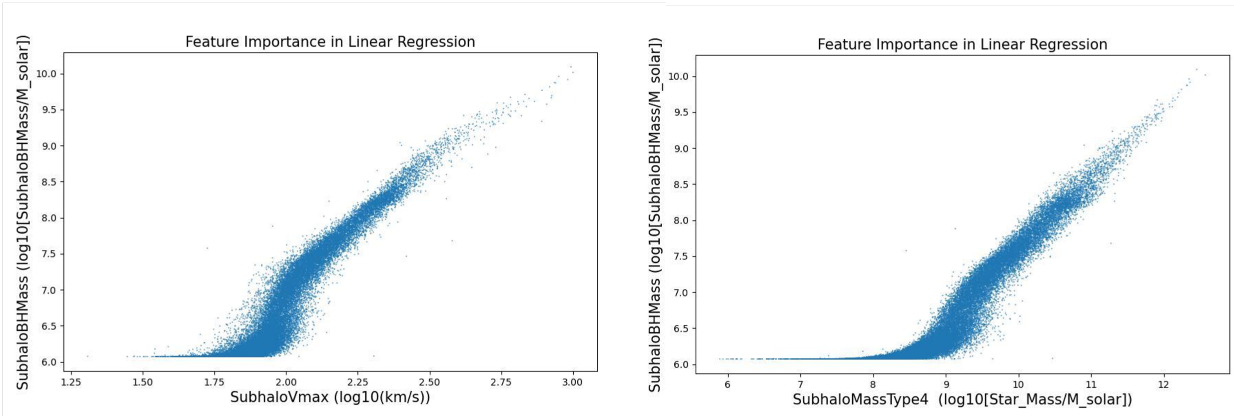


Figure 2: The *SubhaloVmax–SubhaloBHMass* relation (left) and the *SubhaaloMassType4* (stellar mass)–*SubhaloBHMass* relation will all reduced data. Both panels show a non-linear relation between the parameters, indicating that linear regression might not be suitable for our data.

masses. In Figure 5, the MSE value computed for data in each redshift bin is shown in the top left corner of the panels. We see that all MSEs are very small and close to zero, indicating a good quality of predictions.

6 Discussion

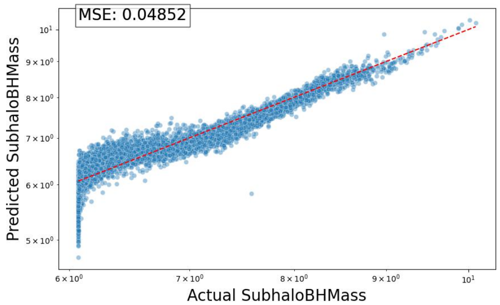
To examine how important each parameter contributes to the final prediction of the black hole mass, we present the feature importance in each redshift bin in Figure 6. The top 9 most influential features are shown in each redshift panel, and the features are ranked in descending order of importance, with the most influential feature at the top.

Interestingly, we see that on the top 2 panels (z = 0.0 and z = 0.5), the most important feature impacting black hole mass prediction is the *logSubhaloMassType4*. However, early in time (meaning at higher redshifts, e.g. z = 1.0, 1.5, and 2.0) the feature *logSubhaloStarMetallicty* dominates. Since metallicity is an indication of star-formation rate and there is a strong correlation between black hole mass and stellar mass, our explanation for this is that earlier in time, an increase in metallicity is an explicit evidence of star-forming (which increases the stellar mass), thus is directly related to black hole mass. However, as time goes on, the stellar metallicity becomes more homogeneous in spacial distribution, so an increase in stellar mass (which would directly impact the black hole mass) would not change the stellar metallicity significantly, i.e. the correlation between metallic and black hole mass becomes weaker over time. But the details are subject to further investigations.

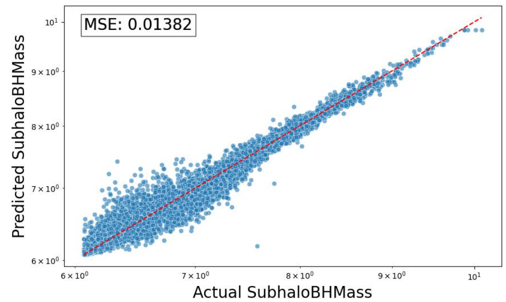
Admittedly, our study has limitations. Potential biases may exist in the reduced data or the data selection process. In this study, we chose specific host dark halo properties that we believed could affect black hole masses. However, this selection may not be comprehensive, as other parameters we overlooked might also play a role in predicting black hole masses. In future research, we aim to explore a broader range of host halo parameters. Secondly, we tested only one model, XGBoost. While XGBoost effectively handles complex, non-linear datasets, comparing our results with those from other machine learning algorithms, such as neural networks, would be beneficial. Such comparisons would enable us to draw more definitive conclusions on the subject matter.

7 Conclusion

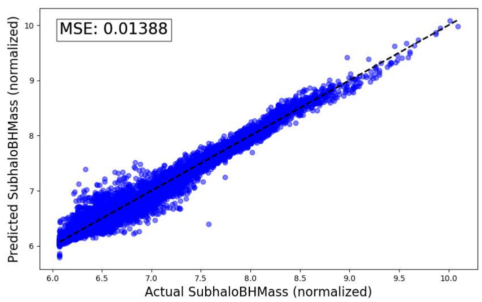
In this work, we examined the features that impact the mass of black holes. As previous works have demonstrated how the environment affects the properties of the black holes resided in, we hypothesize that there exist correlations between black hole masses and host halo properties. With a trained XGBoost classifier and the processed IllustrisTNG data, we demonstrated that such corrections exist: given the properties of host halo properties, the black hole masses can be predicted accurately. We also examined the feature importance in determining the predicted black hole masses, and it shows that the feature dominating the prediction of black hole mass changed over time.



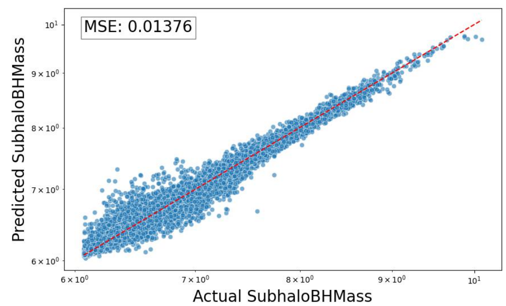
(a) Multi-linear Regression



(b) Random Forest



(c) Neural Network



(d) Neural Network

Figure 3: Predicted black hole (BH) mass vs. actual BH mass, using (a) multi-linear regression, (b) Random Forest Regression (estimator number 50, max depth 12), and (c) Neural Network with PyTorch (4 hidden layers, 64 nodes, RuLU activation function), (d) XGBoost. All halo data for all redshifts are used. MSE is shown in the upper left corner.

For further steps, it is worth investing in more features of the host dark matter halo and the time evolution of feature importance, as well as testing other algorithms such as neural networks.

8 Acknowledgement / Team Contribution

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- Yuxuan Cao: Model comparison, analysis, interpretation of data (contribution: 100/100)
- Joohyun Lee: Data reduction, analysis, interpretation of data (contribution: 100/100)
- Kaile Wang: Report writing and final project presentation (contribution: 100/100)
- Saiyang Zhang: Data reduction/Feature Selection, group coordination, and presentations (contribution: 100/100)

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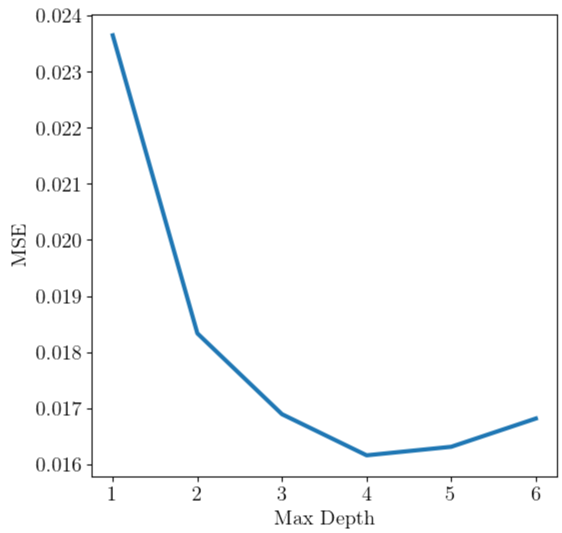

Figure 4: The mean square error (MSE) computed between the predicted and actual black hole mass vs. max depth, with redshift z=0 data. MSE reflects the quality and performance of the XGBoost classifier. From this figure, MSE researches a minimum at "Max Depth" = 4, indicating that it is an optimal value for our data.

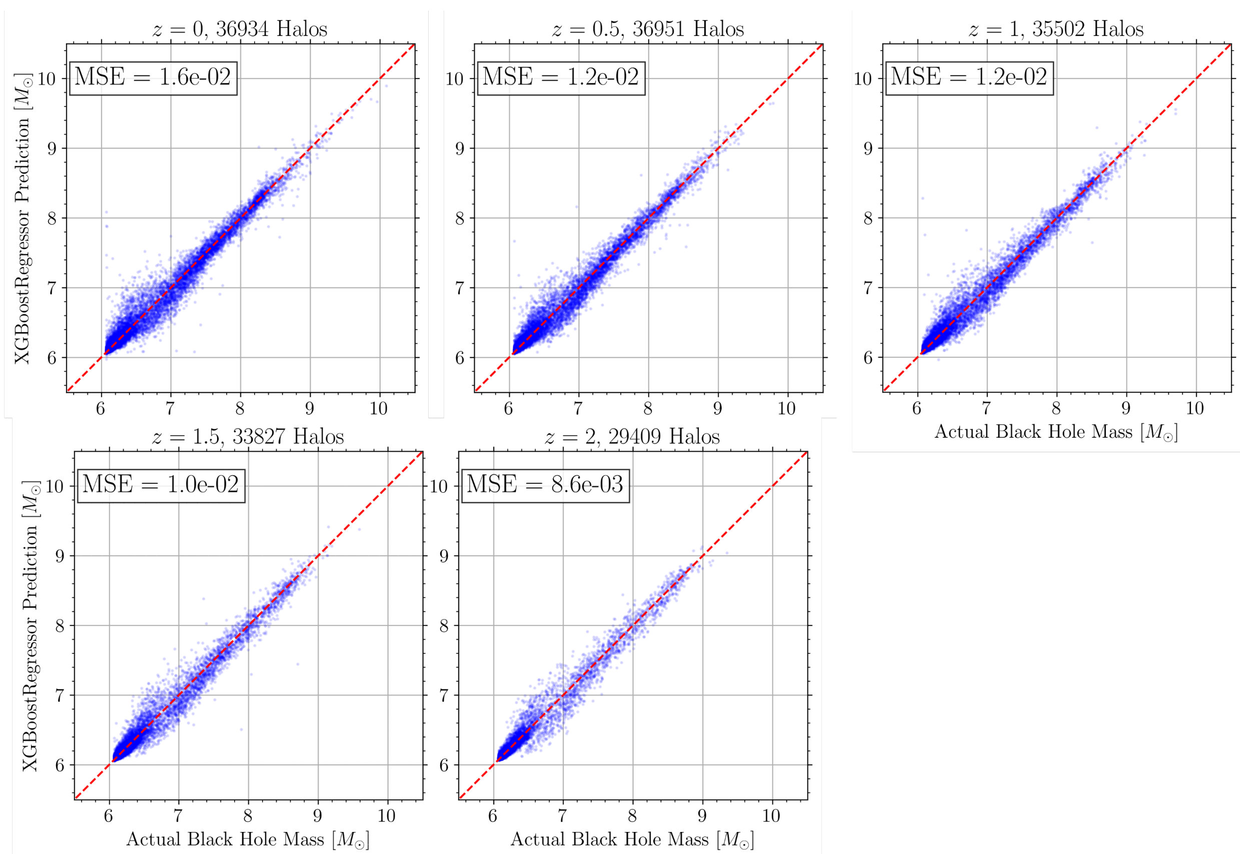

Figure 5: Predicted black hole (BH) mass vs. actual BH mass, using XGBoost classifier. The blue dots represent the black hole data. Data points lie on the red dashed line reflecting perfect prediction. Most of the data is distributed along the line. The mean square error (MSE) of data in each redshift bin is shown in the top left corner of the panels. Towards small black hole mass at $\sim 6 - 7M_\odot$, the predicted mass starts to deviate from the actual mass the most, compared to the prediction results at higher masses.

Figure 6: Feature importance of the XGBoost regressor, displaying the top 9 most influential features. The features are ranked in descending order of importance, with the most influential feature at the top.

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