A Multi-Fidelity Emulator for the Lyman-α Forest Flux Power Spectrum

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ABSTRACT

In this work we extend our recently developed multi-fidelity emulation technique to the simulated Lyman-α forest flux power spectrum. Multi-fidelity emulation allows interpolation of simulation outputs between cosmological parameters using many cheap low-fidelity simulations and a few expensive high-fidelity simulations. Using a test suite of small box (30 Mpc/h) simulations, we show that multi-fidelity emulation is able to reproduce the Lyman-α forest flux power spectrum well, achieving an average accuracy when compared to a test suite of 0.8%. We further show that it has a substantially increased accuracy over single-fidelity emulators, constructed using either the high or low-fidelity simulations only. In particular, it allows the extension of an existing simulation suite to smaller scales and higher redshifts.

Key words: software: simulations – methods: numerical – cosmology: theory – intergalactic medium – methods: statistical

1 INTRODUCTION

The modern and future testbed for cosmology lies in small scales and non-linear structures. Cosmological analyses exploit observations of these scales to explore questions such as the nature of dark matter, the total neutrino mass, and the thermal history of the intergalactic medium (IGM). One of the most powerful probes of small scale structure is the Lyman-α forest, a series of absorption features in the spectrum of quasars (Gunn & Peterson 1965; Theuns et al. 1998; McDonald et al. 2000; Hui et al. 2001; Viel et al. 2002; Fan et al. 2006; Viel & Haehnelt 2006; McDonald et al. 2006). Numerical simulations are required to analyze these observations as they probe the non-linear regime. As these simulations are expensive, cosmologists build emulators (Heitmann et al. 2006; Habib et al. 2007; Heitmann et al. 2009), which interpolate a summary statistic (in this case the 1D Lyman-α forest flux power spectrum) between simulation outputs at different cosmological parameters.

A recent development in cosmology is the application of multi-fidelity emulators, which allow simulations with different particle loads, and thus costs, to be combined together (Ho et al. 2022). Here we adapt the multi-fidelity emulation technique to the Lyman-α forest 1D flux power spectrum. Multi-fidelity emulation is especially useful in this context because the Lyman-α forest probes a range of redshifts, and is sensitive to smaller scales, which require higher resolution simulations, at higher redshifts (Bolton & Becker 2009). The models developed here will allow a single emulator to target the wide range of scales probed by the Lyman-α forest, which would otherwise require a computationally infeasible number of very large simulations (Borde et al. 2014).

The Lyman-α forest is the result of overlapping neutral hydrogen absorption profiles in the spectra from distant luminous quasars, processed through the expansion of the universe (Gunn & Peterson 1965). As light travels from the quasar, it passes through neutral hydrogen gas of varying densities. In the rest frame of those neutral hydrogen islands, light that has been redshifted close to the Lyman-α transition at 1215.67 Å will be absorbed and the rest transmitted. This is repeated as the light continues to intersect more neutral hydrogen islands on its path towards us, the observers. The result is a quasar transmission spectra containing an overlapping field of absorption features that provides a proxy to the dark matter density along that sightline (Croft et al. 1998).

The densities probed by the Lyman-α forest, from redshift 2 – 5, are ~ 1 – 100 × the cosmological mean density. At these densities stellar winds and star formation effects are negligible, although black hole feedback is important (Viel et al. 2013b; Chabanier et al. 2020). The densities along with the range of scales accessed has made the Lyman-α forest popular in cosmological studies, including: constraining the thermal history of the IGM and thus reionization (Bolton et al. 2008, 2014; Nasir et al. 2016; Boera et al. 2019; Wu et al. 2019; Gaikwad et al. 2021; Villasenor et al. 2021), constraining cosmological parameters including the neutrino mass (Viel et al. 2004; McDonald et al. 2005; Viel et al. 2006; Seljak et al. 2005, 2006; Palanque-Delabrouille et al. 2020; Garny et al. 2021), and testing alternatives to cold dark matter (Viel et al. 2005, 2013a; Iršič et al. 2017a; Palanque-Delabrouille et al. 2020; Garzilli et al. 2021; Rogers & Peiris 2021b).

The Lyman-α forest 1D flux power spectrum is the most commonly used summary statistic for Lyman-α forest spectra. It probes small scale structure by measuring the two-point Fourier-space correlation between neutral hydrogen absorption within a sightline (Croft et al. 1998).

Current observational measurements of the Lyman-α forest flux power spectrum come from either a lower resolution, larger sample survey (SDSS, Chabanier et al. (2019)), or various higher resolution, smaller sample surveys (Iršič et al. 2017b; Karaçaylı et al. 2022; Day et al. 2019). In Chabanier et al. (2019), the flux power spectrum constructed from BOSS and eBOSS spectra accesses redshifts from $z = 2.2 - 4.6$ (6% & 18% average uncertainty, respectively) and...
from $k \approx 0.001 - 0.02 \text{ km}^{-1} \text{ s}$ (6% & 14% average uncertainty, respectively). The small sample, higher resolution surveys generally access a similar redshift range, but shift both the largest and smallest scales to higher $k$. For example, in Karaçaylı et al. (2022) (their conservative results), using spectra from multiple surveys (XQ-100, KODIAQ, and SQUAD) they access redshifts from $z = 2 - 4.6$ (7% & 27% average uncertainty, respectively) and scales from $k \approx 0.005 - 0.1 \text{ km}^{-1} \text{ s}$ (12% & 9% average uncertainty, respectively).

The Dark Energy Spectroscopic Instrument (DESI) will soon report its first year results. Ultimately it will increase the number of Lyman-$\alpha$ forest spectra by a factor of four over SDSS. This corresponds to $\sim 50$ quasars per square degree and a total of $7 \times 10^3$ quasars over the 14,000 square degree survey footprint (DESI Collaboration et al. 2016). In addition, DESI is expected to measure the 1D flux power spectrum at smaller scales ($k < 0.035 \text{ km}^{-1} \text{ s}$) and higher redshifts ($z > 4.6$) than SDSS, achieving order of a few percent accuracy (Valluri et al. 2022).

Extracting cosmological information from these observations will require simulations which follow the distribution of gas at relevant densities and on relevant scales. For the Lyman-$\alpha$ forest, box sizes of at least 100 Mpc $h^{-1}$ and mean particle spacing of 100/3072 $\approx 0.03$ Mpc $h^{-1}$ are necessary (Borde et al. 2014). Earlier work has focused on methods which can reduce the cost of such simulations. Borde et al. (2014) used a splicing technique to produce high resolution, large volume outputs from three sets of less computationally intensive simulations: low resolution, large volume; high resolution, small volume; and low resolution, small volume. Lukić et al. (2015) explored the use of Richardson extrapolation to enhance output resolution, in addition to testing the splicing technique.

Parameter inference tasks, such as a direct Markov Chain Monte Carlo analyses, require $\sim 10^5 - 10^6$ model evaluations, indicating the number of simulations required by a naive approach. Even using techniques such as splicing, this is computationally infeasible. However, using a significantly reduced number of simulations ($\sim 30$), an emulator can be constructed that effectively interpolates between this smaller set of simulations. In addition to the Lyman-$\alpha$ forest, emulators have been used extensively in cosmology for studying: the matter power spectrum (Heitmann et al. 2009, 2014; Lawrence et al. 2017; Giblin et al. 2019; Euclid Collaboration et al. 2021; Aricò et al. 2021; Giri & Schneider 2021), weak lensing (Harnois-Déraps et al. 2019; Davies et al. 2021), the halo mass function (McClintock et al. 2019; Nishimichi et al. 2019; Bocquet et al. 2020), and the 21-cm signal (Kern et al. 2017; Cohen et al. 2020; Bevis et al. 2021; Bye et al. 2022). Still, the computational resources required to run $\sim 30$ simulations with the requisite volume and resolution is highly restrictive, especially for the Lyman-$\alpha$ forest.

Here, we use modern machine learning techniques to alleviate the computational resource cost associated with constructing an emulator. Specifically, we are concerned with using machine learning to predict high resolution simulation outputs to a high degree of accuracy, while running a minimal number of high resolution simulations.

One machine learning method that is suited to this task is a Gaussian Process (GP) emulator. Gaussian processes (Rasmussen & Williams 2006) are a means of interpolating between the simulation outputs, providing function prediction in a Bayesian framework. Essentially, a distribution of functions is learned through training on simulations, and the mean (best estimate) and variance (interpolation error) of the output can be returned for arbitrary simulation inputs. While other interpolation methods are possible, Gaussian processes have many benefits: the inherent quantification of prediction uncertainty, the option to incorporate prior knowledge, and the ability to interpolate within high-dimensional parameter space.

Previous uses of GP emulators for the Lyman-$\alpha$ forest have been shown to be effective at predicting summary statistics (Bird et al. 2019; Rogers et al. 2019; Pedersen et al. 2021; Walkert et al. 2021; Rogers & Peiris 2021a,b). Bird et al. (2019) self-consistently showed that the predicted flux power from their GP emulator (trained with 21 simulations) agreed to within 1 – 2% of the corresponding simulation flux power spectrum. These GP emulators still require a substantial computational cost, as the full simulation suite must be run with sufficient volumes and resolutions for the Lyman-$\alpha$ forest.

Recently, Ho et al. (2022) implemented a multi-fidelity GP emulator (Kennedy & O’Hagan 2000) for the matter power spectrum. Here, we combine and expand on the methods outlined in Bird et al. (2019) and Ho et al. (2022), to produce a multi-fidelity GP emulator for the Lyman-$\alpha$ forest flux power spectrum. In our multi-fidelity model, the training simulations are split into two fidelities; a large sample of low resolution simulations (low fidelity, LF), and a small subset of these simulations run at higher resolution (high fidelity, HF). Note that we use fidelity and resolution interchangeably throughout this work. Using these two training sets, the multi-fidelity emulator is trained to predict the 1D flux power spectrum that would be output by a high resolution simulation for arbitrary cosmological and astrophysical parameters.

A multi-fidelity emulator allows us to replace some of the HF simulations that would be needed in a single-fidelity emulator with LF simulations. This can dramatically reduce the computational cost of constructing an emulator, while retaining predictive power across parameter space. Using this method, emulators can be constructed that make use of the full range of scales and redshifts probed by Lyman-$\alpha$ forest observations. This enables analyses which can jointly constrain thermal, astrophysical, and cosmological parameters.

In our high resolution simulations, the Lyman-$\alpha$ forest flux power spectrum is converged to $\approx 5\%$. While the scales we probe in this work are resolved, the box size we use is smaller than required to analyze the full range of scales available in Lyman-$\alpha$ forest data, i.e. we cannot compute a likelihood function using all the real data without larger boxes. We therefore defer a full cosmological likelihood analysis to future work. Our goal is to quantitatively test the accuracy of the emulator output, as compared with the output from a set of testing simulations run at the same resolution as the HF training set, and demonstrate the validity and utility of the multi-fidelity technique. Specifically, we quantify the accuracy of the single- and multi-fidelity emulators with respect to true values from the testing simulations, thus determining how effective the multi-fidelity model is at producing high resolution outputs at minimal computational cost.

2 SIMULATIONS

Simulations were performed using MP-Gadget\(^1\), an N-body and smoothed particle hydrodynamics (SPH) code built on the solid base of Gadget-3 (last described in Springel 2005). MP-Gadget has been substantially modified to include shared-memory parallelism using OpenMP, together with many other algorithmic improvements and new subgrid models, as described in Bird et al. (2022); Ni et al. (2022); Bird et al. (2020). The initial power spectrum and transfer functions are generated with the Boltzmann code CLASS (Lesgourgues 2011). Species-specific initial conditions are generated for baryons and dark matter (Bird et al. 2020; Fernandez et al. 2021). We

\(^1\) https://github.com/MP-Gadget/MP-Gadget
include radiation in the cosmological background model and assume massless neutrinos.

The physics models largely follow those used for the ASTRID simulation, which are described in Bird et al. (2022). Primary sources for these models, as well as changes from Bird et al. (2022) are described below.

We use a cubic kernel for our density estimator (rather than a quintic kernel). For these simulations, the cubic kernel, in addition to running faster, produced a neutral hydrogen column density distribution that was more consistent with observations for column densities between $10^{20}$ and $10^{22}$ cm$^{-2}$ (Ho et al. 2021). We continue to use the pressure-entropy formulation of SPH. The smaller SPH kernel increases the noise within galaxies, but has minimal effect on the Lyman-$\alpha$ forest (Bird et al. 2013).

Star formation follows the model of Springel & Hernquist (2003), with our specific implementation as described in Feng et al. (2016). We lower the number of stars produced per gas particle from 4 (used in ASTRID) to 1 (as in Illustris-TNG), which speeds up the simulation without having an effect on the Lyman-$\alpha$ forest (Bird et al. 2013).

Black holes follow the model of Ni et al. (2022). We found that for the resolutions used here, the dynamic friction from gas led to a few black holes escaping from their dark matter halo, so we only use dynamic friction from dark matter and stars. The black hole feedback factor, which controls the fraction of luminosity that is converted to thermal energy, is an emulator parameter (BHF), with the associated parameter limits in Figure 3. The black hole feedback radius is fixed to 3 kpc h$^{-1}$, selected to be the average black hole feedback radius at the highest tested resolution when using a nearest neighbour distance. To accommodate a lower mass resolution than ASTRID, the minimum stellar mass needed in a halo to seed a black hole was increased to $2 \times 10^4 M_\odot$, and all black hole seeds start with a mass of $5 \times 10^4 M_\odot$.

Stellar winds are modeled following Okamoto et al. (2010). The decoupling distance for the winds is increased from 20 kpc h$^{-1}$ to 1 Mpc h$^{-1}$, which allows the winds to decouple due to density changes rather than travel distance. The density threshold for wind decoupling is set to 10% of the star formation density threshold (which is 57.7 times the critical density). The minimum wind velocity is set to 100 km/s. Finally, metal return (gas enrichment) is disabled as it is not important for the Lyman-$\alpha$ forest and can be computationally expensive.

Gas is assumed to be in ionization equilibrium with a uniform ultraviolet background using the model of Faucher-Giguère (2020). We boost the temperature of the gas to 15000 K the timestep after the gas is reionized, to model impulsive heating during hydrogen reionization from ionization fronts (D’Aloisio et al. 2019).

We implement He $\alpha$ reionization using the model of Upton Sandersbeck & Bird (2020). The input parameters for this model are: quasar mean bubble size and variance, redshifts for the start and completion of He $\alpha$ reionization $z_{\alpha}^s$, $z_{\alpha}^f$, and the quasar spectral index $\alpha_q$ (which effectively scales the peak temperature during He $\alpha$ reionization). The quasar bubble size is reduced from the default of ~ 30 Mpc, motivated by radiative transfer simulations McQuinn et al. (2009), to 5 Mpc, due to our small box size.

Simulations are initialised at $z = 99$ and finish at $z = 2$, and use periodic boundaries. Box volume, particle number, and gas particle mass resolution are reported in Table 1. The range given for the gas resolution is due to the varying value of $h$ in our simulation suite. The gas particle mass resolution for our HF simulations does not meet the resolution that Bolton & Becker (2009) recommend to resolve the forest at all redshifts of interest. However, the Lyman-$\alpha$ forest flux power spectrum from our HF simulations is converged to within $\approx 5\%$ of a simulation that does meet the required resolution of Bolton & Becker (2009). We are interested in the performance of the multi-fidelity GP emulator in learning the mapping from low to high resolution, thus this slight lack of numerical convergence does not affect our results. Examples of the gas density (at $z = 3.6$) for the two resolutions are shown in the top and bottom panels of Figure 1.

Lyman-$\alpha$ forest absorption spectra are generated using Fake Spectra Flux Extractor (Bird 2017)$^2$, described in Bird et al. (2015). We generate 32,000 (seeded) randomly placed skewers for each snapshot, from $z = 5.4$ to $z = 2.0$ in increments of $\Delta z = 0.2$. The pixel

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**Figure 1.** Example Lyman-$\alpha$ forest spectra and corresponding gas density from simulations at redshift 4. The top and bottom panels show the simulated gas surrounding the skewer which produced the spectra shown in the middle panel. Examples are shown for simulations run at high (top panel, yellow line) and low resolution (bottom panel, red line).

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2 https://github.com/sbird/fake_spectra
Table 1. Table of simulation sets

| Simulation | Box Volume | N_part | M_gas (M_☉ h^−1) |
|------------|------------|--------|------------------|
| LF         | (30 Mpc h^−1)^3 | 2 × 256^3 | [1.78, 2.37] × 10^7 |
| HF         | (30 Mpc h^−1)^3 | 2 × 512^3 | [2.22, 2.96] × 10^7 |
| Test       | (30 Mpc h^−1)^3 | 2 × 512^3 | [2.22, 2.96] × 10^6 |

Figure 2. Lyman-α forest flux power spectrum from LF and HF simulations. The top panel shows the flux power spectrum at redshift 3 from an LF simulation (blue), and its HF counterpart (yellow). The lower panels show the ratio of the flux power for these two resolutions, for all LF-HF simulation pairs, at z = 3.8, 4.6, & 5.4. Dashed lines shown the highest k probed by BOSS/eBOSS (Chabanier et al. 2019), and the estimated reach for DESI (Valluri et al. 2022).

Figure 3. Simulation parameter limits and samples. Parameters for the low resolution simulations (crosses) were determined by filling a Latin hypercube. Initially, 30 low resolution samples were generated, then an additional 10 were added while maintaining the Latin hypercube method, hence the non-uniform spacing for the low resolution samples. The optimal subset of low resolution simulations is determined (see Section 3.2.3) and this subset is run at higher resolution (shown as red circles).

While the exact difference between the LF and HF flux power spectra depends on simulation input parameters and redshift, in general the LF differs most from the HF at small scales. The enhanced power on large scales for the LF flux power spectra is consistent with Borde et al. (2014), and is likely due to differences in heating and cooling during H i and He ii reionization.

Figure 3 lists the input parameters that are varied across our suite of simulations, as well as their limits. Two parameters control the primordial power spectrum: n_s is the scalar spectral index (slope) and A_p is the amplitude (see Bird et al. (2019) for more details). Three of the parameters relate to the He ii reionization model: z_f^He ii and z_{f^He ii} are the redshifts for the start and end of He ii reionization, and α_q is the quasar spectral index. We vary the Hubble constant through h, and the total matter density through Ω_{M h^2}. One parameter is varied for H i reionization: z_{f^H i} is the midpoint redshift of H i reionization. Finally, we vary one parameter for the black hole model: BHF is the black hole feedback factor, which controls the fraction of luminosity that is converted to thermal energy. Note that our simulations do not contain a kinetic feedback model. However, at z > 2 it is expected that the thermal mode dominates. Also shown in Figure 3 are the LF and HF training samples. Note that the HF samples are a subset of the LF samples. The selection of the HF samples is described in Section 3.2.3.

3 EMULATORS

In Section 3.1, we will briefly review emulation using a Gaussian process. In Section 3.2, we will review how the Gaussian process emulator can be extended to model simulations with different qualities using a multi-fidelity emulator, MFEmulator. The multi-fidelity emulation technique of Kennedy & O’Hagan (2000) will be reviewed in Section 3.2.1. Section 3.2.2 will discuss the differences in multi-
fidelity emulator design between this paper and Ho et al. (2022). Finally, Section 3.2.3 will outline how we select our training simulations in the parameter space.

3.1 Gaussian process emulator

Gaussian process (GP) regression models (Rasmussen & Williams 2006) have been widely used to build cosmological emulators (Heitmann et al. 2006; Habib et al. 2007; Heitmann et al. 2009). A GP provides closed-form expressions for predictions. In addition, a GP naturally comes with uncertainty quantification, which is useful when building an inference framework. In the context of emulation, a GP can be seen as a Bayesian prior for the simulation response. It is a prior because the emulator model is chosen to ensure smoothness and monotonicity features of the simulation response before data are collected (Santner et al. 2003).

Let \( \theta \in \Theta \subseteq \mathbb{R}^d \) be the input cosmologies for the simulator, where \( d \) is the dimension of the parameters (\( d = 9 \) for our emulator). \( f(\theta) \) is the corresponding output summary statistic. In this work, the summary statistic, \( f(\theta) \), is the Lyman-\( \alpha \) forest flux power spectrum. A GP regression model can be viewed as a prior on the response surface of our simulated Lyman-\( \alpha \) forest flux power spectrum:

\[
f(\theta) \sim \mathcal{GP}(\mu(\theta), k(\theta, \theta')),
\]

where \( \mu(\theta) = \mathbb{E}[f(\theta)] \) is the mean function, and \( k(\theta, \theta') = \text{Cov}(f(\theta), f(\theta')) \) is the covariance kernel function. In this work, we assume a zero mean function, and we used the same covariance function as Bird et al. (2019), which will be defined later in this section.

Suppose we run the simulations at \( n \) carefully chosen input cosmologies, \( \mathcal{D} = \{\theta_1, \cdots, \theta_n\} \), and we generate the corresponding Lyman-\( \alpha \) forest flux power spectrum for each simulation, \( y = \{f(\theta_1), \cdots, f(\theta_n)\} \). Conditioning on this training data, we can get the predictive distribution of \( f \) at a new input cosmology \( \theta \) through the closed-form expression:

\[
f(\theta) \mid y, \mathcal{D} \sim \mathcal{N}(\mu_n(\theta), \sigma_n^2(\theta)),
\]

where the mean and variance are:

\[
\begin{align*}
\mu_n(\theta) &= k(\theta, \mathcal{D})^T K(\mathcal{D})^{-1} y; \\
\sigma_n^2(\theta) &= k(\theta, \theta) - k(\theta, \mathcal{D})^T K(\mathcal{D})^{-1} k(\theta, \mathcal{D}).
\end{align*}
\]

The vector \( k(\theta, \mathcal{D}) = [k(\theta, \theta_1), \cdots, k(\theta, \theta_n)] \) represents the covariance between the new input cosmology, \( \theta \), and the training data. The matrix \( K(\mathcal{D}) \) is the covariance for the training data.

For the covariance kernel function, we choose the same kernel as in Bird et al. (2019), which is a combination of a linear kernel and a radial basis kernel (RBF):

\[
k(\theta, \theta'; \sigma_0, l, \sigma) = k_{\text{RBF}}(\theta, \theta'; \sigma_0, l) + k_{\text{LIN}}(\theta, \theta'; \sigma)
\]

\[
= \sigma_0^2 \exp \left( \sum_{i=1}^d -\frac{(\theta_i - \theta'_i)^2}{2l_i^2} \right) + \sigma^2 \sum_{i=1}^d \theta_i \theta'_i,
\]

where \( \sigma_0^2 \) and \( \sigma^2 \) are the variance hyperparameters for the RBF kernel and the linear kernel, respectively. \( l \) is the lengthscale parameter that controls the smoothness of the Gaussian process function. We applied Automatic Relevance Determination (ARD) for both linear and RBF kernels. That is, we assign one lengthscale \( l_i \) (variance \( \sigma_i^2 \)) hyperparameter for each input dimension \( i \) for the RBF and linear kernels. This allows the GP to dynamically learn the scale over which each input dimension varies, which corresponds to the degree of sensitivity of the flux power spectrum to the input parameter.

Although we do not explicitly write in the notation, \( f(\theta) \) is a single-valued output. Since our target summary statistic is a vector, we model each \( k \)-bin of the flux power spectrum with a separate \( \sigma \). The primary reason for this choice is that the correlation between the low-fidelity and high-fidelity flux power spectrum changes depending on the scale considered. The multi-fidelity method can only capture this scale dependence if we model each scale separately.

3.2 Multi-Fidelity Emulation

We first introduce the Kennedy-O’Hagan model (KO model) (Kennedy & O’Hagan 2000) in Section 3.2.1. Section 3.2.2 describes the changes we have made to adapt the model from Ho et al. (2022) to the Lyman-\( \alpha \) forest. Finally, the strategy we employ for choosing parameters at which to generate high-fidelity training simulations is described in Section 3.2.3.

3.2.1 Kennedy O’Hagan Method

The KO model (Kennedy & O’Hagan 2000) was first introduced to model a sequence of computer codes with increasing fidelity. For simplicity, we assume there are only two fidelities: low-fidelity (LF) simulations with low resolution, and high-fidelity (HF) simulations with high resolution.

We define \( \{y_{LF}, y_{HF}\} \) as the Lyman-\( \alpha \) forest flux power spectra in the training set, \( y_i = \{y_{LF}(\theta_i^L), y_{HF}(\theta_i^H)\} \), where \( n_{LF} \) and \( n_{HF} \) are the number of simulations in the low- and high-fidelity training sets. We use the KO method to model Lyman-\( \alpha \) forest flux power spectra from different fidelities:

\[
f_{HF}(\theta) = \rho \cdot f_{LF}(\theta) + \delta(\theta),
\]

where \( \rho \) is a trainable parameter describing a multiplicative correction between the low- and high-fidelity Lyman-\( \alpha \) forest flux power spectra. \( \delta(\theta) \) is a GP independent of \( f_{LF}(\theta) \), describing an additive correction between fidelities. In other words, Equation 5 assumes the high-fidelity Lyman-\( \alpha \) forest flux power can be decomposed as the low-fidelity flux power multiplied by a correction parameter, \( \rho \), and an additive bias function \( \delta(\theta) \).

As mentioned in Ho et al. (2022), the \( \rho \) parameter has to be scale-dependent (a function of \( k \)) to model the well-known fact that small scales are less well resolved in smaller simulations. Here we use the same method as Ho et al. (2022) and assume Equation 5 is a single-output GP model. We assign a KO model to each \( k \)-bin of the data. In this way, we can model \( \rho \) as a function of \( k \), as shown in Figure 4.

We also assign KO models for each redshift. As shown in Figure 4, \( \rho \) is a non-trivial function of both \( k \) and \( z \), so we cannot simply use an emulator trained on one redshift to apply on another redshift. We note that it is possible to assume a smooth function to model \( \rho(k, z) \). However, validating \( \rho(k, z) \) is out-of-scope for this paper. In practice, observational data are conditioned on a specific redshift, so training emulators on separate redshifts is sufficient for cosmology inference.

Figure 4 shows that \( \rho \) stays close to unity at large scales for most of the redshifts. At small scales, however, different redshifts require different values of \( \rho \). At the middle redshifts (3 ≤ \( z \) < 5), \( \rho \) has a...
large positive deviation from unity. At the low redshifts (2 ≤ z < 3), ρ has a moderate deviation toward ρ > 1. The only exception is at the high redshifts (5 ≤ z ≤ 5.4), which stays close to ρ = 1 for all scales. This indicates that the correction to the Lyman-α forest flux power due to the resolution of the simulation varies with redshift, depending on the over-density probed by the forest.

### 3.2.2 Model differences from Ho et al. (2022)

Here we highlight the ways in which we have adapted the model from Ho et al. (2022), which emulated the non-linear matter power spectrum at z = 0–2, to the Lyman-α forest at z = 2–5.4. Since the redshift range is larger in this work, we employed a new strategy to select the optimal HF training set by averaging over the interpolation loss for all redshift bins. We will describe the strategy in detail in Section 3.2.3.

In Ho et al. (2022), we outlined two multi-fidelity methods: a linear multi-fidelity emulator (the KO model, or the autoregression model (AR1)), and a non-linear multi-fidelity emulator (non-linear autoregressive GP, or NARGP, Perdikaris et al. (2017)). However, we found that NARGP requires more HF training simulations than AR1, perhaps due to the wide range of redshifts used. We use the KO model for our main results, and describe the NARGP results in Appendix A.

In this work, instead of emulating logarithm scaled powers, we adopted the mean-flux normalization strategy proposed in Bird et al. (2019). We normalize all flux power spectra in the training set by the median spectrum:

\[
\begin{align*}
   y_{LF} & = \frac{y_{LF}}{\text{median}(y_{LF})} - 1; \\
   y_{HF} & = \frac{y_{HF}}{\text{median}(y_{HF})} - 1. 
\end{align*}
\]

(6)

The index i refers to one of the spectra in the training set, \( y_{LF} = \{ f_{LF}(g_i)^{n_{LF}} \}_{i=1}^{n_{LF}} \). Equation 6 ensures the training sample distribution is close to having a zero mean, matching the prior of the GP emulator. We found that in practice this normalisation makes training the emulator substantially easier. Note that we normalize the HF training set using the same LF median spectrum. As the HF training set is small, the median spectrum estimate for HF is noisy, and so using it for normalization may introduce some unwanted training bias.

### 3.2.3 Sampling strategy for high-fidelity simulations

The KO model approach can be seen as a Bayesian way to correct an emulator from low-fidelity to high-fidelity. Thus, if \( y \) is the high-fidelity Lyman-α forest flux power spectrum used for training, and \( \mathbf{θ} \) is the corresponding input parameters:

\[
\begin{align*}
   y &= f_{LF}(\mathbf{θ}) + (f_{HF}(\mathbf{θ}) - f_{LF}(\mathbf{θ})) \\
   &= f_{LF}(\mathbf{θ}) + \text{error}(\mathbf{θ}). 
\end{align*}
\]

(7)

The emulation accuracy will be directly affected by how well an autoregressive construction can model error(\( \mathbf{θ} \)). Usually, a large set of low-fidelity simulations are used as training data for \( f_{LF}(\mathbf{θ}) \) because they can be obtained cheaply. The quality of training data for error(\( \mathbf{θ} \)) = \( f_{HF}(\mathbf{θ}) - f_{LF}(\mathbf{θ}) \) thus relies on the choice of high-fidelity simulations.

In Ho et al. (2022), we proposed an optimization strategy to select high-fidelity training simulations. A low-fidelity only emulator (LFEmu)\(^5\) is trained on a subset of low-fidelity training simulations. The posterior means of the trained LFEmu are used to calculate the emulation errors from the remaining LF samples in the Latin Hypercube Sampling (LHS). By minimizing the emulation errors of LFEmu, we can use the selected optimal cosmologies as inputs for the HF training set. By ensuring the HF training set achieves a good interpolation, we mitigate emulation errors for the multi-fidelity emulator.

In practice, we employ a three-stage procedure for building a multi-fidelity emulator:

(i) Prepare LF simulation suite.

(ii) Prepare HF simulation suite. This is done by using LFEmu to find the set of cosmologies that minimizes the interpolation loss.

(iii) Build MFEmulator. If the accuracy is not enough, go back to stage 1 or 2 to run more training simulations.

For stage (ii), to avoid wasting computational resources running more LF simulations, we directly use the LF simulation suite in stage (i) to build and validate the LFEmu. Thus, the cosmologies chosen for the HF set are a subset of the LF simulation LHS, which fulfills the nested training dataset design suggested in Kennedy & O’Hagan (2000). The benefit of using a nested data structure, \( \mathbf{θ}_{HF} \subseteq \mathbf{θ}_{LF} \), is that we can directly compute posterior means from the LF training set for cosmologies \( \mathbf{θ}_{HF} \), without any interpolation in LF.

We note that it is possible to train a MFEmulator without using the LF simulations to optimize the HF points. However, if the selection of HF points are suboptimal (i.e., can barely interpolate in the prior volume), then the MFEmulator accuracy will be suboptimal. This is because the error(\( \mathbf{θ} \)) cannot be decomposed into an autoregressive structure easily.

To find the optimal HF training set across the full redshift range, \( z = 2–5.4 \), we train a LFEmu for each redshift and get the validation loss (we used mean squared errors). We sum up the validation loss for all redshifts and find a subset of cosmologies that minimizes the summed validation loss.

\(^5\) In a similar way, we call a high-fidelity only emulator, HFEmu.
Figure 5. A flowchart for training a multi-fidelity emulator. We start with a low-fidelity (LF) set of simulations. We then select a subset of low-fidelity points to train an emulator, LFEmu, at each redshift. The validation loss for each LFEmu is computed using the rest of the LF simulations as a validation set. Finally, we sum up the validation losses at each redshift, and use the summed loss to propose a set of cosmologies $\theta_{HF}$ which can best minimize the summed loss.

In Figure 5, we summarize the above described procedure in a flowchart. For a formal description, we refer to Ho et al. (2022). The only difference between the proposed procedure in Figure 5 and the procedure in Ho et al. (2022) is that we optimize $\theta_{HF}$ across redshifts $z = 2 - 5.4$ in this work. Thus, we have an additional step to sum the LFEmu validation loss across redshifts.

Training an LFEmu on all possible low-fidelity subsets is computationally intensive. To reduce costs, we employed the greedy optimization strategy from Ho et al. (2022). We first explored all possible subsets for 3 design points within the LF LHS. For the optimal 4 design points, instead of exploring all possible subsets, we grew the subset one point at a time, fixing the previously chosen optimal 3 HF points. In the same line of thought, we grew the subset to 6 optimal design points for HF training cosmologies. Our final simulation suite of 40 LF and 6 HF samples, along with parameter limits, is shown in Figure 3.

4 RESULTS & DISCUSSION

Using the flux power spectra from our LF and HF simulations, we train single-fidelity (one LF only, and one HF only) and multi-fidelity emulators. These trained emulators are used to predict the flux power spectrum output for a set of 10 simulation input parameters. We then compare these predictions to the corresponding testing simulations which were run at the same resolution as the HF simulations (see Table 1).

4.1 Emulator Accuracy

In the following, we only show results for the emulators that use the full available set of training simulations (40 LF and 6 HF). We have verified that using all available training simulations leads to the most accurate emulator. Section 4.2 shows how emulator accuracy degrades when a smaller subset of the available simulations is used.

Using the full set of available simulations, the mean prediction error for the multi-fidelity emulator is $(\frac{P_{\text{pred}}}{P_{\text{true}}} - 1) \approx 0.8\%$ (averaging across all scales, redshifts, and testing simulation outputs). For the LF single-fidelity emulator, the mean prediction error is $\approx 4\%$. This is not unexpected; there are real differences between the flux power spectra output by the low and high resolution simulations that are not being captured with this method. The 4% error may seem quantitatively quite good, considering the simpler methodology and reduced resource cost. However, there is no indication that the error could be reduced further with additional simulations (see Section 4.2).

For the HF single-fidelity emulator, the mean prediction error is $\approx 3\%$. This is likely limited by the sample size of the training set (6 simulations), leading to increased errors when making predictions for inputs that are far away from the training samples. It is important to note that the HF samples are selected to optimize the multi-fidelity emulator, rather than as an independent emulator (i.e. as a Latin hypercube sample). There is some indication that prior information from the LF training samples provides useful information about the best areas of parameter space to sample. To test this, we split our testing set (10 simulations, same resolution as the HF samples) into training and testing sets, then train all 210 combinations of 6 samples, and predict the outputs for the remaining 4 samples. The error range from this exercise is $2.5 - 11.5\%$ (5.5% mean error, 1.5% standard deviation). Though not a direct comparison, the 3% error we obtain from the HF single-fidelity emulator compares favorably with this, indicating that the HF samples selected are an improvement over using a Latin hypercube sampling scheme.

Figure 6 shows the mean prediction error, averaged over all redshifts and 10 test simulations, as a function of wavevector $k$. In this, and the following figures, the shaded region around the curves is the variance in prediction error $(\frac{P_{\text{pred}}}{P_{\text{true}}} - 1)$, to give a sense of how much the error varies beyond the mean. The multi-fidelity emulator outperforms the single-fidelity emulators at all scales, with an error between $0.5 - 1.5\%$. The LF (HF) single-fidelity emulator has error between $2 - 7\%$ ($2 - 6\%$).

Both single-fidelity emulators and the multi-fidelity emulator trend towards higher error for small scales. The LF emulator dips $1 - 2\%$
around \( k \approx 0.02 \text{s/km} \). The dip occurs on scales at which the low resolution flux power spectra goes from overestimating to underestimating the high resolution power (see Figure 2, for \( z \leq 4.6 \)). The uptick in the multi-fidelity emulator error for the largest \( k \)-bins is also present in the HF emulator, indicating that there is a scarcity of large scale modes available in the emulator training.

Figure 7 shows how the emulators perform as a function of redshift and scale. In the following, we define small scales as \( k > 0.02 \text{s/km} \) and large scales as \( k \leq 0.02 \text{s/km} \) (divided at the smallest scale accessible by BOSS/eBOSS data (Chabanier et al. 2019)). On large scales (Figure 7, left panel), the LF emulator error decreases with time until \( z \approx 4 \), then slowly increases. This trend is because, as can be seen in Figure 2 (left of the BOSS/eBOSS dashed line), the low resolution flux power comes into better agreement with the high resolution flux power as it nears \( z \approx 4 \). We also found that the LF simulations do not cool as efficiently as the HF simulations after He II reionization, likely leading to the rise in error for \( z \leq 3.2 \).

On small scales (Figure 7, right panel), the LF emulator error is more variable. The dip in error seen around \( z \approx 4.6 \) occurs as the low resolution flux power crosses from overestimating to underestimating the high resolution flux power (Figure 2 right of the BOSS/eBOSS dashed line). The subsequent rise in error is due to the loss of small-scale power and consequent under-estimation of the flux power spectrum in the low-fidelity simulations.

The trends in redshift and scale seen in the LF emulator performance are due not to interpolation error, but to the different numerical resolution of the two simulation fidelities, since this emulator is not predicting the flux power at the higher resolution. Some differences are connected to temperature differences between the LF and HF simulations. For low densities (\( \sim 1 \) times the mean density), the LF simulations are colder than the HF simulations at high redshift, but come into better agreement leading up to He II reionization, after which they diverge from the HF simulations again. For higher densities (\( \sim 100 \) times the mean density), the LF simulations are once again colder than the HF simulations at high redshift, but at lower redshift they are too hot (with a crossover at \( z \approx 4.6 \)). As higher redshifts probe lower densities, the error initially decreases with redshift, before rising again towards the lowest redshifts.

On both large and small scales the HF emulator errors are around 3.5\%, dominated by sampling variance. During He II reionization the HF emulator has more variation in error, which is probably exacerbated by our small box sizes. The increased variation during He II reionization further indicates that the primary source of error for the HF emulator is the sample size of the training set.

On small scales, the multi-fidelity emulator error is insensitive to redshift and small (0.9\%). On large scales, the multi-fidelity emulator error slightly decreases until \( z \approx 4.2 \), then increases with the onset of He II reionization, before flattening again. The trend is also more variable during He II reionization, indicating that emulator finds it more difficult to learn the mapping during this process. However, the multi-fidelity emulator still outperforms the single-fidelity emulators, with an error between \( \approx 0.4 \% - 1\% \).

### 4.2 Emulator Runtime

While we have shown that the multi-fidelity emulator outperforms the single-fidelity emulators presented here, it still remains to show that it is more computationally cost efficient. We could, for example, add more training simulations to our single-fidelity HF emulator and get a similarly accurate high resolution emulator. However, the computational cost would increase significantly. By comparing the total emulator runtime to prediction error, we can determine the choice that balances computational cost and accuracy. In practice, the important question is to determine the computational cost at which a given emulation technique can achieve a desired accuracy. The computational cost of training the emulators is subdominant (\( O(1) \) cpu-hours) to running the training simulations, so in the following we only consider the runtime for the simulation suites.

Figure 8 shows the mean prediction error (averaged over all redshifts and test outputs) as a function of the number of simulations used in the training set, for small and large scales (as defined in Section 4 and Figure 7). The solid lines show prediction errors for multi-fidelity emulators trained using 6 HF and a varying number of LF simulations. The small and large scale errors flatten out after \( \approx 30 \) LF simulations are used in the training set. The LF simulations allow the emulator to determine how the flux power spectrum depends on the cosmological input parameters, and so this indicates that 30 LF simulations are needed to explore our 9 parameter space. Other emulators range from using \( \approx 6 \) simulations per parameter (e.g. McClintock et al. (2019); Ho et al. (2022)) to \( 30 \) per parameter (e.g. Euclid Collaboration et al. (2021)). The \( 3 \times 4 \) simulations per parameter required here is unusually low, perhaps because the input parameters affect the flux power spectrum close to linearly in much of parameter space.

Dashed lines show prediction errors for multi-fidelity emulators trained using 40 LF and a varying number of HF simulations. Adding extra HF simulations to the training set has a larger impact than adding LF simulations. The addition of each HF simulation generally improves the emulator accuracy for small scales more than for large scales. This is as expected, since the main purpose of the HF simulations is to learn the mapping from low to high resolution output, with small scales being more resolved in the HF simulations.

Figure 9 shows the emulator prediction errors as a function of the total runtime (cost of running the training simulations). All simulations were run on the Frontera supercomputer at the Texas Advanced Computing Center. The cost is divided between the LF training simulations, which cost \( \approx 10 \) node hours each, and the HF training simulations, which cost \( \approx 150 \) node hours each.

The dashed trend shows the same emulators as Figure 8, but no longer divided by scale. Qualitatively it looks the same as both the large scale and small scale results from the previous figure. The error is flat after \( \approx 30 \) LF training simulations, indicating that a similar accuracy can be achieved using the multi-fidelity emulator with \( \approx 30 \) rather than 40 LF simulations. The most efficient 1\% error emulator in this study is a multi-fidelity emulator using 30 LF and 5 HF training simulations (the cost for this was \( \approx 1050 \) node hours). The most accurate emulator is the 40 LF, 6 HF multi-fidelity emulator, with error 0.8\%, and cost \( \approx 1300 \) node hours.

The dotted line (squares) shows the error and runtime for the single-fidelity emulators. Following from the 6 HF single-fidelity emulator result to the dashed (yellow) line, it can be seen that the addition of just a few LF training simulations quickly improves the accuracy. It can also be seen that in terms of computational cost, the multi-fidelity emulator is more efficient. Note that the HF training simulations are not selected to optimize a single-fidelity emulator, but instead are selected to optimize the multi-fidelity emulator. They thus use prior information provided by the LF training simulations and so perform better than a naive Latin hypercube construction of a HF emulator using 6 training samples. Our multi-fidelity scheme

\[\text{At least for errors less than } 4\%, \text{ the approximate amount by which the LF simulations fail to be converged.}\]
Figure 7. Comparing the prediction error as a function of redshift and scale for multi- and single-fidelity emulators. This is mean error across all 10 test simulations. The blue shaded region shows the extent of helium reionization in our simulations (see parameter limits in Figure 3).

Figure 8. Emulator prediction error as a function of the number of simulations used in training the emulator. This is the mean error across all redshifts and 10 test simulation outputs. The prediction error is broken down into large ($k < 0.02 \text{ s/km}$) and small ($k > 0.02 \text{ s/km}$) scales, as in Figure 7. The solid lines show how the average error depends on the number of LF simulations, while the dashed lines show how the average error depends on the number of HF simulations once all LF simulations are included.

Figure 9. Prediction error as a function of total training simulation computational cost. This is the mean error for 10 test simulations over all redshifts and scales. The solid line shows the prediction error when changing the number of HF simulations used in training the multi-fidelity emulator. Also shown are the single-fidelity emulators (red squares), and the multi-fidelity emulator trend with a varying number of LF training simulations (yellow, dashed).

5 CONCLUSIONS

In this work we developed and tested a multi-fidelity emulator for the simulated Lyman-α forest flux power spectrum. Emulators address the growing computational demands of simulations, which must be run at increasingly high resolutions to allow analysis of the increasing quality and quantity of observational data. Here, we use a Gaussian process based emulator that addresses this demand by, in a Bayesian framework, training an interpolating function to predict the output (Lyman-α forest flux power spectrum) for a given input (simulation input parameters). Relatively few simulations are required to accurately predict across the span of input parameter space, making emulators especially useful for parameter inference problems.

The multi-fidelity framework allows a further reduction in computational cost by dividing the emulator training samples into multiple (in our case two) fidelities. The low-fidelity (low-resolution) training
samples allow the emulator to learn how the the outputs depend on input parameters. The high-fidelity (high-resolution) training samples correct numerical errors in the low-fidelity emulator with a (parameter-dependent) mapping from low- to high-fidelity. Thus, the emulator can be trained with a large sample of low-fidelity training simulations and a small subset of high-fidelity training simulations.

Our training suite included 40 low resolution hydrodynamical simulations (30 Mpc/h simulation box length, 256 \(^3\) particles) and 6 high resolution hydrodynamical simulations (30 Mpc/h simulation box length, 512 \(^3\) particles). Using the Lyman-\(\alpha\) forest flux power spectrum extracted from these simulations, we trained single- and multi-fidelity emulators to predict the high resolution flux power spectrum. Ten independent simulations were run to test the prediction accuracy of the trained emulators.

In summary, the multi-fidelity emulator:

- Modelled a redshift range 5.4 – 2 (in 18 redshift bins with \(\Delta z = 0.2\)), on scales ranging from \(k = 1.4 \times 10^{-3}\) to \(k = 5.7 \times 10^{-2}\) s/km (in 25 bins).
- Achieved sub-1% error on most scales and redshifts when averaged over 10 test simulations.
- Reached an average error of 0.8%.
- Achieved 1% average error most cost efficiently using a training set with 30 low resolution and 5 high resolution simulations.

The low resolution single-fidelity emulator (4% average error) predicts the low resolution flux power, so it is limited by real differences between the output of the two resolutions. The high resolution single-fidelity emulator (3% average error) is limited by the small number of training samples. It is likely that the average error for the high resolution single-fidelity emulator could be improved to match the multi-fidelity emulator performance with the addition of more training simulations. However, the high resolution single-fidelity emulator quickly increases in computational cost with additional samples, and we expect it would thus be more expensive than our multi-fidelity emulator.

Some important caveats to our results are that the Lyman-\(\alpha\) forest is converged at the \(\approx 5\%\) level in our high resolution simulations, and the box size is small. In a forthcoming work, a model that uses two different box sizes (rather than two different resolutions) to construct a multi-fidelity emulator will be developed and tested. While there is no direct evidence to suggest that changing the resolution or box size would significantly enhance or diminish the accuracy of the emulators presented here, it still remains to be tested on simulations with higher resolution and larger box sizes. In a forthcoming work, we test the multi-fidelity framework on larger box size, higher resolution simulations, and use this multi-fidelity emulator for cosmological inference.

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DATA AVAILABILITY

Flux power spectra generated from the low resolution, high resolution, and testing sets are available at https://github.com/mafern/MFEmulatorLyaData. HDF5 and plain text (appropriate for multi-fidelity emulation) formats are available. Select single- and multi-fidelity emulator predictions for the 10 testing simulations are also available from the same repository. The spectra underlying the flux power are available upon request.

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APPENDIX A: NON-LINEAR MULTI-FIDELITY EMULATOR

In the main text we have explored the effectiveness of a linear multi-fidelity emulator (the KO model, or AR1). In the linear model, the mapping from LF to HF is \( f_{\text{HF}}(\theta) = \rho f_{\text{LF}}(\theta) + \delta(\theta) \), where \( f_{\text{HF}} \) and \( f_{\text{LF}} \) are the emulator predictions at those resolutions, and \( \rho \) is independent of the input parameters \( \theta \).

Here, we compare those results with the results using a non-linear multi-fidelity emulator (non-linear autoregressive GP, or NARGP). In the non-linear multi-fidelity model, proposed by Perdikaris et al. (2017), the mapping is a function of both the LF output and the input parameters. We model this as:

\[
\hat{f}_{\text{HF}}(\theta) = \rho(\theta, \hat{f}_{\text{LF}}(\theta)) + \delta(\theta),
\]

such that \( \rho \) depends on both the input parameters and LF posterior output. The LF outputs, as is the case with the linear model, are median normalized such that the assumption on the Gaussian process of zero mean is more reasonable, \( \hat{f}_{\text{HF}}(\theta) = f_{\text{LF}}(\theta)/\mu_{\text{LF}} - 1 \).

Following Perdikaris et al. (2017), \( \rho \) is modelled as a Gaussian process with input from both input cosmologies for HF, \( \theta_{\text{HF}} \), and the output from LF, \( f_{\text{LF}}(\theta) \). The NARGP construction results in a deep Gaussian process model (Damianou & Lawrence 2013). We follow the approximation in Perdikaris et al. (2017) and replace \( \hat{f}_{\text{LF}}(\theta) \) with its posterior distribution. Thus, the training reduces to training two regular GPs recursively.

In Figure A1 we show the prediction errors separated into small and large scales, as a function of redshift for both the linear and non-linear multi-fidelity emulators. They perform similarly, with the linear emulator being more accurate at low redshifts on all scales, and high redshifts for small scales. The difference between the average error for the linear and non-linear models (over all scales and redshifts) is 0.08%. This is in contrast to emulation of the matter power spectrum in Ho et al. (2022), where the non-linear model outperformed the linear model.

It is worth noting that the non-linear model agrees closely with the linear model when using the full suite of training simulations, but lags behind the linear model when using fewer HF training simulations. For example, the difference in the average error between linear and non-linear models using 40 LF and 3 HF is ≈ 2% (1.9% error for linear, 3.7% error for non-linear). When using 4 HF the difference is ≈ 1% (1.5%, 2.5%), and when using 5 HF the difference is ≈ 0.4% (0.9%, 1.3%). While differences in the effectiveness of the non-linear model may be due to the quantity being emulated (matter power versus flux power), one likely reason for the difference is the number of input parameters. In Ho et al. (2022), five input parameters are...
used, while in this work we use nine. The non-linear model uses the posterior of the LF output, which requires Monte-Carlo sampling. It is possible that the additional dimensions degrade the performance of the Monte-Carlo integration, and thus the performance of the non-linear model. One other reason may be the larger number of hyperparameters that need to be optimized in the training.

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