



# CHORUS

This is the accepted manuscript made available via CHORUS. The article has been published as:

Matter power spectrum emulator for  $f/R$  modified gravity cosmologies

Nesar Ramachandra, Georgios Valogiannis, Mustapha Ishak, and Katrin Heitmann (LSST Dark Energy Science Collaboration)

Phys. Rev. D **103**, 123525 — Published 10 June 2021

DOI: [10.1103/PhysRevD.103.123525](https://doi.org/10.1103/PhysRevD.103.123525)

# Matter Power Spectrum Emulator for $f(R)$ Modified Gravity Cosmologies

Nesar Ramachandra,<sup>1,\*</sup> Georgios Valogiannis,<sup>2,3,\*</sup> Mustapha Ishak,<sup>4</sup> and Katrin Heitmann<sup>1</sup>

(The LSST Dark Energy Science Collaboration)

<sup>1</sup>*High Energy Physics Division, Argonne National Laboratory, Lemont, IL 60439, USA*

<sup>2</sup>*Department of Astronomy, Cornell University, Ithaca, NY 14853, USA*

<sup>3</sup>*Department of Physics, Harvard University, Cambridge, MA 02138, USA*

<sup>4</sup>*Physics Department, The University of Texas at Dallas, Richardson, Texas 75080, USA*

(Dated: May 5, 2021)

Testing a subset of viable cosmological models beyond General Relativity (GR), with implications for cosmic acceleration and the Dark Energy associated with it, is within the reach of Rubin Observatory Legacy Survey of Space and Time (LSST) and a part of its endeavor. Deviations from GR- $w(z)$ CDM models can manifest in the growth rate of structure and lensing, as well as in screening effects on non-linear scales. We explore the constraining power of small-scale deviations predicted by the  $f(R)$  Hu-Sawicki Modified Gravity (MG) candidate, by emulating this model with COLA (COmoving Lagrangian Acceleration) simulations. We present the experimental design, data generation, and interpolation schemes in cosmological parameters and across redshifts for the emulation of the boost in the power spectra due to Modified Gravity effects. Three preliminary applications of the emulator highlight the sensitivity to cosmological parameters, Fisher forecasting and Markov Chain Monte Carlo inference for a fiducial cosmology. This emulator will play an important role for future cosmological analysis handling the formidable amount of data expected from Rubin Observatory LSST.

## I. INTRODUCTION

The Vera C. Rubin Observatory Legacy Survey of Space and Time (LSST) <sup>1</sup> [1, 2], together with a wide range of current and future surveys of the large-scale structure (LSS) of the universe, such as DESI [3], Euclid [4], the Nancy Grace Roman Space Telescope [5] and SPHEREx [6], will offer a unique opportunity to test our standard cosmological assumptions at an unprecedented level of accuracy. The widely accepted cosmological model,  $\Lambda$  Cold Dark Matter ( $\Lambda$ CDM), attributes the observed accelerated expansion of the universe [7, 8] to the existence of a positive cosmological constant,  $\Lambda$ , corresponding to non-zero vacuum energy. This assumption, combined with the existence of pressure-less cold dark matter and gravity described by Einstein's General Relativity (GR), has been very successful at fitting a large spectrum of cosmological observations [9–14].

Despite these remarkable observational accomplishments,  $\Lambda$ CDM has faced several theoretical challenges, with the cosmological constant problem [15, 16] arguably serving as the primary reason to consider alternative proposals. Furthermore, as our ability to accurately obtain the underlying cosmological parameters from late and early-time observations increases, attention has been drawn to certain tensions between the corresponding extracted values of the Hubble constant,  $H_0$  [17–20], and the amplitude of density fluctuations,  $\sigma_8$  [14, 21–24], which could however be attributed to unknown systematics. Combined with the long-term interest in exploring

deviations from GR in all regimes [25, 26], the above motivate introducing large-scale modifications of gravity as alternative candidates for cosmic acceleration; such theories are called the Modified Gravity (MG) theories [27–30].

In order to be able to evade the existing tight constraints of gravity from observations in the Solar System [25, 26], while at the same time producing detectable large-scale signatures, viable MG candidates typically invoke “screening” mechanisms [31, 32], which suppress deviations in the high-density regime through novel scalar field self-interactions [33–39]. Furthermore, the space of all MG parametrizations that lead to second order equations of motion, the Horndeski class [40–42] has been additionally restricted [43–48] by the simultaneous detection of gravitational waves and electromagnetic counterparts by the LIGO/Virgo collaborations [49–53]. A detailed discussion of viable MG candidates testable by LSST Dark Energy Science Collaboration (DESC) was presented in Ref. [54].

The predicted transition from MG to GR would manifest itself, by means of the dynamical screening mechanism, in the nonlinear regime of structure formation, which will be precisely probed by the Stage-IV surveys of the LSS [55]. As a result, these upcoming observations will offer a unique opportunity to study the large-scale behavior of gravity with unprecedented accuracy. The optimal interpretation of the wealth of upcoming data, however, is conditional upon our ability to produce efficient and reliable theoretical predictions of the expected observable signatures of MG. In the (quasi-)linear regime of structure formation, this can be partially achieved through analytical, perturbation theory approaches, such as Lagrangian Perturbation Theory (LPT) [56–60]. Unfortunately, these approaches break down on nonlinear

\* The two lead authors have contributed equally to this work.

<sup>1</sup> <http://www.lsst.org>

73 scales. Reliable predictions of such small-scale signals  
 74 from MG theories can only be obtained through perform-  
 75 ing full N-body simulations (for a comparison of differ-  
 76 ent codes, see Ref. [61]). These are computationally very  
 77 expensive, particularly in the presence of an additional  
 78 MG-induced force, due to the inherent nonlinearities in-  
 79 troduced by the screening mechanism.

80 As a consequence of the substantial computational  
 81 costs associated with performing full N-body simulations  
 82 for MG models, efficient approaches are essential. To  
 83 that end, the hybrid COmoving Lagrangian Acceleration  
 84 (COLA) method was developed in Ref. [62], expanding  
 85 upon the initial  $\Lambda$ CDM implementation of Ref. [63], for  
 86 efficiently simulating the MG classes of chameleon and  
 87 symmetron screening. Utilizing a combination of 2<sup>nd</sup> order  
 88 Lagrangian Perturbation Theory (2LPT) and a pure  
 89 N-body component, the COLA method provides a great  
 90 trade-off between accuracy and computational efficiency,  
 91 that was found to recover the fractional deviation in the  
 92 nonlinear dark matter power spectra with sufficient ac-  
 93 curacy, at only a fraction of the standard computational  
 94 cost. However, many investigations require even faster  
 95 prediction capabilities to enable the exploration of pa-  
 96 rameter space. For example, Markov Chain Monte-Carlo  
 97 (MCMC) inference relies on tens of thousands of model  
 98 evaluations and even the fast COLA approach, which  
 99 takes  $\sim 1$  hour on a single core for one MG simulation,  
 100 would be too slow to enable such an investigation.

101 To provide faster predictions for, e.g., the power spec-  
 102 trum, fitting functions have been used extensively in the  
 103 past (see, e.g., Refs. [64, 65] for fits capturing  $\Lambda$ CDM  
 104 and  $w$ CDM cosmologies based on the Halofit approach  
 105 or a halo model-based approach to include baryonic ef-  
 106 fects [66] or physics beyond  $\Lambda$ CDM [67]). However, fit-  
 107 ting functions have several drawbacks. First, the accu-  
 108 racy requirements for ongoing and future surveys of a  
 109 few to sub-percent are very difficult to obtain by a single  
 110 functional form and a set of fitting parameters. Second,  
 111 for models outside the range for which the fit was de-  
 112 rived, no error bounds are available and biases can occur.  
 113 Third, a large range of simulations is needed to enable a  
 114 good calibration of the parameters that describe the fit.  
 115 Overall, it has been shown that even for the relatively re-  
 116 stricted case of  $w$ CDM cosmologies, it is very difficult to  
 117 achieve an accuracy of better than 5–10% as pointed out  
 118 in one of the recent Halofit papers [65] and subsequent  
 119 comparisons, e.g., Refs. [68, 69].

120 Because of the above shortcomings of fitting functions  
 121 and the need for very accurate and fast predictions, the  
 122 concept of emulators was introduced to cosmology in  
 123 Refs. [70, 71]. It was shown that with a relatively small  
 124 number of high-quality simulations, prediction schemes  
 125 could be built that provide high-accuracy results for,  
 126 e.g., the matter power spectrum and  $C_{\ell s}$  quickly. The  
 127 **Coyote Universe** project [72–74] then released a stand-  
 128 alone prediction scheme for the matter power spectrum,  
 129 the **CosmicEmu**, based on a set of highly accurate sim-  
 130 ulations. The work was extended in several ways, in-

131 cluding the coverage of a larger  $k$ -range and redshift and  
 132 parameter spaces [68, 75]. The emulation concept itself  
 133 has since then become rather popular and was used in  
 134 several studies concerning the matter power spectrum,  
 135 see, e.g. Refs. [69, 76], a range of other summary statis-  
 136 tics, e.g., galaxy power spectra [77, 78], concentration  
 137 mass relation [77], the halo mass function [79] as well as  
 138 comprehensive simulation efforts that extracted a range  
 139 of emulators, such as the **AEMULUS** project [80–83] and  
 140 **DARK QUEST** [84, 85].

141 In this work we develop a Gaussian Process emulator to  
 142 estimate the fractional deviation of the nonlinear matter  
 143 power spectrum  $P_{MG}(k)/P_{\Lambda CDM}(k)$  (also referred to as  
 144 enhancement/boost in the power spectrum or the power  
 145 spectrum ratio) as a function of cosmological paramet-  
 146 ers and redshift, based on a set of COLA simulations in  
 147 the MG scenario. Given that our focus is to efficiently  
 148 emulate statistics for MG models that will be testable  
 149 by LSST DESC, our target model needs to be one that  
 150 exhibits a well-studied phenomenology (including exist-  
 151 ing full N-body simulations) and will predict detectable  
 152 deviations in the scales of interest to the survey. For  
 153 this reason our chosen candidate is the  $f(R)$  Hu-Sawicki  
 154 model [86], which realizes the chameleon screening mech-  
 155 anism and which we have previously identified as one of  
 156 the prioritized beyond- $w(z)$ CDM candidates testable by  
 157 LSST DESC [54].

158 In this paper we discuss the construction of the em-  
 159 ulator that comprises of an experimental design, train-  
 160 ing data synthesis and the statistical techniques to per-  
 161 form interpolation across cosmological parameters and  
 162 redshifts. After training the emulator on the COLA-  
 163 generated dataset, we validate its ability to recover sim-  
 164 ulated test cosmologies within our target range, before  
 165 proceeding to compare its accuracy against results ob-  
 166 tained by full N-body simulations for the Hu-Sawicki  
 167 model. Having quantified its accuracy, we then illustrate  
 168 the capabilities of our emulator, which delivers a massive  
 169 speed-up by 6 orders of magnitude over COLA simula-  
 170 tions, through three essential applications: a sensitivity  
 171 analysis, obtaining parameter constraints through Fisher  
 172 forecasting and MCMC inference. It is worth noting, at  
 173 this point, that efficient predictions for power spectra in  
 174 the Hu-Sawicki MG model have also been recently pre-  
 175 sented in Refs. [87–89], which however relied upon appro-  
 176 priately designed fitting formulas [87] or semi-analytical  
 177 models [88, 89]. In order to overcome the potential lim-  
 178 itations associated with such approaches, as mentioned  
 179 above, we have developed our emulator based directly on  
 180 the simulations, expanding upon the established  $w$ CDM  
 181 infrastructure of the **CosmicEmu** [90]. In addition to en-  
 182 hancing the variety of available predictive tools in the  
 183 community, which is an important endeavor by itself, this  
 184 contribution is novel. While the above techniques probe  
 185 variations of only one of the two parameters of the Hu-  
 186 Sawicki model, our emulator spans its full 2-dimensional  
 187 parameter space, for the first time in the literature.

188 Our paper is structured as follows: in Sec. II, we de-

scribe the approach to generating our training data set by first introducing our target MG model, then discussing our choices for the experimental design, including cosmological parameters and their ranges, and finally describing the efficient COLA approach we use to generate the simulations. Next, we discuss in Sec. III the details of our emulator development. We then proceed in Sec. IV to validate the emulator results, before presenting three applications in Sec. V. Finally, we conclude and discuss future work in Sec. VI. Technical details on Gaussian Processes and the emulator design can be found in Appendices B and C, respectively.

## II. TRAINING DATA AND DESIGN

### A. Modified Gravity Model

Theoretical investigations of potential departures from Einstein's GR, as well as of their consequent observational implications [25], have been an active research topic, particularly in the last two decades, due to their potential implications on resolving the mystery of cosmic acceleration [27, 29, 30]. One of the most commonly considered classes of MG deviates from GR through the addition of a nonlinear function  $f(R)$  of the Ricci scalar  $R$  to the standard Einstein-Hilbert action. These are the  $f(R)$  gravity theories [91, 92], which are described by the following action  $S$ :

$$S = \int d^4x \sqrt{-g} \left[ \frac{R + f(R)}{16\pi G} + \mathcal{L}_m \right], \quad (1)$$

with  $\mathcal{L}_m$  denoting the matter sector Lagrangian,  $G$  the gravitational constant and using units where the speed of light in vacuum,  $c$ , has been set to unity. The modification of the form (1) activates, in principle, a new additional degree of freedom in the gravitational sector, which could be responsible for driving the cosmic expansion to accelerate, instead of dark energy [93].

The most widely-considered model of this type is the  $f(R)$  Hu-Sawicki model [86], with the functional form:

$$f(R) = -m^2 \frac{c_1 (R/m^2)^n}{c_2 (R/m^2)^n + 1}, \quad (2)$$

where in Equation (2)  $m = H_0 \sqrt{\Omega_m}$ , with  $\Omega_m$  the matter fractional energy density and  $H_0$  the Hubble Constant, both evaluated today and  $n$ ,  $c_1$  and  $c_2$  are free parameters of the model.

Any well-motivated MG parametrization should have the flexibility to match the observed expansion history well-described by  $\Lambda$ CDM, a requirement which gives (for sufficiently small values of  $|f_{R_0}|$ ), the following relationship for the background value of the Ricci scalar,  $\bar{R}$ :

$$\bar{R} = 3\Omega_m H_0^2 \left( 1 + 4 \frac{\Omega_\Lambda}{\Omega_m} \right), \quad (3)$$

and for the derivative  $f_R = \frac{df(R)}{dR}$ ,

$$\bar{f}_{R_0} = -n \frac{c_1}{c_2^2} \left( \frac{\Omega_m}{3(\Omega_m + \Omega_\Lambda)} \right)^{n+1}, \quad (4)$$

where  $\Omega_\Lambda$  is the dark energy fractional density evaluated at the present time. Through relationship (4), one can reduce the number of free parameters of the Hu-Sawicki model, which can be fully characterized by the pair  $\{|f_{R_0}|, n\}$ . We briefly point out here that in the limit of  $|f_{R_0}| \rightarrow 0$  the background cosmology of  $\Lambda$ CDM is recovered. Through an appropriate conformal transformation, the model can be cast into a scalar-tensor theory (with  $f_R$  acting as the MG scalar field) [94] that recovers GR in regions of large Newtonian potential through the chameleon screening mechanism [35, 36].

The Hu-Sawicki model produces novel, distinct signatures which are testable by upcoming cosmological surveys and as a result has been well-explored in the literature through full N-body simulations. It is also known to be free from any physical instabilities [28]. We further note that, despite the increasingly tight observational constraints placed on it over the past decade (see, e.g., [92] for a review), the Hu-Sawicki model remains viable. For all these reasons, it serves as an ideal test-bed for investigating cosmological theories of gravity and is one of the main candidate models to be considered by DESC [54]. The referenced document describes the various beyond- $w(z)$  CDM model prioritized for study by DESC.

### B. Experimental Design

Two main criteria govern the choice of the cosmological parameter space covered by our emulator – first, a consideration of the computational cost incurred in generating a set of COLA simulations, which will determine how many models can be reasonably run, and, second, an estimate for the emulator's target accuracy. The application of these two criteria determines how many parameters we can afford to include and how broad their priors can be.

Our main interest in this paper is the exploration of the two parameters that define the Hu-Sawicki model for  $f(R)$  gravity theories,  $\{f_{R_0}, n\}$ . We aim to vary these parameters over a wide range in order to span a broad array of deviations predicted by the model. We choose

$$-8 \leq \log(f_{R_0}) \leq -4, \quad (5)$$

$$0 \leq n \leq 4, \quad (6)$$

and note that the upper end of the chosen  $f_{R_0}$  range corresponds to a large modification case in which screening is absent, whereas for the low end value, modified gravity forces are very strongly suppressed [86, 95]. Most studies in the MG literature, e.g., Refs. [87, 89], restrict their attention on the subspace of fixed  $n = 1$  and only vary  $f_{R_0}$ , given that deviations are more sensitive to the

latter parameter. In this work, however, we also consider variations with respect to  $n$ , thus allowing a more complete theoretical exploration of the Hu-Sawicki model parameter space. Given the wide dynamical range of  $f_{R_0}$ , over-sampling of large parameter values may occur if the parameter range is sampled linearly. In order to mitigate this problem, we instead use a logarithmic scaling in the experimental design.

Next, we have to decide which additional parameters we want to vary for the CDM component of the model. We want to focus on the parameters that affect the power spectrum the most and at the same time aim to vary only a small number of parameters. An increase in the number of cosmological parameters varied leads to either a less accurate emulator or a much larger number of simulations needed. It is therefore desirable to keep the number of parameters varied small while keeping the needed accuracy.

Figure 10 in Ref. [73] shows a sensitivity analysis for the five parameters of the  $w$ CDM “Standard Model” of cosmology. The image shows the variation of the ratio of the power spectrum to a model that is evaluated at the midpoint of the five Standard Model parameters changing one parameter at a time. The baryon density  $\Omega_b$  clearly does not have much of an effect on the power spectrum ratio, while  $\{\Omega_m h^2, \sigma_8, n_s\}$  all show considerable impact on particularly large scales. While the dark energy equation of state also leads to considerable variations,  $w$  is not of interest here as we fix the background of a  $\Lambda$ CDM model. We note again that the requirement to match a  $\Lambda$ CDM background expansion imposes additional restrictions on the parameter space of the model, which are reflected in Equations (3) and (4) that we introduced Sec II A. As we briefly discuss at the end of Section IV B, variations of  $h$  given current observational bounds do not affect the fractional deviation of the nonlinear matter power spectrum  $P_{MG}(k)/P_{\Lambda CDM}(k)$  considerably. We therefore allow variations of the aforementioned additional three parameters for our emulator. In future work, the parameter space will be extended.

We now proceed to set the range for three of the standard CDM parameters  $\{\Omega_m h^2, \sigma_8, n_s\}$ . We choose the same range used as in the Coyote Universe [73] and the Mira-Titan Universe simulation suites [96]. Both papers provide in-depth discussions about the choices to balance broad parameter coverage and achievable accuracy goals for the emulator, as informed by contemporary and future cosmic microwave background (CMB) and LSS surveys. Choosing the same parameter ranges also has the advantage that results in the future can be compared to the previous work and possibly combined later on. In summary, for the three parameters, we choose:

$$0.12 \leq \Omega_m h^2 \leq 0.15, \quad (7)$$

$$0.85 \leq n_s \leq 1.1, \quad (8)$$

$$0.7 \leq \sigma_8 \leq 0.9. \quad (9)$$

We add that  $\Omega_b h^2 = 0.0223$  (while we ignore the effects of massive neutrinos) and that for the dimensionless Hub-

ble constant we have chosen  $h = 0.67$ . After having decided on the five parameters and their ranges we have to determine the number of simulations needed and pick a sampling scheme that allows us to set up a suitable parameter sampling design. Past experience has shown that roughly 10 simulations per parameter are needed to enable the construction of an accurate emulator (targeting few percent accuracy), leading to a set of  $\sim 50$  COLA simulations.

The next choice to be made concerns the employed sampling scheme. For an excellent discussion on different sampling schemes used in computer experiments, the interested reader is referred to Ref. [97]. Ref. [73] provides an extensive discussion about different methods in the cosmology context. In this paper, we use a symmetric Latin hypercube (SLH) design, introduced in Ref. [98]. Latin hypercube (LH) sampling schemes are statistical stratified sampling methods used to generate near-random samples of values from a multi-dimensional distribution, such that there exists only one sample in each sub-division for each parameter range. Compared to a random space-filling scheme, which does not take into account the previous sampled points in a new sample-point generation, an LH sampling strategy guarantees an optimal representation of the variability of parameters. While sampling on a uniform grid also ensures fair representation, the number of required simulations would be prohibitively large. The SLH offers a space-filling design strategy that allows for flexibility with regard to a number of design points and is computationally inexpensive when optimizing the design itself, when compared to other methods such as Orthogonal Array LH implementations. The SLH imposes additional, specific symmetry requirements compared to other LH designs, as described in detail in e.g. Ref. [73]. Ref. [73] provides concrete examples to illustrate these symmetries. The symmetry imposes a space-filling requirement on the designs considered upfront, which carries through to all projections.

The final choice concerns the proposal distribution for the cosmological parameters. We use uniform distributions for the cosmological parameters  $\theta = \{\Omega_m h^2, \sigma_8, n_s, \log(f_{R_0}), n\}$  to ensure an unbiased exploration of parameter space. The 50 cosmological models that are chosen using the above prescription are shown in Appendix C. In other efforts, the design has been created based on posteriors from surveys see, e.g., the AEMULUS project [99]. This approach reduces the number of required simulations but also restricts the viability of the emulator considerably, because of the limited effective sampling volume and because of potential biases introduced by weighted sampling.

### C. COLA Simulations with Modified Gravity

The signatures introduced by MG models manifest themselves in the nonlinear regime of structure formation, where the screening mechanism is in full effect, as

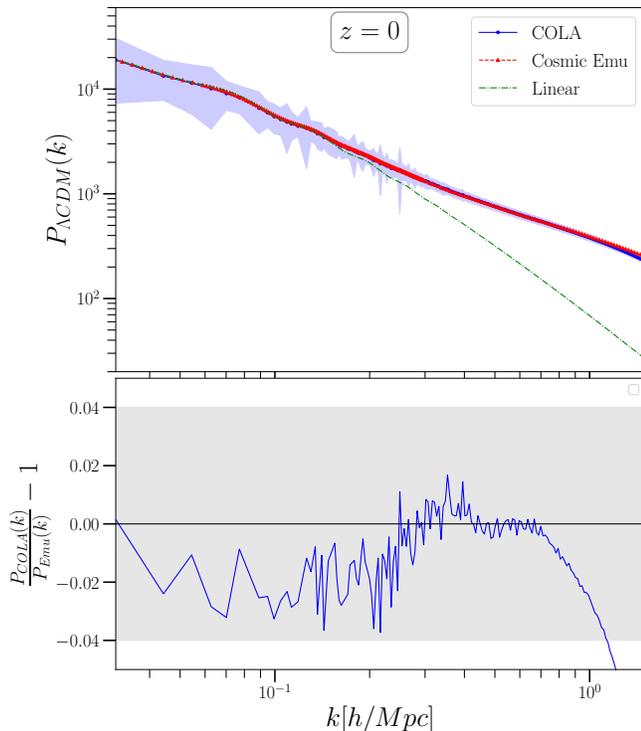


FIG. 1. Top:  $\Lambda$ CDM matter power spectra for the fiducial cosmological parameters at  $z = 0$ , as obtained by the efficient COLA method (blue solid line) and `CosmicEmu` [red dashed line]. The linear matter power spectrum for the same cosmology [green dot-dashed line] is also shown. The shaded blue region represents the standard deviation obtained from the 2000 available  $P(k)$  COLA realizations. Bottom: Fractional difference between the COLA and the `CosmicEmu`-generated power spectra of the upper panel. The shaded gray region highlights the 4% level of accuracy.

well as in the intermediate quasi-linear scales. As a result, perturbation theory approaches fail to capture the full picture of structure formation in the presence of a modification to gravity, which can only be performed through N-body simulations. These are particularly computationally expensive, due to the inherent non-linearity of the scalar-field Klein-Gordon equation. An overview and comparison of different full N-body codes in MG can be found in Refs. [61].

Given the substantial computational cost of running multiple full N-body simulations to train our emulator, we instead utilize the Comoving Lagrangian Acceleration (COLA) hybridization scheme for efficient simulations of chameleon and symmetron screening models developed in Ref. [62], expanding upon the initial  $\Lambda$ CDM implementation of Ref. [63]. Through a combination of 2<sup>nd</sup> order Lagrangian PT (2LPT) that evolves the large scales and a pure N-body component for integrating the nonlinear regime, the COLA approach was found to be able to recover the nonlinear dark matter power spectrum (in  $\Lambda$ CDM) using only a few tens of timesteps [63]. The implementation developed for the  $f(R)$  Hu-Sawicki

TABLE I. Parameters of the COLA MG simulation suite.

Box size, $L$	$200 h^{-1} \text{Mpc}$
Number of particles, $N_p$	$256^3$
Number of grids, $N_g$	$512^3$
Initial redshift $z_i$	49
Final redshift $z_f$	0
Number of time-steps, $N_t$	100
Number of realizations, $N_r$	1
Dimensionless Hubble constant, $h$	0.67

model in Ref. [62], which is the one we employ here, was shown to successfully model the fractional deviation in the dark matter power spectrum,  $P_{MG}(k)/P_{\Lambda\text{CDM}}(k)$ , in the nonlinear regime, using an effective “thin-shell” approach for capturing the chameleon screening effect that was presented in Ref. [100]. The reported accuracy in the estimation of this power spectrum ratio was at the level of 1 percent, compared against N-body simulations at  $z = 0$ . Below we summarize the parameters we choose for our COLA runs, while more details about the COLA MG implementation can be found in Ref. [62].

Our simulations are initialized using the 2LPT initial conditions code (2LPTic) [101] at an initial redshift of  $z_i = 49$ . Given that the effects of MG are assumed to be negligible at early times within the context of cosmic acceleration, we use the same set of  $\Lambda$ CDM initial conditions for both the  $\Lambda$ CDM and the  $f(R)$  runs, as in Ref. [62]. For each of the (50+5) cases in our experimental design (listed in Table III), the linear  $\Lambda$ CDM matter power spectrum is produced with `CAMB` [102], which is used to generate the initial conditions with 2LPTic at  $z_i = 49$ . The COLA simulations are then run using the parameters of Table I, for both the  $\Lambda$ CDM and the  $f(R)$  Hu-Sawicki case with the same initial random seed. At each of the 100 timesteps of the simulations, the matter power spectra are stored, for both  $\Lambda$ CDM and the MG case, with 213 bins equally spaced logarithmically in the  $k$ -range of  $(0.03 - -3.5)h\text{Mpc}^{-1}$ . The choice of 100 timesteps is made so that the target redshift range of our emulator is adequately spanned using only a single run for each case, without at the same time making the simulations too time-consuming<sup>2</sup>. Furthermore, the high number of  $k$  bins ( $n_{bins} = 213$ ) is chosen to guarantee the accuracy of the redshift interpolation. Finally, the exact same specifications are used in the 2000 simulations we perform, each of them for a different randomly chosen initial seed, in order to obtain the covariance matrix of the ratio for the fiducial cosmology of Section V B.

Before we discuss COLA’s accuracy in predicting summary statistics in MG (the matter power spectrum ratio here), which will be addressed in detail in Sec. IV B, we start by presenting the  $\Lambda$ CDM benchmark in Fig. 1. We

<sup>2</sup> We should note here that if one wants to make predictions for an individual redshift, the efficient COLA approach was shown to work well with much fewer timesteps [62, 63]

find that the mean of the 2000 COLA-generated  $\Lambda$ CDM power spectra for the fiducial cosmology remains consistent, within  $\sim 3\%$ , with the nonlinear `CosmicEmu` prediction for the same cosmology down to  $k \sim 1h\text{Mpc}^{-1}$ . It is worth noting that the better agreement compared to the initial COLA implementation in Ref. [63], is attributed to the fact that we are using about 3 times as many time-steps as the runs in that original work, for the reasons discussed in the previous paragraph.

Given that the COLA method is known to perform better at recovering the fractional deviation  $P_{MG}(k)/P_{\Lambda\text{CDM}}(k)$ , rather than the power spectrum itself [62], and also because this quantity is much less sensitive to cosmic variance effects, we choose these ratios as our training data in the Gaussian process emulator. Modeling this quantity has also been the target of interest by other studies in the MG literature [89, 103, 104]. The residual noise in the ratio is later smoothed out using a Savitzky-Golay filter, as explained in Sec. III.

### III. EMULATOR DEVELOPMENT

Based on a carefully chosen design strategy to determine a set of training points, a well-matching interpolating strategy can be selected in order to estimate the summary statistics at intermediate cosmologies. Neural networks [76], polynomial chaos expansions [69] and Gaussian processes [70–74] have been successfully employed to construct emulators for the prediction of astrophysical summary statistics. In particular, Gaussian Processes are an attractive way of performing machine learning tasks with small number well sampled data points. This non-parametric Bayesian regression method provides fast, interpretable and high-fidelity estimations with associated uncertainties. For these reasons, we utilize Gaussian processes, along with Principal Component Analysis and linear interpolation schemes to construct our emulator.

#### A. Gaussian Process Interpolation across Cosmological Parameters

Our emulation strategy for the cosmological parameters  $\theta$  follows a similar routine employed for the `CosmicEmu` [105] construction, using Gaussian processes (GPs) in a representation space [106]. The individual steps, including the data pre-processing are as follows:

1. The individual ratios of the power spectra are noisy since we only perform one realization for each individual COLA simulation. Emulators designed directly based on this data may pick up undesired noise from the data. To avoid this problem, we utilize the Savitzky-Golay filter (or `savgol` filter, [107, 108]) to obtain a smoothed power spectrum ratio  $\chi(k)$ , as detailed in Appendix A.

2. A standardization transformation on both smoothed power spectrum ratio and cosmological parameters is performed, to result in a mean of zero and a standard deviation of one for their respective distributions:

$$\theta_i' = (\theta_i - \mu_{\theta_i})/\sigma_{\theta_i}, \quad (10)$$

$$\chi'(k) = (\chi(k) - \mu_{\chi(k)})/\sigma_{\chi(k)}. \quad (11)$$

The standardized power spectrum ratio  $\chi'(k)$  is re-scaled using the mean  $\mu_{\chi(k)}$  and standard deviation  $\sigma_{\chi(k)}$ . The mean and standard deviations are computed collectively for all the 50 cosmological models. Similarly the individual cosmological parameters  $\theta_i$  are re-scaled to  $\theta_i'$  by their means  $\mu_{\theta_i}$  and standard deviations  $\sigma_{\theta_i}$ .

3. A Singular Value Decomposition (SVD) is performed on the smoothed and normalized power spectrum enhancement  $\chi(k, \theta)$  for dimensionality reduction. This is a generalization of eigenvalue decomposition to any rectangular matrix, whereby a matrix is factorized into a set of orthonormal vectors. Equation (12) below shows the decomposition to the basis  $\phi_m(k)$  and weights  $w_m(\theta)$  of the representation, truncated at  $n_w$  eigenvectors:

$$\chi'(k, \theta') = \sum_{m=1}^{n_w} \phi_m(k) w_m(\theta') + \epsilon. \quad (12)$$

The excess information that is not captured by this decomposition is represented by  $\epsilon$ . The Principal Component Analysis (PCA) of the power spectrum enhancement reveals that a total of  $n_w = 6$  eigenvectors successfully capture over 99.99 percent of the variance in the data, effectively allowing us to truncate the expansion without significant loss of information. In addition to dealing with a reduced dimension (from  $n_{bins} = 213$  to  $n_w = 6$ ) of eigenvectors, this also enables orthogonality in the interpolation space, i.e., the new basis  $\phi_m(k)$  that maximizes variance is an uncorrelated representation of  $\chi'(k, \theta)$ .

4. The weights  $w_m(\theta)$  corresponding to  $n_w = 6$  truncated orthogonal bases  $\phi_m(k)$  are then modeled as functions of the input parameters  $\theta$ . This local interpolation in parameter space is made using multivariate Gaussian Process regression applied to the weights of the Principal Component bases, as explained in Appendix B.

Configuration of the covariance function and determination of the associated hyperparameters are the key components for learning the correct GP fit. We choose a popular Matern-5/2 kernel [109], and check for robustness of the emulator accuracy with different choices of covariance functions. We search

545 for the best combination of hyper-parameters of the  
 546 GP using a fast gradient-based optimization called  
 547 Adagrad [110].

548 The four steps above are applied to all the 100 snap-  
 549 shots, resulting in a suite of 100 emulators for smoothed  
 550 power spectrum deviations. For any new cosmological  
 551 parameters  $\bar{\theta}$ , the trained GP generated 6 corresponding  
 552 weights, and these are multiplied by the PCA basis vec-  
 553 tors to generate new power spectrum enhancement values  
 554 with the  $k$ -range of the emulator.

## 555 B. Redshift Interpolation

The sampling for the redshifts coverage is treated separately from the sampling of the cosmological parameters. The cosmological parameter values are generated using an SLH design to ensure representation across the five dimensional parameter space. In contrast, the COLA snapshots are all created at the same redshifts between  $z_i = 49$  and  $z_f = 0$  with linear spacing in corresponding scale factors. Due to this difference in the training sampling, we do not employ the same interpolation scheme for all the parameters. Instead a separate interpolation routine is executed between the outputs of independent GP emulators. Equation (13) shows a simple linear interpolation for an intermediate redshift  $z$  when emulator results at two nearest redshifts  $z_-$  and  $z_+$  are calculated from the previous section:

$$\chi_{emu}(k; \theta, z) = \chi(k; \theta, z_-) + \frac{z - z_-}{z_+ - z_-} (\chi(k; \theta, z_+) - \chi(k; \theta, z_-)). \quad (13)$$

556 With our emulator suite for 100 individual redshifts,  
 557 a simple linear interpolation works within one per-  
 558 cent accuracy for the redshift interpolation when the  
 559 closest two emulators are used for a given cosmol-  
 560 ogy. Although this requires two independent GP eval-  
 561 uations and PCA reconstructions, this final emulator  
 562  $\chi_{emu}(k, \Omega_m, \sigma_8, n_s, \log(f_{R_0}), n, z)$  is found to be robust  
 563 and fast.

## 564 IV. EMULATOR ACCURACY AND 565 VERIFICATION

566 The accuracy of our emulator is determined by two  
 567 factors. First, limitations of the underlying simulations  
 568 lead to irreducible errors. We have chosen to use La-  
 569 grangian Perturbation Theory for the cosmological sim-  
 570 ulations over a computationally expensive full N-body  
 571 alternative. This choice restricts the accuracy of the em-  
 572 ulator on small scales. Second, an error arises due to the  
 573 limited number of training samples and the nature of the  
 574 sampling and interpolation schemes.

575 We study these effects by carrying out two types of  
 576 verifications. For the first test we compare the emulator

TABLE II. Cosmological parameters for the six additional COLA test simulations.

Model	$\Omega_m h^2$	$n_s$	$\sigma_8$	$\log(f_{R_0})$	$n$
T00	0.125	0.957	0.860	-6.667	0.000
T01	0.136	1.023	0.833	-4.000	2.133
T02	0.150	0.970	0.820	-6.133	3.200
T03	0.132	0.890	0.793	-5.867	2.933
T04	0.129	0.983	0.807	-6.400	3.733
T05	0.127	1.050	0.740	-4.267	0.267

577 against a set of six additional COLA simulations that  
 578 are not part of the design. This allows us to evaluate the  
 579 accuracy of the emulator construction itself. The second  
 580 test utilizes three state-of-the-art N-body simulations for  
 581 beyond  $\omega(z)$ CDM cosmologies and we compare the emu-  
 582 lator performance directly to the measurements from the  
 583 simulations. This test allows us to evaluate the overall  
 584 performance of the emulator, including both errors from  
 585 the limited simulation accuracy and the emulator con-  
 586 struction itself.

587 We restrict the emulator predictions to  $k \leq 1h\text{Mpc}^{-1}$ .  
 588 This choice is mainly driven by the accuracy of the  
 589 COLA simulations. As shown in Fig. 1, the COLA ap-  
 590 proach is in very good agreement with measurements  
 591 from high-resolution N-body simulations, represented by  
 592 the `CosmicEmu` result, out to  $k \sim 1h\text{Mpc}^{-1}$ . At this  
 593 point, the COLA power spectrum starts to deviate from  
 594 the `CosmicEmu` result and underpredicts the power spec-  
 595 trum at the few percent level. Restricting our emulator  
 596 out to this  $k$ -range therefore seems well justified. In ad-  
 597 dition, beyond  $k \sim 1h\text{Mpc}^{-1}$  other effects, like bary-  
 598 onic physics become more and more important (see, e.g.,  
 599 Ref. [111] for a recent discussion of the effects of baryonic  
 600 physics on the power spectrum).

## 601 A. Comparison with COLA Simulations

602 In this section we show the comparison of the emulator  
 603 with COLA results. Our trained emulator is tested on  
 604 parameter values within the limits of our SLH design,  
 605 but not at the exact cosmologies used to construct the  
 606 emulator.

607 In Fig. 2 we show the predictions of the emulator com-  
 608 pared to an additional test set of six COLA simulations.  
 609 The power spectrum ratios for the additional cosmolo-  
 610 gies (T00 – T05, parameters are given in Table II) are  
 611 randomly chosen within the allowed parameter ranges  
 612 specified in Equations. (5) – (9). The gray lines in the  
 613 figure show all power spectrum ratios used to build the  
 614 training set. The lower panel in the figure shows the rel-  
 615 ative error of the emulator output to the corresponding  
 616 COLA results. The relative difference is within 5% for  
 617 our six test models. Sub-percent level accuracy is ob-  
 618 served for models with  $f_{R_0} < 10^{-5}$ . The variation in  
 619 accuracy corresponds to the sampling density of power  
 620 spectrum ratios in the training set. For instance, the

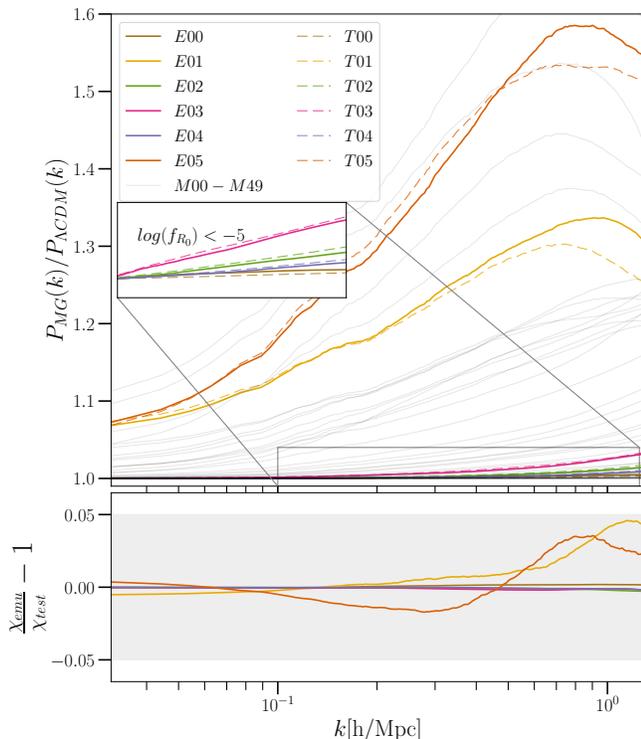


FIG. 2. Test of the emulator accuracy for additional cosmologies. Top: Power spectrum ratios  $P_{MG}(k)/P_{\Lambda\text{CDM}}(k)$  for the six testing COLA simulations at  $z = 0$ ,  $T00 - T05$ , are compared to the corresponding emulator results,  $E00 - E05$ . Training cosmologies,  $M00 - M49$ , are shown in gray. Bottom: Relative errors of the emulator prediction compared to the COLA simulations. For the models with large values for  $f_{R_0}$  ( $T01$  and  $T05$ ) the emulator deviates by up to 5%. The models with  $f_{R_0} < 10^{-5}$  are predicted at sub-percent accuracy (corresponding zoom-in panel shown at the top).

test simulation  $T01$  with  $\log(f_{R_0}) = -4$  is at the very edge of our SLH design used for the training, and the  $T05$  model is also close to the edge of the training design, with  $\log(f_{R_0}) = -4.267$ . By design, we focus more on exploring the modified gravity sector of  $f_{R_0} < 10^{-5}$  that corresponds to smaller boosts in the matter power spectra. We stress that the required accuracy in the estimation of the power spectrum is 1-2 percent [112], down to  $k \sim 1h\text{Mpc}^{-1}$ , which we satisfy for most of the target parameter space.

## B. Comparison with N-body Simulations

Next, we present a comparison of the MG emulator predictions against state-of-the-art N-body simulations for the Hu-Sawicki model. These are the Extended Lensing PHysics using ANalytic ray Tracing ELEPHANT simulations [113], that were performed with a modified version of the RAMSES code, the ECOSMOG module [114, 115]. Power spectra at various redshifts

have been measured for the Hu-Sawicki case of  $n = 1$  and three variations of  $|\bar{f}_{R_0}| = \{10^{-6}, 10^{-5}, 10^{-4}\}$ . We refer to these as F6, F5 and F4, respectively, in the following discussion. The simulations evolved  $1024^3$  dark matter particles, in a simulation volume of  $V_{\text{box}} = (1024h^{-1}\text{Mpc})^3$  and a  $\Lambda\text{CDM}$  cosmology specified by the following parameters:  $\{\Omega_m, \Omega_\Lambda, h, n_s, \sigma_8, \Omega_b\} = \{0.281, 0.719, 0.697, 0.971, 0.82, 0.046\}$ . For each model, five different random realizations are available. More details about these simulations can be found in Ref. [113].

In Fig. 3, we compare the predictions from our emulator to the full N-body simulations from Ref. [113] for the F4, F5 and F6 cases at three different redshifts:  $z = 0$ ,  $z = 0.397$  and  $z = 0.5$ , which span the redshift range in which predicted MG signals are more pronounced. Furthermore, in order to independently illustrate the accuracy of our training set, we show the ratio  $P_{MG}(k)/P_{\Lambda\text{CDM}}(k)$  obtained from COLA simulations that we additionally performed, separately from our design, for these scenarios. COLA is found to recover the simulated ratios at (better than) 1% level of accuracy in the (F6) F5 case for all redshifts, in agreement with previous findings in the literature [62]. For the F4 model, the agreement is still similarly good at  $z = 0$ , but worsens progressively for higher redshifts, with COLA underestimating the predicted deviation. This behavior is most likely attributed to the approximate MG screening implementation [100] used in COLA, which is known to underestimate the ratio particularly in cases that deviate substantially from GR (such as F4) and at high  $z$ . We stress that this tendency is not detrimental, since the deviations typically predicted by cases such as F4 are of substantial magnitude<sup>3</sup>, and effectively ruled out by observations [92, 116]. We do however choose to include larger values of  $f_{R_0}$  in our target range, to enable the exploration of the linearized regime of the Hu-Sawicki MG models. In addition, we also compare a semi-analytical fitting formula provided by Ref. [87] with our emulator. There are two notable differences between our emulator and the fitting formula. First, the fitting formula was trained on a single set of CDM cosmological parameters and a fixed  $n = 1$  whereas our emulator is based on the sampling given in Equations (5) – (9). Second, the  $k$ -range covered by the fitting formula extends to  $k \leq 10h\text{Mpc}^{-1}$ , whereas with our emulator is restricted to  $k \leq 1h\text{Mpc}^{-1}$ .

Our emulator is found to successfully recover the target ratios for F5 and F6 at a very similar level of accuracy as the COLA method, for all three redshifts. The predictions are accurate even for the F4 corner case. All of the above findings are consistent with the levels of accuracy previously found by the accuracy tests shown in Sec. IV A.

We end this section by clarifying that the COLA and full N-body simulations shown in Fig. 3 correspond to

<sup>3</sup> The screening mechanism effectively fails for such large values of  $f_{R_0}$ .

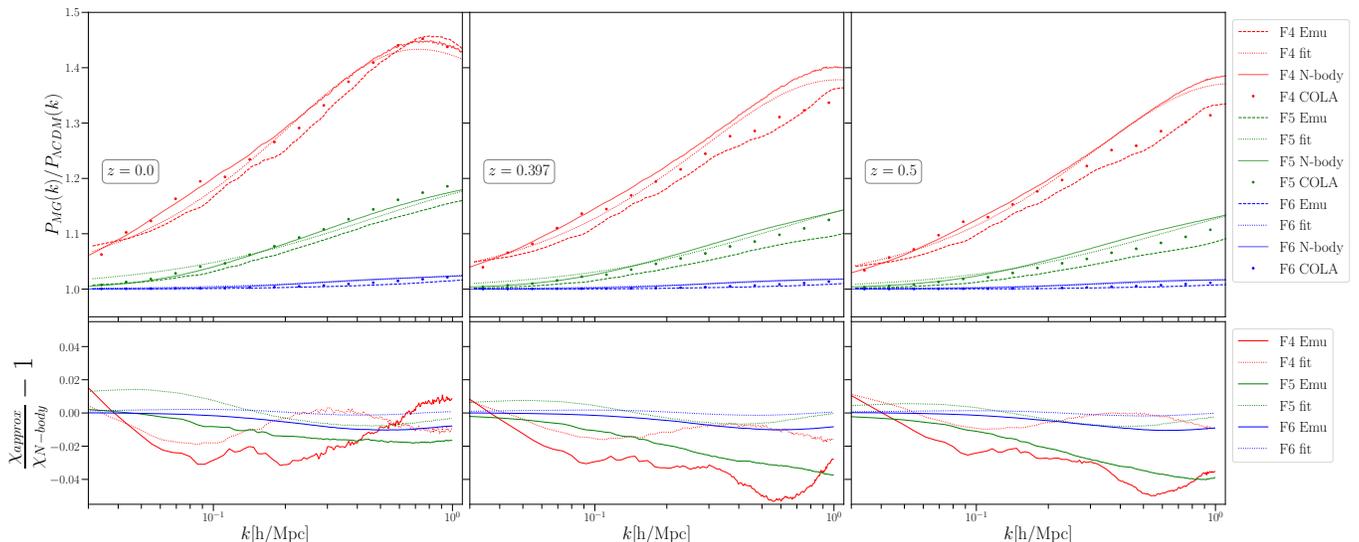


FIG. 3. Comparison of emulator predictions to our corresponding COLA simulations and the N-body simulations of Ref. [113] for the F4 (red), F5 (green) and F6 (blue) models, respectively. Each top panel represents a different redshift:  $z = 0$  (left),  $z = 0.397$  (middle) and  $z = 0.5$  (right). Solid lines are from the three N-body simulations, dashed lines are from the corresponding emulator (with  $z$ -interpolation) output, the dotted lines are the corresponding outputs from the semi-analytical fitting formula given in Ref. [87]

, and the data points are COLA simulations performed for these models. The COLA and N-body runs correspond to a cosmology of  $h = 0.697$  while the emulator was built using  $h = 0.67$ . The ratios of the power spectra are minimally impacted by these different choices. The bottom panels show the relative differences between the fast approximations (our emulator and the fitting formula) and the N-body simulations.

693  $h = 0.697$ , whereas the emulator predictions were gener- 718  
 694 ated from a COLA training set that assumed  $h = 0.67$ , in  
 695 agreement with the Planck constraints [13, 14]. We have 719  
 696 carefully checked and confirmed that this small inconsis- 720  
 697 tency leads to negligible errors in the emulated ratio for 721  
 698 all cases and redshifts of our design. As a result, the di- 722  
 699 rect comparison in Fig. 3 is indeed meaningful, despite 723  
 700 the different underlying values of  $h$  assumed.

## 701 V. EMULATOR PRELIMINARY 718 702 APPLICATIONS

703 We present three preliminary applications for the emu-  
 704 lator developed in this paper. Using the power spectrum 724  
 705 ratio as the summary statistic we first perform a param- 725  
 706 eter sensitivity analysis. Second, we use the emulator 726  
 707 for Fisher forecasting. Finally, results from an MCMC 727  
 708 run for a fiducial cosmology are shown. The evaluation 728  
 709 time for an emulator prediction is less than 0.001 seconds 729  
 710 per computation on an Intel Core i5 Processor, deliver- 730  
 711 ing a massive speed-up over numerical calculation using 731  
 712 COLA, which typically takes about an hour on similar 732  
 713 computational hardware. This is particularly important 733  
 714 for our third application, where our GP emulator is im- 734  
 715 plemented in the MCMC likelihood calculation which re- 735  
 716 quires a very large number of accurate predictions for the 736  
 717 power spectrum ratio. 737

## A. Parameter Sensitivity Analysis

719 In this section we investigate the effect of different  
 720 cosmological parameters on the power spectrum ratio  
 721  $P_{MG}(k)/P_{\Lambda CDM}(k)$  using the emulator. For this study,  
 722 we choose a base model at redshift  $z = 0.0$ . The base  
 723 model is evaluated at parameters shown in Equation (14):

$$\begin{aligned}
 \Omega_m h^2 &= 0.142, \\
 n_s &= 0.967, \\
 \sigma_8 &= 0.816, \\
 \log(f_{R_0}) &= -5, \\
 n &= 1.0.
 \end{aligned} \tag{14}$$

724 We then measure the sensitivity of the power spectrum  
 725 ratio to changes in one cosmological parameter at a time  
 726 while keeping the others at their base values. We stress  
 727 that the MG parameters span a much broader range than  
 728 the  $\Lambda$ CDM parameters and therefore we expect a much  
 729 larger impact on the power spectrum ratio for varying  
 730  $\log(f_{R_0})$  and  $n$ . The results are presented in Fig. 4.

731 Primarily, and in agreement with the literature [86, 95],  
 732 we observe that  $\log(f_{R_0})$  has the highest impact on the  
 733 matter power spectrum ratios, showing up to 40 percent  
 734 variation just around  $0.3h\text{Mpc}^{-1} \lesssim k \lesssim 1h\text{Mpc}^{-1}$  for  
 735 the range  $-6 \leq \log(f_{R_0}) \leq -4$ . Larger  $\log(f_{R_0})$  results  
 736 in enhancement of the power spectrum ratios, due to the  
 737 progressive weakening of the screening mechanism, and

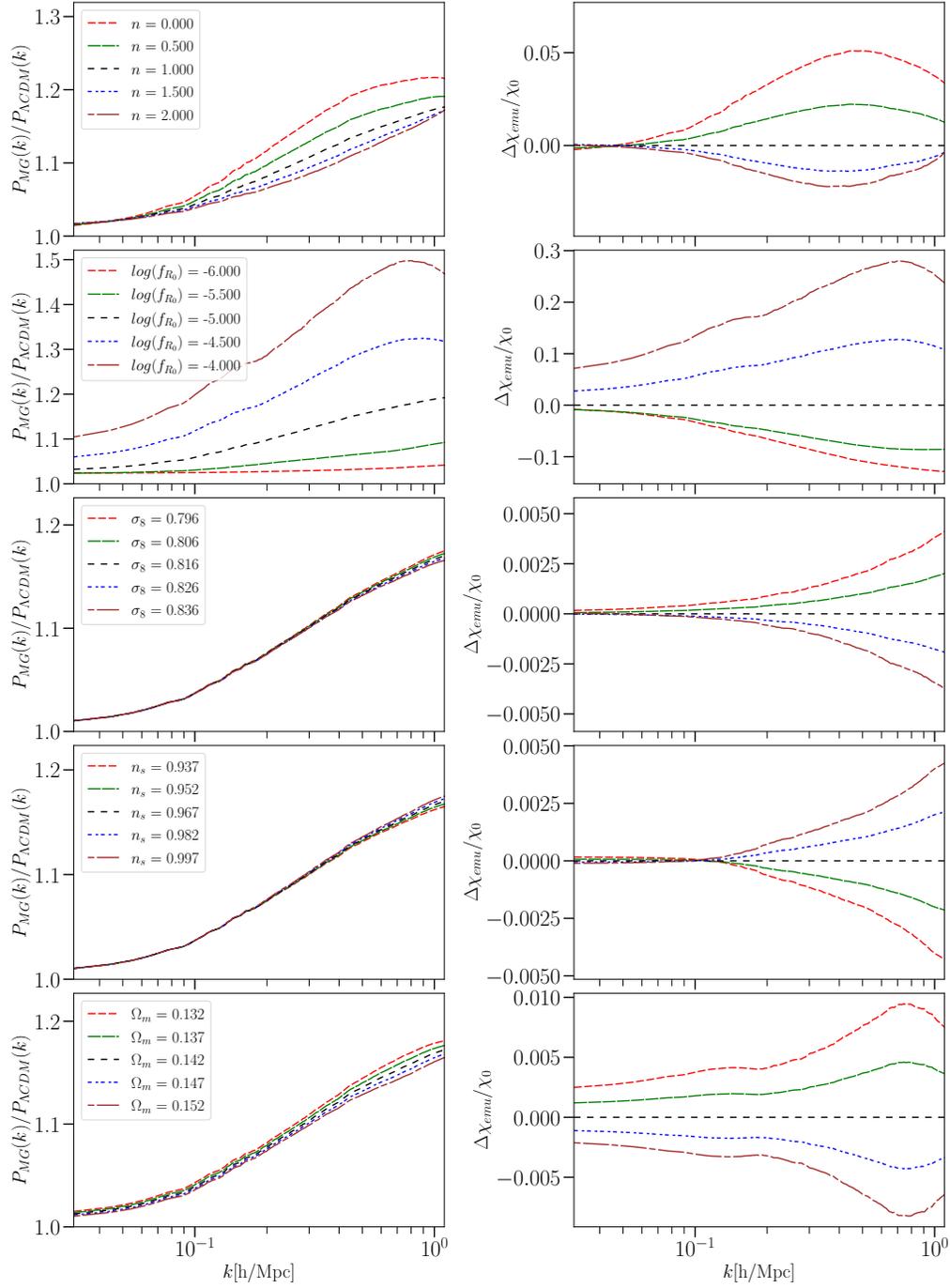


FIG. 4. Results for the sensitivity analysis for the power spectrum ratios using emulator predictions. The impact of five cosmological parameters is investigated. The left panels show the emulator outputs from linearly varying one parameter while keeping the rest at the base cosmology. The right panels show the relative variation of the the power spectrum ratios  $\Delta\chi_{emu}/\chi_0$  with respect to the emulator output  $\chi_0$  at base cosmology parameters listed in Equation (14). From top to bottom the parameter sensitivity analysis with respect to  $n$ ,  $\log(f_{R_0})$ ,  $\sigma_8$ ,  $n_s$  and  $\Omega_m h^2$  is shown respectively. Note that the scales on the  $y$ -axes for the relative variation differ by up to two orders of magnitude. Given the wide range we allowed for  $\log(f_{R_0})$  it is not surprising that its impact is by far the largest on the power spectrum ratio.

738 the increase is monotonous across the full range of test-  
 739 ing cosmologies. The analysis also suggests that with  
 740  $\log(f_{R_0}) > -5$  the modified gravity matter power spec-  
 741 trum  $P_{MG}(k)$  is up to 50 percent higher than  $P_{\Lambda CDM}(k)$ .  
 742 This shows that models in this range are disfavored by  
 743 current data, which is consistent with previous studies  
 744 constraining  $f(R)$  models using available data sets, see  
 745 for example Refs. [92, 116].

746 The second highest contribution to the changes in the  
 747 summary statistic is due to the second Hu-Sawicki MG  
 748 parameter,  $n$ . The variation is under 10% from the base  
 749 cosmology for the range  $0 \leq n \leq 2$ . However, the peak of  
 750 the departure occurs at slightly larger length scales, be-  
 751 tween  $0.1h\text{Mpc}^{-1} \lesssim k \lesssim 0.9h\text{Mpc}^{-1}$ . For  $k \lesssim 1h\text{Mpc}^{-1}$ ,  
 752 larger values of  $n$  cause higher suppression of the mat-  
 753 ter power spectrum ratios. This trend reverses beyond  
 754  $k \gtrsim 1h\text{Mpc}^{-1}$ . Unfortunately, there are currently no N-  
 755 body Hu-Sawicki simulations for  $n \neq 1$  available in the  
 756 literature, and thus a thorough comparison on nonlinear  
 757 scales is not possible. Nevertheless, our observed large-  
 758 scale trend seems to be in qualitative agreement with  
 759 the linear considerations in Ref. [86]. Even though we  
 760 do not expect the behavior of the model to be substan-  
 761 tially different for  $n \neq 1$ , we defer a detailed study of the  
 762 emulator accuracy for such values to future work, when  
 763 corresponding N-body simulations become available.

764 Finally, the relative change of the emulator output  
 765 when varying the  $\Lambda$ CDM parameters is more restricted.  
 766 Both  $\sigma_8$  and  $n_s$  reveal sub-percent variation within their  
 767 respective ranges of  $0.796 \leq \sigma_8 \leq 0.836$  and  $0.937 \leq$   
 768  $n_s \leq 0.997$ . Moreover, both their peak departures from  
 769 the base model occur at  $k \gtrsim 1h\text{Mpc}^{-1}$ , where the accu-  
 770 racy of the training COLA simulations with respect  
 771 to full N-body simulations reduces at higher redshifts.  
 772 Also, the variations of  $\sigma_8$  and  $n_s$  beyond  $k \lesssim 0.1h\text{Mpc}^{-1}$ ,  
 773 are opposite of each other, i.e, increasing  $\sigma_8$  reduces the  
 774  $P_{MG}(k)/P_{\Lambda CDM}(k)$  ratio, whereas  $n_s$  has the opposite  
 775 effect. Variations of the final emulator parameter,  $\Omega_m h^2$ ,  
 776 lead to a monotonic change in the matter power spec-  
 777 trum ratios, where increasing the values from 0.132 to  
 778 0.152 shows a decrease in  $P_{MG}(k)/P_{\Lambda CDM}(k)$ . This re-  
 779 duced sensitivity of the ratio with respect to variations of  
 780 the  $\Lambda$ CDM parameters (relative to the response of MG  
 781 parameters) was also found using the fitting formula ap-  
 782 proach in Ref. [87].

## 783 B. Fisher Forecasting

784 The likelihood  $\mathcal{L}(\chi|\theta)$  is defined as the probability  
 785 distribution function of an observed summary statistic  
 786  $\chi$  for a given model with parameters  $\theta$ . The emula-  
 787 tor output  $\chi_{\text{emu}}(k; \theta) = P_{MG, \text{emu}}(k)/P_{\Lambda CDM, \text{emu}}(k)$  at  
 788 a given redshift itself can be considered as the forward  
 789 model in the computation of the likelihood. In the  
 790 case of the observed power spectrum ratio  $\chi_{\text{obs}}(k) =$   
 791  $P_{MG, \text{obs}}(k)/P_{\Lambda CDM, \text{obs}}(k)$  for a set of cosmological pa-  
 792 rameters  $\theta = \{\Omega_m h^2, \sigma_8, n_s, \log(f_{R_0}), n\}$ , the likelihood

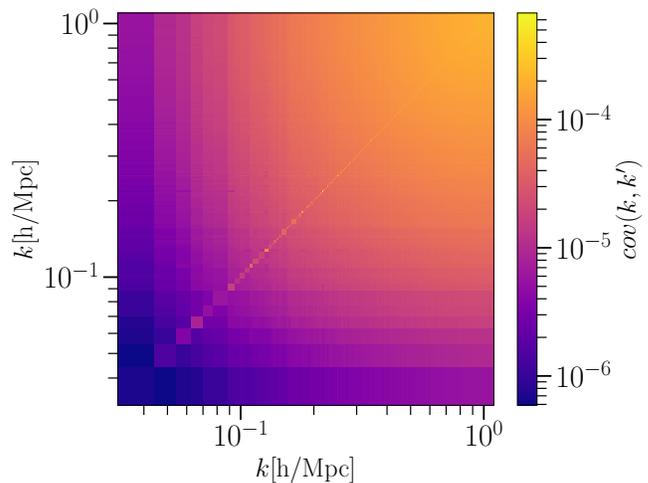


FIG. 5. Covariance matrix for the ratio  $P_{MG}(k)/P_{\Lambda CDM}(k)$  obtained from 2000 COLA realizations for our fiducial cosmology parameters  $\theta_{fid}$  at redshift  $z = 0.02$  as an example. The likelihood obtained using this covariance matrix is used for both Fisher analysis and posterior estimation of the cosmological parameters via MCMC sampling.

793 is computed using Equation (15) assuming it is of a Gaus-  
 794 sian form:

$$\log \mathcal{L}(\chi|\theta) \propto -\frac{1}{2} [\chi_{\text{emu}}(k; \theta) - \chi_{\text{obs}}(k)] \widehat{C_{ij}^{-1}} [\chi_{\text{emu}}(k; \theta) - \chi_{\text{obs}}(k)]^T. \quad (15)$$

795 We construct a mock data set for the power spectrum  
 796 ratios with an associated mean,  $\chi_{\text{obs}}(k)$ , and a covariance  
 797 matrix  $C_{ij}$ , which captures the effects of cosmic variance.  
 798 This data set is computed using 2000 COLA simulation  
 799 realizations run at a fiducial cosmology  $\theta_{fid} \equiv \{\Omega_m h^2 =$   
 800  $0.142, n_s = 0.967, \sigma_8 = 0.816, \log(f_{R_0}) = -5, n = 1.0\}$ ,  
 801 shown in Figure 5. The unbiased estimator for the inverse  
 802 covariance matrix  $\widehat{C_{ij}^{-1}}$  is then computed using Equation  
 803 (16) given by Ref. [117]. This correction accounts for the  
 804 number of COLA simulations used ( $N = 2000$ ) and the  
 805 size of the data vector  $D$ , which depends on our range of  
 806 wavenumbers used in calculating the likelihood:

$$\widehat{C_{ij}^{-1}} = \frac{N - D - 2}{N - 1} C_{ij}^{-1}. \quad (16)$$

807 The box size, mass resolution and other simulation  
 808 specifications for these additional COLA simulations are  
 809 the same as the ones listed in Table I. We choose a single  
 810 redshift of  $z = 0.02$  for this analysis.

811 The Fisher information matrix assesses how well a cos-  
 812 mological parameter can be inferred from a summary  
 813 statistic. It is defined in terms of the likelihood  $\mathcal{L}$  of  
 814 the data in the following equation:

$$F_{ij} = - \left\langle \frac{\partial^2 \log \mathcal{L}}{\partial \theta_i \partial \theta_j} \right\rangle. \quad (17)$$

815 The Fisher matrix can be calculated directly using the  
816 emulator, either using numerical derivatives, or using the  
817 analytical derivatives of Gaussian Processes propagated  
818 through the emulator. We choose the former method  
819 and calculate the second order partial derivatives numerically.  
820 The corresponding confidence ellipses are shown in  
821 Figure 6. The numerical derivatives are evaluated with  
822 multiple step sizes to ensure consistency.

823 The Fisher information obtained from the power spec-  
824 trum ratio analysis reveals correlations between MG  
825 parameters and  $\Lambda$ CDM parameters. We present re-  
826 sults using 4 different wavenumber thresholds ( $k_{max} =$   
827  $0.15h\text{Mpc}^{-1}$ ,  $0.25h\text{Mpc}^{-1}$ ,  $0.5h\text{Mpc}^{-1}$  and  $1.0h\text{Mpc}^{-1}$ )  
828 corresponding to increasing scales of nonlinear growth of  
829 structure. The tightest constraints for forecasts across all  
830 parameters are achieved when including nonlinear scales  
831 up to  $k_{max} = 1.0h\text{Mpc}^{-1}$ , and the constraints weaken  
832 with decreasing nonlinearity. This is expected, given  
833 that including more modes gives us increasingly more in-  
834 formation about the underlying cosmological parameters  
835 (including the MG parameters), resulting in increased  
836 constraining power.

837 It should be noted that the aim of this exploratory  
838 set-up is not to perform a thorough study of forecasted  
839 MG constraints, but rather to highlight the diverse ap-  
840 plications of our emulator. As a result, these constraints  
841 only provide an approximate view. For a more realis-  
842 tic approach, one would need to combine the emulated  
843 ratio with a prediction for  $P_{\Lambda\text{CDM}}(k)$  (e.g. from the  
844 `CosmicEmu`), as well as fold in prescriptions for the galaxy  
845 bias and/or redshift-space distortions [60], in order to ob-  
846 tain a prediction for the observed galaxy power spectrum  
847 in MG (as for example was done in [87]). This step goes  
848 beyond the scope of this paper, but will be studied in  
849 detail in future work. As a consequence, our constraints  
850 are not directly comparable to the ones obtained by the  
851 fitting formula approach in [87].

### 852 C. Parameter Constraints Using MCMC

853 The speed and precision of our emulator enables quick  
854 parameter inference using traditional Bayesian inference  
855 schemes like Markov Chain Monte Carlo (MCMC) meth-  
856 ods. We illustrate the application of such emulator-based  
857 posterior estimation for mock data, the same as shown in  
858 Sec. VB. The Gaussian likelihood is computed via Equa-  
859 tion (15), using the emulator and the mock covariance  
860 matrix shown in Fig. 5 from 2000 COLA realizations  
861 for the fiducial cosmology parameters  $\theta_{fid}$ . Our aim is to  
862 demonstrate the recovery of the original parameter values  
863 within appropriate error margins. In addition, the explo-  
864 ration of the posterior distribution allows us to study the

865 covariance between the parameters that arises from the  
866 data vector and sensitivity of the parameters.

867 We execute two MCMC sampling schemes. First with  
868 fixed values for the  $\Lambda$ CDM parameters at  $\{\Omega_m h^2 =$   
869  $0.142, n_s = 0.967, \sigma_8 = 0.816\}$ , we evaluate the posterior  
870 distributions of the 2 MG parameters. The logarithmic  
871 value for  $f_{R_0}$  is chosen to reduce the dynamical range  
872 of the MCMC sampling, and a flat prior in the range  
873  $-8 \leq \log(f_{R_0}) \leq -4$  is selected. For  $n$  we also use a  
874 flat prior within the limits of our experimental design:  
875  $0 \leq n \leq 4$ . While the choice of priors could be more  
876 stringent, we select such uninformative priors spanning  
877 the entire parameter range of the emulator in order to  
878 avoid obtaining prior-dominated constraints for the MG  
879 parameters. The likelihood  $\mathcal{L}(\chi|\theta)$  of the mock data vec-  
880 tor is computed up to  $k < 1.0h\text{Mpc}^{-1}$ .

881 We utilize an MCMC approach to approximate the  
882 posterior distribution using an affine-invariant ensemble  
883 sampling [118] method implemented in the `emcee`  
884 [119] sampler. An ensemble of 300 walkers or Markov  
885 chains with 3000 evaluations or steps per walker only  
886 takes about 4000 seconds on a single processor, hence  
887 enabling quick explorations of the posterior space of the  
888 parameters of interest. The final constraints obtained  
889 were  $\theta_{MCMC} \equiv \{\log(f_{R_0}) = -5_{-0.04}^{+0.05}, n = 1.18_{-0.20}^{+0.20}\}$ ,  
890 as shown in the top panel of Fig. 7, and a recovery  
891 of parameters within the  $2\text{-}\sigma$  margin of error is found.  
892 While the 2000 realizations for fiducial covariance matrix  
893 have enabled tight parameter constraints via MCMC  
894 sampling compared to the broad priors, overcoming the  
895 offset within  $2\text{-}\sigma$  margin of error from the fiducial targets  
896 may require further reduction in noise. The emulator  
897 outputs at the  $\theta_{fid}$  and  $\theta_{MCMC}$  are matched well with  
898 the  $P_{MG}(k)/P_{\Lambda\text{CDM}}(k)$  ratio of the fiducial cosmology  
899 simulations. Moreover, the direction of the covariance  
900 from the Fisher forecasts in Section VB also matches  
901 with the contours of the posteriors. The consistent re-  
902 sults are shown in the bottom left panel of Fig. 7.

903 In addition, we also sample the combined posterior dis-  
904 tribution of the  $\Lambda$ CDM parameters  $\{\Omega_m h^2, \sigma_8, n_s\}$  and  
905 the  $f(R)$  Hu-Sawicki model parameters  $\{\log(f_{R_0}), n\}$  us-  
906 ing an MCMC approach. The fiducial cosmology  $\theta_{fid}$ ,  
907 the covariance information and the likelihood function re-  
908 main the same, with a  $k$ -range limited to  $k < 1.0h\text{Mpc}^{-1}$   
909 for the computation of the likelihood. The priors are  
910 again chosen to be flat within the full range covered  
911 by the emulator. The corresponding posterior distribu-  
912 tion functions are shown in Fig. 8, along with the tar-  
913 get cosmological parameters corresponding to the mock  
914 data set. The final constraints corresponding to the  
915 MCMC sampling are  $\theta_{MCMC} \equiv \{\Omega_m h^2 = 0.15_{-0.01}^{+0.01},$   
916  $n_s = 0.91_{-0.04}^{+0.06}, \sigma_8 = 0.79_{-0.05}^{+0.05}, \log(f_{R_0}) = -5.05_{-0.05}^{+0.05},$   
917  $n = 1.22_{-0.19}^{+0.25}\}$ .

918 The MCMC sampling of the parameter space is re-  
919 stricted to the parameter range in our SLH design. Es-  
920 pecially for  $\Omega_m h^2$ ,  $\sigma_8$  and  $n_s$ , this results in a partial  
921 coverage of the posterior distribution. This is displayed  
922 in the individual panels of Fig. 8, where the posteri-

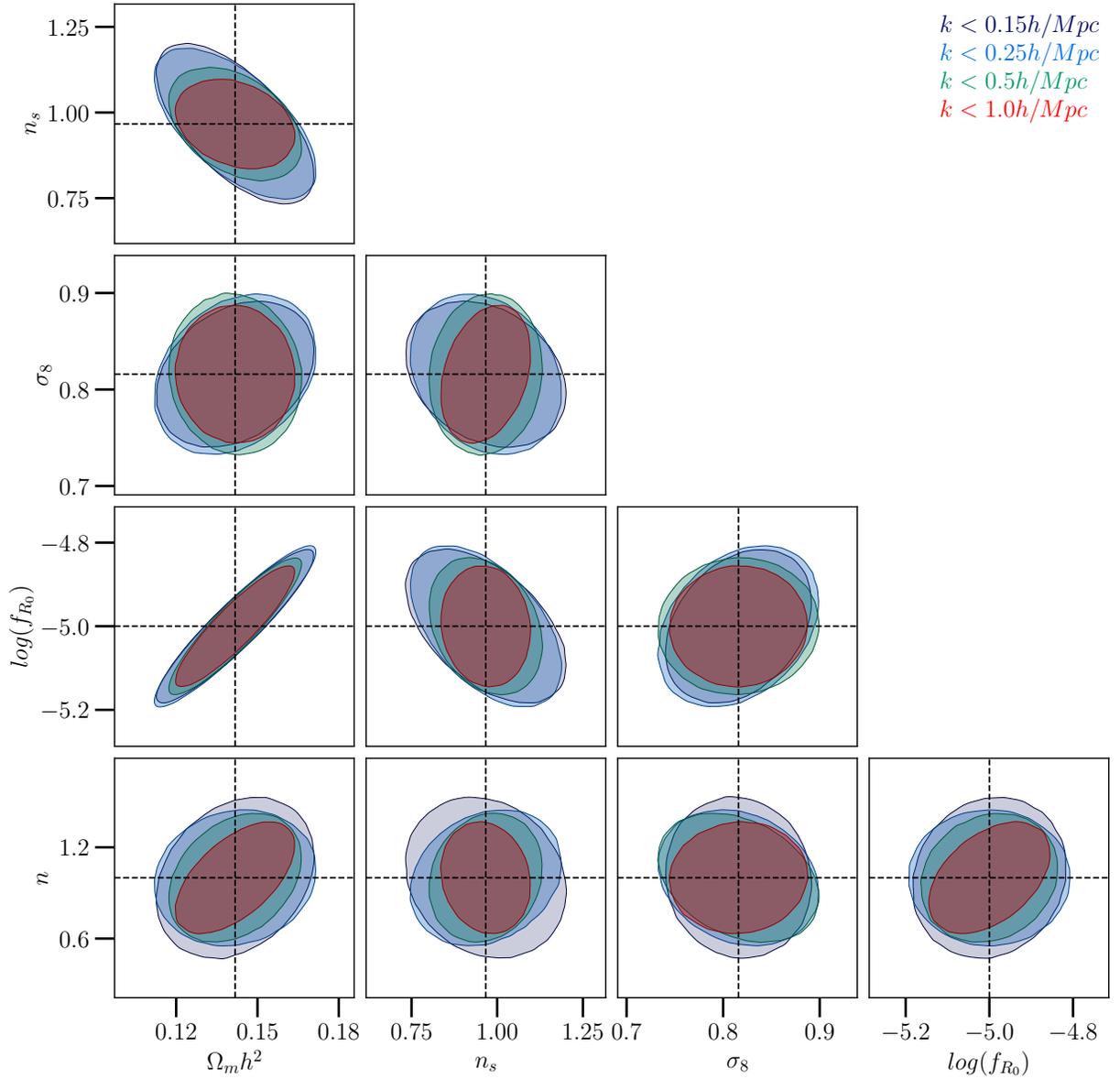


FIG. 6. Confidence ellipses from the Fisher information matrix  $F_{ij}$  for the cosmological parameters considered and using the emulator to provide the power spectrum ratio information. Each panel shows the covariance between the  $\Lambda$ CDM and MG parameters. The thresholds for the wave-numbers used in the computation of the likelihood, i.e.,  $k_{max} = 0.15h\text{Mpc}^{-1}$ ,  $0.25h\text{Mpc}^{-1}$ ,  $0.5h\text{Mpc}^{-1}$  and  $1.0h\text{Mpc}^{-1}$  correspond to the four 2- $\sigma$  level confidence ellipses in each panel. The dashed lines in each panel correspond to the fiducial cosmological parameters  $\theta_{fid}$ .

923 ors are limited to the parameter range of the emulator.  
 924 These constraints would be tightened using a joint anal-  
 925 ysis (with CMB data, for instance). In this study we  
 926 restrict our attention to explorations of the constrain-  
 927 ing power of  $P_{MG}(k)/P_{\Lambda\text{CDM}}(k)$  alone, and reserve com-  
 928 bined analyses for future studies. We additionally note  
 929 that MCMC constraints for the HS model were also pre-  
 930 sented in [89, 120], but using the power spectrum. For  
 931 this reason, our results are not directly comparable with  
 932 the ones in these studies.

933 The 1, 2 and 3- $\sigma$  contours for the MG parameters  
 934  $\{\log(f_{R_0}), n\}$  are within the range of our experimental

935 design, as seen in both Fig. 7 and Fig. 8. We note that the  
 936 constraints obtained from sampling a parameter space of  
 937 just 2 parameters are tighter than those for 5 paramet-  
 938 ers. Posterior estimation restricted to fewer parameters  
 939 removes possible degeneracies, resulting in reduced sam-  
 940 pling space.

941 The original parameters corresponding to the mock  
 942 data vectors are recovered in both the sample MCMC  
 943 runs, indicating that the boost in the matter power spec-  
 944 tra is a powerful statistic for constraining MG param-  
 945 eters, especially when coupled with robust emulators as  
 946 presented in this work. In both posterior approximations,

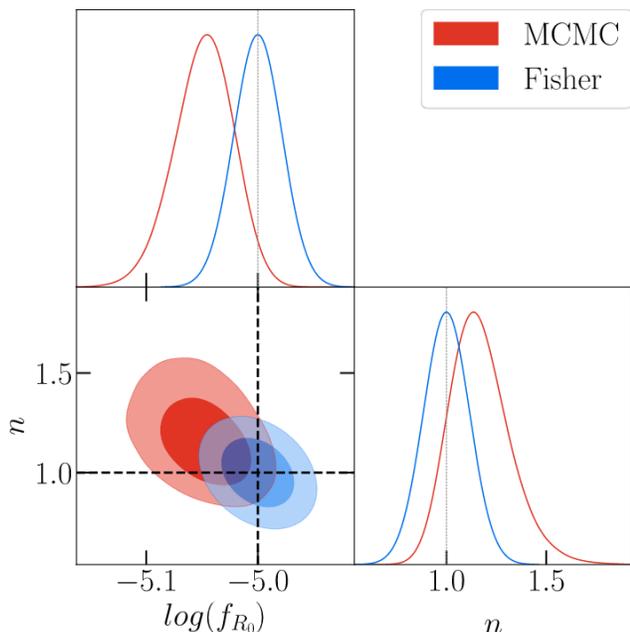


FIG. 7. Bayesian posterior distribution for  $\{\log(f_{R_0}), n\}$  obtained using MCMC sampling. The data vector, emulator output and likelihood computation are carried out for wavenumbers  $k < 1.0h\text{Mpc}^{-1}$ . The two shades of red correspond to 1-, 2- $\sigma$  confidence intervals of the posterior. Dotted lines are the target cosmologies of the mock data,  $\log(f_{R_0}) = -5$  and  $n = 1$ . The constraints are obtained from uniform priors in the ranges  $-8 \leq \log(f_{R_0}) \leq -4$  and  $0 \leq n \leq 4$ . The blue contours are the 1- and 2- $\sigma$  confidence ellipses from the Fisher information constraints for the same  $k$ -range at the fiducial cosmology, showing the consistency between the two applications in space and direction of correlation.

the chosen prior probability distributions are highly uninformative, i.e., they are uniform with coverage of the entire training limits. Posterior contours in Figure 7 display a shift from the fiducial values, and a partial coverage of posterior distribution is seen in Figure 8. These constraints on the cosmological parameters would be improved either using a tomographic or multi-probe analysis, along with more realistic data vectors and covariance matrices. We reserve these for a future study of modeling cosmological observables and associated forecasting in MG scenario.

## VI. CONCLUSIONS

In this paper, we present an emulator for efficiently predicting the enhancements in the nonlinear matter power spectrum due to beyond-GR effects. This emulator is based on the  $f(R)$  Hu-Sawicki model, a MG candidate prioritized for further studies in near-future Stage-IV surveys such as the LSST and Euclid. We aim at simplifying the tasks of model selection and cosmological parameter inference by the use of fast and robust generation of

the power spectrum ratio  $P_{MG}(k)/P_{\Lambda\text{CDM}}(k)$ . The emulator provides estimations across the redshift range of  $0 < z < 49$ , for a combination of cosmological parameters  $\{\Omega_m h^2, \sigma_8, n_s, \log(f_{R_0}), n\}$ . This way, we enable the full exploration of the parameter space that defines the Hu-Sawicki model.

Our emulator is based on simulations produced by the efficient COLA method, which effectively captures the chameleon screening mechanism through a phenomenological thin-shell factor attached to the scalar field Klein-Gordon equation. The matter power spectrum ratios extracted are computed by running two consistent COLA simulations at each training point – one for MG and the other for the corresponding  $\Lambda\text{CDM}$  scenario, reducing the effect of cosmic variance while at the same time highlighting the effects of MG. Our fully trained emulator is validated on additional cosmologies within our target parameter space and is found to achieve sub-percent levels of accuracy for models with  $f_{R_0} < 10^{-5}$  and up to 5% agreement when  $f_{R_0} > 10^{-5}$ . The computation time is less than 0.001 seconds, delivering thus a massive speed-up by 6 orders of magnitude compared to the COLA simulations.

In order to explore and validate the diverse capabilities of our emulator, we further proceed to utilize its predictions for three preliminary applications. First, we perform a sensitivity study of the target summary statistic with respect to the variation of the five cosmological parameters. We find that the power spectrum ratio exhibits the highest sensitivity for the MG parameter  $\log(f_{R_0})$  followed by the  $n$  parameter, in agreement with previous studies [86, 95]. Next, we produce constraints around a fiducial cosmology using Fisher forecasting as well as MCMC parameter inference. The confidence contours obtained are consistent between the two methods and also consistent with the corresponding analytical expressions. The emulated ratio is thus found to enable accurate constraints for both MG parameters as well as the values of the background  $\Lambda\text{CDM}$  cosmological parameters.

We conservatively limit the use of the emulator to  $k \leq 1.0h\text{Mpc}^{-1}$  throughout the analysis of this paper. Our tests shows that the COLA prescription agrees with available N-body simulations within a relative error of 5% up to  $k \sim 1.0h\text{Mpc}^{-1}$ , and hence we advocate the use of this emulator only up to this limit.

We also advise the reader to exercise caution in extrapolating the emulator beyond the limits of cosmological parameters and redshifts used in the experimental design. Gaussian Processes, like any interpolation schemes, may give estimates with large extrapolation uncertainties beyond the training range. We note again that our tests on additional COLA simulations show that models with  $\log(f_{R_0}) < -5$  agree within 1%, while the estimation error rises up to 5% for larger values of  $\log(f_{R_0})$ . We also note that the emulator is trained on one realization per cosmology, with just 50 training points. With a large training sample with better sampling and larger

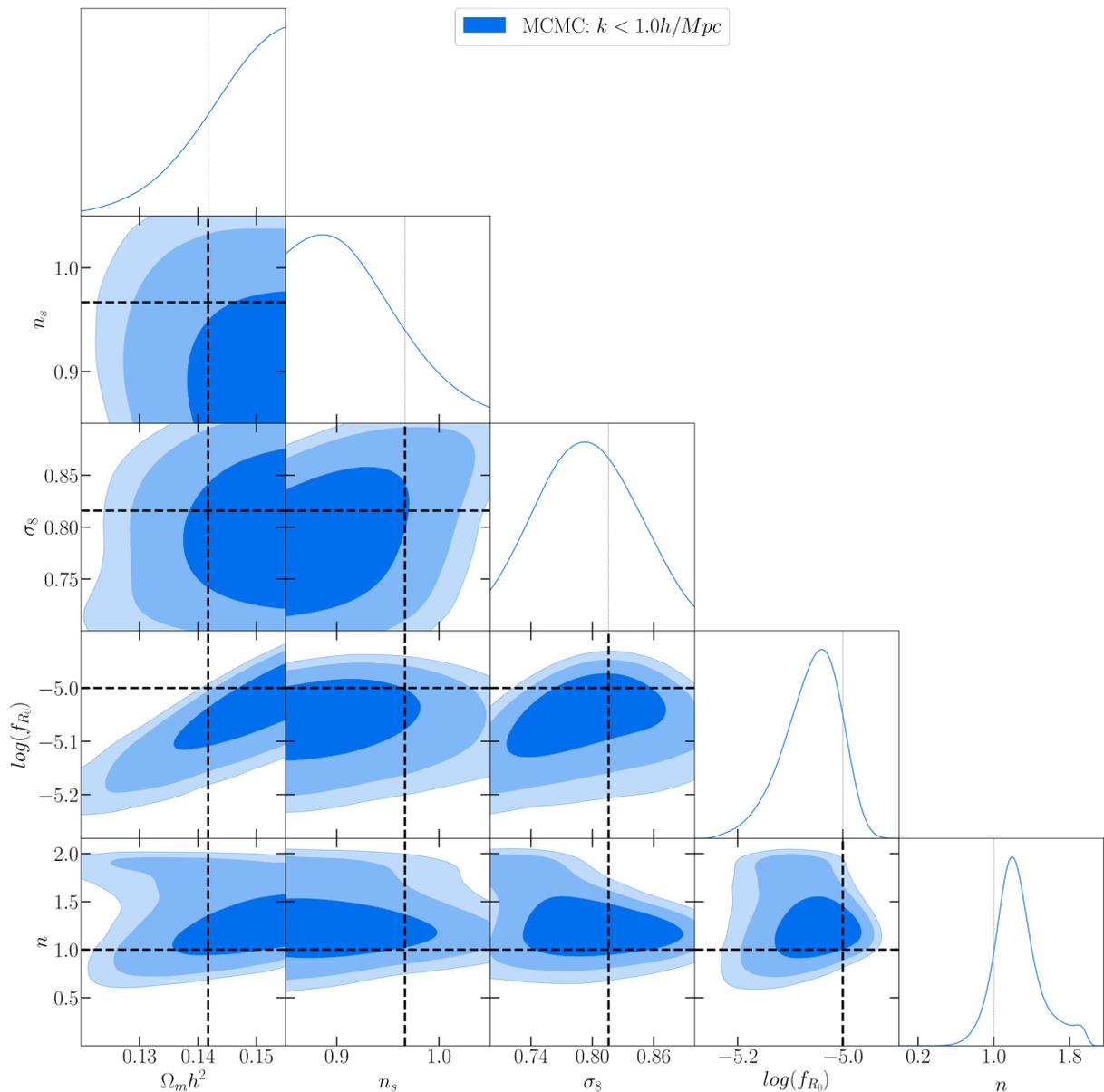


FIG. 8. Posterior distribution evaluated from an MCMC sampling for five cosmological parameters. The data vector, emulator output and likelihood function are computed for wave-numbers  $k < 1.0h\text{Mpc}^{-1}$ . The three shades of blue correspond to 1-, 2- and 3- $\sigma$  confidence intervals. Dotted lines are the target cosmological parameters of the mock data set  $\theta_{fid}$ . It is very satisfactory to observe that the target cosmological parameters fit well within the 2- $\sigma$  confidence intervals, despite the relatively limited constraining power of the ratio of power spectra when used with no additional cosmological information.

1025 number of realizations per cosmology, the relative error  
 1026 with respect to COLA simulations is naturally expected  
 1027 to reduce.

1028 In addition to enabling an efficient exploration of the  
 1029 deviations predicted by MG, our emulator also serves as a  
 1030 stepping stone to allow a broad portfolio of future appli-  
 1031 cations. Through a simple multiplication by the  $\Lambda\text{CDM}$   
 1032 power spectrum (from emulators like `CosmicEmu`), the  
 1033 emulated power spectrum ratio can straightforwardly  
 1034 provide a prediction for the MG nonlinear matter power  
 1035 spectrum itself. The latter can then also be utilized to

1036 incorporate the effects of galaxy bias and Redshift Space  
 1037 Distortions (RSD) in MG (for example as in Ref. [60]),  
 1038 which are crucial for comparing with observations, or to  
 1039 enable obtaining MG constraints from weak lensing cos-  
 1040 mic shear measurements. Such predictions should how-  
 1041 ever take into account the accuracy and sensitivity of the  
 1042 estimators at corresponding length scales, and we reserve  
 1043 this for future studies. Furthermore, the emulator will be  
 1044 a useful standardized routine to be included in the Core

1045 Cosmology Library (CCL<sup>4</sup>, [121]) in order to calculate 1095  
 1046 basic cosmological observables, specifically for Rubin Ob-  
 1047 servatory LSST analyses. We also intend in a follow-up 1096  
 1048 work to employ the emulator in providing forecasts using 1097  
 1049 a detailed joint probes cosmological parameters analysis. 1098  
 1050 Last but not least, we plan to expand our emulator’s ca- 1099  
 1051 pabilities in order to incorporate the effects of massive 1100  
 1052 neutrinos, and also to support the more general class of 1101  
 1053 Horndeski MG models prioritized by our collaboration. 1102  
 1054 The necessary modifications to achieve these steps with 1103  
 1055 the efficient COLA approach are already underway. The  
 1056 combined outcome of these efforts will be a diverse set of  
 1057 tools that will allow efficient and reliable explorations of  
 1058 the broad spectrum of beyond- $w(z)$ CDM candidates.

1059 It is worth emphasizing the multitude of ways in which  
 1060 our work expands upon the previous ones in the litera-  
 1061 ture. While the matter power spectrum ratio in the Hu-  
 1062 Sawicki scenario has already been modeled using fitting 1104  
 1063 formulas or semi-analytical approaches [87–89], our em- 1105  
 1064 ulator is the first predictive tool purely based on numer- 1106  
 1065 ical simulations. Not having to rely on a single functional 1107  
 1066 form of the modeled observable, emulators are guaran- 1108  
 1067 teed to maintain consistent levels of accuracy in their pre- 1109  
 1068 dictions across the full target parameter space. Fitting 1110  
 1069 formulas, on the other hand, may have reduced accuracy 1111  
 1070 outside the particular parameter choices used for their 1112  
 1071 calibration, introducing unknown systematic biases to 1113  
 1072 their predictions, even in the less complicated extension 1114  
 1073 of  $w$ CDM cosmologies [65, 68, 69]. Furthermore, while 1115  
 1074 previous approaches focused their attention on variations 1116  
 1075 of only one the two MG parameters of the Hu-Sawicki se- 1117  
 1076 nario, our emulator spans the full 2-dimensional param- 1118  
 1077 eter space of the model, being the first one of its kind in 1119  
 1078 that regard. Last but not least, given the ever increasing 1120  
 1079 interest in testing theories of gravity with cosmological 1121  
 1080 surveys, a wide range of complementary predictive tools 1122  
 1081 available in the community is very desirable. In order to 1123  
 1082 contrast different methods, we compared our predictions 1124  
 1083 against the ones made by the fitting formula approach 1125  
 1084 of Ref. [87], finding good agreement over the parameter 1126  
 1085 and  $k$ -range that can be compared.

1086 In this decade, precise cosmological observations 1129  
 1087 will offer a unique opportunity to constrain beyond- 1130  
 1088  $w(z)$ CDM models at an unprecedented level of accu- 1131  
 1089 racy. Emulators like the one developed in this work 1132  
 1090 will be essential and necessary to perform cosmological 1133  
 1091 analyses with accurate and fast theoretical predictions in 1134  
 1092 the nonlinear regime, and to take full advantage of the 1135  
 1093 formidable data expected from Rubin Observatory LSST, 1136  
 1094 DESI, Euclid, SPHEREx and Roman Space Telescope. 1137

## Appendix A: Savitzky-Golay smoothing

1104 The Savitzky-Golay smoothing filter [107, 108] per-  
 1105 forms convolution operations on adjacent data points  
 1106 with a polynomial function, which gives us the effect  
 1107 of smoothing the input dataset. The window size and  
 1108 the order of the polynomial are the two parameters that  
 1109 specify the smoothing operation. Equation (A1) shows  
 1110 the value of  $j$ -th bin of the smoothed power spectrum  
 1111 ratio  $\chi(k)$ :

$$\chi(k_j) = \sum_{i=\frac{1-m}{2}}^{\frac{m-1}{2}} C_i \frac{P_{MG}(k_{j+i})}{P_{\Lambda\text{CDM}}(k_{j+i})}. \quad (\text{A1})$$

1104 The individual convolution coefficients  $C_i$  are defined  
 1105 by the analytical expression given in Ref. [107]. Within  
 1106 every window, a polynomial (of order  $p$ ) is fitted, which  
 1107 provides a smoothing effect of the input dataset. The  
 1108 window size  $m$  is the number of data points chosen for  
 1109 individual regression.

1110 The tuning of the two free parameters  $m$  and  $p$  de-  
 1111 pends on the largely on the type of data and the desired  
 1112 level of smoothing. These parameters are hand-tuned for  
 1113 smoothing the power spectrum ratios, and checked for  
 1114 consistency with various choices of smoothing filters and  
 1115 window sizes. As the ratio of window width to polyno-  
 1116 mial order,  $m/p$  increases the amount of smoothing in-  
 1117 creases. First, the window width was appropriately tuned  
 1118 to be effective against the noise and is set to be  $m = 51$   
 1119 points. For this window width, a third order polyno-  
 1120 mial ( $p = 3$ ) is fitted. A polynomial of order  $p > 3$  would  
 1121 closely follow the undesired noise resulting from the single  
 1122 realizations of the COLA simulations. For a given poly-  
 1123 nomial order, decreasing the window length has a similar  
 1124 effect, i.e., while the bias decreases (the smoothing func-  
 1125 tion closely follows the raw data power spectrum ratios  
 1126 from the COLA simulations), the estimation variance in-  
 1127 creases, resulting in an over-fitted smoothing function.

1128 Smoothing near the boundaries requires additional  
 1129 considerations. The data points at the edges cannot be  
 1130 placed at the center of a symmetric window, hence the  
 1131 Equation (A1) is applied for  $\frac{m-1}{2} \leq j \leq n_{bins} - \frac{m-1}{2}$   
 1132 only. We use a separate treatment for smoothing at the  
 1133 boundaries, where the polynomial fitted to the windows  
 1134 near the edges of the data is used to evaluate the first and  
 1135 the last  $m/2$  smoothed outputs of  $\chi(k_j)$ . The effect due  
 1136 to the edge effects is less significant at low- $k$  boundary  
 1137 (i.e.,  $k < 0.17hMpc^{-1}$ ) since the raw  $P_{MG}(k)/P_{\Lambda\text{CDM}}(k)$   
 1138 is less noisy. On the higher end, this near-boundary ef-  
 1139 fects smoothing at  $k > 2.35hMpc^{-1}$ . Since our emulator  
 1140 outputs are restricted to  $k \leq 1hMpc^{-1}$ , this does not  
 1141 effect our estimations directly. However, the consistency  
 1142 of the smoothing results across all the 213 bins (up-to  
 1143  $k = 3.5hMpc^{-1}$ ) is considered whilst tuning the free-  
 1144 parameters.

<sup>4</sup> <https://github.com/LSSTDESC/CCL>

## Appendix B: Gaussian Processes

A parametric regression task [122] involves an estimation of finite number model parameters that fit the data. For  $n$  training targets  $\{y_1, \dots, y_n\}$  at training locations  $\{x_1, \dots, x_n\}$ , one may define a polynomial regression relationship and estimate the finite number of polynomial coefficients. With a frequentist approach, point estimates of these parameters can be estimated. Alternatively, a Bayesian approach treats these model parameters as probability distributions which are to be inferred using the training points. With these either a point estimation or distribution of a test target  $y_*$  can be made at a new location  $x_*$ .

In contrast, Gaussian process [109] regression is a non-parametric approach i.e., one finds a distribution of possible functions  $f(x)$  that are consistent with observed data. GPs are remarkably good Bayesian tools that perform regression tasks with associated uncertainties. Although the inference is fast, computational cost of GP regression can be very expensive and grows cubically with the training set size and dimension. Due to this constraint, dimensionality reduction is usually performed on the training data, as is the case with our approach of building the emulator. We employ a data reduction technique called Principal Component Analysis (PCA) to reduce computational expenses during GP training. With a PCA decomposition (in Equation 12), the bases  $\phi_i(k)$  are independent of the cosmological parameters, and only the weights  $w_i(\theta)$  are used in GP interpolation. Thus the training locations are the set of parameters  $\theta$  (tabulated in Appendix C) where 50 COLA simulations are computed, and the training targets are the corresponding weights  $w_i(\theta)$ .

With GP, we first assume that the joint probability distribution  $p(f(x_1), \dots, f(x_n))$  are jointly Gaussian with mean  $\mu(x)$  and covariance  $\mathbf{K}$ , where the elements  $\mathbf{K}_{ij} = k(x_i, x_j)$  with  $k(x_i, x_j)$  being the covariance kernel. For simplicity, the GP prior can be defined using a zero mean and covariance as  $p(f(x)) = GP(0, \mathbf{K})$ . In our emulator construction, the weights are essentially sampled from this distribution, i.e.,  $w_i(\theta) \sim GP(0, \mathbf{K})$ , where the covariance  $\mathbf{K} = k(\theta, \theta')$ .

The kernel function  $k$  is usually selected depending on how smooth the function is expected to be. One popular choice is the squared exponential or the Radial basis function kernel:  $k_{RBF}(x, x') = \sigma^2 \exp\left(-\frac{(x-x')^2}{2\theta^2}\right)$  with hyperparameters  $(\sigma^2, \theta)$  corresponding to the process variance and lengthscale, respectively. These hyperparameters can be inferred based on the maximum likelihood or other more Bayesian techniques. Once optimized, the GP model has learned a distribution of functions that fits the training data.

Using the GP assumption that our data can be represented as a sample from a multivariate Gaussian distribution, the above definition can also be extended to a hold-out target  $y_*$  at a new location  $x_*$  in terms of the

trained covariance  $\mathbf{K}$ . The joint probability of training targets  $y$  and test targets  $y_*$  shown on Equation (B1) is also a Gaussian Process:

$$p(y, y_*) = \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K} & \mathbf{K}^T \\ \mathbf{K}_* & \mathbf{K}_{**} \end{bmatrix}\right). \quad (\text{B1})$$

The covariance  $\mathbf{K}$  is obtained by  $\mathbf{K}_{ij} = k(x_i, x_j)$  is the matrix we get by applying the trained kernel function to our training values, i.e., the similarity of each observed  $x$  to each other observed  $x$ .  $\mathbf{K}_* = k(x_i, x_*)$  shows the similarity of the training values to the test value whose output values were trying to estimate.  $\mathbf{K}_{**} = k(x_*, x_*)$  gives the similarity of the test values to each other.

The desired posterior of our prediction is the conditional probability distribution the test target  $p(y_*|y)$ . This is finally derived using the joint probability distribution in Equation (B1) using marginalization:

$$p(y_*|y) = \frac{p(y, y_*)}{p(y)} = \mathcal{N}(\mathbf{K}_* \mathbf{K}^{-1} y, \mathbf{K}_{**} - \mathbf{K}_* \mathbf{K}^{-1} \mathbf{K}_*^T). \quad (\text{B2})$$

Hence the mean of our estimation at new test location is simply given by  $\mu(y_*) = (\mathbf{K}_* \mathbf{K}^{-1} y)$ , and the uncertainty of this prediction is  $\sigma(y_*) = (\mathbf{K}_{**} - \mathbf{K}_* \mathbf{K}^{-1} \mathbf{K}_*^T)$ . In the prediction phase of our emulator, this mean and variance for the predictive weights  $w_{i_*}(\theta_*)$  are calculated for any new set of cosmological parameters  $\theta_*$ . Since the form of  $\mathbf{K}$  is already determined from training points using hyperparameter optimization, the GP prediction is simply matrix operations. This makes GP inference extremely fast and easily parallelizable.

## Appendix C: Parameters of COLA simulation

Table of all parameters of each COLA simulation.

## ACKNOWLEDGMENTS

1227  
 1228 This paper has undergone internal review by the LSST  
 1229 Dark Energy Science Collaboration. The internal re-  
 1230 viewers were Tessa Baker, Francois Lanusse and Danielle  
 1231 Leonard. The authors would like to thank them for useful  
 1232 feedbacks.

1233 The two lead authors, NR and GV have contributed  
 1234 equally to this work. NR was involved in development  
 1235 and applications of the emulator, and contributed to the  
 1236 text of the paper. GV was involved in providing the idea  
 1237 for this paper, producing the COLA and N-body MG  
 1238 simulations and contributed to the writing of the text.  
 1239 MI was involved in developing the idea for the paper,  
 1240 the MG part of the design, contributed to the analysis  
 1241 of Fisher and MCMC results, mentored the project, and  
 1242 contributed to the text of the paper. KH was involved in  
 1243 developing the idea for the paper, provided the design,  
 1244 and contributed to the text of paper.

1245 LSST DESC acknowledges ongoing support from the  
 1246 Institut National de Physique Nucléaire et de Physique  
 1247 des Particules in France; the Science & Technology Fa-  
 1248 cilities Council in the United Kingdom; and the Depart-  
 1249 ment of Energy, the National Science Foundation, and  
 1250 the LSST Corporation in the United States. LSST DESC  
 1251 uses the resources of the IN2P3 / CNRS Computing Cen-  
 1252 ter (CC-IN2P3–Lyon/Villeurbanne - France) funded by  
 1253 the Centre National de la Recherche Scientifique; the  
 1254 Univ. Savoie Mont Blanc - CNRS/IN2P3 MUST com-  
 1255 puting center; the National Energy Research Scientific  
 1256 Computing Center, a DOE Office of Science User Fa-  
 1257 cility supported by the Office of Science of the U.S.  
 1258 Department of Energy under contract No. DE-AC02-  
 1259 05CH11231; STFC DiRAC HPC Facilities, funded by UK  
 1260 BIS National E-infrastructure capital grants; and the UK  
 1261 particle physics grid, supported by the GridPP Collab-  
 1262 oration. This work was performed in part under DOE  
 1263 contract DE-AC02-76SF00515.

1264 Argonne National Laboratory’s work was supported  
 1265 under the U.S. Department of Energy contract DE-  
 1266 AC02-06CH11357. GV recognizes financial support  
 1267 by DoE grant DE-SC0011838, NASA ATP grants  
 1268 NNX14AH53G and 80NSSC18K0695, NASA ROSES  
 1269 grant 12-EUCLID12-0004 and funding related to the  
 1270 WFIRST Science Investigation Team. MI acknowledges  
 1271 that this material is based upon work supported in part  
 1272 by the Department of Energy, Office of Science, under  
 1273 Award Number DE-SC0019206.

1274 We would like to thank Salman Habib and Eske Ped-  
 1275 ersen for useful discussions related to this project. We  
 1276 also would like to thank Baojiu Li, for kindly providing  
 1277 us with the MG N-body simulation data. GV would also  
 1278 like to thank Rachel Bean and Hans Winther for use-  
 1279 ful discussions related to this project. NR would like to  
 1280 thank Andrew Hearin for assistance with Python pack-  
 1281 aging.

1282 The emulator is built using the following Python pack-  
 1283 ages: `GPflow` [123], `TensorFlow` [124] and `Scikit-learn`

1284 [125]. The analyses performed in this paper utilize the  
 1285 following: `Numpy` and `Scipy` [126], `Matplotlib` [127],  
 1286 `emcee` [119] and `GetDist` [128]. The final emulator is pro-  
 1287 vided at <https://github.com/LSSTDESC/mgemu> [129].

TABLE III. Cosmological parameters of the all the COLA simulations in the suite. 50 training (M00-M49) cosmologies are tabulated.

Model	$\Omega_m h^2$	$n_s$	$\sigma_8$	$\log(f_{R_0})$	$n$
M00	0.142	1.038	0.818	-6.367	1.878
M01	0.152	0.911	0.884	-7.102	2.286
M02	0.154	1.034	0.778	-6.612	0.816
M03	0.135	0.891	0.827	-4.245	1.061
M04	0.141	0.952	0.724	-4.980	1.224
M05	0.149	0.964	0.896	-4.490	2.041
M06	0.146	0.928	0.769	-7.184	1.633
M07	0.139	0.977	0.851	-7.265	0.327
M08	0.124	0.960	0.765	-4.327	3.429
M09	0.151	0.874	0.757	-6.939	1.388
M10	0.138	1.030	0.892	-5.878	3.347
M11	0.146	0.956	0.814	-4.408	0.082
M12	0.143	0.981	0.871	-4.163	3.592
M13	0.144	0.854	0.741	-6.694	0.898
M14	0.141	0.887	0.847	-6.857	4.000
M15	0.139	0.850	0.806	-6.286	2.449
M16	0.150	1.042	0.720	-5.551	2.531
M17	0.154	0.895	0.863	-7.347	1.796
M18	0.147	1.021	0.712	-7.918	3.837
M19	0.131	0.903	0.700	-5.224	3.510
M20	0.127	0.985	0.761	-5.959	0.735
M21	0.130	1.017	0.810	-7.429	1.306
M22	0.120	0.932	0.867	-6.531	0.980
M23	0.122	0.907	0.798	-4.000	0.245
M24	0.149	1.001	0.855	-6.204	1.143
M25	0.126	0.899	0.745	-5.796	2.857
M26	0.153	0.993	0.802	-8.000	3.755
M27	0.155	0.968	0.733	-5.469	3.020
M28	0.145	0.883	0.790	-4.571	2.694
M29	0.148	0.915	0.839	-6.041	3.265
M30	0.144	0.997	0.900	-6.776	0.490
M31	0.128	0.879	0.888	-4.082	0.163
M32	0.121	1.005	0.737	-4.653	2.204
M33	0.125	0.858	0.880	-6.449	1.469
M34	0.136	1.050	0.794	-5.714	1.551
M35	0.134	1.013	0.753	-5.143	0.000
M36	0.131	1.046	0.859	-5.306	3.102
M37	0.132	0.919	0.729	-7.837	0.408
M38	0.129	0.944	0.786	-7.592	3.918
M39	0.137	0.870	0.708	-6.122	0.653
M40	0.124	1.026	0.843	-5.061	2.612
M41	0.151	0.940	0.835	-7.673	0.571
M42	0.136	0.923	0.749	-4.735	3.673
M43	0.129	0.972	0.831	-4.816	2.367
M44	0.126	0.936	0.704	-7.510	1.959
M45	0.134	0.948	0.876	-7.020	2.776
M46	0.140	1.009	0.773	-7.755	2.939
M47	0.121	0.866	0.822	-5.388	3.184
M48	0.123	0.989	0.716	-4.898	1.714
M49	0.133	0.862	0.782	-5.633	2.122

- [1] P. A. Abell et al. (LSST Science Collaborations, LSST Project), (2009), arXiv:0912.0201 [astro-ph.IM].
- [2] A. Abate et al. (LSST Dark Energy Science), (2012), arXiv:1211.0310 [astro-ph.CO].
- [3] M. Levi et al. (DESI collaboration), (2013), arXiv:1308.0847 [astro-ph.CO].
- [4] R. Laureijs et al. (EUCLID Collaboration), (2011), arXiv:1110.3193 [astro-ph.CO].
- [5] D. Spergel, N. Gehrels, J. Breckinridge, M. Donahue, A. Dressler, et al., (2013), arXiv:1305.5422 [astro-ph.IM].
- [6] O. Dor et al., (2014), arXiv:1412.4872 [astro-ph.CO].
- [7] S. Perlmutter et al. (Supernova Cosmology Project), *Astrophys. J.* **517**, 565 (1999), arXiv:astro-ph/9812133 [astro-ph].
- [8] A. G. Riess et al. (Supernova Search Team), *Astrophys. J.* **607**, 665 (2004), arXiv:astro-ph/0402512 [astro-ph].
- [9] D. J. Eisenstein et al. (SDSS Collaboration), *Astrophys. J.* **633**, 560 (2005), arXiv:astro-ph/0501171 [astro-ph].
- [10] W. J. Percival et al., *Monthly Notices of the Royal Astronomical Society* **381**, 1053 (2007), arXiv:0705.3323 [astro-ph].
- [11] W. J. Percival et al., (2009), arXiv:0907.1660 [astro-ph.CO].
- [12] E. A. Kazin, J. Koda, C. Blake, and N. Padmanabhan, (2014), arXiv:1401.0358 [astro-ph.CO].
- [13] P. Ade et al. (Planck Collaboration), (2013), arXiv:1303.5076 [astro-ph.CO].
- [14] P. A. R. Ade et al. (Planck Collaboration), *Astron. Astrophys.* **594**, A13 (2016), arXiv:1502.01589 [astro-ph.CO].
- [15] S. Weinberg, *Rev. Mod. Phys.* **61**, 1 (1989).
- [16] S. M. Carroll, *Living Reviews in Relativity* **4**, 1 (2001), arXiv:astro-ph/0004075 [astro-ph].
- [17] G. Efstathiou, *Monthly Notices of the Royal Astronomical Society* **440**, 1138 (2014), <https://academic.oup.com/mnras/article-pdf/440/2/1138/18498204/stu278.pdf>.
- [18] A. G. Riess, S. Casertano, W. Yuan, L. M. Macri, and D. Scolnic, *Astrophys. J.* **876**, 85 (2019), arXiv:1903.07603 [astro-ph.CO].
- [19] B. R. Zhang, M. J. Childress, T. M. Davis, N. V. Karpenka, C. Lidman, B. P. Schmidt, and M. Smith, *Monthly Notices of the Royal Astronomical Society* **471**, 2254 (2017), <https://academic.oup.com/mnras/article-pdf/471/2/2254/19491062/stx1600.pdf>.
- [20] L. Lombriser, *Physics Letters B* **803**, 135303 (2020).
- [21] C. Heymans et al., *Monthly Notices of the Royal Astronomical Society* **432**, 2433 (2013), <https://academic.oup.com/mnras/article-pdf/432/3/2433/12627095/stt601.pdf>.
- [22] H. Hildebrandt et al., *Monthly Notices of the Royal Astronomical Society* **465**, 1454 (2016), <https://academic.oup.com/mnras/article-pdf/465/2/1454/24243465/stw2805.pdf>.
- [23] T. Abbott et al. (DES), *Phys. Rev. D* **98**, 043526 (2018), arXiv:1708.01530 [astro-ph.CO].
- [24] W. Lin and M. Ishak, *Phys. Rev. D* **96**, 083532 (2017).
- [25] C. M. Will, *Living Rev. Rel.* **9**, 3 (2006), arXiv:gr-qc/0510072 [gr-qc].
- [26] C. M. Will, *Living Rev. Rel.* **17**, 4 (2014), arXiv:1403.7377 [gr-qc].
- [27] K. Koyama, *Rept. Prog. Phys.* **79**, 046902 (2016), arXiv:1504.04623 [astro-ph.CO].
- [28] T. Clifton, P. G. Ferreira, A. Padilla, and C. Skordis, *Phys. Rept.* **513**, 1 (2012), arXiv:1106.2476 [astro-ph.CO].
- [29] M. Ishak, *Living Rev. Rel.* **22**, 1 (2019), arXiv:1806.10122 [astro-ph.CO].
- [30] P. G. Ferreira, (2019), arXiv:1902.10503 [astro-ph.CO].
- [31] J. Khoury, arXiv e-prints, arXiv:1011.5909 (2010), arXiv:1011.5909 [astro-ph.CO].
- [32] J. Khoury, (2013), arXiv:1312.2006 [astro-ph.CO].
- [33] A. Vainshtein, *Physics Letters B* **39**, 393 (1972).
- [34] E. Babichev and C. Deffayet, *Class. Quant. Grav.* **30**, 184001 (2013), arXiv:1304.7240 [gr-qc].
- [35] J. Khoury and A. Weltman, *Phys. Rev. D* **69**, 044026 (2004).
- [36] J. Khoury and A. Weltman, *Phys. Rev. Lett.* **93**, 171104 (2004).
- [37] K. Hinterbichler and J. Khoury, *Phys. Rev. Lett.* **104**, 231301 (2010).
- [38] K. A. Olive and M. Pospelov, *Phys. Rev.* **D77**, 043524 (2008), arXiv:0709.3825 [hep-ph].
- [39] G. Dvali, G. F. Giudice, C. Gomez, and A. Kehagias, *JHEP* **08**, 108 (2011), arXiv:1010.1415 [hep-ph].
- [40] G. W. Horndeski, *International Journal of Theoretical Physics* **10**, 363 (1974).
- [41] C. Deffayet, X. Gao, D. A. Steer, and G. Zahariade, *Phys. Rev. D* **84**, 064039 (2011).
- [42] T. Kobayashi, M. Yamaguchi, and J. Yokoyama, *Prog. Theor. Phys.* **126**, 511 (2011), arXiv:1105.5723 [hep-th].
- [43] L. Lombriser and A. Taylor, *JCAP* **1603**, 031 (2016), arXiv:1509.08458 [astro-ph.CO].
- [44] L. Lombriser and N. A. Lima, *Phys. Rev. Lett.* **B765**, 382 (2017), arXiv:1602.07670 [astro-ph.CO].
- [45] J. Sakstein and B. Jain, *Phys. Rev. Lett.* **119**, 251303 (2017), arXiv:1710.05893 [astro-ph.CO].
- [46] J. M. Ezquiaga and M. Zumalacarregui, *Phys. Rev. Lett.* **119**, 251304 (2017), arXiv:1710.05901 [astro-ph.CO].
- [47] P. Creminelli and F. Vernizzi, *Phys. Rev. Lett.* **119**, 251302 (2017), arXiv:1710.05877 [astro-ph.CO].
- [48] T. Baker, E. Bellini, P. G. Ferreira, M. Lagos, J. Noller, and I. Sawicki, *Phys. Rev. Lett.* **119**, 251301 (2017), arXiv:1710.06394 [astro-ph.CO].
- [49] B. A. Abbott et al. (Virgo, LIGO Scientific), *Phys. Rev. Lett.* **119**, 161101 (2017), arXiv:1710.05832 [gr-qc].
- [50] A. Goldstein et al., *Astrophys. J.* **848**, L14 (2017), arXiv:1710.05446 [astro-ph.HE].
- [51] V. Savchenko et al., *Astrophys. J.* **848**, L15 (2017), arXiv:1710.05449 [astro-ph.HE].
- [52] B. P. Abbott et al. (Virgo, Fermi-GBM, INTEGRAL, LIGO Scientific), *Astrophys. J.* **848**, L13 (2017), arXiv:1710.05834 [astro-ph.HE].
- [53] B. P. Abbot et al., *ApJLett* **848**, L12 (2017), arXiv:1710.05833 [astro-ph.HE].
- [54] M. Ishak et al., (2019), arXiv:1905.09687 [astro-ph.CO].
- [55] A. Albrecht et al., (2006), arXiv:astro-ph/0609591.
- [56] A. Aviles and J. L. Cervantes-Cota, *Phys. Rev. D* **D96**, 123526 (2017), arXiv:1705.10719 [astro-ph.CO].

- [57] A. Aviles, M. A. Rodriguez-Meza, J. De-Santiago, and J. L. Cervantes-Cota, *JCAP* **1811**, 013 (2018), arXiv:1809.07713 [astro-ph.CO].
- [58] A. Aviles, J. L. Cervantes-Cota, and D. F. Mota, *Astron. Astrophys.* **622**, A62 (2019), arXiv:1810.02652 [astro-ph.CO].
- [59] G. Valogiannis and R. Bean, *Phys. Rev.* **D99**, 063526 (2019), arXiv:1901.03763 [astro-ph.CO].
- [60] G. Valogiannis, R. Bean, and A. Aviles, *JCAP* **01**, 055 (2020), arXiv:1909.05261 [astro-ph.CO].
- [61] H. A. Winther et al., *Monthly Notices of the Royal Astronomical Society* **454**, 4208 (2015), arXiv:1506.06384 [astro-ph.CO].
- [62] G. Valogiannis and R. Bean, *Phys. Rev.* **D95**, 103515 (2017), arXiv:1612.06469 [astro-ph.CO].
- [63] S. Tassev, M. Zaldarriaga, and D. Eisenstein, *JCAP* **1306**, 036 (2013), arXiv:1301.0322 [astro-ph.CO].
- [64] R. E. Smith, J. A. Peacock, A. Jenkins, S. D. M. White, C. S. Frenk, F. R. Pearce, P. A. Thomas, G. Efstathiou, and H. M. P. Couchman, *MNRAS* **341**, 1311 (2003), arXiv:astro-ph/0207664 [astro-ph].
- [65] R. Takahashi, M. Sato, T. Nishimichi, A. Taruya, and M. Oguri, *Astrophys. J.* **761**, 152 (2012), arXiv:1208.2701 [astro-ph.CO].
- [66] A. J. Mead, J. A. Peacock, C. Heymans, S. Joudaki, and A. F. Heavens, *Monthly Notices of the Royal Astronomical Society* **454**, 19581975 (2015).
- [67] A. J. Mead, C. Heymans, L. Lombriser, J. A. Peacock, O. I. Steele, and H. A. Winther, *Monthly Notices of the Royal Astronomical Society* **459**, 14681488 (2016).
- [68] E. Lawrence, K. Heitmann, J. Kwan, A. Upadhye, D. Bingham, S. Habib, D. Higdon, A. Pope, H. Finkel, and N. Frontiere, *Astrophys. J.* **847**, 50 (2017), arXiv:1705.03388 [astro-ph.CO].
- [69] M. Knabenhans et al. (EUCLID Collaboration), *MNRAS* **484**, 5509 (2019), arXiv:1809.04695 [astro-ph.CO].
- [70] K. Heitmann, D. Higdon, C. Nakhleh, and S. Habib, *ApJLett* **646**, L1 (2006), arXiv:astro-ph/0606154 [astro-ph].
- [71] S. Habib, K. Heitmann, D. Higdon, C. Nakhleh, and B. Williams, *Phys. Rev. D* **76**, 083503 (2007), arXiv:astro-ph/0702348 [astro-ph].
- [72] K. Heitmann, M. White, C. Wagner, S. Habib, and D. Higdon, *Astrophys. J.* **715**, 104 (2010), arXiv:0812.1052 [astro-ph].
- [73] K. Heitmann, D. Higdon, M. White, S. Habib, B. J. Williams, E. Lawrence, and C. Wagner, *Astrophys. J.* **705**, 156 (2009), arXiv:0902.0429 [astro-ph.CO].
- [74] E. Lawrence, K. Heitmann, M. White, D. Higdon, C. Wagner, S. Habib, and B. Williams, *Astrophys. J.* **713**, 1322 (2010), arXiv:0912.4490 [astro-ph.CO].
- [75] K. Heitmann, E. Lawrence, J. Kwan, S. Habib, and D. Higdon, *Astrophys. J.* **780**, 111 (2014), arXiv:1304.7849 [astro-ph.CO].
- [76] S. Agarwal, F. B. Abdalla, H. A. Feldman, O. Lahav, and S. A. Thomas, *Monthly Notices of the Royal Astronomical Society* **439**, 21022121 (2014).
- [77] J. Kwan, S. Bhattacharya, K. Heitmann, and S. Habib, *The Astrophysical Journal* **768**, 123 (2013).
- [78] B. D. Wibking, D. H. Weinberg, A. N. Salcedo, H.-Y. Wu, S. Singh, S. Rodriguez-Torres, L. H. Garrison, and D. J. Eisenstein, *Monthly Notices of the Royal Astronomical Society* **492**, 28722896 (2019).
- [79] S. Bocquet, K. Heitmann, S. Habib, E. Lawrence, T. Uram, N. Frontiere, A. Pope, and H. Finkel, arXiv e-prints (2020), arXiv:2003.12116 [astro-ph.CO].
- [80] J. DeRose, R. H. Wechsler, J. L. Tinker, M. R. Becker, Y.-Y. Mao, T. McClintock, S. McLaughlin, E. Rozo, and Z. Zhai, *The Astrophysical Journal* **875**, 69 (2019).
- [81] T. McClintock, E. Rozo, M. R. Becker, J. DeRose, Y.-Y. Mao, S. McLaughlin, J. L. Tinker, R. H. Wechsler, and Z. Zhai, *The Astrophysical Journal* **872**, 53 (2019).
- [82] Z. Zhai, J. L. Tinker, M. R. Becker, J. DeRose, Y.-Y. Mao, T. McClintock, S. McLaughlin, E. Rozo, and R. H. Wechsler, *The Astrophysical Journal* **874**, 95 (2019).
- [83] T. McClintock, E. Rozo, A. Banerjee, M. R. Becker, J. DeRose, S. McLaughlin, J. L. Tinker, R. H. Wechsler, and Z. Zhai, arXiv e-prints (2019), arXiv:1907.13167 [astro-ph.CO].
- [84] T. Nishimichi et al., *The Astrophysical Journal* **884**, 29 (2019).
- [85] Y. Kobayashi, T. Nishimichi, M. Takada, R. Takahashi, and K. Osato, arXiv e-prints, arXiv:2005.06122 (2020), arXiv:2005.06122 [astro-ph.CO].
- [86] W. Hu and I. Sawicki, *Phys. Rev.* **D76**, 064004 (2007), arXiv:0705.1158 [astro-ph].
- [87] H. A. Winther, S. Casas, M. Baldi, K. Koyama, B. Li, L. Lombriser, and G.-B. Zhao, *Phys. Rev. D* **100**, 123540 (2019), arXiv:1903.08798 [astro-ph.CO].
- [88] B. Giblin, M. Cataneo, B. Moews, and C. Heymans, *MNRAS* **490**, 4826 (2019), arXiv:1906.02742 [astro-ph.CO].
- [89] B. Bose, M. Cataneo, T. Trster, Q. Xia, C. Heymans, and L. Lombriser, (2020), arXiv:2005.12184 [astro-ph.CO].
- [90] K. Heitmann, E. Lawrence, J. Kwan, S. Habib, and D. Higdon, *Astrophys. J.* **780**, 111 (2014), arXiv:1304.7849 [astro-ph.CO].
- [91] A. De Felice and S. Tsujikawa, *Living Rev. Rel.* **13**, 3 (2010), arXiv:1002.4928 [gr-qc].
- [92] C. Burrage and J. Sakstein, *Living Reviews in Relativity* **21**, 1 (2018), arXiv:1709.09071 [astro-ph.CO].
- [93] S. M. Carroll, V. Duvvuri, M. Trodden, and M. S. Turner, *Phys. Rev.* **D70**, 043528 (2004), arXiv:astro-ph/0306438 [astro-ph].
- [94] P. Brax, C. van de Bruck, A.-C. Davis, and D. J. Shaw, *Phys. Rev.* **D78**, 104021 (2008), arXiv:0806.3415 [astro-ph].
- [95] G.-B. Zhao, B. Li, and K. Koyama, *Phys. Rev. D* **83**, 044007 (2011), arXiv:1011.1257 [astro-ph.CO].
- [96] K. Heitmann et al., *Astrophys. J.* **820**, 108 (2016), arXiv:1508.02654 [astro-ph.CO].
- [97] T. Santer, B. Williams, and W. Notz, *Analysis of Computer Experiments* (Springer, New York, 2003).
- [98] K. Q. Ye, W. Li, and A. Sudjianto, *Journal of Statistical Planning and Inference* **90**, 145 (2000).
- [99] J. DeRose, R. H. Wechsler, J. L. Tinker, M. R. Becker, Y.-Y. Mao, T. McClintock, S. McLaughlin, E. Rozo, and Z. Zhai, *Astrophys. J.* **875**, 69 (2019), arXiv:1804.05865 [astro-ph.CO].
- [100] H. A. Winther and P. G. Ferreira, *Phys. Rev.* **D91**, 123507 (2015), arXiv:1403.6492 [astro-ph.CO].
- [101] R. Scoccimarro, *Monthly Notices of the Royal Astronomical Society* **299**, 1097 (1998), arXiv:astro-ph/9711187 [astro-ph].
- [102] A. Lewis, A. Challinor, and A. Lasenby, *Astrophys. J.*

- 1538 **538**, 473 (2000), arXiv:astro-ph/9911177 [astro-ph]. 1574
- 1539 [103] M. Cataneo, L. Lombriser, C. Heymans, A. J. 1575
- 1540 Mead, A. Barreira, S. Bose, and B. Li, Monthly 1576
- 1541 Notices of the Royal Astronomical Society **488**, 1577
- 1542 2121 (2019), [https://academic.oup.com/mnras/article-](https://academic.oup.com/mnras/article-pdf/488/2/2121/28967640/stz1836.pdf) 1578
- 1543 [pdf/488/2/2121/28967640/stz1836.pdf](https://academic.oup.com/mnras/article-pdf/488/2/2121/28967640/stz1836.pdf). 1579
- 1544 [104] H. A. Winther, S. Casas, M. Baldi, K. Koyama, B. Li, 1580
- 1545 L. Lombriser, and G.-B. Zhao, Phys. Rev. D **100**, 1581
- 1546 123540 (2019). 1582
- 1547 [105] K. Heitmann, D. Higdon, C. Nakhleh, and S. Habib, 1583
- 1548 ApJLett **646**, L1 (2006), astro-ph/0606154. 1584
- 1549 [106] D. Higdon, J. Gattiker, B. Williams, 1585
- 1550 and M. Rightley, Journal of the Ameri- 1586
- 1551 can Statistical Association **103**, 570 (2008), 1587
- 1552 <https://doi.org/10.1198/016214507000000888>. 1588
- 1553 [107] A. Savitzky and M. J. E. Golay, Analytical Chemistry 1589
- 1554 **36**, 1627 (1964). 1590
- 1555 [108] W. H. Press and S. A. Teukolsky, Computers in Physics 1591
- 1556 **4**, 669 (1990). 1592
- 1557 [109] C. E. Rasmussen and C. Williams, 1593
- 1558 Gaussian Processes for Machine Learning (MIT Press, 1594
- 1559 2006). 1595
- 1560 [110] J. Duchi, E. Hazan, and Y. Singer, Journal of Machine 1596
- 1561 Learning Research **12**, 2121 (2011). 1597
- 1562 [111] V. Springel *et al.*, MNRAS **475**, 676 (2018), 1598
- 1563 arXiv:1707.03397 [astro-ph.GA]. 1599
- 1564 [112] D. Hutner and M. Takada, Astropart. Phys. **23**, 369 1600
- 1565 (2005), arXiv:astro-ph/0412142. 1601
- 1566 [113] M. Cautun, E. Paillas, Y.-C. Cai, S. Bose, J. Armijo, 1602
- 1567 B. Li, and N. Padilla, Monthly Notices of the Royal As- 1603
- 1568 tronomical Society **476**, 3195 (2018), arXiv:1710.01730 1604
- 1569 [astro-ph.CO]. 1605
- 1570 [114] B. Li, G.-B. Zhao, R. Teyssier, and K. Koyama, Jour- 1606
- 1571 nal of Cosmology and Astroparticle Physics **2012**, 051 1607
- 1572 (2012). 1608
- 1573 [115] S. Bose, B. Li, A. Barreira, J.-h. He, W. A. Hellwing, 1609
- 1610 K. Koyama, C. Llinares, and G.-B. Zhao, JCAP **1702**, 050 (2017), arXiv:1611.09375 [astro-ph.CO].
- [116] L. Lombriser, Annalen der Physik **264**, 259 (2014), arXiv:1403.4268 [astro-ph.CO].
- [117] J. Hartlap, P. Simon, and P. Schneider, A&A **464**, 399 (2007), arXiv:astro-ph/0608064 [astro-ph].
- [118] J. Goodman and J. Weare, Communications in Applied Mathematics and Computational Science, Vol. 5, No. 1, p. 65-80, 2010 **5**, 65 (2010).
- [119] D. Foreman-Mackey, D. W. Hogg, D. Lang, and J. Goodman, Publications of the Astronomical Society of the Pacific **125**, 306 (2013), arXiv:1202.3665 [astro-ph.IM].
- [120] A. Schneider, A. Refregier, S. Grandis, D. Eckert, N. Stoira, T. Kacprzak, M. Knabenhans, J. Stadel, and R. Teyssier, Journal of Cosmology and Astroparticle Physics **2020**, 020 (2020).
- [121] N. E. Chisari *et al.*, ApJS **242**, 2 (2019), arXiv:1812.05995 [astro-ph.CO].
- [122] R. A. Fisher, in Breakthroughs in statistics (Springer, 1992) pp. 66–70.
- [123] A. G. d. G. Matthews, M. van der Wilk, T. Nickson, K. Fujii, A. Boukouvalas, P. León-Villagrà, Z. Ghahramani, and J. Hensman, Journal of Machine Learning Research **18**, 1 (2017).
- [124] M. Abadi *et al.*, arXiv preprint arXiv:1603.04467 (2016).
- [125] F. Pedregosa *et al.*, Journal of Machine Learning Research **12**, 2825 (2011).
- [126] T. Oliphant, “Python for Scientific Computing,” (2007).
- [127] J. D. Hunter, “Matplotlib: A 2D Graphics Environment,” (2007).
- [128] A. Lewis, (2019), arXiv:1910.13970 [astro-ph.IM].
- [129] G. Valogiannis, N. Ramachandra, M. Ishak, and K. Heitmann, “MGemu: An emulator for cosmological models beyond general relativity,” (2020).