INTELLIGENT DESIGN: ON THE EMULATION OF COSMOLOGICAL SIMULATIONS

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Draft version February 1, 2011

ABSTRACT

Simulation design is the choice of locations in parameter space at which simulations are to be run and is the first step in building an emulator capable of quickly providing estimates of simulation results for arbitrary locations in the parameter space. We introduce an alteration to the “OALHS” design used by Heitmann et al.(2006) that reduces the number of simulation runs required to achieve a fixed accuracy in our case study by a factor of two. We also compare interpolation procedures for emulators and find that interpolation via Gaussian Process models and via the much-easier-to-implement polynomial interpolation have comparable accuracy. A very simple simulation-building procedure consisting of a design sampled from the parameter prior distribution, combined with interpolation via polynomials also performs well. Although our primary motivation is efficient emulators of non-linear cosmological N-body simulations, in an Appendix we describe an emulator for the cosmic microwave background temperature power spectrum publicly available as computer code.

Subject headings: cosmic background radiation – cosmological parameters – methods: numerical – methods: statistical

1. INTRODUCTION

Many data analysis problems in cosmology require the repeated computation of the power spectrum, or other summary statistic, expected for a given point in the model parameter space. These range from the very expensive, such as the calculation of weak lensing shear power spectra via ray tracing through N-body simulations, to the relatively cheap, such as the calculation of cosmic microwave background (CMB) power spectra from Einstein–Boltzmann (EB) equation solvers. Decreasing the computer resources and time required for performing these calculations has benefits across this range of problems.

The benefits of speed are perhaps most obvious at the more expensive end of the cost spectrum. As Heitmann et al.(2009) have recently argued, a “brute-force” analysis to produce constraints on cosmological parameters from “Stage IV” weak lensing shear power spectra\(^1\) would take a 2048-processor machine 20 years. Techniques that can dramatically reduce the compute resource demands are not merely beneficial, but absolutely necessary. The “Cosmic Calibration” (CC) framework introduced by Heitmann et al. (2006) and developed in a series of papers (Habib et al. 2007; Heitmann et al. 2008; Schneider et al. 2008; Heitmann et al. 2009; Lawrence et al. 2009) has largely been motivated by this problem.

\(^1\) Such as from the Large Synoptic Survey Telescope (LSST) or a future space-based dark energy mission

Even at the relatively cheap end there are benefits to increased speed. Although EB solvers are relatively fast (Seljak & Zaldarriaga 1996), and can take as little as tens of seconds on a single processor, much effort has gone into making power spectrum calculation even faster. Early work exploited the angular-diameter distance degeneracy at small angular scales to reduce pre-compute requirements (Tegmark & Zaldarriaga 2000; Kaplinghat et al. 2002). Later work used more sophisticated training and interpolation procedures, and a lot of pre-computing, to achieve very high accuracy at very fast post-compute speeds (Fendt & Wandelt 2007b,c; Auld et al. 2007, 2008).

Following the terminology of Heitmann et al. (2006), by emulator we mean a machine that can estimate the results of a power spectrum calculation, without actually doing the calculation. Typically emulator construction includes a pre-computing stage in which the calculation of the power spectrum is performed at some finite set of locations in the parameter space. The choice of this set of points (or the “simulation design”) is a critical step in the emulator’s construction. It can have a significant impact on the number of calculations required to achieve a given accuracy. The focus of this paper is on the development of simulation designs that minimize the computer resource demands of the pre-compute stage.

The new design technique we introduce includes an application of the highly efficient “Orthogonal Array Latin Hypercube Sampling (OALHS)” which is part of the CC framework. The essential new elements are the choice of the parameter basis in which to perform the OALHS and the volume reduction in the parameter space achieved by constructing designs in a hypersphere rather than a hypercube. This choice is informed by the (appropriately-weighted) use of information about the rates of change of the power spectrum with respect to parameter variations.

We also consider the interpolation procedures used for estimating the power spectrum at arbitrary locations in the parameter space, from those pre-computed at the design locations. We compare results from the Gaussian process (GP) models used in the CC framework with those from fitting a second-order polynomial. In all cases we study we find the (much-simpler-to-implement) second-order polynomial fitting performs similarly to the GP interpolation. Their relative merits will vary from problem to problem however, and we speculate as to when GP will have advantages. We find that simulated
annealing is an enormously useful step to include for calibrating the GP parameters.

From our case study we draw conclusions that will be useful for application to other problems. Most importantly we demonstrate that the simulation design, rather than the choice of an interpolation method, is most critical for emulator construction. We also consider the choice of basis functions for reducing the dimensionality of the statistics to be interpolated, calibration of GP parameters for interpolation (and how this is affected by the choice of design algorithm), and the convergence of interpolation errors as the number of design points is increased.

As a testing and development ground for our work on emulators we have chosen to work with CMB temperature power spectra. Although we are also motivated by weak lensing applications, the relative speed of a Boltzmann-code calculation compared to an $N$-body simulation makes the CMB temperature power spectrum quite convenient for testing and development. Accurate calculation of non-linear matter power spectra is sufficiently expensive as to make their use for development of emulation strategies a practical impossibility. Heitmann et al. (2009) circumvented this problem by developing and testing their design strategy using an approximate (but fast) method for calculating the matter power spectra (HALOFIT Smith et al. 2003).

While existing CMB emulators are very fast and sufficiently accurate, they do have very heavy pre-compute requirements. The PICO code relies on tens of thousands of evaluations. The heavy pre-compute needs make it difficult to extend an existing emulator’s capabilities to include additional physical effects, such as isocurvature modes or completely new physical models. Improved designs can greatly reduce these difficulties. As a demonstration we describe and validate a publicly available emulator in Appendix A called EMU CMB, that can calculate CMB temperature power spectra out to $\ell = 5000$ at sub-percent accuracy as a function of six cosmological parameters. The development of the emulator, utilizing the efficient design techniques we discuss here, only required running an EB solver (CAMB Lewis et al. 2000) at 100 design points. We also show in Appendix A the emulator performance for the CMB polarization power spectra, which still have large errors at low $\ell$. The large number of training points required for previous CMB emulators is in part driven by improving the accuracy for the low-$\ell$ polarization spectra (as well as covering a larger parameter space).

The structure of this paper is as follows. We describe each aspect of our emulator in Section 2. We lay out the physical model for CMB power spectra that we use as a case study for the emulator construction in Section 2.1. We consider 3 simulation design methods that are described in Section 2.2. The basis decomposition of the simulation design runs and the 2 interpolation methods we compare are given in Section 2.3 and 2.4. We present the results of our case study in Section 3 and draw conclusions about the performance and practicality of the different design and interpolation methods in Section 4. We present an example of a CMB temperature power spectrum emulator that meets the requirements for analysis of modern CMB experiments in Appendix A. Code to construct emulators similar to the one in this section can be downloaded from http://www.emucmb.info. In Appendix B we compare the performance of quadratic polynomial interpolation in the matter power spectrum design of Heitmann et al. (2009) with the GP interpolation errors presented in their paper.

There are three steps to constructing an emulator.

1. Choose a “simulation design,” i.e., the set of points in the parameter space at which the summary statistic (henceforth assumed to be a power spectrum) will be calculated.

2. Perform a reduction in the number of dimensions of the power spectrum, via an (incomplete) mode decomposition.

3. Specify an interpolation procedure to allow one to estimate the power spectrum that one would have calculated at any point in the parameter space.

Here we review how these three steps are implemented in the “CC” work of Heitmann et al. (2006); Habib et al. (2007); Heitmann et al. (2008); Heitmann et al. (2009); Lawrence et al. (2009) and also with PICO (Fendt & Wandelt 2007)[a].

2.1. CMB Temperature Power Spectrum For Our Case Study

The very low expense of CMB temperature power spectrum calculations makes them convenient to use for testing and development of new emulation techniques. For this reason, we pursue emulation of a CMB temperature power spectrum calculator for our case study.

We set ourselves the goal of building an emulator with sufficient accuracy for analyzing the temperature power spectrum constraints that are expected from Planck, and to do so in the simplest possible manner with the fewest possible “simulations.” To inform the emulator construction, we assume prior constraints on cosmological parameters of similar quality to those from WMAP5 (Nolta et al. 2009). We consider the following six cosmological parameters:

$$\theta = (n_s, 100\theta^*, \ln(10^{10} A), \omega_c, \omega_b, \tau)^T,$$  \hspace{1cm} (1)

where $n_s$ is the scalar spectral index, $\theta^*$ is the angular size of the sound horizon at last scattering (in radians), $A$ is the amplitude of the primordial power spectrum defined at the pivot scale $k = 0.002$ Mpc$^{-1}$, $\omega_c \equiv \Omega_c h^2$ is the dark matter density, $\omega_b \equiv \Omega_b h^2$ is the baryon density, and $\tau$ is the optical depth. Our fiducial values for these parameters are given in the first column of Table 1 and are derived from a Markov Chain Monte Carlo (MCMC) chain using the WMAP5 likelihood\(^3\). We use a Fisher matrix to compute constraints on these six cosmological parameters given a signal power spectrum computed with CAMB and a model for the noise power spectrum,

$$C^\ell_{\text{noise}} = \frac{a(\ell \sigma_{\text{unr}})^2}{W_{\text{noise}}},$$  \hspace{1cm} (2)

[\footnote{http://sci.esa.int/planck/}]

[\footnote{Provided by Alexander van Engelen and Gil Holder}]

\begin{table}[h]
\centering
\caption{Fiducial cosmological parameter values and 1-σ marginal errors derived from the Fisher matrix.}
\begin{tabular}{|l|l|l|l|}
\hline
Parameter & Fiducial value & WMAP5 error & Planck error \\
\hline
$n_s$ & 0.959932 & 0.0139280 & 0.0048435 \\
$100\theta^*$ & 1.039648 & 0.0033038 & 0.0003797 \\
$\ln(10^{10} A)$ & 3.049634 & 0.0475892 & 0.0346602 \\
$\omega_c$ & 0.1079211 & 0.0069907 & 0.0017480 \\
$\omega_b$ & 0.0224900 & 0.0006217 & 0.0001885 \\
$\tau$ & 0.086429 & 0.0175253 & 0.0162973 \\
\hline
\end{tabular}
\end{table}
with noise weights $w_{\text{noise}} = 1.43 \times 10^{14}$ for WMAP5, $w_{\text{noise}} = 4.7 \times 10^{16}$ for Planck, beam smearing $\sigma_{\text{beam}} \equiv \text{FWHM}/2.355$, and FWHM = 0.00378 for WMAP5 (at 90 GHz) and 0.0021 for Planck (at 143 GHz).

We further include in our Fisher matrix a prior on a combination of polarization data with temperature data and the main contribution of the polarization data to parameter constraints. In Figure 1 we show the size of the power spectrum error bars for our WMAP5-like observations, and those for our Planck-like observations. In Figure 2 we show the corresponding two-dimensional Fisher matrix contours.

![Fig. 1.— Error models for the CMB temperature power spectrum used in the Fisher matrix predictions for WMAP5 (black) and Planck (yellow).](image)

![Fig. 2.— 2-D marginal parameter constraints predicted by the Fisher matrices for Planck (red, solid) and WMAP5 (black, dashed) noise and beam models.](image)

We were sufficiently satisfied with the accuracy and simplicity of the emulator we developed, that we are releasing a version of it as a publicly available code, called EMU CMB, described in Appendix A. There is another fast and accurate code available (PICO Fendt & Wandelt 2007b[a]) that has some advantages. Most notably, PICO is a more complete emulator that provides predictions for polarization as well as temperature power spectra and includes models with non-zero spatial curvature. EMU CMB’s advantages are (1) its significantly simpler algorithm that has made it very easy for us to make available implementations in multiple languages with no need for external libraries, (2) the simple training algorithm can be reimplemented quickly (using our public code if desired) for revised CMB models, and (3) it extends to higher multipole moment ($\ell_{\text{max}} = 5000$). The latter quality is especially important for analysis of high-resolution data, such as from the Atacama Cosmology Telescope or the South Pole Telescope (SPT).

The design runs for this paper were all calculated using CAMB (2008 June release Lewis et al. 2000) with accuracy settings $\text{accuracy\_boost} = 4$, $\text{l\_accuracy\_boost} = 4$, $\text{l\_sample\_boost} = 8$, and without including gravitational lensing. With this accuracy setting, numerical integration errors are negligibly small. We modified CAMB to extract the power spectra only at multipoles where they are actually computed, skipping the default interpolation to all multipoles. For a maximum multipole of $\ell = 3000$, this gives 448 power spectrum values using the default multipole spacing in CAMB.

### 2.2. Simulation design construction

Here we review two design procedures: that used for CC and that used for PICO. We also introduce our new design procedure. We compare results from these three design procedures in Section 3.

The CC design approach is “Orthogonal Array Latin Hypercube Sampling”, or OALHS (Tang 1993; Morris & Mitchell 1995; Leary et al. 2003; Carnell 2009). It begins with defining the boundaries of a hypercube in a scaled parameter space – all parameter dimensions rescaled to fit in an interval between 0 and 1. A grid in this hypercube is then defined. In a two-dimensional parameter space the $n_d$ design points are assigned to the grid in such a way that each design point is the only occupant of its row and the only occupant of its column. In a 3-dimensional space, the occupation of site $\{i,j,k\}$ means that sites $\{l,j,k\}$ are empty for all $l \neq i$, sites $\{i,l,k\}$ are empty for all $l \neq j$ and sites $\{i,j,l\}$ are empty for all $l \neq k$. The generalization to $n$-dimensional spaces is straightforward. The final step is to then set the exact location of each design point within its grid cell. This is done using various criteria that generally aim to maximize the distance between points in any lower-dimensional projection. The fact that the points are well spread out, in many different ways of quantifying “spread out”, improves interpolation to non-design points.

The design for PICO is constructed from samples from a prior probability distribution for the parameters and hence we
call this design procedure PS for “Prior Sampling”. In particular, the PICO design is a draw of samples from a converged MCMC run. The design is motivated by the fact that the samples are drawn from exactly the region of the parameter space where we desire accurate emulation (i.e., the region with non-negligible prior probability).

The parameter bounds used in our OALHS design are given in Table 2. The bounds have a width of eight times the marginal Fisher matrix errors for the WMAP5 noise model, centered on the fiducial point given in Column 2 of Table 1. Given these bounds and the number of design points, \( n_d \), we draw a realization of an OALHS using the \texttt{maximinLHS} function of the \texttt{Lhs} package (Carnell 2009), which maximizes the minimum distance between the design points within the Latin hypercube. All two-dimensional projections of a 100-point OALHS design are shown in the upper triangle of panels of Figure 3. If necessary, the OALHSFS design can be adjusted with a PS design as we have done in the lower panels of Figure 3. The design points are located within the hypersphere of radius 4 in the decorrelated parameter space (note that each parameter has unit variance in this space). We chose a radius of 4-\( \sigma \) because this encloses over 98% of the volume of a six-dimensional Gaussian distribution, which we judged to be sufficient for our emulator. (Note that this is covering 98% of the volume of the prior distribution. The fraction of the posterior distribution covered will be much larger.) The points of a 100-point PS design selected as random samples from an MCMC chain using the CMB power spectrum with the same WMAP5 noise model are overplotted as red crosses for comparison. It is readily apparent that the OALHSFS design points are confined to the region of high prior probability as defined by the MCMC samples.

As shown in Figure 3 the PS design gives similar volume savings over the OALHS design as does the OALHSFS. However, the PS designs do not consistently cover the design space and can lead to very large interpolation errors in regions where the design points are sparse. The Fisher matrix approximates the shape of the likelihood about its peak at quadratic order in the cosmological parameters. Our OALHSFS design will fail to encompass a region of constant probability if higher order corrections to the shape of the likelihood are significant. The PS design does not suffer from this problem. In practice, it will be possible to measure the accuracy of the OALHSFS probability contours by comparing with a PS design as we have done in the lower panels of Figure 3. If necessary, the OALHSFS design can be adjusted to allow for different ranges along the different axes in the “de-correlated” parameter space. That is, some axes might extend for, e.g., \( \pm 4 \sigma \) while some might extend for \( \pm 12 \sigma \), etc. (where \( \sigma \) is the marginal error determined from the Fisher matrix).

![Figure 3](image)

**Figure 3.** Location of 100 simulation design runs in the 6-dimensional parameter space. Upper triangle is for the OALHS design and the lower triangle is for the OALHSFS design (black triangles) and the PS design (red crosses).

Both the OALHS and PS design procedures have their advantages. The OALHS design fills the parameter space in an efficient way, providing well-spaced anchor points for interpolation. The PS design, on the other hand, concentrates design points only in the region of parameter space where we are actually interested in evaluating the emulator. We now present a design procedure that captures the advantages of both.

If \( p_o \) is the number of input parameters to our simulation, we can compute a Fisher information matrix (based on the data error distribution determining the parameter prior) from the summary statistic of the simulations we wish to emulate using \( 2p_o + 1 \) additional simulation runs; that is via \( p_o \) two-point numerical derivatives of the summary statistic and one fiducial point used to calculate the summary statistic covariance model. We use this Fisher matrix to rotate the input parameter axes to a less-correlated set of input parameters. We then build an OALHS design in this de-correlated parameter space, but reject all samples of the OALHS design that are outside of a hypersphere of constant probability (at quadratic order) centered on the fiducial parameter location. We call this design OALHSFS for OALHS samples inside a “Fisher sphere”. We also use this decorrelated space for performing the interpolation of the simulation design runs.

The two-dimensional projections of a 100-point OALHSFS design constructed from a Fisher matrix using the WMAP5 noise model are shown as the black triangles in the lower panels of Figure 3. The design points are located within the hypersphere of radius 4 in the decorrelated parameter space (note that each parameter has unit variance in this space). We chose a radius of 4-\( \sigma \) because this encloses over 98% of the volume of a six-dimensional Gaussian distribution, which we judged to be sufficient for our emulator. (Note that this is covering 98% of the volume of the prior distribution. The fraction of the posterior distribution covered will be much larger.) The points of a 100-point PS design selected as random samples from an MCMC chain using the CMB power spectrum with the same WMAP5 noise model are overplotted as red crosses for comparison. It is readily apparent that the OALHSFS design points are confined to the region of high prior probability as defined by the MCMC samples.

### Table 2

| Parameter | Minimum | Maximum |
|-----------|---------|---------|
| \( n_d \) | 0.9042  | 1.0156  |
| 1000*     | 1.0264  | 1.0529  |
| \( \ln (10^{10} \text{A}) \) | 2.8592  | 3.2340  |
| \( \omega_c \) | 0.07996 | 0.1359  |
| \( \omega_m \) | 0.02000 | 0.02498 |
| \( \tau \) | 0.01633 | 0.15653 |
In addition to the prior parameter ranges, the parameter ranges along each axis of the simulation design could also be informed by the curvature of the mode amplitude surfaces to be interpolated. In the case that a design axis has a range much shorter than the response surface curvature scale along a given coordinate axis the design will provide an estimate of the curvature scale. This could result in, e.g., the response surface being modeled as less smooth than it really is. Information about the curvature of the response surface is contained in the second derivatives of the power spectra with respect to the cosmological parameters (while the Fisher matrix uses the first derivatives of the power spectra). The range of the design axes could then be increased in directions where the curvature is very small (e.g., using the mode amplitude with the smallest curvature scale). This could result in, e.g., the response surface being modeled as less smooth than it really is. Because the emulators for our case study and Emu CMB work to an acceptable precision we have not explored these ideas further.

It is always possible that when inferring parameter constraints from a data set via MCMC, the MCMC chain will move some steps out of the region of parameter space covered by the emulator design. If the MCMC chain spends very little time in the region outside the design, it may be possible to fall back on evaluating the actual Boltzmann code for analyzing the CMB. For applications with more expensive simulations (such as N-body simulations) the emulator’s predictions can be extrapolated to get an initial MCMC chain that can then be used to inform the construction of a new design.

2.3. Dimensional Reduction

To reduce the dimensionality of the function to be interpolated, both the CC and PICO emulators perform a principal component decomposition of the \( n_d \times n_p \) matrix of simulation design runs \( y_i = \ell(\ell+1)/(2\pi)C_\ell \) where \( i = 1 \) to \( n_p \) and \( \ell \) takes \( n_d \) values in the range \( 2 \leq \ell \leq \ell_{\text{max}} \). The principal components that contribute least to the variance over the design are discarded. We have found that keeping the 20 most-important modes is more than sufficient for our purposes, i.e., the errors made from neglecting the other \( (n_p - 20) \) modes are insignificant. We quantify the errors from the truncated mode decomposition in two ways. First, we have verified that using 20 PC modes allows us to reconstruct the power spectra at all design points in several OALHS design sets to within 0.1%. Second, we used the Fisher matrix to estimate the cosmological parameter biases that would be induced from the systematic errors in the reconstructed power spectra (see Huterer & Takada [2005] for details on the Fisher matrix methods). For \( p_\mu = 20 \), the distribution of parameter biases had first and third quartiles < 10% for all six of our cosmological parameters. This means that in the case of perfect interpolation of the power spectra, the inferred parameter constraints using our emulator would have biases less than 10% of the \( 1 - \sigma \) marginal errors for both the OALHS and OALHSFS designs.

Following Heitmann et al. [2006], Habib et al. [2007], Schneider et al. [2008] we first subtract the \( \ell \)-dependent mean of the design runs from each design power spectrum and then scale the result by a single number so that the combined entries of our \( n_d \times n_p \) matrix of design runs have variance one. Denoting this centered and scaled matrix \( \eta \), we then perform a singular value decomposition, \( \eta = \mathbf{U} \mathbf{B} \mathbf{V}^T \) where \( \mathbf{U} \) has dimension \( n_d \times p \) with \( \mathbf{V}^T \mathbf{V} = \mathbf{I}_p \) and \( \mathbf{B} \) is a diagonal matrix of singular values. Finally we define the matrix of basis vectors, \( \Phi = \frac{1}{\sqrt{n_d}} \mathbf{U} \mathbf{B} \mathbf{V}^T \) so that \( \frac{1}{n_d} \mathbf{w}_\mu \mathbf{V}^T \mathbf{w} = \mathbf{I}_p \).

Retaining only the \( p_\mu \geq p \) most significant columns of \( \Phi \) we can write the scaled power spectrum as a sum over \( p_\mu \) modes

\[
\eta_\ell(\theta) = \sum_{\mu=1}^{p_\mu} w_\mu(\theta) \Phi_{\ell \mu},
\]

where \( \Phi_{\ell \mu} \) is the entry of the matrix \( \Phi \) in row \( \ell \) and column \( \mu \), and \( w_\mu(\theta) \) is the \( \mu \)-th (parameter-dependent) mode amplitude.

In Figure 4 we show the first four PC basis functions for the power spectra in the three different design types, PS, OALHS, and OALHSFS. Because of the very different volumes of parameter space covered, application of the PC algorithm to the design runs yields very different basis functions for the OALHS design versus the PS and OALHSFS designs. This is a crucial difference because the basis functions must accurately describe the design spectra at all multipoles in order to meet the accuracy targets over the large dynamic range we are simulating. Note that modes 1 and 2 derived from the PS and OALHSFS designs have several oscillations, but are much smoother when derived from the OALHS design. This difference can be seen later in the interpolation errors from the different designs (Figure 7) where the OALHS design has larger, and more oscillatory, errors at large multipoles indicating that the missing oscillatory structure in the OALHS design basis functions leads to missing structure in the reconstructed power spectra. In Appendix A we address the choice of basis functions again when we extend the emulator for the CMB temperature power spectrum to \( \ell = 5000 \).

2.4. Interpolation

We compare two methods for interpolating the mode amplitudes \( w_\mu(\theta) \) between design points in the cosmological parameter space.

For the first interpolation method we again follow the CC framework and model \( w_\mu(\theta) \) as independent GPs for each
value of \( \mu \). We refer the reader to Habib et al. (2007); Heitmann et al. (2009) for details about the construction of the GP model for the mode amplitudes. In summary, for a fixed set of points \( \theta_i (i = 1, \ldots, n_d) \), the amplitudes \( w_{\mu}(\theta_i) \) are modeled to have a multivariate Gaussian distribution with mean zero and a parametrized covariance structure that determines the smoothness of the interpolation. The covariance parameters are calibrated from a likelihood model conditioned on the simulation design runs. Because the GP framework infers distributions for the covariance parameters rather than best fit values, the error in the GP fit and interpolation can be propagated through to the final cosmological parameter constraints.

Our second interpolation method is to fit a \( p_\theta \)-dimensional linear or quadratic polynomial to the design runs. Compared to the GP model, this has the advantage of being very fast to compute, but the disadvantage of not propagating any interpolation error. For small numbers of design points, the order of the polynomial is limited (in order to obtain a well-conditioned fit) and this can further limit the accuracy of the polynomial interpolation. We therefore expect GP interpolation to outperform global polynomial fits when the curvature of the mode amplitude surfaces (in any parameter direction) exceeds the maximum polynomial order that can be fit with \( n_d \) design points. A caveat is that GP models with our chosen covariance will also yield unacceptably large interpolation errors for extremely rapidly varying surfaces unless the number of design points is significantly increased. So there is a general limit on the smoothness of the mode amplitudes as functions of cosmological parameters for such high-dimensional parameter spaces and limits on the practical number of design runs.

Figure 5 shows the first and fourth mode amplitudes in the PC decomposition of the power spectra in the OALHS 100-point design as a function of \( n_t \) with all other cosmological parameters fixed at their central values. The range of \( n_t \) covers the marginal 4-\( \sigma \) error as derived from the Fisher matrix with the WMAP5 noise model. The first mode amplitude in this case is a very smooth function of \( n_t \), while the less significant modes have a higher degree of curvature. (Note that the size of the residuals in the mode amplitudes does not obviously translate into power spectrum errors because of the centering and scaling of the power spectra done before performing the mode decomposition.)

For our case study we have found the step of calibrating the GP parameters to have intensive computational and human-labor requirements. With the GP covariance parametrization used in the CC framework there are \( p_\mu \) variance parameters and \( p_\mu \times p_\theta \) correlation parameters. To calibrate the GP model we must then find the maximum of the likelihood in this high-dimensional parameter space. We used MCMC to find the vicinity of the GP likelihood peak, but found the most difficult step to be initializing the chains in regions of non-negligible probability. A simulated annealing algorithm with a constant cooling schedule turned out to be quite effective in getting our GP calibration chains started. Because the calibration of the GP model can be a large computational obstacle in constructing an emulator we highly recommend the use of a simulated annealing or similar algorithm. We do not, however, know of any algorithm that can replace the human labor of assessing the convergence of the multiple MCMC chains required to optimize the GP model. We demonstrate the performance of our simulated annealing algorithm for calibrating the GP interpolation parameters in Figure 6.

We also found the choice of the proposal distribution for the GP correlation parameters in the MCMC algorithm to be crucial to efficient calibration of the GP model. We used independent uniform distributions for each correlation parameter, but initially allowed the width of the uniform proposal to be adjusted according to the variance in the previous 1000 steps in the chain. Because this breaks the detailed balance requirement for convergence of the MCMC chain, we fix the widths of the proposal distribution after a preset number of chain steps (of order \( 10^3 \)).

Because the evaluation of the GP likelihood at each chain step requires inversion of an \( n_d \times n_d \) matrix, the GP interpolation method becomes unpractical as \( n_d \) becomes very large. This is unfortunate because the interpolation accuracy should improve as \( n_d \) increases! We therefore expect GP models to provide a preferable interpolation method for small \( n_d \) and polynomial interpolation to be preferred for large \( n_d \). For our case study, we actually find that polynomial interpolation provides smaller interpolation errors for a wide range of \( n_d \). We demonstrate the performance of polynomial interpolation for a different case study matching that of Heitmann et al. (2009) in Appendix B.

Our C++ code for calibrating GP models for interpolation (built with the Scythe Statistical library) is available for download at \( \text{http://www.emucmb.info} \).

3. EMULATOR RESULTS COMPARED

3.1. Designs Compared

In Figure 7 we show the fractional interpolation error for 100 test spectra using the three design methods under consideration. The test spectra were computed at points in our six-dimensional cosmological parameter space drawn from the posterior distribution for our WMAP5 noise model. Each interpolation method was trained on 100 design points. (Note that we always show the expected value of the emulator; we do not compute the random draws that are part of a complete GP prediction.) At these test points, the OALHSFS design has interpolation errors approximately two times smaller than the OALHS design at all multiples and for both interpolation methods. Using quadratic polynomial interpolation, the PS design has comparable interpolation errors to the OALHSFS design, but has very poor performance using GP interpolation. As we mentioned in Section 2.2, the OALHSFS design is built in a parameter-space volume that is \( 1/12 \) the size of the OALHS volume. If the increased density of simulation points is the dominant difference between the OALHSFS and OALHS designs, then Figure 7 gives some indication of how the interpolation accuracy improves with the increased density. However the interpretation is not straightforward as the shape of the designs (spherical versus cubic) may also be important. That is, the design points outside the Fisher sphere in the OALHS design could, in principle, be helpful in reducing the interpolation accuracy, but we have not pursued the separation of these effects further. The main result that the OALHSFS design gives improved performance is sufficient for our purposes. We show similar results, but for \( n_d = 50 \) in Figure 8. The interpolation errors using quadratic polynomials have similar relative performance between the three design types as in Figure 7. The GP interpolation results, however, now show smaller errors using the PS design than using the OALHS design. The OALHSFS design using GP interpolation generally gives smaller errors than the OALHS design, but there are a few test points where the OALHSFS design

The GP correlation parameters in the MCMC algorithm to be crucial to efficient calibration of the GP model. We used independent uniform distributions for each correlation parameter, but initially allowed the width of the uniform proposal to be adjusted according to the variance in the previous 1000 steps in the chain. Because this breaks the detailed balance requirement for convergence of the MCMC chain, we fix the widths of the proposal distribution after a preset number of chain steps (of order \( 10^3 \)).

Because the evaluation of the GP likelihood at each chain step requires inversion of an \( n_d \times n_d \) matrix, the GP interpolation method becomes unpractical as \( n_d \) becomes very large. This is unfortunate because the interpolation accuracy should improve as \( n_d \) increases! We therefore expect GP models to provide a preferable interpolation method for small \( n_d \) and polynomial interpolation to be preferred for large \( n_d \). For our case study, we actually find that polynomial interpolation provides smaller interpolation errors for a wide range of \( n_d \). We demonstrate the performance of polynomial interpolation for a different case study matching that of Heitmann et al. (2009) in Appendix B.

Our C++ code for calibrating GP models for interpolation (built with the Scythe Statistical library) is available for download at \( \text{http://www.emucmb.info} \).

3. EMULATOR RESULTS COMPARED

3.1. Designs Compared

In Figure 7 we show the fractional interpolation error for 100 test spectra using the three design methods under consideration. The test spectra were computed at points in our six-dimensional cosmological parameter space drawn from the posterior distribution for our WMAP5 noise model. Each interpolation method was trained on 100 design points. (Note that we always show the expected value of the emulator; we do not compute the random draws that are part of a complete GP prediction.) At these test points, the OALHSFS design has interpolation errors approximately two times smaller than the OALHS design at all multiples and for both interpolation methods. Using quadratic polynomial interpolation, the PS design has comparable interpolation errors to the OALHSFS design, but has very poor performance using GP interpolation. As we mentioned in Section 2.2, the OALHSFS design is built in a parameter-space volume that is \( 1/12 \) the size of the OALHS volume. If the increased density of simulation points is the dominant difference between the OALHSFS and OALHS designs, then Figure 7 gives some indication of how the interpolation accuracy improves with the increased density. However the interpretation is not straightforward as the shape of the designs (spherical versus cubic) may also be important. That is, the design points outside the Fisher sphere in the OALHS design could, in principle, be helpful in reducing the interpolation accuracy, but we have not pursued the separation of these effects further. The main result that the OALHSFS design gives improved performance is sufficient for our purposes. We show similar results, but for \( n_d = 50 \) in Figure 8. The interpolation errors using quadratic polynomials have similar relative performance between the three design types as in Figure 7. The GP interpolation results, however, now show smaller errors using the PS design than using the OALHS design. The OALHSFS design using GP interpolation generally gives smaller errors than the OALHS design, but there are a few test points where the OALHSFS design
gives worse performance for several multipoles. These results are consistent with our expectation that at a fixed number of design points \( n_d \) the reduction in the mean distance between design points in the OALHSFS and PS designs (see Figure 3) should improve the interpolation accuracy. Indeed we do see an improvement by a factor of \( \sim 2 \) in the interpolation accuracy. However, the poor performance of the PS design with 100 design points and using GP interpolation demonstrates that the PS design is a less reliable algorithm than OALHS-based designs for building an emulator using GP interpolation. This could be because the PS design leaves regions of parameter space very sparsely covered compared to the OALHS designs (especially in higher dimensions).

Next we investigate how the accuracy gains of OALHSFS over OALHS at fixed \( n_d \) translate into a reduction in \( n_d \) at fixed interpolation accuracy. In Figure 2 we show the quartiles and maxima of the average fractional interpolation error in a band from \( l = 1500 \) to \( l = 2000 \) (that is, we averaged the absolute value of the error over \( l = 1500 \) to 2000) versus \( n_d \) for 100 test points taken from a PS design. We plot the interpolation errors for both the OALHS and OALHSFS designs using GP interpolation. Comparing the solid and dashed lines at fixed interpolation accuracy (i.e., along a horizontal axis) we see the OALHSFS design requires \( \sim 25-70\% \) fewer design points than the OALHS design (with larger savings at low \( n_d \)). One possible explanation for this trend is that some of the design points in the OALHS design are not significantly contributing to the reconstruction of the mode amplitude surfaces in the (high-probability) region where the test points are actually located. When \( n_d \) is small, every design point should be important for reducing the interpolation errors, so wasting even one point in the OALHS design would degrade the emulator. This demonstrates a main point of the paper that the design space volume reduction offered by the OALHSFS design is significant in minimizing \( n_d \) to achieve a fixed error tolerance.

In order to understand when the errors in the truncated mode decomposition of the power spectra are significant relevant to the interpolation errors, we plot the fractional errors in the reconstructed power spectra as functions of \( p_{\mu} \) at each design point (i.e., without any interpolation) in Figure 10. The reconstruction errors are rapidly decreasing functions of the number of retained PC modes, as expected. For the choice used throughout this paper of \( p_{\mu} = 20 \) for \( n_d \geq 50 \), the errors from the truncated mode decomposition are adequate for our error tolerance of \( 10^{-3} \) for both the OALHS and OALHSFS designs. However, from Figure 3 we can see that with \( p_{\mu} = 20 \) the mode reconstruction errors are non-negligible for the \( n_d = 100, 200 \) designs, which would explain why the total fractional power spectrum errors (mode reconstruction + interpolation) do not steadily decrease for \( n_d > 100 \).

### 3.2. Interpolation Methods Compared

In Figure 11 we compare the mean interpolation errors in the band \( 1500 < l < 2000 \) using the GP model and a quadratic polynomial fit to the OALHSFS and PS designs as functions
FIG. 7.— Fractional power spectrum interpolation errors using 3 different 100-point simulation designs: PS (left), OALHS (center), OALHSFS (right). The interpolation is performed using GP (top) and quadratic polynomial (bottom) fits to the 20 most significant principal components in each design, and is tested against 100 points in an additional PS design. The dark grey bands show the minimum and maximum errors out of the 100 design points for each \( l \) while the red (inner) band shows the errors within the first and third quartiles. The central black line shows the median interpolation error.

FIG. 8.— Same as Figure 7 except for \( n_d = 50 \).

of \( n_d \). In all of the designs considered polynomial interpolation provides smaller interpolation errors than GP interpolation.
We demonstrate one such practical emulator in Appendix A

The (first or second order) polynomial interpolation performs so well because the response surfaces of each mode amplitude are so smooth as functions of the six active cosmological parameters. The GP models also require smooth response surfaces, but we expect the low-order polynomial fits to be worse than the GP fits for a given correlation length in the response surface as the correlation length is decreased. This is because the covariance structure in the GP model has more flexibility than a (global) second order polynomial. Therefore, for some applications the fast-to-compute polynomial interpolation will no longer suffice. The relative performance of different interpolation methods will always be problem-specific. However, we explore designs for the matter power spectrum in Appendix B and show that the polynomial interpolation is again comparable to the GP interpolation demonstrated in [Heitmann et al. (2009)] for similar designs for most of the dynamic range in the simulated power spectra (except for the smallest scales). So, for both the CMB and matter power spectrum, an emulator constructed using an OALHSFS design and quadratic polynomial interpolation has similar performance to an emulator using an OALHS design and GP interpolation. As the number of design points increases, both interpolation methods should converge to arbitrary accuracy as higher-order polynomial fits become well-conditioned.

4. CONCLUSIONS

We have demonstrated an improved method for generating simulation designs for interpolation based on selecting OALHS inside a spherical (rather than cubical) volume in a whitened cosmological parameter space defined by the Fisher matrix. Our improved design algorithm (OALHSFS) offers a significant improvement in design efficiency over the OALHS algorithm; giving a factor of ∼ 2 reduction in the number of design points (n_d) required to reach a fixed emulator accuracy. We also compared the OALHS-based designs with designs constructed by drawing samples from the prior distribution for the cosmological parameters (which we call prior sampling or PS designs). Because both PS and OALHSFS designs concentrate design points in the volume of parameter space with significant prior probability, they both yield smaller interpolation errors for a fixed n_d than OALHS designs when n_d is large. When n_d is small, the PS designs give poor coverage of the parameter space; giving erratic interpolation errors depending on the particular PS design realization. This is not surprising because it is exactly the problem that OALHS designs are meant to solve. However, we take the superior performance of both the PS and OALHSFS designs in the large n_d limit (n_d = 100 for our case study in six-dimensional parameter space), as evidence that the OALHSFS design retains the advantages of the OALHS design while also capturing the benefit of limiting design points to regions of significant prior probability.

We compared the GP interpolation methods used in previous literature of the emulator framework for cosmological simulations with simple, global polynomial interpolation over the design space. We find that second order polynomial interpolation gives interpolation errors that are only slightly worse than a GP model with optimized correlation parameters. This is a useful discovery because the GP models can be computationally challenging to calibrate while a polynomial fit via least-squares minimization is very fast. For PS designs we found it is not always possible to fit a GP model, while second order polynomial interpolation still gives errors similar to those using an OALHSFS design. For applications where low-order polynomial interpolation does not provide sufficient precision, we note that the GP model calibration done via MCMC can be significantly hastened by using a simulated annealing algorithm to search for regions of high likelihood in the GP parameters.

Making use of the simplicity of polynomial interpolation, we are releasing code to generate emulators of the CMB power spectra whose computational limitation is only the time it takes to run the Boltzmann code to generate spectra at the design points (available at [http://www.emucmb.info](http://www.emucmb.info)). We demonstrate one such practical emulator in Appendix A.
for the TT power spectrum reaching ℓ > 5000 and including lensing contributions. This emulator uses 100 design points to achieve interpolation errors less than 0.6% in the power spectrum for all ℓ. Python and IDL scripts as well as a module for CosmoMC (Lewis & Bridle 2002) for generating predicted power spectra from this emulator are available at the same URL.

Because of the similar performance of the two interpolation methods we investigated, we conclude that the simulation design is the most significant component of the emulator framework introduced in Heitmann et al. (2006); Habib et al. (2007); Heitmann et al. (2009). The mathematically consistent GP framework becomes important when it is necessary to propagate the errors in the design interpolation or when optimizing the interpolation for a given OALHS-based design.

As mentioned by other recent work (Heitmann et al. 2006; Habib et al. 2007; Heitmann et al. 2009) the simulation emulator technology becomes most interesting for emulating computationally expensive simulations such as those needed for predicting tracers of the matter power spectrum (e.g., weak lensing or galaxy spectra). In this case N-body simulations of the dark matter distribution can take days or weeks to run, which puts severe constraints on the number of design points that can be considered. In addition to the matter power spectrum, the need for predicting the outputs of suites of simulations over cosmological parameter space has recently been recognized for understanding the deviation from universality of the halo mass function (Manera et al. 2009), the distribution of progenitor masses in the conditional mass function (Neistein et al. 2010), computing the 1-point probability distribution function of the Lyα flux (Viel et al. 2009), and mapping the input space of semi-analytic models of galaxy formation (Bower et al. 2009, 2010). We expect the methods developed here to be useful for the first three applications. However, the problem of mapping the input space for simulations with a large number of parameters is qualitatively different. Our design based on the Fisher matrix assumes that the prior probability distribution in the input parameter space is unimodal and that the maximum of the prior probability distribution is known a priori. The success of the interpolation methods discussed in this paper also assume that the ranges of input parameters are sufficiently small that the outputs are (quite) smooth functions of the input parameters. Both of these assumptions are broken when mapping the input space for semi-analytic galaxy formation models so this should be considered a separate problem for emulator construction (see Bower et al. 2010, for how OALHS designs are useful for such problems).

Recently, Angulo & White (2010) have shown that statistics such as the power spectrum (as well as mass functions and merger trees) can be obtained at different cosmological parameter values using appropriate rescalings of a single N-body simulation. If this method proves to be successful in further tests, it could alleviate the strict bounds on the number of design points that are feasible for statistics derived from cosmological N-body simulations. In this case, the advantages of GP interpolation methods would become less useful (namely the ability to optimize the GP model to achieve minimal interpolation errors and to propagate the interpolation errors). Alternatively, using the methods of Angulo & White (2010) could make it feasible to construct emulators of more sophisticated statistics derived from light cones requiring many N-body simulations for a single point in parameter space. We plan to pursue this in future work.

We thank David Higdon, Charles Nakhleh, Salman Habib, Katrin Heitmann, Ian Vernon, Richard Bower, and Shaun Cole for useful conversations. We also thank Chad Fendt for reviewing our work and helping us understand how it relates to PICO and Alexander van Engelen and Gil Holder for providing their MCMC chain sampling from the WMAP5 posterior distribution. We thank the anonymous referee for many useful suggestions to improve the manuscript. This work was supported at UC Davis by NSF grant 0709498 and an award from NASA’s Jet Propulsion Laboratory.

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APPENDIX

EMU CMB: A CMB TT power spectrum emulator for current experiments

In this section we present a CMB TT power spectrum emulator suitable for use in parameter estimation algorithms from Planck\(^6\), ACT\(^7\), SPT\(^8\), or similar experiments. We use CAMB (Lewis et al. 2000) to generate CMB TT power spectra with the same six cosmological parameters as in the main body of the paper\(^9\), but out to \(\ell_{\text{max}} = 5238\) and including the lensing distortion of the power spectrum. We have not concerned ourselves with modeling uncertainties such as those due to recombination. Instead, we regard this emulator as proof that a practical tool for current data analyses can easily be constructed. Emulators for revised models can be quickly constructed using the same algorithm. We provide scripts for this purpose as well as details of the exact CAMB settings that generated the results presented in this section at [http://www.emucmb.info](http://www.emucmb.info).

Building the emulator

We use an OALHSFS design with \(n_d = 100\) covering the WMAP5 4-\(\sigma\) error bounds as determined by our Fisher matrix described in Section 2.1. The design runs for EMU CMB use the 2009 October release of CAMB (different from the case study in the main body of the paper) with the “curved correlation function” lensing implementation including nonlinear corrections calculated by HALOFIT (Challinor & Lewis 2005). We again use accuracy settings \(\text{l\_accuracy\_boost} = 4\) and \(\text{l\_accuracy\_boost} = 4\), but build the emulator from the power spectra as output by CAMB at every multipole rather than extracting only the uninterpolated power spectra values. We set \(\text{l\_sample\_boost} = 4\) to determine the number of multipole values where the power spectra are actually computed. See [http://www.emucmb.info](http://www.emucmb.info) for the complete CAMB parameter files.

Also in contrast to the main body of the paper, we perform the dimension reduction of the design runs on \(y_i \equiv \log (\ell (\ell + 1)/(2\pi)^2 C_{\ell i})\) (\(i = 1, n_d\)). Performing a PC decomposition on the logarithm of the power spectra yields basis functions that better describe the lensing variations at \(\ell \gtrsim 3000\) across the design points as shown in Figure A1.

As in the main text, we fit global second order polynomials to each of the first 20 mode amplitudes to perform the interpolation over the design space. Using only the first 20 PCs allows reconstruction of the power spectra at the design points to less than 0.1% accuracy for \(\ell \lesssim 100\) and to less than 0.01% accuracy for \(\ell \gtrsim 100\).

EMU CMB accuracy

We validated the emulator by running CAMB at an additional 100 points in a new realization of an OALHSFS design. (Note the validation plots in the main body of the paper use points from a PS design.) The interpolation errors for the spectra at these 100 test points are shown in Figure A2. For all test points, the emulator is accurate to less than 0.6% out to \(\ell = 5238\). The errors are less than 0.2% for \(\ell < 3000\), which is consistent with Figure 7.

Note that while EMU CMB uses significantly fewer training runs of CAMB than PICO, unlike PICO this EMU CMB example does not predict polarization power spectra. We have verified with simple tests that interpolation of the low-\(\ell\) parts of the EE and TE CMB power spectra is more challenging than the TT spectra demonstrated here. In addition, many of the training runs for PICO were required to include cosmological models with nonzero spatial curvature, which we have not considered\(^{10}\).

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\(^{6}\) [http://www.esa.int/esaMI/Planck/index.html](http://www.esa.int/esaMI/Planck/index.html)

\(^{7}\) [http://www.physics.princeton.edu/act](http://www.physics.princeton.edu/act)

\(^{8}\) [http://pole.uchicago.edu](http://pole.uchicago.edu)

\(^{9}\) We revert to the more common definition of the primordial amplitude defined at the pivot scale \(k = 0.05\hMpc^{-1}\).

\(^{10}\) C. Fendt private communication.
In this section we compare the polynomial interpolation errors for OALHS designs for the dark matter power spectrum to the GP interpolations demonstrated in Heitmann et al. (2009). Following Heitmann et al. (2009) we use the HALOFIT (Smith et al. 2003) algorithm as provided in CAMB (Lewis et al. 2000) to generate nonlinear dark matter power spectra as functions of the five cosmological parameters: $\Omega_c h^2$, $\Omega_b h^2$, $n_s$, $w$, $\sigma_8$. The reduced Hubble parameter $h$ is determined from $\omega_c$ and $\omega_b$ assuming spatial flatness and a fixed angular size of the sound horizon at last scattering ($\theta_s = \pi/302.4$ steradians as defined in Heitmann et al. 2009). The prior parameter ranges defining the boundaries of the OALHS design are the same as Heitmann et al. (2009).

The fractional interpolation errors for three designs with $n_d = 10, 37, 100$ are shown in Figure A1. Heitmann et al. (2009) built an OALHS design with $n_d = 37$ and demonstrated sub-percent interpolation errors using GP interpolation over the same range in wavenumber as shown in Figure A1. Using quadratic polynomial interpolation, the errors are worse, but are still under 2% for all wavenumbers. Increasing $n_d$ to 100 points reduces the interpolation errors to sub-percent levels for all but a few test points in the design. For the matter power spectrum over this design space, the GP interpolation developed by Heitmann et al. (2009) therefore requires three times fewer design points to achieve the same accuracy as a naive quadratic polynomial fit. However, we note that the OALHSFS design demonstrated in Section 3.1 can achieve the same reduction in the required number of design points to reach a fixed accuracy while using the much simpler polynomial interpolation.

We take these results as confirmation that the good performance of polynomial interpolation in the CMB designs in the main body of the paper is not limited to a single physical example. More generally, the success of a simulation emulator depends strongly on the simulation design (including the form of the mode decomposition of the power spectrum) while optimized GP interpolation can also significantly improve the performance of a given Latin-hypercube-based design (in contrast to a PS-based design).
Fig. A2.— Fractional errors in the interpolation of the power spectra for the EMU CMB design. See Figure 7 caption for the meaning of the colors.
Fig. B1.— Fractional error in the interpolated matter power spectra using polynomial interpolation for 3 OALHS designs with different $n_d$. The parameters and widths of the OALHS designs match those in Heitmann et al. (2009). For $n_d = 10$ the mode amplitudes in the decomposition of the power spectra are fit with linear polynomials. For $n_d = 37, 100$ the mode amplitudes are fit with quadratic polynomials.