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Comment on Article by Vernon et al.

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1 General Comments

We congratulate the authors on an excellent example of collaborative work that combines Bayesian statistics with computational and observational cosmology. We appreciate the effort it takes to grow this collaboration into a relationship that can produce the results shown in this paper. In particular, the process of determining the likelihood, eliciting the form of a discrepancy, or visualizing the results is easy enough to put in a paper, but the time and effort to get to that point is substantial. This has certainly been our experience in cosmological applications.

Like Vernon, Goldstein and Bower (VGB) describe, we have also invested much effort over the past few years collaborating with cosmologists at Los Alamos National Laboratory. Our approach uses a more fully Bayesian formulation and carries out the multivariate emulation using a basis representation. We make an initial comparison of the posterior distribution produced by our approach to the non-implausible regions in the input space presented in this paper. We then go on to describe the approach we have developed for emulating the dark matter power spectrum. In particular, we consider two ways in which our handling of the output differs from that of VGB.

2 Comparison to the Posterior Distribution using a Fully Bayesian Approach

First, we compare a part of the VGB analysis to the fully Bayesian approach described in Higdon et al. (2008). Briefly, our approach decomposes the multivariate computer output using principal components. Independent, constant-mean Gaussian processes with a squared-exponential covariance function are fit to the weights for each basis function. The observed data are assumed to follow a Gaussian distribution with specified covariance and mean given the by the simulation model plus discrepancy. In this case, rather than estimate the discrepancy as described by Higdon et al. (2008), we fix the discrepancy at the values estimated and provided by VGB in the the form shown in VGB's Equation (20). This likelihood, plus flat priors on the inputs and other appropriate priors on nuisance parameters, provides a way to calibrate simulator inputs that produce best-fitting simulator outputs. Estimation proceeds using MCMC. The methodology is applied to VGB's Wave 2 suite. The resulting posterior distribution for the model parameters are given in Figure 1.

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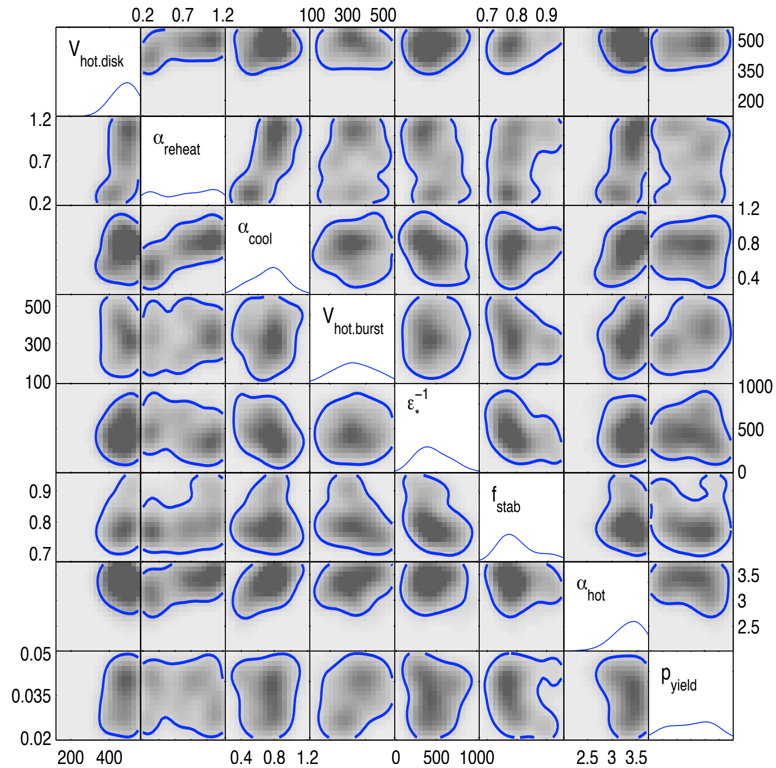

Figure 1: Posterior distribution of the input parameters using the fully Bayesian formulation of Higdon *et al.* (2008). Here the observational data are combined with the wave 2 simulations. Compare this figure with Figure 11 from VGB which gives the plausibility region of the input parameters using the same information. Here the lines show an estimated 95% hpd region for each of the bivariate margins of the posterior; the diagonal shows estimates of the univariate marginal densities.

Our fully Bayesian approach appears to more strongly constrain the parameters, but the results are fairly similar. Any conclusions made from this comparison should be tentative since there are major differences between the two formulations. The fully Bayesian approach uses an emulator with a constant mean, with most of the structure captured by using the covariance function, as opposed to the VGB approach which captures structure mostly with the mean. Also, the multivariate emulator is constructed using basis functions, as opposed to the carefully chosen function locations in VGB. Perhaps most importantly, our full Bayesian specification assumes that the observations have a Gaussian distribution around the simulation, which could produce very different results than the implausibility function used by VGB. We haven't explored how these differences affect the resulting posterior.

The results suggest that a fully specified Bayesian approach can be applied to VGB's problem, although we note that the computational burden is quite significant. Nevertheless, as we are sure VGB can attest, the vast majority of the effort in this type of problem is not spent in deriving or implementing a particular model, but in understanding the scientific issues well enough to represent them statistically. Further, we were able to implement the fully Bayesian procedure quickly only because our own similar efforts have given us extensive experience and resulted in the creation of a software package that readily handles this type of problem.

3 Emulating the Dark Matter Power Spectrum

Lawrence et al. (2010) is also interested in estimating or constraining cosmological parameters, particularly the dark energy equation of state. To achieve this goal, we use a large simulation suite called the Coyote Universe. This suite contains nearly 1000 n-body gravitational simulations of dark matter for 37 cosmologies that span that currently acceptable ranges of five cosmological parameters. The goal is to produce an emulator that captures the best available theory for comparison with upcoming observations from new probes. For output, Lawrence et al. (2010) considers the nonlinear dark matter power spectrum. Like the luminosity functions from VGB, the power spectrum summarizes the distribution of objects in space, making it useful for evaluating models of structure formation. Here we describe the approach taken in Lawrence et al. (2010) for handling the output and how it differs from the methodology described in VGB.

3.1 Modeling the Output

Figure 1 from VGB shows the luminosity results from the initial set of runs. These runs demonstrate a large variance and lack of smoothness, both of which present potential difficulties for emulator fitting. Further, smoothness is an expected property in the actual Universe. Similarly, our Figure 2 demonstrates the same issues from the Coyote Universe. This plot shows the power spectra (on a transformed scale) for the high resolution simulations of 37 cosmologies at six redshifts. The large variation and lack of smoothness arise from uncertainty in initial conditions and numerical issues related to the finite size of the simulation. These issues do not appear to be a detriment to the scientific goals from VGB. In our case, these issues wash out important features in the output, notably a series of systematic bumps in the vicinity of $k = 0.1$ known as the baryonic acoustic oscillations (BAO) that are very important in understanding structure formation. As such, we need to spend some effort in resolving these issues.

In order to overcome these difficulties, we use the simulations to estimate the smooth power spectra, which are then used to build the emulator. The estimation uses replicate simulations for each set of cosmological parameters at three levels of resolution starting from different draws of the initial condition. Figure 3 shows the results for a single cosmology. The red line is the spectrum from the single high resolution run (higher resolution runs have larger volumes and more particles), the black lines are from the four medium resolution runs, and the gray lines are from the 16 low resolution runs.

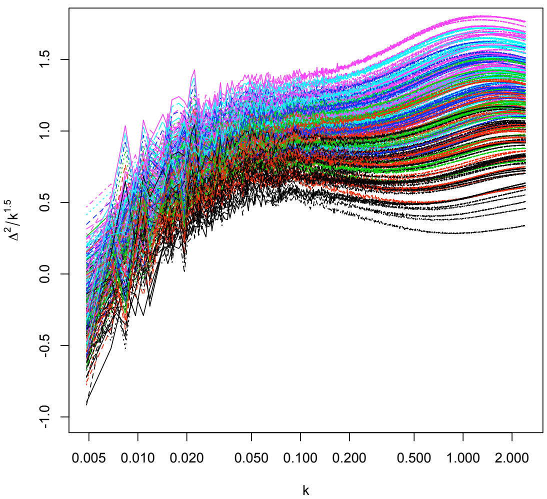

Figure 2: Transformed power spectra from the high resolution Coyote Universe simulations. The simulations span 37 cosmological parameter settings and 6 redshift values. The spectra are very jagged with large variation, particularly at low k. This is both unrealistic and a detriment to answering important scientific questions.

The lower two resolutions have limited or no utility at high k values (accordingly, this part has already been removed), but do provide information in the low k region where the variance is large and the mid k regions where the important features are located.

Lawrence et al. (2010) describes the power spectrum estimation in detail, so we only give a brief overview here. The smooth power spectrum is assumed to be a process convolution (Higdon 2002): a smooth class of functions built by kernel smoothing a random process. Because this model can be specified constructively, it allows great flexibility. In particular, the kernel can be changed over the domain to create a nonstationary function. The function class for the smooth power spectrum estimates is specified as process convolution built out of Brownian motion observed on a fixed grid and smoothed by a Gaussian kernel whose width is allowed to vary smoothly over the domain. The kernel width function is described by a second process convolution built from Gaussian impulses on a small grid, smoothed by a Gaussian kernel with a fixed width, and assumed to be common across cosmologies. The observed simulated power spectra are assumed to be normally distributed with a smooth mean given by the power spectrum process convolution and known variances. Priors on the variances for the latent random processes (the Brownian motions and the Gaussian impulses) and the kernel width of the second process convolution complete the specification. The Brownian motions are integrated out of the posterior and estimation proceeds using MCMC to sample from the posteriors of the parameters and the impulses comprising the kernel-width process

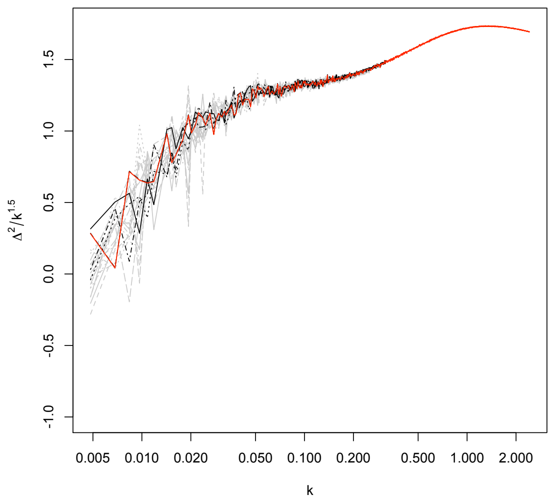

Figure 3: Replicate outputs for a fixed cosmology and redshift at three resolutions. Red is high resolution, black is medium resolution, and gray is low resolution.

convolution. The results, as shown in Figure 4, are more realistic, less influenced by random fluctuations in the initial condition, and easier to model. Importantly, the estimation procedure is able to pick out the BAO.

Ultimately, this approach is one choice for balancing a number of considerations. Estimating the BAO would have been impossible without replicates, but we might have reduced the replication and explored a larger number of parameters, used larger parameters ranges, and/or more thoroughly filled in the design space. This choice is, of course, governed most strongly by the scientific questions at hand.

3.2 Decomposing the Output

Many of the luminosity plots in VGB show vertical lines indicating the points along the luminosity functions that were used to compare observation and simulation. For the Wave 1 analysis, seven points (three from the bj curves and four from the K curves) are used as outputs for the emulator and for history matching. The number of points is increased as the analysis progresses.

Lawrence et al. (2010) uses the approach discussed in Higdon et al. (2008) of a principal component decomposition on the smooth power spectra estimates. In this case, the first five principal components capture 99.99% of the variation. Figure 5 shows the resulting basis functions (the nearly repeating patterns in this plot are created by combining the 6 redshifts for each cosmology in order to simplify the emulator estimation).

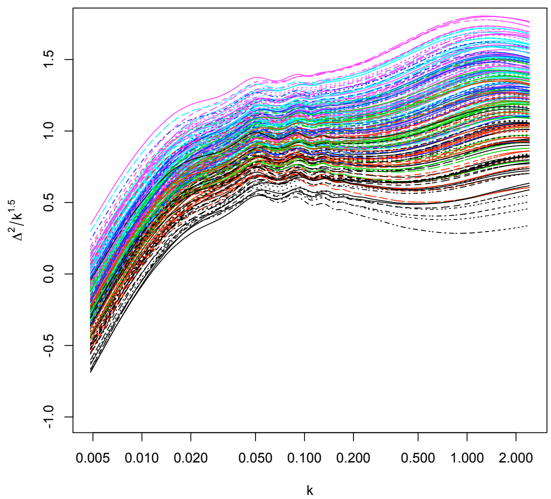

Figure 4: Estimates of the unknown smooth power spectra. Compare to Figure 2 and note the BAO near $k = 0.1$.

Five independent emulators are built to model the weights for each of the five basis functions. This approach achieves a similar size reduction to the VGB approach, but still attempts to model the entire functional output. In part, this decomposition is aided by the earlier estimation of the smooth spectra which greatly reduces the variance.

4 Conclusion

We spent much of our computational effort on finding a more ideal, smooth representation of the power spectrum, while VGB spent their computational effort on better exploration of the parameter space. These different approaches put different demands on the emulator. Thus, it is not surprising that we have different emulation strategies. The more general issue of determining how best to use limited computational resources is an open question in the general topic of simulation-aided inference. As the authors point out, this general topic has no shortage of open research directions. We thank the authors for their bold effort. The paper is full of new ideas and perspectives for augmenting statistical inference with physically-based computational models.

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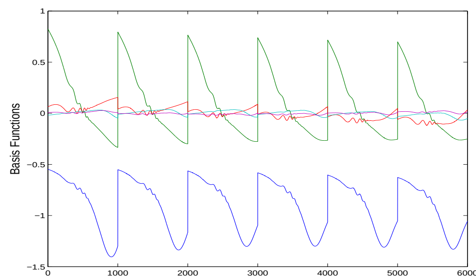

Figure 5: Basis functions used for emulation. The emulator is built by combining the six redshift spectra for each cosmology. This causes the sawtooth effect in this plot as the spectra change subtly across redshifts.

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