Diagnostics for Stochastic Emulators

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Abstract

Computer models, also known as simulators, can be computationally expensive to run, and it is for this reason that statistical surrogates, also known as emulators, have been developed for such computer models. Gaussian processes are commonly used to emulate deterministic simulators, and they have also been extended to emulate stochastic simulators that have input-dependent noise. Any statistical model, including an emulator, should be validated before being used. We discuss how current methods of validating Gaussian process emulators of deterministic models are insufficient when applied to Gaussian process emulators of stochastic computer models. We develop tools for diagnosing problems in such emulators, based on independently validating the mean and variance predictions using out-of-sample, replicated, simulator runs. To illustrate these ideas, we apply them to a simple toy example, and a real example of a building performance simulator.

Keywords: Gaussian process; Computer Experiment; Validation; Heteroscedastic; Surrogate

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1 Introduction

Computer models, also known as simulators, can take non-trivial amounts of time to run. If one wants to use a simulator to learn about a system in some way, whether this is to infer some parameter or maximise an output, many simulator runs may be required. This can often be computationally expensive or infeasible. Such problems can be overcome by building a surrogate model that represents the simulator, while also being quick to run. One such surrogate model is the Gaussian process emulator; this takes given outputs from a few runs of the simulator, a training set, and constructs a probabilistic model of the outputs of future runs. Because this model is probabilistic we get a measure of the uncertainty of the predictions. In this setting we gain computational speed at the expense of certainty.

A lot of effort has been spent on using Gaussian process emulators to model deterministic simulators (Sacks et al., 1989; Kennedy and O’Hagan, 2001; Oakley and O’Hagan, 2002), that is to say: simulators that return the exact same output values when the same input values are used. in more recent years some attention has shifted to emulating stochastic simulators which can yield different outputs even when the same inputs are used (Ankenman et al., 2010; Boukouvalas, 2010). This often involves modelling how both the mean and variance of the simulator changes for different input values.

As pointed out by Bastos and O’Hagan (2009) “building an emulator requires some assumptions and approximations”. This obligates us to check the quality of an emulator once constructed, as an emulator must adequately represent the simulator if it is to be used as a surrogate model. This article will outline why stochastic emulators require more diagnostic checks compared to their deterministic counterparts, and will also present some suitable additional diagnostics.

Section 2 will review heteroscedastic Gaussian processes as a tool for stochastic emulation. Section 3 will then summarise typical diagnostic checks that can be used to validate a deterministic emulator, and how these checks alone can be insufficient for stochastic emulators. Sections 4 and 5 discuss techniques for identifying some of the unique problems resulting from stochastic emulation. Then in Section 6 we showcase these techniques on a real simulator from the engineering design of buildings.

2 Stochastic Emulation

In this section an increasingly common methodology for emulating stochastic simulators will be outlined; detailed descriptions of deterministic emulation via Gaussian processes are abundant (see O’Hagan, 2006 for one such example).

The principle of deterministic emulation is that the simulator η(x) is modelled as a Gaussian process - for every set of input values, x₁, ..., xₙ, the output values η(x₁), ..., η(xₙ) have a multivariate normal distribution. To build a Gaussian process emulator; a mean function m(x) is constructed, usually in the form m(x) = h(x)^T β where h is a set of basis functions and β is a vector of unknown parameters. A covariance function K(x, x’) is also constructed to model local divergences from the mean function, usually in the form K(x, x’) = α²C(x, x’), where α is a scale parameter, and C(x, x’) is a function for the correlation between output values. An additional variance term δ²(x)Iₓ=x’ can be used as
well, representing normally distributed intrinsic variance of the simulator. For deterministic
emulators this additional variance is either set to zero because a deterministic simulator
definitionally does not have any intrinsic variance; or it is known as the nugget and is set as
a near zero constant, often included for computational reasons (Andrianakis and Challenor
2012).

For stochastic simulators, this nugget $\delta(x)$ no longer needs to be near zero as the
simulator does indeed have some intrinsic variance. Similarly, it no longer needs to be
constant as the intrinsic variance of a computer model may well not be fixed, it could be
different for different input values $x_i$.

Just as the simulator output is modelled as a Gaussian process, the same can then be
done for the intrinsic variance $\delta(x)$. To prevent negative values of $\delta(x)$ appearing, the log
intrinsic variance can be modelled as a Gaussian process instead. This is a modelling choice
made by many (Goldberg et al., 1997; Kersting et al., 2007; Boukouvalas et al., 2014; Binois
et al., 2016), but simpler variance functions can also be chosen (Boukouvalas et al., 2014).

The overall model structure is then given by equation (1)

$$
\eta(x) \sim GP( m(x), K(x,x') + \delta^2(x)I_{x=x'} )
$$

$$
m(x) = h(x)^T \beta
$$

$$
K(x,x') = \alpha^2 C(x,x')
$$

$$
\log(\delta^2(x)) \sim GP( m_\delta(x), K_\delta(x,x') + \sigma^2 I_{x=x'} )
$$

$$
m_\delta(x) = h_\delta(x)^T \beta_\delta
$$

$$
K_\delta(x,x') = \alpha_\delta^2 C_\delta(x,x')
$$

For predictions we condition on observed simulator runs $y = [(y_1) = \eta(x_1), \ldots, (y_n) = \eta(x_n)]$ where $\eta(x_i)$ refers to the $i^{th}$ run of the simulator at input
coordinate $x_i$. Equation (2) gives the predictive equations for the simulator output given
observed runs of the simulator and predicted values for the log intrinsic variances (Binois
et al., 2016), and equation (3) gives predictions for the log variances given estimated values
of the log variance at the input points.

$$
\eta(X^*) | \bar{y}, \delta^2(X^*) \sim \mathcal{N}( h(X^*)^T \beta + K(X^*,X)(K(X,X) + \delta^2(X)R)^{-1}(\bar{y} - h(X)^T \beta),
K(X^*,X^*) + \delta^2(X^*)I - K(X^*,X)(K(X,X) + \delta^2(X)R)^{-1}K(X,X^*) )
$$

$$
\log(\delta^2(X^*)) | \log(\delta^2(X)) \sim \mathcal{N}( h_\delta(X^*)^T \beta_\delta + K_\delta(X^*,X)(K_\delta(X,X) + \sigma^2 I)^{-1}(\delta^2(X) - h_\delta(X)^T \beta_\delta),
K_\delta(X^*,X^*) - K_\delta(X^*,X)(K_\delta(X,X) + \sigma^2 I)^{-1}K_\delta(X,X^*) )
$$

$X$ is the matrix with rows corresponding to input points $x_i$, $X^*$ is the analogous matrix
but for predictive input points $x_i^*$, $\bar{y}$ are the sample means of the simulator outputs at the

$\eta$
Goldberg et al. (1997) initially proposed estimating the numerous unknown parameters of this model via an MCMC / Gibbs sampling scheme. This proves to be too costly in practice, and so numerous efforts have been made to provide faster alternatives, which often rely on fixed ‘plug-in’ estimates in some way (Kersting et al., 2007; Boukouvalas et al., 2014; Binois et al., 2016). In this article, Maximum a Posteriori estimates for the parameters are used, via the optimizing function provided by Stan (Stan Development Team, 2015). Similarly, to maintain an analytic solution for the predictions, $\delta^2(X^*) | \delta^2(X)$ is taken as fixed at its expectation $E[\delta^2(X^*) | \delta^2(X)]$. These modelling choices are done for practical purposes, but a full Bayesian acknowledgement of uncertainty would be preferable if it were computationally feasible. The mean functions are both taken to be linear ($h(x)^T \beta = \beta_0 + x^T \beta ; h_\delta(x)^T \beta_\delta = \beta_{\delta 0} + x^T \beta_\delta$) and the correlation functions are both taken to be the squared exponential ($K(x,x') = \prod_{i=1}^d \exp(-\frac{(x_i-x'_i)^2}{l_i^2})$; $K_\delta(x,x') = \prod_{i=1}^d \exp(-\frac{(x_i-x'_i)^2}{l_{\delta i}^2})$ where $d$ is the dimension of the input points, and $l_i$ is known as a length scale parameter).

Multiple assumptions have been made in the above model formulation. Firstly, a stationary covariance function is often chosen for both $K(x,x')$ and $K_\delta(x,x')$; it is assumed that the intrinsic variance of the simulator is Gaussian; it is also assumed that our uncertainty about the log variance and the simulator output can be modelled as Gaussian processes; and finally, we have also estimated a considerable number of parameters - which includes the estimates for the intrinsic variances at the input points. These are all assumptions and estimates which may or may not be reasonable, and so it is required that any emulator constructed with assumptions like these must be validated before it is used.

In subsequent sections, it will be useful to be able to distinguish between two types of uncertainties that are present in stochastic emulators. There is epistemic uncertainty, which is our own personal uncertainty about the simulator response, which is also present in deterministic emulators. For stochastic emulators there is also the intrinsic variance that the stochastic simulator has, which for simplicity shall be referred to as the aleatoric uncertainty, which is not present in deterministic emulators. Another way of viewing these two different uncertainties is that the epistemic uncertainty is uncertainty the statistician has brought in by using an emulator to model the simulator; and the aleatroic uncertainty is uncertainty the practitioner has brought in by using stochasticity in their simulator to model the real world. Kennedy and O’Hagan (2001) refer to the epistemic uncertainty instead as “code uncertainty”. We do not use this term in this article, because it can be conflated with “uncertainty within the code”, rather than “uncertainty about the code”.

\begin{equation}
\beta_i \sim N(0,10) ; \quad \beta_{\delta i} \sim N(0,10) \\
\alpha \sim \text{Gamma}(4,1) ; \quad \alpha_\delta \sim \text{Gamma}(4,1) \\
l_i \sim \text{Gamma}(4,4) ; \quad l_{\delta i} \sim \text{Gamma}(4,4) \\
\sigma^2 \sim \text{HalfNormal}(0,1)
\end{equation}
The chosen term “epistemic uncertainty” could be conflated with the discrepancy between the simulator and the real world, but such model discrepancy is not discussed in this article, and so the chosen term remains acceptable.

3 Deterministic Diagnostics

Bastos and O’Hagan (2009) presented several diagnostic tools for identifying problems with a deterministic emulator. Separate simulator runs, \( y^* = [(y^*_1)_1 = \eta(x^*_1)_1, \ldots, (y^*_r)_r = \eta(x^*_r)_r], \) which were not used to fit the emulator, are compared to emulator predictions. If these observed validation data points seem reasonable compared to emulator predictions, then confidence is gained in the emulator’s ability to represent the simulator. The diagnostics presented included the Mahalanobis distance; plots of the individual standard errors, uncorrelated standard errors (such as the pivoted Cholesky errors); the QQ plot; and credible interval statistics. More recently, Al-Taweel (2018) added the graphical coverage interval diagnostic as an extension of the credible interval diagnostic.

As an example of one of these diagnostics developed for deterministic emulators, the individual standard errors are given by

\[
D_{i,j}^I(y^*) = \frac{(y^*_i)_j - E[\eta(x^*_i)|\bar{y}]}{\sqrt{V[\eta(x^*_i)|\bar{y}]}}
\]  

where \( V[\eta(x^*_i)|\bar{y}] \) is the variance of the predictions at \( x^*_i. \) These should be normally distributed with mean 0 and variance 1. Any \( D_{i,j}^I(y^*) \) with absolute value greater than 2 is thus an unlikely value, with less than a 1 in 20 chance of happening, and potentially suggests a local problem with the emulator. Similarly, in a large sample of validation points, very few standard errors with values greater than 2 suggests the emulator’s uncertainty is too large as we do expect roughly 5% of points to be outside 2 standard deviations.

These diagnostics all work well for the deterministic emulators they were designed for, and they can also be applied to stochastic emulators, as the response distribution is still a Gaussian process (equation 2). However, just as stochastic simulators are more difficult to model, they are also more difficult to validate, and diagnostics are less easy to interpret - a single simulator run \( \eta(x^*_i)_j \) is less informative for the simulator at \( x^*_i \) compared to a single run \( \eta(x^*_i)_j \) of a deterministic simulator.

To provide an example for this, a stochastic emulator will be constructed for the toy simulator given by equation 6.

\[
\eta(x) = \sin(16x) + \cos(24x) + 8x + 2x\epsilon \\
\epsilon \sim N(0, 1)
\]  

Using 30 training points, stochastic emulator predictions can be obtained (top of figure 1). Because the toy simulator is simple and cheap to evaluate, the true function is also superimposed.

Clearly this emulator does not capture the detail from the simulator, and instead has a simple, approximately linear predicted mean function, with a predicted variance function
Figure 1: Emulator predictions of the toy simulator using only 30 training points (top), and the respective noiseless mean emulator predictions (bottom). Emulator predictions are in blue, with 95% prediction intervals shaded. The true simulator is in black with 95% prediction intervals shaded where relevant. Black points represent simulator runs used to fit the emulator, red points represent runs used to validate the emulator.

that is consistently too large. This emulator may not be particularly useful due to its simplicity, but a large amount of epistemic uncertainty is not grounds to invalidate an emulator. In this case however, the emulator has in fact overestimated the aleatoric variance and is overconfident in its simplistic mean function. Figure 1 also plots the emulator’s predictive interval for the mean function alone, excluding the aleatoric variance, using the noiseless predictive equations given in equation 7.

$$
\eta(X^*) \mid \bar{y}, \delta^2(X^*) \sim \\
N( h(X^*)^T \beta + K(X^*, X)(K(X, X) + \delta^2(X)R)^{-1}(\bar{y} - h(X)^T \beta), \\
K(X^*, X^*) - K(X^*, X)(K(X, X) + \delta^2(X)R)^{-1}K(X, X^*) )
$$

These are the same as the ‘stochastic kriging’ equations [Ankenman et al. 2010], and the only difference to the previous predictive equations from equation 2 is that the additional noise at the prediction points $\delta^2(X^*)I$ is missing. This gives us the predictions for what the
emulator believes the mean of the simulator output could be for different input points, and so the only uncertainty here is the *epistemic* uncertainty surrounding this mean function.

Here, the true mean function is outside the 95% interval for the emulator mean 45% of the time, and so the emulator is far too confident in the mean being quite linear. The simplicity in the emulator is not because of a large degree of *epistemic* uncertainty, the emulator is instead fairly certain but about the wrong mean-variance structure. Because of this, it is difficult to call this emulator ‘valid’, so ideally diagnostics should detect some issues. This problem is similar to that found in deterministic emulation where the nugget parameter can be estimated to be too large, allowing local features of a deterministic simulator to be disregarded as observational noise (Andrianakis and Challenor, 2012).

Figure 2 shows select graphical diagnostic plots from Bastos and O’Hagan (2009) produced using 20 validation points. The exact input and output values of these points can be seen in figure 1. None of these plots seem to identify any problems - the standard errors seem like white noise, with only 1 standard error with absolute value greater than 2, and only by a small margin. There similarly doesn’t seem to be any significant patterns or extreme values in the Cholesky errors, and the QQ plot appears like a straight line with no huge systematic deviations. Also shown in figure 2 is the coverage diagnostic from Al-Taweel (2018), which likewise has no huge deviations from the straight line, and no points outside their respective intervals. The Mahalanobis distance is 1.180, which is within the inter-quartile range of the reference distribution (0.743, 1.315).

These diagnostics do not identify any problems with the emulator, despite it being clear from direct observation of predictions that the emulator does not adequately recreate the simulator. In higher dimensions it becomes harder to directly observe the predictions, and in practical examples the emulator cannot simply be compared with the truth as done here (as otherwise there was little reason to construct an emulator to begin with). As such, without additional tools, an emulator like the one in figure 1 could be validated, leading to inaccurate conclusions being made about the simulator.

If confidence in a stochastic emulator’s ability to represent a simulator is needed, new tools are required to check the fit of an emulator. In the next section we will discuss some additional techniques that help identify the problems found above.

### 4 Stochastic Diagnostics

The goal of this section is to outline methods for separately validating an emulator’s fit of the mean and an emulator’s fit of the heteroscedastic variance. As the previous section showed, attempting to only validate the overall performance of the emulator can fail to identify specific problems with the mean fit and/or the variance fit, which can then disguise each other. Not only may this still lead to a poor assessment of the emulator’s overall fit; but the individual accuracy of the emulator’s mean (or the emulator’s variance) may be of specific interest if subsequent analysis relies on this particular component being accurately modelled.

At this point it is important to note that the heteroscedastic emulator model from equation 1 assumes the additional noise of the simulator is normally distributed. The QQ
plot used by Bastos and O’Hagan (2009) is one way of testing this normality assumption, and such normality checks should still be conducted just as they should be done any time data is assumed to be normal.

4.1 Mean Validation

The previous diagnostics relied on obtaining values of the simulator output at new validation points $x^*_i$, and then checking whether the emulator’s predictions agreed with these observed true values. We are unable to directly observe the true simulator mean at $x^*_i$ to validate the emulator’s predictions for the mean, but with at least one repeat validation run, the sample mean $\bar{\tilde{y}}^*_i = \frac{1}{r^*_i} \sum_{j=1}^{r^*_i} \tilde{y}^*_{i,j}$ can be calculated. These observed sample means then contain information about what the true mean is, albeit with some observational noise.

If a random variable $Z$ is normally distributed ($Z \sim N(\mu, \sigma^2)$), then the sample mean $\bar{Z}$ calculated from $n$ samples is also normally distributed but with a smaller variance ($\bar{Z} \sim N(\mu, \sigma^2/n)$).
Therefore, the emulator’s prediction for the sample mean remain Gaussian, and can be obtained via the equation given by $^8$

$$
\bar{\eta}(X^*) \mid \bar{y},\, \delta^2(X^*) \sim \n( h(X^*)^T \beta + K(X^*, X)(K(X, X) + \delta^2(X)R)^{-1}(\bar{y} - h(X)^T \beta),
K(X^*, X^*) + \delta^2(X^*)R^* - K(X^*, X)(K(X, X) + \delta^2(X)R)^{-1}K(X, X^*) )
$$

$R^*$ is a diagonal matrix with entries $1/r_i^*$ corresponding to the reciprocal of the number of simulator runs used to calculate the validation data sample means $\bar{y}_i^*$. This equation can either be viewed as: the same as the original stochastic emulator predictions from equation $^2$ but with the noise variance greatly reduced (by dividing $\delta^2(x_i^*)$ by $r_i^*$); or the equation can be viewed as the noiseless mean predictions from equation $^7$ but with a portion of the additional noise at the prediction points $(\delta^2(x_i^*)/r_i^*)$ re-added. Regardless, as the number of repeats increases, the additional noise contributed from $\delta^2(X^*)R^*$ decreases towards 0 and the equations become like those for the noiseless mean predictions; and if no repeats are used ($r_i^* = 1$), then the predictive equation is exactly equivalent to the emulator predictions for the raw simulator output.

Because the sample mean predictions still have a Gaussian distribution, the diagnostic tools developed by Bastos and O’Hagan (2009) and Al-Taweel (2018) can now also be applied to the sample means. With many repeats $r_i^* - 1$, this almost becomes equivalent to using values of the true mean to validate the emulator’s predictions for the mean, using the same diagnostics previously used to validate the overall performance of the emulator. Even with very few repeats these diagnostics can still identify issues that may not have been discovered applying the diagnostics to raw simulator runs with no repeats.

For example, say that simulator runs $y_{i,1}^*$ and $y_{i,2}^*$ are both obtained using the same input values. Both are observed to be much larger than expected, but not quite large enough for either to yield an individual standard error with value larger than 2, because the predictive standard deviation for the simulator runs is also large. The sample mean $\bar{y}_i^* = (y_{i,1}^* + y_{i,2}^*)/2$ will also be larger than expected, but the respective predictive standard deviation will be smaller. This causes the standard error for the sample mean to be larger and thus more likely to have a value greater than 2. In this way, the individual standard errors of the sample means acknowledge that it is unlikely for several simulator runs obtained from the same input values to all have unexpectedly large or small values, whereas individual standard errors of the raw simulator runs ignore this information.

In this way, sample mean diagnostics can more easily identify issues - the idea being that as $r_i^*$ increases, we tend towards attempting to validate the predictions in the bottom of figure $^2$ as opposed to the predictions in the top of figure $^1$. This is an easier task because a greater percentage of the truth lies completely outside the respective emulator predictive interval.
4.2 Variance Validation

It is also desirable to validate the emulator’s predictions for the variance. Just as before, we also cannot observe the true variances, but with repeats the sample variances $\hat{S}^2(x^*_i) = \frac{1}{r^*_i - 1} \sum_{j=1}^{r^*_i} (y_i^* - \bar{y}^*_i)^2$ can be calculated. These sample variances then contain information about the true variance at $x^*_i$, which can be compared to the predictions of the aleatoric variance $\delta^2(x^*_i)$.

Predictive values of the sample variance $S^2(x^*_i)$, given $\delta^2(x^*_i)$, can be generated via:

$$\frac{(r^*_i - 1)S^2(x^*_i)}{\delta^2(x^*_i)} \sim \chi^2_{r^*_i - 1}$$

This yields predictions of the sample variances at $x^*_i$ as if they were calculated using $r^*_i$ simulator runs. The observed $\hat{S}^2(x^*_i)$ can then be compared to this predictive distribution for $S^2(x^*_i)$.

$S^2(x^*_i)$ does not have a Gaussian distribution, so detailed diagnostics like those from Bastos and O’Hagan (2009) are more difficult. However, the credible interval diagnostic is still applicable. A credible interval diagnostic is a check to see whether a sensible number of observed validation points lie within their respective credible intervals. If too few (or too many) observed points lie inside the credible interval, then that suggests the credible interval maybe too small (or too large), and thus there is a problem with the emulator predictions. Because our primary motivation is to check whether the intrinsic variance $\delta^2(x^*_i)$ is in general overestimated (or underestimated), the number of observed sample variances $\hat{S}^2(x^*_i)$ less than the median of the emulator’s predictive sample variance distribution $S^2(x^*_i)$ is a descriptive statistic. This diagnostic is given by:

$$D_S(y^*) = \frac{1}{v} \sum_{i=1}^{v} \mathbb{1}(\hat{S}^2(x^*_i) < M_i)$$

Where $\mathbb{1}(\cdot)$ is an indicator function, and $M_i$ is the emulator’s predictive median for $S^2(x^*_i)$. We expect this credible interval diagnostic $D_S(y^*)$ to be close to 0.5. If $D_S(y^*)$ is much larger than 0.5, and therefore much more than 50% of observed sample variances lie beneath the median, then we can assume, in general, that the median is estimated to be too large and thus the intrinsic variance $\delta^2(X^*)$ is, in general, too large. Too small predictions for $\delta^2(X^*)$ can similarly be identified. This ‘less than median’ diagnostic $D_S(y^*)$ provides an overall measure of whether $\delta^2(X^*)$ is more often overestimated than underestimated (and vice-versa).

This $D_S(y^*)$ diagnostic only checks, across the whole of the input space, whether the predicted variance is bigger than the truth as often as it is smaller, or vice-versa. For more local problems, a check for whether there are specific regions of the input space where the variance is likely to be overestimated (or underestimated) can be useful. The probability that the emulator’s sample variance predictions are larger than the observed sample variances:

$$D^P_S(y^*) = P(S^2(x^*_i) > \hat{S}^2(x^*_i))$$

can be useful. These probabilities $D^P_S(y^*)$ can be calculated by obtaining many predictive samples of $S^2(x^*_i)$ and calculating the proportion that are greater than $\hat{S}^2(x^*_i)$. These
\(D_i^P(y^*)\) probabilities can be plotted against the input values \(x^*_i\), and should look like noise around 0.5. Extremely large (or extremely small) values for the probability indicate that the emulator believes the observed sample variance was surprisingly small (or surprisingly big). Regions where \(P(S^2(x^*_i) > \hat{S}^2(x^*_i))\) is frequently larger (or smaller) than 0.5 therefore imply local issues with overestimated (or underestimated) predictive aleatoric variance. This is because observing many nearby sample variances that are smaller (or bigger) than expected is an unlikely event to occur, and is thus more likely to be due to poor predictions of the variance than it is to be because of random chance.

### 4.3 Example

For the same poorly fitting emulator from before, using a set of 20 validation points again, but this time made up of 10 unique coordinates each with one repeat (\(r^*_i = 2\) for all \(i\)), we can obtain these new mean and variance diagnostics.

Figure 3 provides graphical diagnostics for the sample means. These seem to identify issues with the emulator - the individual standard errors and Choleksy errors both have 2 points with absolute values greater than 2. Considering this validation data set only has 10 unique coordinates in total, this is a very high proportion. The QQ plot and coverage diagnostic also both show some (but not huge) divergences from the straight line \(y = x\).

8 out of the 10 observed sample variances have values less than the predicted median \((D_S(y^*) = 0.8)\), which is much more than the expected 5, suggesting that the variance function is overestimated. The plot of \(P(S^2(x^*_i) > \hat{S}^2(x^*_i))\) is given in figure 4. This plot also shows how in general the variance is overestimated as there are clearly more points with \(P(S^2(x^*_i) > \hat{S}^2(x^*_i))\) greater than 0.5. Another trend that can be seen from this plot is that the variance appears to be more overestimated towards the boundaries of the input space, with the predictions of the variance possibly more accurate closer to \(x = 0.5\). With only 10 unique input coordinates this conclusion is difficult to make with much confidence, but in this instance, this observation is nonetheless representative of the truth, as we can see from figure [1] that the variances are in fact overestimated by a larger margin towards the boundaries of the input space.

These diagnostics do indeed now bring some attention to the idea that the mean function might be poorly estimated, and the variances overestimated, something which previous diagnostics did not identify. With only 10 unique validation coordinates, confidence in such conclusions is decreased, but for problems as severe as the one above, fewer unique coordinates proves to be an acceptable cost.

It is important to acknowledge that utilising repeat points will take up part of the validation data budget that could be used for more unique validation coordinates, but this previous example shows how this can be a necessary trade off - despite only 10 unique validation locations, as opposed to the 20 from before, the poorly estimated mean and overestimated variance in the emulator is now more easily diagnosed.
Figure 3: Sample mean graphical diagnostics for the emulator of the toy simulator using only 30 training points. diagnostics are: standard errors against input point (top left), pivoted Cholesky errors against pivoting order (top right), QQ plot (bottom left), and the coverage diagnostic (bottom right).

5 Validation Design

The obvious question is then: how should validation points be chosen? How many repeats should be used, and where should they be placed? At least one repeat is required per unique validation coordinate for the above diagnostic methods to be used. Additional repeats provide more accurate sample mean and sample variance estimates, and are thus more informative as to how well fitting the emulator is at that point. On the other hand, more repeats will result in fewer unique validation coordinates, yielding a less space filling validation design. In this section, one method for choosing the number and location of repeated validation runs is outlined.

The sampling standard deviation of the sample mean is $\sqrt{\delta^2(x^*_i)/r^*_i}$, and the sampling standard deviation of the sample variance is $\delta^2(x^*_i)\sqrt{2/(r^*_i - 1)}$. Both of these decrease approximately with respect to $\sqrt{r^*_i}$, therefore, adding additional repeat points improves the accuracy of the sample mean and sample variance by approximately the same amount.

As the sample mean has a simpler, Gaussian, distribution repeats will be chosen to
Figure 4: $P(S^2(x^*_i) > \hat{S}^2(x^*_i))$ for the emulator of the toy simulator using only 30 training points using 20 validation points (10 unique coordinates each with one repeat).

improve the quality of the sample mean diagnostics. However, this should also result in improvements in the accuracy of the sample variances.

To visualise the benefit additional repeats provide, figure 5 plots the predicted emulator mean, emulator mean 95% prediction intervals, and the emulator sample mean 95% intervals. This is done for each prediction point having 2 repeats, and each point having 10 repeats. Superimposed on this plot is the true mean and the true sample mean 95% intervals.

The true sample mean distribution and the emulator sample mean predictions are evidently more noticeably different when 10 repeat points are used to calculate the sample means. With 10 repeat points, there are a numerous locations where the true mean lies completely outside the sample mean prediction intervals, and a few locations where the true sample mean 95% interval and the emulator sample mean interval do not overlap at all. This makes it far more likely that randomly selected validation coordinates will clearly show an emulator misspecification. This is because the epistemic uncertainty is no longer dominated by the aleatoric uncertainty from the sample mean, and so differences between the truth and the predictions are no longer ‘hidden’ by the additional uncertainty.

This plot also demonstrates the risk in interpreting the mean diagnostics if too few
Figure 5: Emulator mean and sample mean predictions of the toy simulator using only 30 training points, using 2 repeats at each prediction point (top), and 10 repeat points (bottom). Emulator predictions are in blue, with 95% prediction intervals shaded dark blue, sample mean predictions shaded light blue, and the true simulator is in black with 95% prediction intervals also shaded black.

repeat validation points are used - with only one repeat, the sample mean predictions are not too dissimilar to the raw simulator predictions, and thus the sample mean diagnostics are only marginally preferred to the default diagnostics when no repeats are used.

A very large number of uniform repeat points is clearly not viable for most practical cases, but the example proves helpful in understanding why extra repeat points can be useful - it is desirable to not have the *aleatoric* uncertainty that arises from our sampling of validation sample means and sample variances dominate the *epistemic* uncertainty we actually want to validate. Because an important part of the sample mean diagnostics (and the above plots) is the interval constructed by 2 standard deviations, this will be the quantity used to select repeat points. Other values and thresholds can be used instead, ultimately the aim is only to construct a design that adds more repeats where the aleatoric uncertainty is predicted to be large compared to the epistemic uncertainty.

The constructed validation design scheme chooses the number of repeats \( r_i^* \) at the validation coordinate \( x_i^* \) such that the inequality \( \sigma_\delta(x_i^*) < 2\sigma_\eta(x_i^*) \) holds. \( \sigma_\delta(x_i^*) \) is the
standard deviation of the noiseless predictions of the mean at a validation point \( \mathbf{x}_i^\ast \) (which can be calculated from equation 7) and \( \sigma_{\eta}(\mathbf{x}_i^\ast) \) is the standard deviation of the noisy predictions of the sample mean (predictions given by equation 8). If this inequality holds, then the total emulator uncertainty of the sample mean is no more than twice the total emulator uncertainty for the true mean. The predictive uncertainty of the sample mean will clearly always be larger than the predictive uncertainty for the true mean, because the uncertainty surrounding the sample mean includes the epistemic uncertainty surrounding the true mean as well as the aleatoric sampling uncertainty; but the inequality limits how much more uncertainty can be included by only observing sample means rather than the true mean. Increasing the number of validation repeat points \( r_i^\ast \) will decrease the value of \( 2\sigma_{\eta}(\mathbf{x}_i^\ast) \), which will in turn increase the chance that the inequality holds. Therefore, using this inequality to choose the number of repeats \( r_i^\ast \) will add additional repeat points to validation points where the aleatoric uncertainty is initially large compared to the epistemic uncertainty.

In visual terms referring back to figure 5, the inequality \( \sigma_{\delta}(\mathbf{X}_i^\ast) < 2\sigma_{\eta}(\mathbf{X}_i^\ast) \) forces the light blue intervals to be less than twice the size of the dark blue intervals. This inequality can be rewritten as \( \sigma_{\eta}(\mathbf{X}^\ast) - \sigma_{\delta}(\mathbf{X}^\ast) < \sigma_{\delta}(\mathbf{X}^\ast) \), which is equivalent to ensuring the light blue intervals excluding the dark blue intervals must be smaller than the dark blue intervals alone.

Other thresholds could be chosen for the inequality - the chosen threshold was selected to force the additional aleatoric uncertainty to be, at most, equivalent in magnitude to the epistemic uncertainty, but it is by no means the only choice. The inequality could instead be \( \sigma_{\delta}(\mathbf{x}_i^\ast) < 1.5\sigma_{\eta}(\mathbf{x}_i^\ast) \) which would weight towards more repeat points being chosen, or \( \sigma_{\delta}(\mathbf{x}_i^\ast) < 0.5\sigma_{\eta}(\mathbf{x}_i^\ast) \) which would weight towards less repeat points being chosen, for example.

There are then a few possible ways to incorporate this inequality into a validation design scheme. In this work, the following scheme is used: a unique validation coordinate is chosen; the minimum number repeats needed to ensure that \( \sigma_{\delta}(\mathbf{X}^\ast) < 2\sigma_{\eta}(\mathbf{X}^\ast) \) is calculated (and constrained to at least 1 repeat); and then the next coordinate point is chosen. This is repeated until the validation budget is exhausted. If at any step the number of required repeats would exceed the validation budget, then that coordinate point is assigned the remainder of the validation budget instead.

Doing this for the poorly fitting toy emulator example, using a Sobol sequence (Bratley and Fox, 1988) to choose the validation coordinates, and a total validation budget of 20, yields a validation design of 5 unique coordinates, with the number of repeats roughly increasing as \( \mathbf{x}_i^\ast \) increases. (Going from the smallest \( \mathbf{x}_i^\ast \) to the largest: \( r_i^\ast = 3, 4, 4, 5, 4 \). The largest \( \mathbf{x}_i^\ast \) would’ve been assigned an additional repeat point if not for the validation budget being exhausted). The respective sample mean diagnostics are then plotted in figure 6.

With only 5 coordinates the QQ plot and coverage plot become less informative, but the trade-off for this is that the individual and Cholesky error plots more confidently identify issues in the emulator - 2 out of 5 individual standard errors have absolute value greater than 2, one of which has an incredibly high value of \( \sim 4 \). It is thus more clear that the emulator is definitely not a good representation of the simulator.

This idea of using more repeat validation runs in areas of high aleatoric variances can be
very effective at identifying local problems with a stochastic emulator. There is a concern however, that the number of space filling points will then not be sufficient - validation coordinates must check the quality of the fit of the emulator throughout the input space, otherwise local issues of the emulator may be missed. Similarly, the QQ plot and the coverage diagnostic rely on there being an acceptably ‘large’ number of data points, and so become less informative as the number of unique validation coordinates decreases. A similar requirement exists for the sample variance diagnostics $D_S(y^*)$ and $D_P^i(y^*)$, hence their exclusion in the most recent example.

Accordingly, a constraint can also be applied requiring a minimal number of unique validation coordinates be chosen. If this minimum would not normally be reached, then the simulator can be run at the minimum number of unique validation coordinates instead. Repeats can then be distributed one at a time to each validation coordinate, until that coordinate’s required number of repeats is reached, or until the budget is exhausted. This is what is done in practice in the next section.

In cases where the validation budget is small, such as in the previous example, it can be
preferable to constrain the number of unique validation coordinates to be disproportionally large compared to the total budget. Without such a constraint, the QQ plot, coverage plot, $D_S(y^*)$, and $D_P(y^*)$ become much less informative; and the diagnostic value of the mean standard error plots depends highly on the specific locations of a few unique validation coordinates. When a larger validation budget is available, which one would expect for higher dimensional simulators, a smaller percentage of the validation budget needs to be intentionally constrained as unique validation coordinates before the QQ plot, coverage plot and sample variance diagnostics become viable again. Because of this, any validation design that attempts to make use of a larger number of repeats (such as the above scheme) is naturally more suited to situations where the validation budget is sufficiently large.

6 Building Performance Simulator

In this section, a building performance simulator will be used to showcase these diagnostic tools on a “real” example. A building performance simulator models output variables of a building, such as the internal temperature, given the physical shape and design of the building, and a description of the weather. EnergyPlus is one such building performance simulator ([US Department of Energy] [2010]). One use of this simulator is to estimate how much energy a planned building may use in a given time frame. We have ‘designed’ a very simple building using a reference hospital design ([Field et al.] [2010]). The building is given an “ideal loads” heating and cooling system, and we are interested in seeing how selected variables can affect the total energy usage of the building over a year. The simulator takes approximately a minute to run, and there are 5 input variables we would like to investigate: wall concrete thickness (input 1), wall insulation thickness (input 2), roof insulation thickness (input 3), floor concrete thickness (input 4), and the height of the windows as a ratio of the wall height (input 5). All the inputs are rescaled to be between 0 and 1. Of particular interest for this study is to also see how varying weather affects the variability of the output, and so the weather input is sampled randomly each time the simulator is run, resulting in a simulator that provides a different output value each time it is run regardless of whether the other input variables remain the same.

As the simulator takes a non trivial amount of time to run, and we wish to run this simulator many times, we model the simulator using the emulator described in section 2. 150 training data points are simulated, using a maximin Latin hypercube design ([McKay et al.] [2000]), which are used to fit the emulator. Validation points are chosen via the adaptive scheme, with a constraint of at least 10 unique coordinates, and a maximum of 100 validation points. This resulted in 43 unique validation coordinates, only six of which were given more than 1 repeat value (i.e. 2 runs); 2 receiving 2 repeats, and 2 receiving 3 repeats, 1 received 5 and 1 received 6. To validate the fit of the emulator, the diagnostics outlined previously are then used. Figure 7 shows the individual sample mean standard errors against each of the inputs. Figure 8 shows $P(S^2(x^*_i) > \hat{S}^2(x^*_i))$ against each of the inputs.

The sample variance diagnostic $D_S(y^*)$ has a value of 0.23, which is very small, suggesting that the predicted $\delta^2(x^*_i)$ values are too small on average. The plot of $P(S^2(x^*_i) > \hat{S}^2(x^*_i))$
Figure 7: Sample mean standard errors against the inputs for the emulator of the building simulator using 150 training points and 100 validation points (43 unique validation coordinates) chosen via the adaptive scheme. Black points represent validation points generated using 1 repeat, blue represents 2 repeats, and purple represents 3 or more repeats.

\( \hat{\sigma}^2(x^*_i) \) for input 2 shows a significant spatial trend for the underestimated variance. For very low values of input 2, the variance seems to be overestimated, and for higher values it is certainly underestimated. The individual sample mean standard error plots in figure 7 show 6 standard errors with absolute values greater than 2, and one standard error has a very high value of 5.05, which is an extremely unlikely event. Together, this information suggests some significant issues with the emulator, and thus the emulator should be improved before it is used.

With only one highly extreme sample mean standard error in a 5 dimensional space, it becomes difficult to identify if any one input dimension is responsible for the emulator’s poor fit. Input 2 also has a trend of increasing standard errors as the input value gets very small, and all of the validation coordinates with more than one repeat have very small values for input 2. This, coupled with the previously discussed trend from the sample variance plots, suggests that the emulator misspecification may mostly be related to input 2. The variance appears overestimated for low values of input 2, the extremely large standard error for the mean function is for a low value of input 2, and the standard errors for the
mean are increasing for low values of input 2. Because of this, we could conclude that
the emulator has failed to identify a large change in the mean function and was instead
‘tricked’ into believing large observed training simulator values for low values of input 2
arose because of an increased variance. This would cause the emulator’s mean function to
be poorly estimated for low values of input 2 as it fails to capture the large change in the
mean, and the variance would then also be overestimated for low values of input 2, which
is indeed what we see from the diagnostics.

If we were to believe such conclusions, the rest of the emulator then appears acceptable,
albeit with an underestimated variance. Therefore, if the recommended modifications to
this emulator were not feasible, using this emulator to come to conclusions about the
simulator’s mean for non-small values of input 2 might be tolerated, even though this
would not be ideal.

For this example, underestimated variances is an easier problem to detect, and might be
identified by the diagnostics from [Bastos and O’Hagan (2009)] because individual standard
errors would likely be large (as the predictive variance would be too small). However, even
in this case, the mean and variance diagnostics are more informative - providing additional insight into how the emulator fails to represent the truth, and to what extent it still does recreate the simulator.

Regardless, we conclude that this emulator is not adequate, and so the validation data is merged with the training data, and an additional set of 100 data points chosen via a maximin Latin hypercube design is added. This increase in training data should then yield a better fitting emulator. Instead of requiring additional simulator runs, we could have instead tried modifying the prior mean structure \( h(x) \), say by adding a logarithmic transformation of input 2 term (or similar), which would incorporate our belief that the simulator response changes rapidly for low values of input 2. If this were to work, this would be an efficient solution, making use of the additional information obtained from the diagnostics. For simplicity and clarity, and because this simulator is not restrictively expensive, additional input points are instead the chosen solution.

The new emulator, trained using this larger data set, can again be used to adaptively generate another validation data set of size 100 (with a minimum of 10 unique coordinates), continuing the Sobol sequence used to generate the previous validation dataset so that validation coordinates remain separate to the training data coordinates. This resulted in 37 unique validation coordinates, twenty of which have more than 1 repeat. This already suggests that the aleatoric variance is estimated as larger than before.

Figures 9 and 10 show the graphical diagnostics for the emulator fitted to this larger dataset.

The percentage of sample variances beneath the predicted median is now 54%, which is not too far from 50%, and so overall the variance does not appear to be significantly overestimated or underestimated. Neither figure 10 or 9 suggest any major issues with the emulator either. There is only one standard error with absolute value larger than 2, and it is only marginally so. This corresponds to 2.7% of the validation coordinates having absolute value larger than 2, which is somewhat smaller than 5%, which suggests the mean prediction may be slightly underconfident. The plots of \( P(S^2(x^*_i) > \hat{S}^2(x^*_i)) \) show no notable patterns either.

With these diagnostics we could then conclude that this emulator adequately represents the simulator. In practice we could alternatively choose to add more points if desired, to further improve the fit of the emulator, and we may want to also add the validation points to the training data and refit a final emulator to this merged dataset, but this is not essential.

7 Conclusions

We have shown that stochastic emulators can be difficult to validate, just as they can be difficult to fit. The principle idea given is that repeat validation simulator runs at validation coordinates provide greater insights into the performance of an emulator, and this can be more useful than simply increasing the number of unique validation coordinates.

We showed how applying previously developed emulator diagnostics to the sample means, instead of individual simulator runs, can be valuable in diagnosing problems in the emulator’s mean predictions. We also implemented additional diagnostics for the sam-
Figure 9: Sample mean standard errors against the inputs for the emulator of the building simulator using additional training points and 100 validation points (37 unique validation coordinates) chosen via the adaptive scheme. Black points represent validation points generated using 1 repeat, blue represents 2 repeats, and purple represents 3 or more repeats.

An added benefit of the diagnostics here is that they separately check the mean and variance functions. Thus if we are more interested in the mean than the variance, we can prioritise the importance of one set of diagnostics over the other, and vice versa.

An issue with these diagnostics is that local issues with the variance function are harder to diagnose. As well as this, it can still be possible to validate an invalid emulator: validation coordinates can, by chance, be chosen in areas where the emulator is indeed valid, but problems may exist in other areas of the input space. Similarly, although a validation coordinate may be correctly chosen in an area where the emulator has poor fit, the valida-
Figure 10: $P(S^2(x^*_i) > \hat{S}^2(x^*_i))$ against the inputs for the emulator of the building simulator using additional training points and 100 validation points (37 unique validation coordinates) chosen via the adaptive scheme. Black points represent validation points generated using 1 repeat, blue represents 2 repeats, and purple represents 3 or more repeats.

This simulator runs for this coordinate may, simply by chance, provide sample means and sample variances that agree with the emulator’s predictions. These problems in validation mostly arise due to the difficulty in such a task. Given such difficulty, the diagnostics presented here do appear to be capable and economical; when used in conjunction with previously developed diagnostics for deterministic emulators, these stochastic diagnostics provide a varied and descriptive set of tools for assessing the fit of a stochastic emulator.

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