# GP Emulator for FE simulator

## Overview

Currently, our aim is to produce a Gaussian process emulator trained on the output of the finite element model of tip deflection, rotation, and cost of a wind turbine blade. The Gaussian process emulator will be used to estimate the optimal calibration parameters to minimize tip deflection and rotation. The calibration parameters currently under consideration are volume fraction and thickness. The optimization of the calibration parameters will be effected by use of a Markov chain Monte Carlo algorithm.

## Background: Gaussian processes

Gaussian processes can be thought of as generalizations of multivariate normal random variables. Whereas a multivariate normal random variable is a random vector of finite length, a Gaussian process is a random function. The value of the function at any finite selection of points is itself a multivariate normal random variable. Just as a multivariate random variable is characterized by its mean vector and covariance matrix, a Gaussian process is fully characterized by its mean function and covariance function , where is the domain of the process. Thus for any points in the domain of the Gaussian process, gives the mean of the Gaussian process at , and gives the covariance between the values of the Gaussian process at points and . As a special case, then, gives the marginal variance of the Gaussian process at .

## Background: Gaussian process regression

The use of Gaussian processes to produce a computationally efficient predictor   of expensive computer code given observations of code output at is promulgated by (Sacks, Welch, Mitchell, & Wynn (1989) and explored at length by Santner, Williams, & Notz (2003). When using a Gaussian process as an emulator for a finite element model, we essentially perform Gaussian process regression on some observations from the finite element simulator. In this way, the Gaussian process is “trained” on the observations coming from the finite element model; i.e., the mean function and covariance function of the Gaussian process are updated to accommodate those observations . The resulting Gaussian process interpolates the observations from the finite element model, and allows prediction at points not observed. Uncertainty at unobserved points is quantified by the updated covariance function.

Suppose, for example, that we have observations at points . We may begin with a Gaussian process with constant mean function . Notice that we may use our covariance function to define an matrix such that the entry of is equal to . We may wish to train our Gaussian process on these observations, and then examine the resulting Gaussian process at the points . Recall that the Gaussian process at the points is a multivariate normal random variable of length , which is fully characterized by its mean vector and covariance matrix . We can find these as:

A visualization of this example can be found in Figure 1. Here, .

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| C:\Users\carle\AppData\Local\Temp\gp2.png  Figure 1: Gaussian process trained on five observations. The mean function is given in red, and 100 draws are given in gray. The spread of the gray draws illustrates the uncertainty at each point. |

## Gaussian processes for computer model calibration

Often, when creating a simulator of some phenomenon , the simulation will depend upon some unknown quantity . For example, consider modeling the physics of particle interactions in an environment in which the outcomes are extremely sensitive to small changes in the strength of gravity in the locale of the experiment, such that the computer model output depends upon knowing the value of to a higher precision than the standard value of m/s2 (Thompson & Taylor, 2008). Then we may model

where for some . Here, the simulator requires an input the value of which is uncertain, and which is not controlled or observed as part of any field observations. In order to model as successfully as possible, we must calibrate the above model, by approximating the true value of , which we may call the calibration parameter.

However, notice that the above model description assumes that where is the true value of the calibration parameter, we will have that is an unbiased predictor of . This will often not be the case. Thus where model bias is known or suspected to exist, we must replace the above model with

where is a discrepancy function describing the bias of as an approximation of . In this case, both and may be modeled as independent Gaussian processes, following the framework established by Kennedy & O’Hagan (2001). In that work, the authors effect a Bayesian calibration of unknown parameters while estimating model discrepancy and undertaking uncertainty quantification of the results. The importance of model discrepancy is discussed further by Brynjarsdóttir & O’Hagan, (2014). The work done in the present project closely follows that of Higdon et al. (2004) and Williams et al., (2006), who use the framework established by Kennedy & O’Hagan to calibrate uncertain parameters by combining scant field observations with computer code observations .

The primary difference between the present work and the previous work referenced above is that we replace field observations with what we may call *desired data*. The intent is to calibrate elements of the model, not to observed reality, but rather to our design targets.

## The model for our emulator

The example given in Figure 1 is univariate. By contrast, our model has three inputs (temperature, volume fraction, and thickness) and three output (tip deflection, tip rotation, and cost). A fourth, dummy input variable is used to select which output is desired; thus we formalize the model as having four-dimensional input and univariate output.

The inputs are divided into control inputs (dummy variable, temperature) and calibration inputs (volume fraction, thickness). This reflects the fact that we wish to calibrate our choice of volume fraction and thickness (and not, e.g., a “choice” of at which temperature to operate). Notice that while volume fraction and thickness of the blade material is clearly under our control during the manufacturing process, we treat these parameters as uncertain calibration parameters rather than as control parameters. This is because we seek to use the basic framework described in the previous section to aid in the design process; thus our uncertainty with respect to volume fraction and thickness is uncertainty with respect to which values best serve our design priorities.

The covariance function used in our model is given by

where is the control input of the dummy variable and the temperature, and is the calibration input of the volume fraction and thickness.

For convenience, we reparameterize the parameters as

Using 504 observations from the finite element model, the resulting covariance matrix for the observation points is , and the resulting likelihood function is numerically unstable. Efforts to estimate via MCMC or similar methods run afoul of this numerical instability. The instability can be avoided by instead working with the log-likelihood, which may be optimized by gradient methods. Doing so, we estimate:

## Using the model for calibration via MCMC

We use the emulator to find optimal values of volume fraction and thickness, respectively. The methodology for achieving this is calibrate the emulator to “desired” data . That is, given a (fabricated) “observation” of desired tip deflection, rotation and cost, we use an MCMC routine to find posterior distributions on (given uniform prior densities on each). We take to be constant with respect to temperature.

Using the above estimations of , we use the likelihood of the “desired observation” to perform the MCMC routine to find these posterior distributions. Numerical instability can again be controlled by calculating the log-likelihood of each point of the calibration space considered in the MCMC routine.

Thus, the likelihood for the desired data is given by

where is the covariance matrix of the Gaussian process (which has been trained on the observations from the finite element model) at the points where are the dummy variable and temperatures at which is “observed”, and .

Uniform priors are placed on : and . Thus, since are found via empirical Bayes methods, we have that the (unnormalized) posterior distribution of is simply the above likelihood function restricted to the supports of the uniform distribution on :

In the MCMC routine, samples of are drawn componentwise. A univariate normal proposal distribution is used for each of volume fraction and thickness. Thus, for example, given a previous sample , a new proposal is drawn with . We then compute:

(where the log scale is used for computational stability), and we accept as a new volume fraction draw with probability . If we do not accept , then we treat as a new (repeated) draw. This process is then repeated to obtain a new draw of .

The proposal variances and are adaptive, in that during the burn-in period of the MCMC routine, the proposal variances are adjusted to optimize the rate of acceptance of new samples. Specifically: for every 100 draws during the burn-in period, if either of volume fraction and thickness has an acceptance rate out of the range then the corresponding proposal variance is adjusted by a factor of .75 or 1.25 (depending on whether the acceptance was too low or too high).

## MCMC results

Three MCMC chains of 10,000 draws apiece were obtained, with randomly selected initial positions. 2,000 draws from each chain were discarded as burn-in.

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| C:\Users\carle\AppData\Local\Microsoft\Windows\INetCache\Content.Word\Picture2.png  Figure 2: Summaries of MCMC chains |

The three chains show good convergence qualities. In each of the three chains, volume fraction immediately moves to its upper boundary of .6 and stays there. Thickness in each chain shows the same posterior mean of approximately 16.58mm.

Summaries of each of the three chains is shown in Figure 2. Notice that posterior means, quantiles, and standard deviations are in close agreement in each chain.

The three starting locations of the chains are, respectively: (0.5259, 12.5132), (0.5074, 23.5869), and (0.4470, 18.9989).

The posterior variance of volume fraction is much smaller than that of thickness. This is because volume fraction, constrained by its upper boundary, has higher acceptance with an extremely small proposal density variance. During the burn-in period, the adaptive proposal density variance thus shrinks much more than does that of thickness.

Correspondingly, trace plots of the three chains show a skewed distribution for volume fraction (with shortened tail against the upper boundary of .6), and a roughly symmetric distribution for thickness. See Figure 3.

We may also examine the partial averages of these chains; early in the burn-in they each converge to the posterior means displayed in Figure 3. See Figure 4.

We may also examine the Gelman-Rubin diagnostic statistic for the three chains to assess convergence. Approximate convergence of MCMC chains entails that the potential scale reduction factor for each calibration parameter be near 1. A rule of thumb is that values below 1.1 indicate convergence. For volume fraction, we have that the 95% upper confidence interval for this statistic is 1.04, and for thickness, it is approximately 1.00. See Figure 5.

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| Figure 3: Trace plots and densities of draws |

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| Figure 4: Weighted partial sums |

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| Figure 5: Gelman-Rubin statistic |

# References

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