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Case Study in Combining Physical and Computer Experiments

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Case Study in Combining Physical and Computer Experiments

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I. Introduction

Computer models (CM) are often used to evaluate potential measurement systems. For example, a simple chemical reaction observed over time allows us to estimate a reaction rate parameter in a very simple "computer model" in Section 3 below. Even the most elaborate model is a simplification of a complex system so a key question is whether a particular CM is sufficiently accurate to adequately predict system performance. In our Section 3 example, 1.5 units remain unreacted in the real experiment, which is a feature of the true system that is not captured by the simple model.

Model bias can be an important component of CM uncertainty. Allowing for model bias while simultaneously calibrating computer model parameters has been shown to reduce the RMSE when predicting a response (Higdon et al., 2008; Unal et al., 2011; Vanli et al., 2010). Two related issues are examined in Burr and Hamada (2012): (1) to what extent does simultaneous calibration and bias fitting lead to "better" model parameter estimation, and (2) to what extent does the choice of basis functions for the bias fitting impact parameter estimates. Burr and Hamada (2012) show that simultaneous estimation of computer model parameters and model bias does not necessarily improve model parameter estimation, and that standard model choice methods such as the Bayesian information criterion cannot always reliably indicate the best basis functions or the number of basis functions.

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This paper examines whether simultaneous CM calibration and bias estimation leads to better response prediction, where response prediction is measured in one of the most common ways, using the root mean squared prediction error (RMSE).

The following sections include background for CMs and measurement system error modeling, one example, and discussion.

II. Model Validation in The Presence of Model Bias

We assume the true value of a response $y^T(x)$ is modeled with a model value $y^M(x,\theta)$ and that the model has a bias term $b_\theta(x)$ satisfying

$$y^T(x) = y^M(x,\theta) + b_\theta(x). \qquad (1)$$

The model parameters are divided into a "user-controlled" group x and calibration parameters θ following Bayarri et al. (2007), Higdon et al. (2008), and Wang et al. (2009). Examples of user-controlled parameters are physical dimensions of a nuclear measurements experimental setup that might include radiation source terms, attenuation terms, and detection system (including geometry) properties. Calibration parameters often include fundamental constants such as nuclear cross sections that define nuclear interaction probabilities. Such cross sections are often well measured but still have non-negligible measurement error in some contexts such as in estimating the neutron multiplication coefficient (Kawano et al., 2006).

Also assume the field (measured) data varies around $y^T(x)$ with random errors R satisfying

$$y^F(x) = y^T(x,\theta) + R. \qquad (2)$$

In practice, any bias in the measurement method will be confounded with model bias so to avoid indeterminacy, assume the measurement R errors have mean 0 (zero bias) and variance σ_R^2.

Equations (1) and (2) capture the notion that comparisons of measurement data to model predictions can be used to estimate model bias $b_\theta(x)$ and simultaneously to find good values of calibration parameters θ. Code accuracy is defined by the magnitude of $b_\theta(x)$. After comparing model

predictions to measured values, bias-adjustment together with estimation of θ ("calibration") can lead to more accurate predictions at new x values. These more accurate predictions should have higher accuracy as a result of such bias-adjustment and calibration.

Another goal for code validation is to predict accuracy prior to data collection by using "similar" problems that have been "validated." That is, a truly predictive science requires predicting $b_\theta(x)$ prior to observing new data, by appealing to an archived collection of "similar" problems, which is beyond our scope here (Oden et al., 2010). Our scope is to use field data and corresponding code output at various values of θ as in Eqs. (1) and (2) to simultaneously estimate $b_\theta(x)$ and θ. Burr and Hamada (2012) assessed whether the estimate $\hat{\theta}$ of θ has smaller RMSE than an estimate of θ that does not simultaneously estimate $b_\theta(x)$. Wang et al. (2009) took a somewhat different view and interpreted model validation as meaning that confidence bands around the estimate of $b_\theta(x)$ provide high confidence that a pre-specified tolerance threshold (the maximum allowable model bias) is not exceeded.

Our goal here is to assess whether the estimate $\hat{y}$ of y that arises from simultaneously estimating $b_\theta(x)$ and θ has smaller RMSE than an estimate of y that does not simultaneously estimate $b_\theta(x)$ and θ.

III. Example : Simulated Data from the Model

$$y(t) = 3.5\ \exp(-1.7t) + 1.5 + R(t)$$

A simple example with a nonlinear regression model substituting for a CM is given in Bayarri et al. (2007). Consider a nonlinear regression model $y(t) = \mu(t) + R(t)$, where $\mu(t)$ is the mean and $R(t)$ is the error at time t. Let the hypothesized (and wrong) "computer" model for $\mu(t)$ be $\mu(t) = 5\ \exp(-\theta t)$ with θ unknown. This models a chemical reaction process with initial chemical concentration 5 and reaction rate θ, both in arbitrary units, so $5\ \exp(-\theta t)$ is a standard model for the amount of chemical remaining at time t and $y(t)$ are the measured values, measured with measurement errors $R(t)$.

Let the *true model* be

$$y(t) = 3.5\ \exp(-1.7t) + 1.5 + R(t), \qquad (3)$$

Which captures the fact that 1.5 units remain unreacted in the real experiment. Figure 1 plots data simulated from this model for values of t equally spaced from 0.11 to 3.01 with residual variance $\sigma_R^2 = 0.3^2$ and fits from several models to be described. The estimated θ is $\hat{\theta} = 0.62$ with an estimated error variance $\hat{\sigma}_R^2 = 0.31$ and the solid line is the fitted values $5\ \exp(-0.62t)$. *Notice the tendency for the estimate* $\hat{\theta}$ *to be wrong in a way to attempt to compensate for the model bias. Notice however that the fit still exhibits a bias* and that $\hat{\sigma}_R^2 = 0.31$ is much larger than the true value $0.3^2 = 0.09$. The bias is also evident in the bottom plot, which plots the residuals and a linear fit to the residuals. All simulations and analyses are performed in R (R Core Development Team, 2004). For example, $\hat{\theta}$ was estimated using nls to implement nonlinear constrained least squares using the function call nls (yvals~5*exp(θ*tvals), data=dataframe1, start= list (a=1)) in R where the data (3 reps at each of 10 time values) is in the data frame named dataframe1.

Now allow for the bias $b(\theta,t)$ as in Eq. (1) and *fit the wrong model*

$$y(t) = 5\ \exp(-1.7t) + b(\theta,t) + R(t) \qquad (4)$$

to estimate θ and σ_R^2 assuming $\mu(t) = 5\ \exp(-\theta t)$. The bias $b(\theta,t)$ was fit in this example by using nls (yvals ~ 5*exp (-a*tvals) + s(tvals), data=dataframe1, start= list(θ =1)) which allows for a smooth bias term by using the default spline fit available in nls via s(tvals). Alternatively, in the 6-step procedure below, user-supplied basis functions to fit $b(\theta,t)$ are described.

When fitting $b(\theta,t)$ as just described, in 1000 simulations the average $\hat{\theta}$ is 1.69 which is within the replication error associated with 1000 simulations of the true value (1.70). However, the average (over 1000 simulations) estimated σ_R^2 is 0.64, which is considerably larger than the true value of $0.3^2 = 0.09$. Also, Figure 2 (top plot) shows that a bias adjustment to the fitted value does not adequately remove the bias. Similarly, the bottom plot of Figure 2 shows that the estimated bias $b(\theta,t)$ does not estimate the true bias very well.

Although Bayarri et al. (2007) use a prior distribution for model parameters including the bias function $b(\theta,t)$ and also report good performance of $\hat{\theta}$, it appears to be difficult to simultaneously find good estimates of $b(\theta,t)$ and θ. In fact, Bayarri et al. (2007) state and we concur that in general one cannot expect to always get good estimates of true model parameters such as θ using a "wrong" model and a bias adjustment. For example, if the coefficient of 5 in the fitted model $y(t) = 5\ \exp(-\theta t) + b(\theta,t) + \varepsilon(t)$ where $\theta = 1.7$ is changed to $\theta = 2.5$, then the average of $\hat{\theta}$ is 2.5 in 1000 simulations. Also, if the true coefficient is changed from 5 to 4.1 and the true constant is changed from 1.5 to 0.5, then the average of $\hat{\theta}$ is 3.03 in the model *with* $b(\theta,t)$ and the average of $\hat{\theta}$ is 1.69 (very close to the true value) in the model *without* $b(\theta,t)$. Because all models are "wrong" in the sense that they

are an intentional simplification of a complex reality, such findings call into question whether it is generally possible to find estimates of $b(\theta,t)$ and θ that are simultaneously close to their true values.

So it appears that the numerical example presented in Bayarri et al. (2007) is a case of getting lucky regarding estimation of θ when a bias term $b(\theta,t)$ is accommodated. Although estimation of fundamental constants θ in Eq. (1) is sometimes a goal for CMs and associated experiments, adding a bias term does not always improve estimation of θ, as this example illustrates. Nevertheless, adding the bias adjustment essentially combines a reasonable physical model (the CM or in this example an exponential term with a wrong coefficient) with a reasonable empirical model (the fitted bias). Combining two models is likely to improve interpolation and possibly extrapolation in selected circumstances outside the range of the inputs used to calibrate the model. For example, the experimenter could probably reliably create other initial concentrations and use a calibrated (but wrong) model to estimate how the initial concentration will change with time. Interpolation and extrapolation are common goals for CM.

This example can also illustrate Bayesian modeling, which is heavily used in CM evaluation. First, the model parameter θ in $\mu(t) = 5\ \exp(-\theta t)$ is known to be nonnegative and possibly also less than some reasonable upper limit. Such constraints are easily handled by using a prior probability distribution for θ that puts all of its probability on positive values, perhaps favoring a particular range of values. Second, the bias function $b(\theta,t)$ can be constrained to be a smoothly varying function of t or not. One effective way to impose a smoothness constraint is to assume that $b(\theta,t)$ is well-modeled by a Gaussian process, which typically forces $b(\theta,t)$ to be smooth by assuming nearby t values have highly positively correlated (very similar) $b(\theta,t)$ values. By varying prior assumptions regarding $b(\theta,t)$, it is possible to also model nonsmooth functions $b(\theta,t)$. However, more field data is required to model nonsmooth functions. In most applications, CM output is a "black box," with unknown functional form, so Bayarri et al. (2007) and Higdon et al. (2008) describe using basis functions to fit the response/output from CM evaluations at multiple input settings. The bias term $b_\theta(x)$ can also be fit using basis functions.

a) Simultaneous estimation of CM parameters and model bias

Following Bayarri et al. (2007) and Myers et al. (2008), we use principal components (PCs) as a basis for the CM output and Gaussian kernels as a basis for $b_\theta(x)$, and reanalyze the example. The inference steps are:

1) Evaluate the model output $y^M(x,\theta)$ at N values of θ. In the example, x is time (one dimensional) and θ is the reaction rate (a scalar).
2) Usethe values $y^M(x,\theta_1), y^M(x,\theta_2),..., y^M(x,\theta_N)$ to calculate PCs, denoted PC_Y. Mean-centering and scaling prior to PC calculation is always an option. Fit each $y^M(x,\theta_i)$ to PC_Y to choose a good dimension (usually 2 or 3 PCs are required for a good fit). In the example, $y^M(t,\theta) = 5\exp(-\theta t)$ so time t is used as the predictor which is often denoted as x, depending on context. Use a range of θ values that is broad enough for $y^M(x,\theta_1), y^M(x,\theta_2),..., y^M(x,\theta_N)$ to span the observed $y^F(x)$ values.
3) Choose a basis Z_B to fit the bias term. We used 10 equally-spaced Gaussian kernels across the range of x (t in the example), and then used the Bayesian information criterion (BIC, see below) to select a subset of 2 to 7 from the 10 available kernels.
4) Fit the experimental data $y^F(x)$ simultaneously to PC_Y and Z_B. In the example, there are three repeats for each value of t, so the error variance σ_ε^2 should be fairly well estimated unless the prior probability density is strongly concentrated away from the true value of 0.3^2.
5) Partition the fit from (4) into fit_{PCY} due to PC_Y and fit_{ZB} due to Z_B. *Use fit_{PCY} to estimate θ.* [Note: alternatively and more simply, we could use the known functional form for the computer model, $\mu(t) = 5\ \exp(-\theta t)$, to estimate θ. But in practice, one rarely knows the functional form of the computer model.] Intuitively, if model run $y^M(x,\theta_k)$ is closest in some distance measure to fit_{PCY}, then $\hat{\theta} = \theta_k$. We implemented this intuitive approach using Euclidean or Manhattan distance (the sum of absolute values of individual component differences, see the distfunction in R), and also implemented a similar approach involving fits of θ to PC_Y.
6) The results of the fit are $\hat{\sigma}_R^2, \hat{\theta}$, fit_{ZB}, and fit_{PCY}.

To implement this Bayesian approach that follows Bayarri et al. (2007) and Higdon et al. (2008), we use Markov Chain Monte Carlo (MCMC) as implemented in the metrop function in the mcmc package for R (Geyer, 2009). All MCMC results throughout this paper were obtained using metrop. The main Bayesian feature required is to constrain coefficients of PC_Y and Z_B to reasonable values. For the coefficients of PC_Y, reasonable values are determined from the range of coefficient values in Step 2. For the coefficients of Z_B, reasonable values are determined by

requiring the fitted values to be within a range determined by the experimental data $y^F(x)$.

For this example, we fixed the CM output basis to be PC_Y as described, and fixed the $b_\theta(x)$ basis to be Z_B (Gaussian kernels spread across the range of x) as described. We then tried 0 to 7 components for PC_Y and for Z_B and evaluated whether the BIC (a well-known option for model selection, see Aitken (2010), defined as BIC= - 2log(maximum likelihood) + p log(n) where p is the number of fitted parameters and n is the sample size), appeared to be effective in the sense of choosing models that gave better estimates of $b_\theta(x)$ and of θ. Because in this example there are 3 repeated measurements at each of the 10 values of x, each method can compare its estimate of σ_ε^2 to the sample variance. We found $\hat{\theta}$ to be sensitive to both the prior probability distribution for σ_ε and sensitive to the dimension of PC_Y and Z_B. See Burr and Hamada (2012) for more detail, but briefly, in each of 100 simulations we used a gamma prior distribution with mean equal to the true value 0.3 and differing standard deviations (0.01, 0.1, 10, 100) for σ_R and two PCs to fit the CM output and 0, 1, 2, 3, or 5 Gaussian kernels to fit the model bias $b_\theta(x)$ (0 kernels means that we did not allow for model bias). The resulting $\hat{\theta}$ values (where $\hat{\theta}$ is the posterior mean as estimated from the MCMC observations) varied wildly from near 0 to near 100. Average $\hat{\theta}$ values were given in Burr and Hamada (2012).

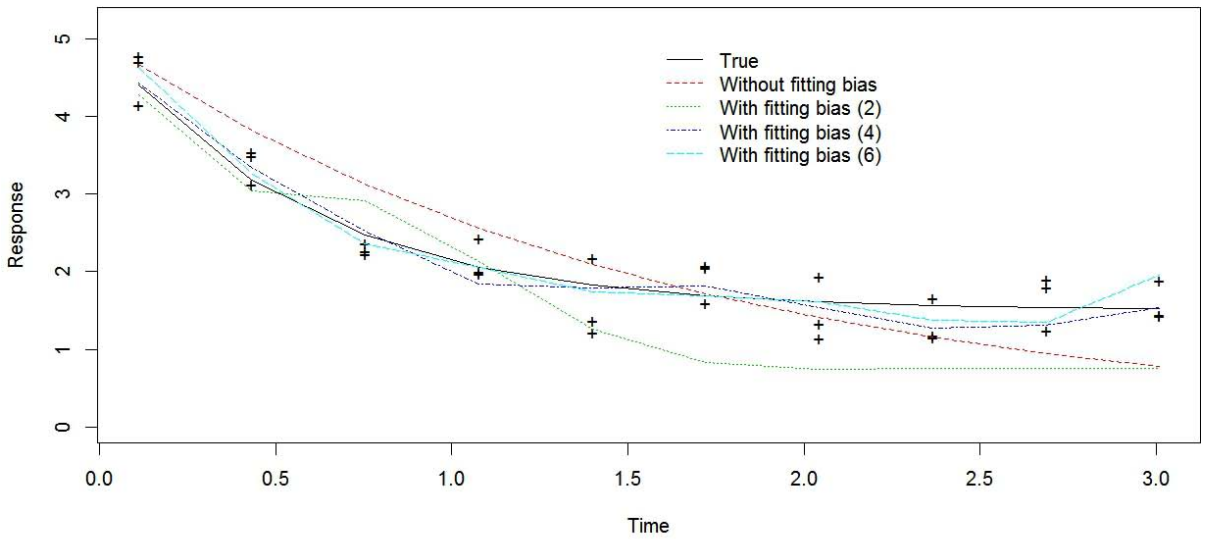

Figure 1 : Simulated data from the example using the true model $y(t) = 3.5\exp(-1.7t) + 1.5 + R(t)$ to generate data and $y(t) = 5\exp(-1.7t)$ as the CM. The predicted values without fitting a bias term and with fitting a bias term for 2, 4, or 6 basis functions are shown.

As an aside, we also used the constrained nonlinear least squares function nls as previously described, using the same type of constraints, but had convergence problems for about 20% of the realizations so we do not report nls results. In some applications however, simple application of nls is adequate for parameter estimation. Because MCMC is straight forward and easily provides posterior credible intervals for parameters, we prefer MCMC. Of course ensuring MCMC realizations have converged is time consuming, and on the basis of a several auxiliary realizations we chose proposal step sizes to get approximately a 20% acceptance rate (Geyer, 2009).

b) Root mean squared error of prediction (RMSE) in a simulation study

All RMSE results in this subsection are based on 10^4 simulations, are repeatable to ± 0.005, and $\sigma_R = 0.1$ and $\sigma_R = 0.3$ were used. The RMSE for simultaneous estimation (SE) of CM parameters and model bias and for local kernel smoothing (KS) (using lokerns) are given. The boldface entries below indicate options for which the RMSE for SE was smaller than the RMSE for KS.

First, consider predictions at the 10 times when the response is observed.

For σ_R = 0.1, the RMSE is 0.10 for SE and 0.08 for KS.
For σ_R = 0.3, the RMSE is 0.17 for SE and 0.22 for KS.

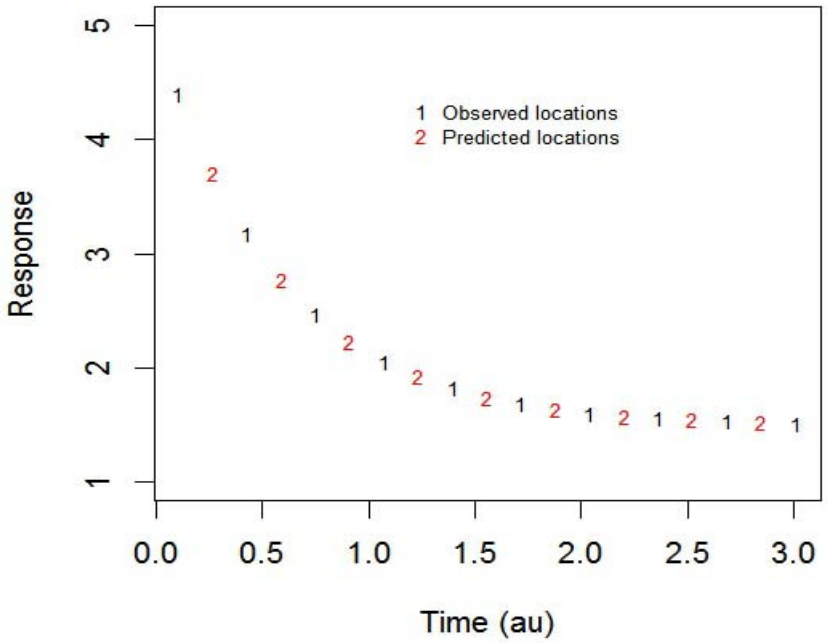

Figure 2 : The 10 times at which the response is observed, and 9 additional times where the response will also be predicted.

Next, consider predictions at the 9 new times in Figure 2, and there are several options for this type of prediction.

Option 1: Linearly interpolate the values at original 10 times to the 9 new times.

For $\sigma_R = 0.1$, the RMSE is 0.11 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 0.15 for SE and 0.18 for KS.

Option 2 : Linearly interpolate the basis functions from the original 10 times to the 9 new times.

For $\sigma_R = 0.1$, the RMSE is 0.11 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 0.15 for SE and 0.17 for KS.

Option 3 : Assume the true bias is known exactly, so exactly interpolate the true values at the original 10 times and then interpolate to the 9 new times. This option is not available in practice but serves as a basis for comparison in the unrealistic case that the true values could be known exactly at the original 10 times. The 0.03 RMSE for SE does not depend on σ_R in option 3, because the true values at the original 10 times are simply interpolated to estimate the true values at the 9 new times.

For $\sigma_R = 0.1$, the RMSE is 0.03 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 0.03 for SE and 0.18 for KS.

Option 4 : Similar to option 3, but use the observed data to estimate bias, so exactly interpolate the mean of the 3 observations at each of the 10 original times. This option is available in practice.

For $\sigma_R = 0.1$, the RMSE is 0.10 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 0.27 for SE and 0.17 for KS.

Option 5 : Use the estimate $\hat{\theta}$ of θ in the assumed known functional form $5\exp(-\hat{\theta}t)$ where $\hat{\theta}$ depends on the realization of the random noise.

For $\sigma_R = 0.1$, the RMSE is 0.80 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 1.56 for SE and 0.17 for KS.

Option 6 : The same as option 5, but use $= 1.7$, the true value of θ.

For $\sigma_R = 0.1$, the RMSE is 1.05 for SE and 0.08 for KS.
For $\sigma_R = 0.1$, the RMSE is 1.52 for SE and 0.17 for KS.

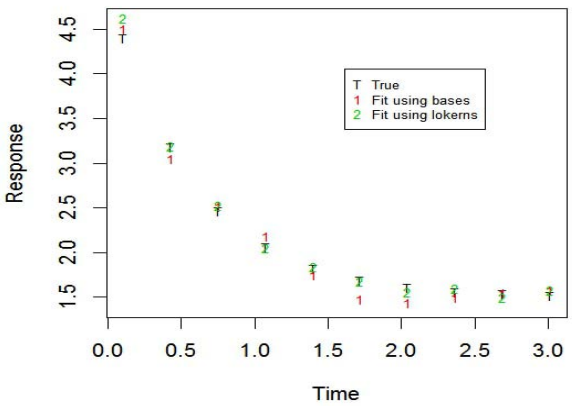

Figure 3 : The true response at each of the 10 times, and the predicted response using simultaneous estimation of CM parameters and CM bias and using local kernel smoothing, lokerns.

c) Example summary

Summary points 1-3 are found in Burr and Hamada (2012). Point 4 is the focus of this paper.

1) One can degrade performance by simulating from the same true model as assumed in the fitting, $\mu(t) = 5\exp(-\theta t)$, letting $y(t) = \mu(t) + R(t)$, and allowing for a bias term in the fit. That is, allowing for CM bias when none exists will change the inference on θ.
2) As reported in Bayarri et al. (2007), fitting a bias term does impact $\hat{\theta}$, but the bias term does not necessarily make $\hat{\theta}$ closer to θ.
3) The basis choices and the dimensions of the basis matter (for example, the value of $\hat{\theta}$ varies as the bases and dimensions of the bases change) so some sort of model selection should be considered. However, the Bayesian Information Criterion (BIC) for model selection did not perform very well. Residual diagnostics to detect patterns in residuals can be automated and appears to have more potential to guide model selection.
4) As shown above, simultaneous estimation of θ and b does not necessarily reduce the RMSE in predicting y.

Summary points 1-4 combine to suggest that simultaneous estimation of θ and b requires considerable attention to detail and careful analysis. It is is still "part art" to do a good job in simultaneous fitting of θ and b. Also, because the functional output in this example was a one-dimensional function of time, local kernel smoothing can be very competitive as a purely empirical prediction option. In higher dimensions, kernel smoothing is not as effective, although recent research suggests that nonparametric smoothing with an iterative bias correction can be effective even in high dimensions as a purely empirical smoothing and interpolation option for prediction (Cornillon et al., 2011; Burr et al., 2010 and 2011).

IV. Summary and Conclusion

Most model validation efforts include comparison of real data to corresponding code predictions. There will be iterative improvement to the models and ultimately we need apriori (prior to the next data collection) "error bars" for bias between field data and CM prediction to have defensible predictive science in this context, including in the simple reaction-rate example provided here.

Simultaneous fitting of model parameters and model bias leads to an underdetermined problem, so prior information regarding bias shape can be crucial. Even with good agreement between prior assumptions and the true state of nature, our example suggests that simultaneous estimation of model bias and model parameters does not necessarily give better estimates of model parameters nor good estimates of model bias, nor reduce the RMSE for predicting the response y. However, it can as advertized lead to better "combined model" predictions, where the combined model is the CM with fitted parameters and fitted bias. A follow-on study to investigate the effects of varying the relative sizes of error variance σ_R^2 and model bias $b(\theta, t)$ would be valuable.

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