FBC: Full Bayesian Calibration

Contents

Introduction

FBC is a package that uses the data from both field experiment and computer simulation to calibrate the simulator model [1]. A field experiment relates a set of experimental variables as inputs to a response as output. A computer simulation also relates the same experimental variables as inputs to the response as output but also include calibration inputs. These inputs either represent unknown but fixed physical properties that are governed by the physical system in field experiments (and therefore need not be specified in field experiments) or represent various aspects of the simulation model such as tuning hyperparameter of the model. In both cases, the calibration parameters must be estimated for a simulator model to mimic the physical system adequately. The goal of the calibration is to estimate calibration parameters by fitting a statistical model to the observed data using both field and simulator data. Estimated parameters of the calibration model can be used for inference or calibrated prediction.

The FBC package is a based on the well-known Kennedy and O'Hagan (KOH) calibration model (2001). In the KOH model, field and simulator data are stacked in a single model, where simulator response is fitted using a Gaussian Process (GP) that models the simulator model and field response is fitted using a three-component model that accounts for simulator model using simulator GP, bias-correction using another independent GP, and a Gaussian random error term representing measurement error. Using two independent GPs and a Gaussian random error introduces new hyperparameters to the calibration model that must be estimated along with calibration parameters. In its original formulation, KOH formulates a hierarchical Bayesian framework with two sequential phases. In the first phase, model hyperparameters are predicted using maximum likelihood estimation (MLE) method. In the second phase, Bayesian analysis is employed to derive the posterior distribution of calibration parameters while fixing the hyperparameters found in the first phase.

[1] *The first q columns of matrix* `Phi` *in* `calibrate` *output represent the MCMC samples of posterior densities for calibration parameters. In our ball example, there is only one calibration parameter (gravity), which is denoted by* κ_1 *and represented by* `kappa1` *in* `Phi`*..*

Neither KOH's original formulation nor later suggestions are fully Bayesian as they use MLE methods to estimate hyperparameters and fix the hyperparameters in the second phase which ignores the added uncertainty of the estimated hyperparameters, largely due to computational infeasibility (Kennedy & O'Hagan, 2001; Higdon et al., 2004; Liu et al., 2009). On the other hand, `FBC` runs a fully Bayesian model that includes both calibration parameters and model hyperparameters in its Bayesian framework. Implementation of the package optimizes the calibration process and memory management to increase computational efficiency. Moreover, the fully implemented Bayesian framework, enables the user to apply the expert knowledge about any of the model parameters using prior specifications. All common prior distribution are implemented in `FBC` to allows for high degree of flexibility in specifying the prior information or the lack thereof. `FBC` runs a variation of Markov Chain Monte Carlo (MCMC) algorithm called Metropolis-Within-Gibbs algorithm to find the posterior distribution of calibration parameters and model hyperparameters. Furthermore, `FBC` enables calibrated prediction for new input configurations using the calibration model.

The current vignette is structured into following sections: The first section, Using `FBC`, explains the package functionality through a simple pedagogic example. Also in this section, the notation for inputs and outputs of both computer and physical experiments are introduced. In the second section, Calibration Model, generalizes the example introduced in the first section to build model components and shows how a calibration model based on KOH model is built internally. Using the general notation, while referencing the example, modelling choices are justified. In the third section, Parameter Estimation, the theoretical results to characterize the posterior distribution of model parameters are presented along with procedure for MCMC-based estimation of parameters. In the fourth section, Calibrated Prediction, the theoretical results to derive calibrated predictions for new input configuration using the estimated parameters are offered. In the fifth section, Implementation, some of the implementation features and choices of `FBC` package are explained along with its limitations. In the sixth and last section, Applications, three more examples are presented to demonstrate the full functionality and limitations of the `FBC` package. And finally, the Appendix provides deeper discussion and further details to some of the concepts presented in the sections.

1. Using `FBC`

`FBC` package has two main public functions: `calibrate()` and `predict()`. As function names suggest, `calibrate()` takes the field and simulation training data to calibrate the simulator model and `predict` takes a new field input configuration and the calibration model object to predict the field response and its associated uncertainty. In addition, `FBC` has four more public functions to help with prior specifications, summarizing, and visualization of calibration. Furthermore, there are three more public function that are not directly used by user to build calibration model but provide functionalities that are not offered by base R. This section explains how to use the mentioned functions and what to expect in their use and results using a simple pedagogic example. Throughout this section, the user is expected to be well-versed with calibration model in general and KOH model in particular. It is designed to be a self-contained section on the usage of `FBC` package but can be augmented with section six, Applications, to further examine the functionalities and limitation of the package. Less experienced users are encouraged to start from next section which aims to explain the theory behind calibration models and calibrated predictions in more details.

1.1 Setup

The simplest and safest method to obtain `FBC` package is through CRAN using following command.

```
install.packages(FBC)
```

Alternatively, the development version of the `FBC` package can be installed directly from Github using `devtools` package. Note that, current vignette is based on published version of the package on CRAN and the development version may contain further functionalities.

```
devtools::install_github("parpishro/FBC")
```

After installing the package, it must be loaded into the R session.

```
library(FBC)
```

1.2 Data:

Building a calibration model requires data from both field experiment and computer simulation. To focus on the functionality of the package, we use a simple pedagogic example as experimental setting. In the field setting, a wiffle ball is dropped from different heights and the time it takes to hit the ground is measured. The experimental input is height (h). and the response is time (t). In the simulation setting, the physical process of a falling ball is modelled by a mathematical equation that relates h to t, however, one must also provide gravity (g) as calibration input. Note that in the field experiment, the earth's gravity is fixed but unknown to the experimenter [2]. The field experiment has been performed by Derek Bingham and Jason Loeppky and it is provided by Robert Gramacy in his book "surrogates" [3]. The mathematical model used in simulation of the ball drop experiment can be easily derived from introductory physics results.

$$t = \sqrt{\frac{2h}{g}}$$

The simulation code takes h and g are taken as experimental and calibration inputs and returns t as simulator response based on above mathematical equation. A common method to choose the different combination of the inputs from acceptable ranges is Latin Hypercube Sampling (LHS) method (McKaThe `FBC` package requires the training data to be in matrix format, where for both matrices, the first column always represents response vector and following columns represent experimental inputs (for both data matrices) and calibration inputs (only for simulation data matrix). The data matrices for ball example are produced in advance and loaded into the package environment under the name of `ballField` and `ballSim` [4].

Below, the structures and dimensions of both data matrices can be inspected.

```
head(ballField, 3)
>         t     h
> [1,] 0.27 0.178
> [2,] 0.22 0.356
> [3,] 0.27 0.534
dim(ballField)
> [1] 63  2
head(ballSim, 3)
>          t     h      g
> [1,] 0.404 0.998 12.220
> [2,] 0.487 0.940  7.909
> [3,] 0.450 0.886  8.736
dim(ballSim)
> [1] 100   3
```

[2] *In ball example there is only one experimental input and therefore* $\mathbf{x_f}$ *is a vector of length one or scaler. Similarly, in its matrix notation,* $\mathbf{X_f}$ *is a* $(n \times 1)$ *matrix or a vector of length* n*..*

[3] *Note that calibration parameters* κ *are often assumed to be unchanged throughout field experiment. Therefore, same* (κ) *vector is augmented to all of the field input configurations..*

[4] *Note that the range of Beta distribution is the span of [0, 1], which is the range of calibration inputs for simulator after scaling .*

Figure 1 shows the distribution of time versus height for both physical and simulation experiments. Note that for higher height values, the simulation responses (blue) underestimate their corresponding field response (red), displaying a systemic bias for simulation model.

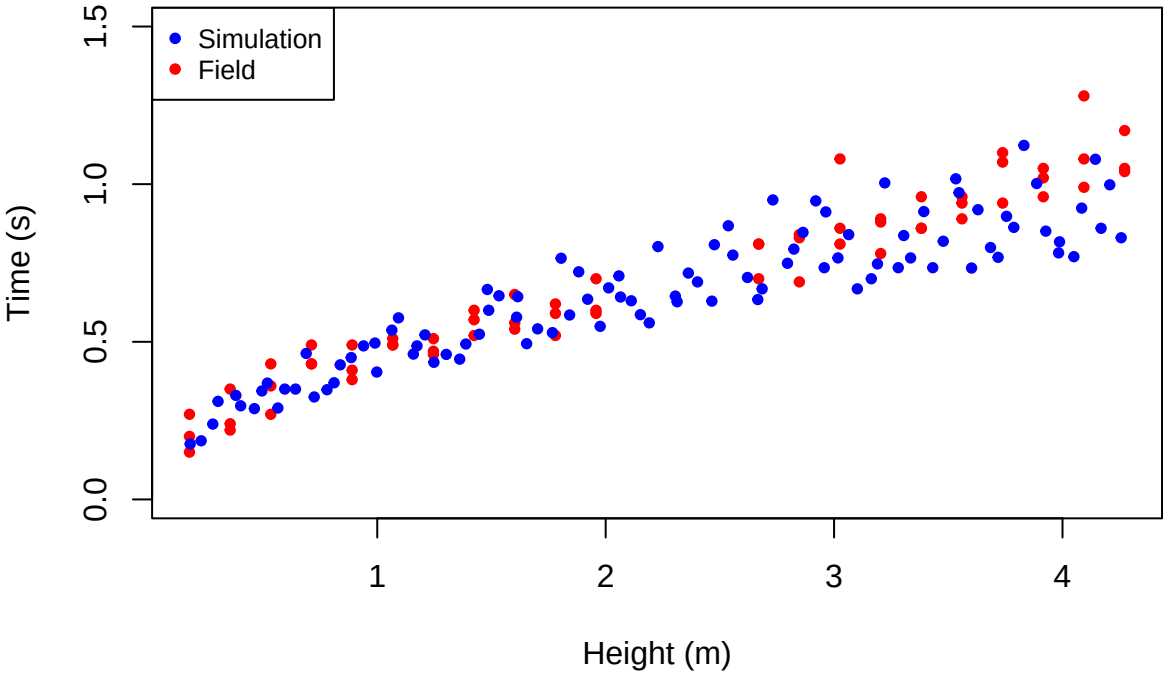


Figure 1: The time versus height plot for both field experiment and simulation.

The ball example is a simple pedagogical example as it has only one experimental input and one calibration input. Using this toy example, we demonstrate the functionality of the package without getting to the details of a complex mathematical model. More complex and real-world examples are covered in the last section.

1.3 Building a Calibration Model:

The `calibrate()` function takes three sets of arguments from user: data, MCMC, and prior specification parameters. Other than data arguments which must be supplied by user, all other arguments have reasonable default values for ball example [5].

```
calMod <- calibrate(sim = ballSim, field = ballField,                                  # Data
                    nMCMC = 11000, nBurn = 1000, thinning = 50,                        # MCMC
                    kappaDist = "beta", kappaInit = NA, kappaP1 = 1.1, kappaP2 = 1.1, # Priors
                    hypers = set_hyperPriors(),
                    showProgress = FALSE)
```

The first and second arguments `sim` and `field` must be supplied by user. As mentioned earlier, both must be either in matrix format representing the simulation and field data respectively. In both `ballSim` and `ballField` of our ball example, the first column represent the response **t** and the second column represent experimental input **h**. Additionally, `ballSim` has a third column that represents calibration input **g**. Calibration inputs are implicit in field experiment and are absent in the data matrix `ballField`.

[5] *Boundary values of [0, 1] corresponds to* $-\infty$ *and* ∞ *in the original scale of calibration parameters.* .

$$
\begin{array}{lccccc}
 & & \text{Response} & & \text{Experimental} & \text{Calibration} \\
\texttt{ballSim} & = \Big[& \mathbf{t} & & \mathbf{h} & \mathbf{g} \Big] \\
 & & & & & \\
\texttt{ballField} & = \Big[& \mathbf{t} & & \mathbf{h} & \Big]
\end{array}
$$

The second set of arguments consists of MCMC parameters: `nMCMC` represents the number of total MCMC iterations , `nBurn` represent the number of burn-in iterations to be removed from the beginning of the chain, and `thinning` indicate the sampling rate to remove the autocorrelation from the sampled draws. For example, when `thinning = 50`, for every 50 draws from the result only one will be kept in order to remove the autocorrelation between draws.

The third and last set of arguments consists of prior specification for each parameter of the model. The main goal of calibration is to estimate the calibration parameters (g in ball example). However, employing KOH calibration model introduces eight additional classes of hyperparameters to the model. The parameters in all eight classes are not known in advance and must be estimated. As `FBC` employs a full Bayesian framework, the priors for all model parameters must be specified in advance. Throughout the package implementation and current guide a consistent notation is used to denote parameters: κ, $\theta_{\mathbf{s}}$, $\alpha_{\mathbf{s}}$, $\theta_{\mathbf{b}}$, $\alpha_{\mathbf{b}}$, σ_s^2, σ_b^2, σ_e^2, and μ_b denote calibration parameters, correlation scale parameters of simulator GP, correlation smoothness parameters of simulator GP, correlation scale parameters of bias-correction GP, correlation smoothness parameters of bias-correction GP, marginal variance of simulator GP, marginal variance of bias-correction GP, measurement error variance, and mean of bias-correction GP respectively.

For each class of parameters, there are four associated arguments. 1) distribution type, which is a character string determining the prior distribution family (suffixed with "dist" in argument names). Currently, `FBC` supports almost all common distributions and can be chosen from "uniform", "gaussian", "gamma", "beta", "lognormal", "logistic", "betashift", "exponential", "inversegamma", "jeffreys", and "fixed" [6]. 2) Initial value, which is double representing starting point of the parameter in MCMC algorithm (suffixed with "init" in argument names). 3) First distribution parameter (suffixed with "p1" in argument names) and 4) second distribution parameter (suffixed with "p2" in argument names) are doubles representing the two parameters of the chosen distribution [7], [8]. Table 1 summarizes all classes of parameters along with their corresponding argument names for prior specifications.

Table 1: *Argument names to specify priors for each parameter class.*

Parameter Class	Distribution	Initial Value	Shape Parameters
True field calibration inputs (κ)	`kappaDist`	`kappaInit`	`kappaP1` & `kappaP2`
Simulation GP scale (θ_s)	`thetaSDist`	`thetaSInit`	`thetaSP1` & `thetaSP2`
Simulation GP smoothness (α_s)	`alphaSDist`	`alphaSInit`	`alphaSP1` & `alphaSP2`
Bias-correction GP scale (θ_b)	`thetaBDist`	`thetaBInit`	`thetaBP1` & `thetaBP2`
Bias-correction GP smoothness (α_b)	`alphaBDist`	`alphaBInit`	`alphaBP1` &`alphaBP2`

[6] *"betashift" refers to a beta distribution that is shifted one unit to right to cover [1 2] interval and it is used to specify the priors for correlation smoothness parameters which must be constrained to [1 2] interval. Moreover, choosing "fixed" as distribution will exclude that class of parameters from the MCMC sampling. In this case, the given initial value will be used as fixed parameter value and p1 and p2 arguments will be used.*

[7] *For example, if "gaussian" distribution is used, p1 and p2 represent mean and variance of the distribution and if "uniform" distribution is used, p1 and p2 represent lower and upper bound of the distribution.*

[8] *Not all distribution types require two arguments. In particular, "exponential" distribution only requires rate parameter (p1) and "jeffreys" requires none. In these cases the unused arguments are ignored.*

Parameter Class	Distribution	Initial Value	Shape Parameters
Simulation marginal variance (σ_s^2)	`sigma2SDist`	`sigma2SInit`	`sigma2SP1` & `sigma2SP2`
Bias-correction marginal variance (σ_b^2)	`sigma2BDist`	`sigma2BInit`	`sigma2BP1` & `sigma2BP2`
Measurement error variance (σ_ϵ^2)	`sigma2EDist`	`sigma2EInit`	`sigma2EP1` & `sigma2EP2`
Bias-correction mean (μ_b)	`muBDist`	`muBInit`	`muBP1` & `muBP2`

From the classes of parameters mentioned, the prior for calibration parameters should be specified by user based on field knowledge as these parameters are problem-specific [9]. In contrast, all other parameters have reasonable default values based on KOH calibration model literature (Kennedy & O'Hagan, 2001; Higdon et al. 2004; Chen et al. 2017). For this reason and to avoid unwanted complexity, the priors for all other classes of parameters are specified with `hypers` argument and using a helper function `set_hyperPriors()`. In particular, the default value of `hypers` argument is `set_hyperPriors()` without any argument. Nevertheless, expert knowledge about one or more of these parameters can be supplied using arguments of the `set_hyperPriors()` function, which are defined in Table 1, to change the default prior specifications.

Note that some classes of parameters may contain more than one parameters. In this case, the argument values can be vector instead of default scaler. In this case all four fields of that parameter class must be also in vector format with same length as number of parameters in the class. For example, if there are five calibration parameters, `kappaDist` can either be a scaler, in which case the distribution for all calibration parameters will be set to that scaler value and `kappaInit`, `kappaP1`, and `kappaP2` must be also scaler, or can be a vector of length five that supplies the distribution types for all calibration parameters and `kappaInit`, `kappaP1`, and `kappaP2` must also be vector of length 5.

Moreover, there is a logical argument `showProgress` that indicate whether function must show the progress in calibration on console. This will put the `calibrate()` in interactive mode and will show the percentage of the MCMC draws along with sample draws [10].

The output of the `calibrate()` function is an object of class `fbc` that contains the samples from posterior joint distribution of parameters, along with other model information. Below, the components of the a `fbc` object is displayed.

```
names(calMod)
>  [1] "Phi"        "estimates"  "logPost"    "priors"     "acceptance" "vars"       "data"
>  [8] "scale"      "indices"    "priorFns"   "proposalSD"
```

The first and main component of the `calMod` is matrix `Phi` whose columns represent the sample of posterior densities for each unknown parameter of the model in the same order as parameter classes in table 1. Since κ, θ_s, α_s, θ_b, α_b parameter classes may contain more than one parameter, they are suffixed by a number that represents the index of the parameter in the class. For example, if there are 3 calibration inputs, the first 3 columns of the matrix `Phi` represent posterior density of calibration parameters and the column headers will be `kappa1`, `kappa2`, and `kappa3`. In the ball example, there is only one calibration parameter g, which is denoted by κ_1 and represented by `kappa1` in matrix `Phi`. Each row of the matrix `Phi` represents a MCMC draw.

[9] *Although a vague prior is specified as default for calibration parameters values, the user is encouraged to specify the prior based on the field knowledge. The default vague prior is specified using a uniform distribution with lower bound of 0 and upper bound of 1, which characterize the lower and upper bound of parameter domain after standardization ($U(0,1)$).*

[10] *Running `calibrate()` with high number of parameters or MCMC runs will be a lengthy process. This argument shows the progress of algorithm on percentage basis, along with sample of results, which can be useful for debugging purposes.*

```
head(calMod$Phi, 3)
>   kappa1 thetaS1 thetaS2 alphaS1 alphaS2 thetaB1 alphaB1 sigma2S sigma2B sigma2E   muB
> 1   6.16    5.14    0.69    1.94    1.84    0.68    1.90    0.09    0.30    0.09 -0.35
> 2   8.72    4.92    1.04    1.94    1.97    0.17    1.81    0.09    0.66    0.09  0.24
> 3  13.70    4.35    0.76    1.90    1.93    0.43    1.79    0.10    0.44    0.08  0.15
```

Table 2 provides an overview of the model parameters and the notation to represent them in ball example. Later sections will explain in detail why are these hyperparameters introduced, what do they represent, and how they are estimated.

Table 2: Notation used in matrix `Phi` to represent parameters in ball example.

Column	Notation	Description
`kappa1`	κ_1	Unknown value of true calibration input g
`thetaS1`	θ_{s1}	Scale parameter of h input for simulator correlation
`thetaS2`	θ_{s2}	Scale parameter of g input for simulator correlation
`alphaS1`	α_{s1}	Smoothness parameter of h input for simulator correlation
`alphaS2`	α_{s2}	Smoothness parameter of g input for simulator correlation
`thetaB1`	θ_{b1}	Scale parameter of h input for bias-correction correlation
`alphaB1`	α_{b1}	Smoothness parameter of h input for bias-correction correlation
`sigma2S`	σ_s^2	Marginal variance of simulator covariance
`sigma2B`	σ_b^2	Marginal variance of bias-correction covariance
`sigma2E`	σ_ϵ^2	Variance of random measurement error in field
`muB`	μ_b	bias-correction mean

There are ten more elements in `caqlMod` other than matrix `Phi`, which are listed here along with a brief description. The data frame `estimates`, which provides a summary table of all model parameters, includes the mean, mode, median, standard deviation, and 50% and 80% upper and lower quantiles of the marginal distribution of all parameters. The vector `logPost` contains the posterior log likelihood given a parameter draw from `Phi` matrix. The nested list `priors` contains prior specifications for all parameters. The vector `acceptance` represent the acceptance rate of each parameter after running the MCMC algorithm with adaptive proposal. It is important to note that, the current implementation of MCMC algorithm employs Metropolis-Within-Gibbs variation, which is a one-dimensional proposal scheme and the optimal acceptance rate must be close to 0.44. The vector of strings `vars` contains the parameter notation used in code and as `Phi` column headers. The rest of the components in `Phi` are not of great importance for user, however, they are needed for calibrated prediction. The list of matrices and vectors `data` includes the training data in the forms that match KOH model components. The numeric vector `scale` contains scaling factors that are used to scale the training data during calibration. The named list `indices` contain the indices of parameters in each row of `Phi` matrix. The function list `priorFns` includes the prior functions that are created during calibration based on given prior specifications. And finally, `proposalSD` is a numeric vector that represents the final standard deviation of proposal for each parameter.

1.4 Calibrated Prediction

Similar to any other predict function, `predict()` requires a model object argument called `object`, which in `FBC` package must be a `fbc` object, along with an argument representing a new input configuration called `newdata`. Moreover, current implementation of the `predict()`, support two different methods of prediction: Maximum A Posteriori ("MAP") and MCMC-based fully Bayesian ("Bayesian") methods. The method can be selected using `method` argument that can take a character string value of either "MAP" or "Bayesian".

```
predsMAP   <- predict(object = calMod, newdata = matrix(c(2.2, 2.4), ncol = 1), method = "MAP")
predsBayes <- predict(object = calMod, newdata = matrix(c(2.2, 2.4), ncol = 1), method = "Bayesian")
```

The return value of `predict()` is a list consisting of two fields: `pred`, which is a vector of the predicted response for every new input configuration (rows of `newdata`), and `se`, which is a vector of the predicted response's standard errors.

```
predsMAP
> $pred
> [1] 0.6922523 0.7301342
>
> $se
> [1] 0.077 0.077
predsBayes
> $pred
> [1] 0.695 0.733
>
> $se
> [1] 0.071 0.071
```

In "Bayesian" method, which is the default value of `method` argument, MCMC draws of calibration model parameters are used to form a distribution of each predicted value. In particular, each rows of matrix `Phi` from the output of the calibration model, is used to predict the response for every row of `newdata`. Therefore, a distribution of response is created for each new input configuration. Then, the predictive mean and variance of the resulting distribution are used to compute the point predictions as well as standard errors for predictions.

In "MAP" method, the row of `Phi` matrix that results in maximum log posterior, is extracted and taken as model parameters to compute both point estimates and standard errors. This method is much faster than the "Bayesian" method as it only computes the prediction for each row of observation once.

1.5 Specifying Parameter Priors:

As mentioned hyperparameters of the calibration model can be set using `set_hyperParameters()` function. All arguments of this function, which collectively specify the priors for all hyperparameters, have reasonable default values. Therefore `set_hyperParameters()` can be used without arguments to set the hyperparameters. In fact, the default value of the `hyper` argument in `calibrate()` is the function `set_hyperParameters()` without any argument. Nevertheless, when there is prior belief about structure of correlation structures (either simulator GP or bias-correction GP), these beliefs can be applied to the model in the form of prior specification using `set_hyperPriors()`. For example in the following snippet, only correlation scale parameters of the simulation GP are set to "beta" distributions and the second parameter of beta distribution is set to 6. The first parameter of the beta distribution, the initial value for these parameters, and all other parameter specification remain unchanged.

```
priors <- set_hyperPriors(thetaSDist = "beta", thetaBP2 = 6)
```

1.6 Summarizing the Calibration Model:

Both `summary()` and `print()` generic functions are implemented to work with the output of `calibrate()` function. In particular, given a `fbc` object, `summary()` returns the `estimate` component of `calibrate()` output, which is a data frame containing statistical summary of calibration parameters. Similarly, `print()` will display the same summary data frame in the console.

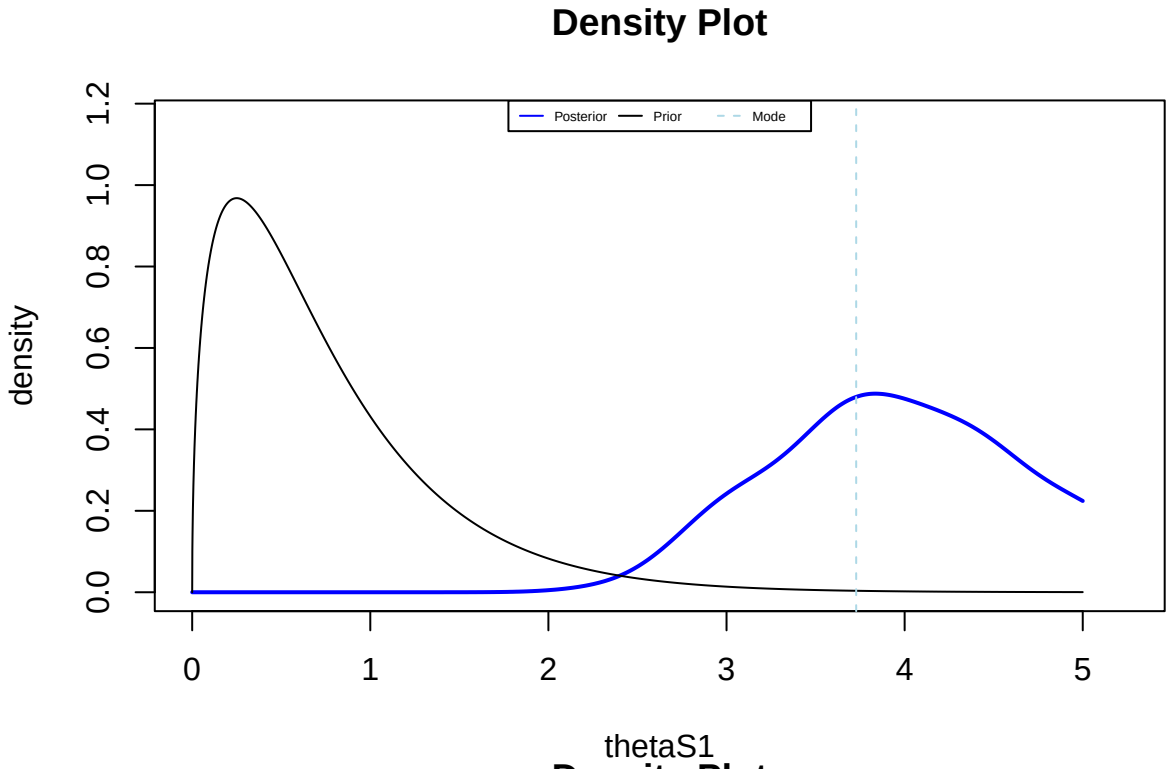
```
calModSum <- summary(calMod)
print(calMod)
>           mean median   mode  lwr50  upr50  lwr80  upr80    sd
> kappa1   9.118  8.594  7.221  7.521 10.233  6.914 12.316 1.995
> thetaS1  4.120  4.044  3.728  3.545  4.576  3.049  5.223 0.837
> thetaS2  0.741  0.710  0.610  0.599  0.839  0.510  1.017 0.210
> alphaS1  1.896  1.906  1.921  1.865  1.927  1.837  1.946 0.046
> alphaS2  1.862  1.862  1.817  1.817  1.911  1.780  1.946 0.065
> thetaB1  0.601  0.520  0.196  0.287  0.791  0.170  1.190 0.418
> alphaB1  1.793  1.824  1.772  1.719  1.905  1.572  1.961 0.147
> sigma2S  0.091  0.089  0.082  0.082  0.098  0.076  0.107 0.012
> sigma2B  0.785  0.611  0.280  0.354  0.984  0.267  1.545 0.627
> sigma2E  0.100  0.100  0.103  0.089  0.109  0.081  0.120 0.016
> muB     -0.119 -0.118 -0.140 -0.257  0.021 -0.349  0.136 0.192
```

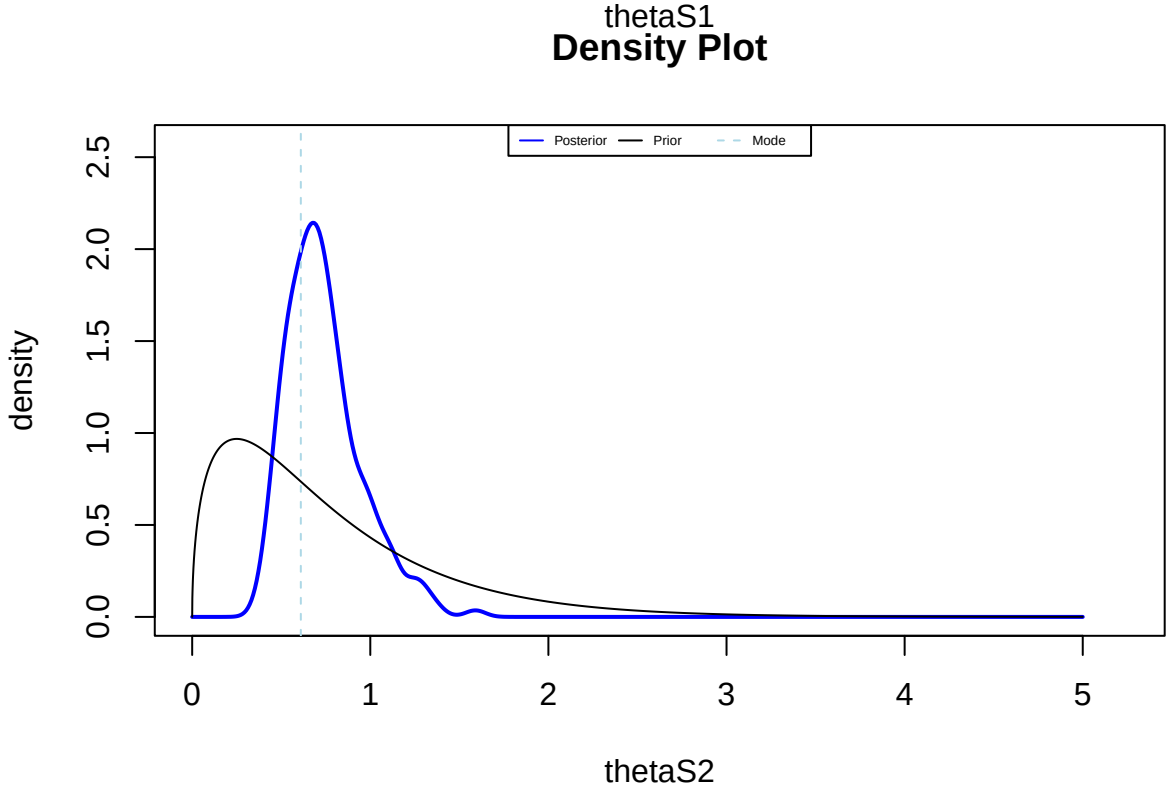
1.7 Visualization of Calibration Model

The implementation of this generic function `plot()` in `FBC` package enables visualization of a calibration model results. Given a calibration model in the form of a `fbc` object using argument `x`, `plot()` can visualize the model in three different mode, which can be chosen by supplying the `type` argument.

In particular, `type` must be a character string form "density", "trace", and "fits". Using "density", which is the default value of the `type` argument, `plot()` will plot the marginal posterior density distribution for the given parameter using `parameter` argument. It does so by estimating a density function given the MCMC-based posterior draws of the parameter. It also plots the prior distribution of the given parameter in the same plot for ease of comparison and visualizes the empirical mode of the posterior density. The `parameter` argument must be a character string consistent with the notation used throughout the package and current vignette , namely from "kappa", "thetaS", "alphaS", "thetaB", "alphaB", "sigma2S", "sigma2B","sigma2E", or "muB". The default value for `parameter` argument is "kappa" or calibration parameters, which usually are the parameters of the interest. Note that `parameter` argument characterizes the class of parameters and when there is more than one parameter in that class,`plot()` will plot the density distribution for all parameters in that class in separate plots.

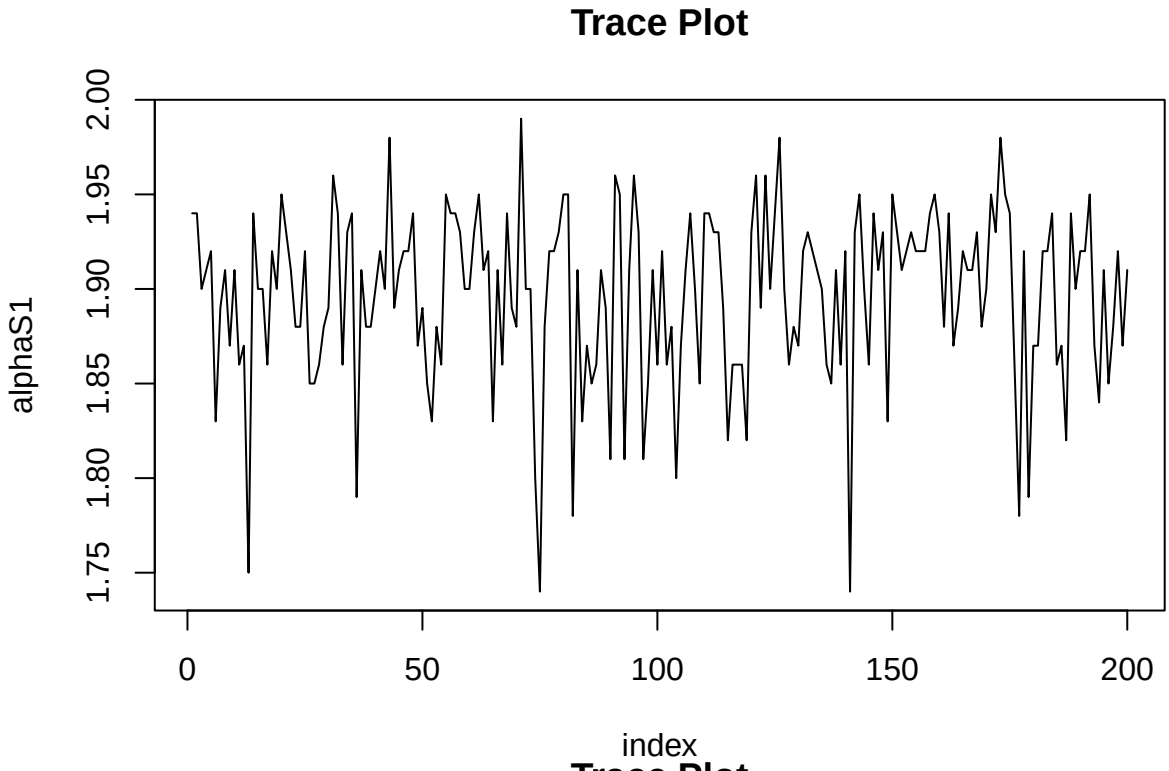
```
# Note that there are two correlation scale parameters in simulator GP and there will be two plots
plot(calMod, parameter = "thetaS")
```

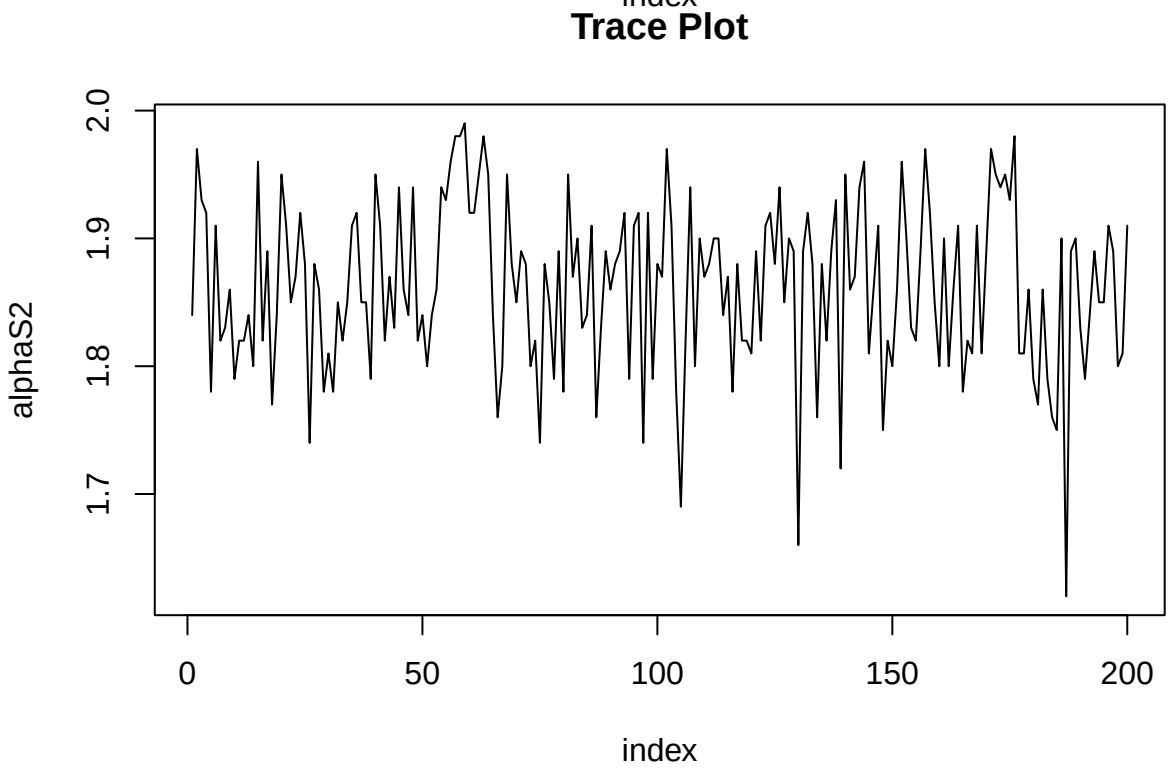




Using "trace" as `type` argument, `plot()` will plot the progression of the given parameter as MCMC draws are taken. It is similar to the time series of the parameter but indexed with number of iteration in MCMC rather than time. The trace plot can be used to determine whether there is good mixing in MCMC draws. Using "trace" as `type` argument also requires supplying the `parameter` from aforementioned list of possible parameter classes. And similar to density plots, trace plots will be plotted for all of the parameters in the given class in separate plots.

```
# Note that there are two correlation smoothness parameters in simulator GP and there will be
# two plots
plot(calMod, parameter = "alphaS", type = "trace")
```

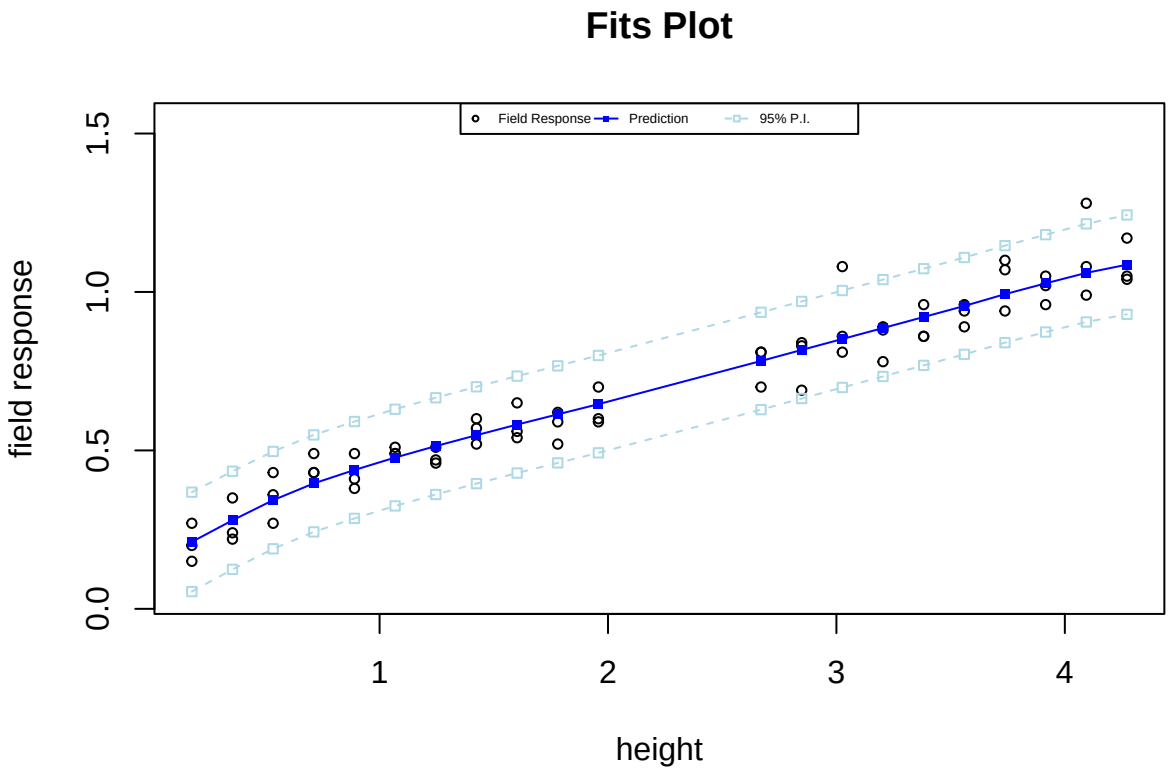




And finally using "fits" as `type` argument, `plot()` will plot the fitted values of the response versus all experimental variables in separate plots. The `parameter` argument is not required for this type and will

be ignored. Fits plots can be used to visually determine the goodness of fits versus actual response during interpolations. Internally, `plot()` will use `predict()` function (using "MAP" method) to compute the fitted values for the training input configurations and will plot them in along with actual values. Furthermore, `xlab` argument can be supplied with a character string to characterize the experimental variables' names. If not supplied, the x-axis will labelled by "x1", "x2", until last experimental variable.

```
# Plots the fitted values versus all experimental inputs along with actual values in separate plots
plot(calMod, type = "fits", xlab = "height")
```



There are also three more exported functions in `FBC` package that are not required to build calibration models or to perform calibrated prediction. These functions are used internally in the package but since they offer functionalists that are not supported in base R, they are exported for use.

1.8 Computing Correlation:

This function is used to compute the correlation between rows of two given matrices assuming a power exponential correlation family structure. This family is a generalization of correlation, where distinct scale and smoothness hyperparameters are used for different dimensions of the given data (columns of given matrices) when computing the correlation. In `FBC`, `correlation()` function treats different dimensions using separate scale and smoothness parameters. Note that only the first matrix, characterized by argument `X` must be supplied and the default value for the second matrix, characterized by `Y` is `NULL`. When only a single matrix is supplied, `correlation()` will compute the correlation of that matrix with itself. Other than the given matrix or matrices, which must have same number of columns, user must supply two vectors with `theta` and `alpha` arguments to characterize scale and smoothness parameters. The length of both vectors either must be same and equal to the number of columns in given matrices, or they must be scaler in which case for all dimensions same values of scale or smoothness will be used.

```
X     <- matrix(c(1, 3, 5,
                  2, 2, 6,
                  1, 4, 1), nrow = 3, byrow = TRUE)

Y     <- matrix(c(7, 3, 0,
                  2, 2, 4), nrow = 2, byrow = TRUE)

sc    <- c(1, 2, 3) # scale parameters of correlation structure
sm    <- c(2, 1, 2) # smoothness parameters of correlation structure

# correlation of a matrix with itself
round(correlation(X, theta = sc, alpha = sm), 5)
>          [,1]    [,2] [,3]
> [1,] 1.00000 0.00248    0
> [2,] 0.00248 1.00000    0
> [3,] 0.00000 0.00000    1

# correlation between two matrices
round(correlation(X, Y, theta = sc, alpha = sm), 5)
>       [,1]    [,2]
> [1,]    0 0.00248
> [2,]    0 0.00001
> [3,]    0 0.00000
```

1.9 Building Prior Functions:

This function will create a prior function based on given distribution and distribution parameters. The function arguments are `prior`, which characterize the distribution family of the prior and two other the arguments, `p1` and `p2` that characterize the parameters of the chosen distribution. The `prior` argument can take a character string value from "uniform", "gaussian", "gamma", "beta", "lognormal", "logistic", "betashift", "exponential", "inversegamma", "jeffreys", "fixed". For example for `prior = "gamma"`, `p1` and `p2` determine shape and scale of the gamma distribution, or for Gaussian distribution, `p1` and `p2` determine mean and standard deviation of the Gaussian distribution. When "fixed" is used for `prior`, the prior function is simply `x = 1`. The output of `prior_builder()` is a function that given a value, computes the probability density of the chosen distribution. To reduce the load of internal computation during creation of the calibration model, `prior_builder()` computes the log of density and if used externally must be transformed.

```
# create a prior function for beta(2, 5). Note that the function compute log of priors and must be tran
pr_fun <- prior_builder(prior = "beta", p1 = 2, p2 = 5)
round(exp(pr_fun(c(-1, 0, 0.1, 0.5, 0.9, 1, 2))), 3)
> [1] 0.000 0.000 1.968 0.938 0.003 0.000 0.000

# create a prior function for a Uniform distribution with lower bound of -10, and upper bound of 10
pr_fun <- prior_builder(prior = "uniform", p1 = -10, p2 = 10)
round(exp(pr_fun(c(-11, -5, 0, 4, 10, 12))), 3)
> [1] 0.00 0.05 0.05 0.05 0.05 0.00

# create a prior function for Gaussian distribution with mean of 1 and standard deviation of 2
pr_fun <- prior_builder(prior = "gaussian", p1 = 1, p2 = 2)
round(exp(pr_fun(c(-9, -5, -3, -1, 1, 3, 5, 7, 11))), 3)
> [1] 0.000 0.002 0.027 0.121 0.199 0.121 0.027 0.002 0.000
```

1.10 Estimating the Mode of a Continious Variable

The function `pmode()` computes an estimate of the mode for a continuous distribution. It works similar to a histogram, in which the domain of the distribution is broken into same length bins. For each bin, the draws of the distribution that fall within that bin is counted and at the end the mean of the bin with highest count is returned as estimated mode. The function also takes the number of bins through `breaks` argument. The default value is `NULL`, which makes `pmode` to determine the number of required bins dynamically based on number of data points and the domain of the distribution.

```
# find the estimated mode of a vector
vec <- runif(100, 0, 10)
pmode(vec)
> [1] 9.668813
pmode(vec, breaks = 10)
> [1] 8.401239
```

2. Calibration Model

Calibration model is statistical model that represent both field and simulator response as function of input configuration. In this section, we explain the theory behind building a calibration model and relate the notation used in the formulation of calibration model and in the package implementation to our ball example.

2.1 Data

A computer experiment or simulation is simply running a computer code at different input configurations and recording the response. The code is an implementation of the mathematical model that is intended to mimic the physical experiment. In general, a simulation has p experimental inputs but also has q additional calibration inputs that are either tuning parameters or unknown physical properties that are not controllable by field experimenter. Table 2 describes the response and inputs of a computer experiment with m observations using matrix notation. The subscript s is used to denote simulation.

Table 2: Notation used to represent simulation data component of calibration model.

Notation	***Description***	***Ball Example***
m	Number of simulation runs	100
p	Number of experimental inputs	1
q	Number of calibration inputs	1
$\mathbf{x_s}$	Simulation input vector containing $(p+q)$ inputs	(h, g) (vector of length 2)
y_s	Univariate simulation response	t (scaler)
$\mathbf{X_s}$	$(m \times (p+q))$ simulation input matrix	[**h g**] ((100×2) matrix)
$\mathbf{y_s}$	Vector of m univariate simulation response	**t** (vector of length 100)

On the other hand, a physical experiment consists of n observations of a physical property, each with p experimental inputs. The calibration inputs are implicit in physical experiment and their values are unknown

but assumed to be fixed throughout observations. To represent both experiments in a unified structure, the unknown calibration inputs of field experiment κ must be augmented to experimental inputs, so that both physical and computer experiments have $(p+q)$ inputs (h and g in ball example) and a univariate response (t in ball example). Assuming vector $\mathbf{x_f}$ represent experimental input, the augmented input vector is denoted by $\mathbf{x}_\kappa$. Since $\mathbf{x_f}$ has p elements and κ has q elements, both will have $(p+q)$ elements similar to $\mathbf{x_s}$. Stacking the input vectors, we can represent all field and augmented input vectors using $\mathbf{X_f}$ and $\mathbf{X}_\kappa$. Similarly, vector $\mathbf{y_f}$ represents all field observations. Subscripts f and $\kappa$are used to denote field and augmented data respectively.

Elements of vector κ are parameters of the calibration model and will be estimated by `calibrate()` [11].

[11] *The first q columns of matrix* `Phi` *in* `calibrate` *output represent the MCMC samples of posterior densities for calibration parameters. In our ball example, there is only one calibration parameter (gravity), which is denoted by* κ_1 *and represented by* `kappa1` *in* `Phi`*..*

Table 3: Notation used to represent field data component of calibration model.

Notation	***Description***	***Ball Example***
n	Number of field observations	63
p	Number of experimental inputs	1
$\mathbf{x_f}$	Field input vector containing p experimental inputs	h (scaler)[12]
κ	Vector of unknown true calibration inputs in field experiment	true value of gravity κ_1
$\mathbf{x}_\kappa$	Augmented field input vector containing $(p+q)$ inputs[13]	$(h, \kappa_1)^2$ (vector of length 2)
y_f	Univariate field response	t (scaler)
$\mathbf{X_f}$	$(n \times p)$ field input matrix	$\mathbf{h}$ (vector^2 of length 63)
$\mathbf{X}_\kappa$	$(n \times (p+q))$ augmented field input matrix	$[\mathbf{h} \quad \kappa_\mathbf{1}]$[14]
$\mathbf{y_f}$	Vector of n univariate field response	$\mathbf{t}$ (vector of length 63)

All of the data components in Table 2 and 3 are generated internally to build the calibration model. The user is only required to provide two matrices representing the field and simulation datasets in their entirety through `sim` and `field` arguments of `calibrate()`.

2.2 KOH Model

Random Functions: KOH models the functional relationship between simulation input and output as a realization of a random function $\eta(\mathbf{x_s})$. Similarly, KOH models the functional relationship between field input and output as a realization of random function $\eta(\mathbf{x}_\kappa)$ but acknowledges a systemic model discrepancy and measurement errors. As a result, KOH models the discrepancy by adding a bias-correction term as realization of another random function $\delta_\kappa(\mathbf{x_f})$. The error term ϵ is considered to be an independent draw from a normal distribution with zero mean and unknown variance σ^2_ϵ.

$$\epsilon \quad \sim \mathcal{N}(0, \sigma^2_\epsilon)$$

$$y_f = \eta(\mathbf{x}_\kappa) + \delta_\kappa(\mathbf{x_f}) + \epsilon$$

$$y_s = \eta(\mathbf{x_s})$$

Therefore other than κ and σ^2_ϵ parameters, the random functions $\eta(.)$ and $\delta_\kappa(.)$ are also unknown and must be specified. KOH models $\eta(.)$ and $\delta_\kappa(.)$ by two independent Gaussian Processes (GP).

[12] *In ball example there is only one experimental input and therefore* $\mathbf{x_f}$ *is a vector of length one or scaler. Similarly, in its matrix notation,* $\mathbf{X_f}$ *is a* $(n \times 1)$ *matrix or a vector of length* n*..*

[13] *Note that calibration parameters* κ *are often assumed to be unchanged throughout field experiment. Therefore, same* (κ) *vector is augmented to all of the field input configurations..*

[14] *Since calibration input is fixed for all field observation,* $\kappa_\mathbf{1} = (\kappa_\mathbf{1}, ..., \kappa_\mathbf{1})$ *vector of length 63}] (*(100×2) *matrix)..*

$$\eta(.) \sim GP\ (0,\ \sigma_s^2.R_s(.,.))$$
$$\delta_\kappa(.) \sim GP\ (0,\ \sigma_b^2.R_b(.,.))$$

Where σ_s^2 and σ_b^2 are marginal variance of simulator and bias-correction GPs, and $R_s(.,.))$ and $R_b(.,.))$ are correlation matrix of simulator GP (using full input matrix $\mathbf{X_s}$ or $\mathbf{X}_\kappa$) and bias-correction GP (using field input matrix X_f).

Note that means of GPs are considered to be zero because `calibrate()` function first standardizes simulation response $\mathbf{y_s}$ (mean zero and standard deviation of one) and then scales field response according to $\mathbf{y_s}$'s scaling factors. Furthermore, the simulator inputs (both experimental and calibration) are scaled to span $[0, 1]$ and the scaling factors of simulation experimental inputs are used to scale field experimental inputs. As a result considering zero mean for both processes seem reasonable. (TODO: look into the effect of constant mean for discrepancy GP).

Correlation Structure: `FBC` employs a power exponential correlation family to represent the correlation structure of both GPs. Assuming $\mathbf{x}$ and $\mathbf{x}'$ are two rows of full input matrix (either $\mathbf{X_s}$ or $\mathbf{X}_\kappa$) and $\mathbf{x_f}$ and $\mathbf{x_f'}$ are two rows of field experimental input matrix ($\mathbf{X_f}$), the correlation matrices $R_s(\mathbf{x}, \mathbf{x}')$ and $R_b(\mathbf{x_f}, \mathbf{x_f'})$ are defined as following:

$$R_s(\mathbf{x},\ \mathbf{x}') = \prod_{i=1}^{p+q} e^{-\theta_i |x_i - x_i'|^{\alpha_i}}$$

$$R_b(\mathbf{x_f},\ \mathbf{x_f}') = \prod_{j=1}^{p} e^{-\theta_j |x_j - x_j'|^{\alpha_j}}$$

Using separable power exponential correlation family introduces two new hyperparameters for each input: scale (θ_i) and smoothness (α_i). Together, they flexibly determine the shape of correlation structure. Table 4 introduce the notation used for hyperparameters of $\eta(.)$ and $\delta_\kappa(.)$.

Table 4: *New Parameters To Build KOH Calibration Model.*

GP	Hyperparameters	Ball Example (Columns of `Phi`)
$\eta(.)$	$(\theta_{s1}, ..., \theta_{s(p+q)}, \alpha_{s1}, ..., \alpha_{s(p+q)}, \sigma_s^2)$	(`thetaS1`, `thetaS2`,`alphaS1`,`alphaS2`, `sigma2S`)
$\delta_\kappa(.)$	$(\theta_{b1}, ..., \theta_{bp}, \alpha_{b1}, ..., \alpha_{bp}, \sigma_b^2)$	(`thetaB1`, `alphaB1`, `sigma2B`)

Full Model: After augmentation of true calibration inputs (vector κ to field data, both simulation and field experiment have the same input. KOH combines both components to build a joint model. The joint vector of all parameters in the final calibration model is denoted by:

$$\phi = (\kappa_1,\ ...,\ \kappa_q,\ \theta_{s1},\ ...,\ \theta_{s(p+q)},\ \alpha_{s1},\ ...,\ \alpha_{s(p+q)},\ \theta_{b1},\ ...,\ \theta_{bp},\ \alpha_{b1},\ ...,\ \alpha_{bp},\ \sigma_s^2,\ \sigma_b^2,\ \sigma_\epsilon^2)$$

Note that in the ball example, the column headers of matrix `Phi` exactly match to model parameters.

```
#head(output$Phi, 3)
```

2.3 Model Parameters

Table 5 provides a general overview of all model parameters, the notations, and corresponding parameters in the ball example.

Table 5: General notation used to represent model parameters and an example of corresponding identifiers in `Phi` matrix.

Parameter	General Notation	Ball Example
True field calibration inputs	$\kappa = (\kappa_1, ..., \kappa_q)$	(`kappa1`)
Simulation GP scale	$\theta_s = (\theta_{s,1}, ..., \theta_{s,p+q})$	(`thetaS1 thetaS2`)
Simulation GP smoothness	$\alpha_s = (\alpha_{s,1}, ..., \alpha_{s,p+q})$	(`alphaS1 alphaS2`)
Bias-correction GP scale	$\theta_b = (\theta_{b,1}, ..., \theta_{b,p})$	(`thetaB1`)
Bias-correction GP smoothness	$\alpha_b = (\alpha_{b,1}, ..., \alpha_{b,p})$	(`alphaB1`)
Simulation marginal variance	σ_s^2	`sigma2S`
Bias-correction marginal variance	σ_b^2	`sigma2B`
Measurement error variance	σ_ϵ^2	`sigma2E`

Each row of matrix `Phi` represents a draw from joint distribution of parameters (MCMC run) and each column represents a parameter in the model. User-given initial values for parameters are used to initialize the first row of the `Phi` matrix. Then, each row will be used to find another sample from joint parameter space to fill the next row of `Phi` until matrix `Phi` is complete.

3. Parameter Estimation

`FBC` employs a full Bayesian approach to jointly estimate all parameters. To find the marginal posterior density distribution for each parameter, we need prior specification for each parameter (prior knowledge) and the joint likelihood estimation (full data).

3.1 Bayesian Analysis

Because `FBC` uses a full Bayesian framework, expert knowledge or opinion can be applied to the model parameters as prior specification. Variety of common prior distributions are implemented in `FBC` and can be used to specify the priors for each parameter (see section 1.2). There are seven classes of parameters and all have been specified in `calibrate()` using default values. Of those seven classes, calibration parameters (vector κ) and perhaps measurement error variance (scaler σ_ϵ^2) are application-dependent. It is recommended for user to specify the prior arguments for these parameters based on prior knowledge or consensus. Nevertheless, prior for calibration parameters is defaulted to Beta(1.1, 1.1) distribution [15]. It is close to standard uniform distribution (U(0, 1)) but densities approach to zero sharply as samples approach boundaries. This default

[15] *Note that the range of Beta distribution is the span of [0, 1], which is the range of calibration inputs for simulator after scaling .*

choice has been made to ensure a somewhat non-informative prior while de-emphasizing on boundary values[16]. For all other classes of parameters reasonable priors have been specified using default values. Priors for correlation scale parameters (vectors θ_s and θ_b) have been set to Gamma(1.1, 0.1) distribution. Similarly, the priors for correlation smoothness parameters (vectors α_s and α_b) have been set to Beta(5, 2) distribution that is shifted one unit to right to span [1, 2] as is the acceptable range for moothness parameters. This choice emphasizes higher (closer to 2 than 1) smoothness parameters. Finally, the priors for marginal simulator and bias-correction and measurement error variances (scalers σ_s^2, σ_b^2, and σ_ϵ^2) are set to be Inverse Gamma(1.5, 1.5). This emphasizes very low variances and de-emphasizes higher values.

By representing both data in a joint calibration model, we can compute the conditional likelihood of response given a parameter vector (See Appendix). Therefore, given the prior specifications above, we can derive joint posterior distribution of parameters given data:

$$\mathcal{P}[\phi|\mathcal{D}] \;\propto\; L(\mathcal{D}|\phi)\;.\;\mathcal{P}[\phi]$$

Where $\mathcal{D}$ represent full data (field and simulation). However, the above formulation is intractable and thus we need a simulation-based method to sample from joint posterior distribution. `FBC` implements a version of Markov Chain Monte Carlo (MCMC) simulation.

3.2 MCMC Simulation

MCMC simulation algorithm is used to draw samples from joint posterior distribution of the parameter space and build `Phi` matrix row by row. MCMC algorithm creates a Markov chain by updating parameters in each iteration according to a proposal scheme. Then given this parameter vector ($\phi^{(i)}$) and data ($\mathcal{D}$), the posterior likelihood can be computed. If posterior probability density of the parameters is larger than the density of a random draw from standard uniform distribution, the algorithm keeps the that parameter configuration by writing the next row of matrix `Phi`, otherwise updates the new row by last parameter vector. In either case, the new row will be used to generate the next proposal. Note that the first row of `Phi`, which is needed to start the algorithm, is supplied by user through initial values for the parameters. The detailed algorithm is presented in the Appendix.

3.3 Parameter Posterior Distributions

At the end of the MCMC run, sample of the joint posterior distribution for each parameter (a column in matrix `Phi`) can be used as an approximation of marginal posterior distribution. Center measures such as mean, mode, or median are provided as parameter estimate depending on the application and distribution shape. Furthermore, 50% and 80% credible sets are formed for each parameters to quantify the uncertainty in estimation. These statistics are provided in `summary` element in the output of `calibrate()` and additionally. (TODO: fix estimate->summary)

```
#output$estimates
```

Alternatively, posterior density kernels can be visualized over their assumed prior to investigate the effect of data on priors for each parameter.

```
# plot(output)
```

[16] *Boundary values of [0, 1] corresponds to $-\infty$ and ∞ in the original scale of calibration parameters.* .

4. Prediction

TODO

5. Implementation

TODO

6. Application

Ball Example

Data:

Spot Weld Example

Description:

Experimental Input: The physical model has three inputs: gauge (G), load (L), and current (C):

- Gauge (G):
- Load (L):
- Current (C):

Calibration Input: The simulation model has one additional input, τ that affects the amount of heat produced in the metal sheets. τ cannot be controlled in the physical experiment and its value is unknown. However it has to be specified for the simulation model as calibration input t:

- Heat generation factor τ: Factor affecting amount of heat produced

Mapping Parameters: To map the spot weld data (both field and simulation data) and parameters to `FBC` input configuration, we use the dagger † superscript to distinguish process parameters and variables with `FBC` variables and parameters:

$$\begin{aligned} \mathrm{x}_1 &\longrightarrow G^\dagger \\ \mathrm{x}_2 &\longrightarrow L^\dagger \\ \mathrm{x}_3 &\longrightarrow C^\dagger \\ \kappa_1 &\longrightarrow \tau^\dagger \end{aligned}$$

Kinetic Example

Appendix

MCMC Algorithm

Implementation of Metropolis within Gibbs algorithm

Let Φ be the matrix of parameter values (columns) indexed by MCMC iterations. Each column represents (after MCMC completes) the posterior density of a parameters. Since all parameters are included in Φ but have overlapping indices, the parameter densities (columns) are renamed to $(\phi_1, ..., \phi_d)$, where $d = 4p+3q+3$ is total number of parameters to have a unique index:

$$\Phi = \begin{array}{c} \begin{matrix} (\mathbf{1}) & & ... & & ... & & (\mathbf{d}) \end{matrix} \\ \begin{matrix} \mathbf{k}_1^* \ ... \ \mathbf{k}_q^* & \mathbf{t}_{s1}^* \ ... \ \mathbf{t}_{s(p+q)}^* & \mathbf{a}_{s1}^* \ ... \ \mathbf{a}_{s(p+q)}^* & \mathbf{t}_{b1}^* \ ... \ \mathbf{t}_{bp}^* & \mathbf{a}_{b1}^* \ ... \ \mathbf{a}_{bp}^* & \mathbf{v}_s^* & \mathbf{v}_b^* & \mathbf{v}_e^* \end{matrix} \\ \begin{bmatrix} k_1^{(1)} \ ... \ k_q^{(1)} & t_{s1}^{(1)} \ ... \ t_{s(p+q)}^{(1)} & a_{s1}^{(1)} \ ... \ a_{s(p+q)}^{(1)} & t_{b1}^{(1)} \ ... \ t_{bp}^{(1)} & a_{b1}^{(1)} \ ... \ a_{bp}^{(1)} & v_s^{(1)} & v_b^{(1)} & v_e^{(1)} \\ ... & ... & ... & & ... & & & ... \\ k_1^{(N)} \ ... \ k_q^{(N)} & t_{s1}^{(N)} \ ... \ t_{s(p+q)}^{(N)} & a_{s1}^{(N)} \ ... \ a_{s(p+q)}^{(N)} & t_{b1}^{(N)} \ ... \ t_{b(p+q)}^{(N)} & a_{b1}^{(N)} \ ... \ a_{b(p+q)}^{(N)} & v_s^{(N)} & v_b^{(N)} & v_e^{(N)} \end{bmatrix} \end{array}$$

- Initialize the first row with user-given initial values:

$$\begin{aligned} \phi^{(1)} &= (\phi_1^{(1)},\ ...,\ \phi_d^{(1)}) \\ &= (k_1,\ ...,\ k_q,\ \theta_0^{(1)},\ ...,\ \theta_0^{(p+q)},\ \alpha_0^{(1)},\ ...,\ \alpha_0^{(p+q)},\ \theta_0^{(1)},\ ...,\ \theta_0^{(p)},\ \alpha_0^{(p)},\ ...,\ \alpha_0^{(p)},\ v_{s0},\ v_{b0},\ v_{e0}) \end{aligned}$$

- At each iteration $i \in (2, ..., N)$, and to update j-th parameter ($j \in (1, ..., d)$ and first $(j-1)$ parameters are already updated):

  1. Propose a new value for $\phi_j^{(i)}$ based on its last update [17]. $\phi_j^{(i-1)}$, called Metropolis Update (MU):

  $$\phi_j^* = \mathcal{N}(\phi_j^{(i-1)}, \sigma_p^2)$$

  where σ_p^2 is adaptively adjusted [18] to ensure (faster) convergence.

  2. Form the parameter vector ϕ^* based on MU:

  $$\begin{aligned} \phi^{(last)} &= (\phi_1^{(i)}, ..., \phi_{j-2}^{(i)},\ \phi_{j-1}^{(i)},\ \phi_j^{(i-1)},\ ...,\ \phi_d^{(i-1)}) \\ \phi^* &= (\phi_1^{(i)}, ..., \phi_{j-1}^{(i)},\ \phi_j^*,\ \phi_{j+1}^{(i-1)},\ ...,\ \phi_d^{(i-1)}) \end{aligned}$$

  3. Draw a random sample u from $U(0, 1)$ and take its log: $\ln(u)$

[17] If it is first parameter, the last update is the last row ($\phi^{(i-1)}$

[18] Every 50 iterations, acceptance rate (AR) is computed. If $AR < 0.44$, proposal variance σ_p^2 is decreased, and vice versa.It has been shown that for one-dimensional proposals used in Metropolis within Gibbs algorithm, the optimal acceptance rate is 0.44 (TODO: citation).

4. Compute the difference between the log of joint posterior density given current and last parameter vectors:

$$h(\phi^*,\ \phi^{(last)}) = \ln(L(\mathrm{y}|\phi^*)) + \ln(\mathcal{P}[\phi^*]) - \ln(L(\mathrm{y}|\phi^{(last)})) + \ln(\mathcal{P}[\phi^{(last)}])$$

5. If $h(\phi^*,\ \phi^{(last)}) > \ln(u)$, set:

$$\phi_j^{(i)} = \phi_j^*$$

otherwise,

$$\phi_j^{(i)} = \phi_j^{(i-1)}$$

6. The update vector now is:

$$\phi^{(last)} = (\phi_1^{(i)}, ..., \phi_{j-1}^{(i)},\ \phi_j^{(i)},\ \phi_{j+1}^{(i-1)},\ ...,\ \phi_d^{(i-1)})$$

- If all parameters are updated, go to next iteration of i
- When iterations of i is completed, return the matrix of Φ that contains joint posterior density distribution of all parameters. Marginal distribution of each parameter can be used for point prediction and uncertainty quantification (credible interval).

Bayesian Analysis

In the Bayesian framework, the joint probability distribution of all parameters and hyperparameters of the calibration model given data ($\mathcal{P}[\phi|\mathrm{y}]$) can be derived:

$$L(\mathrm{y}|\phi) = |C|^{-\frac{1}{2}} \,.\, e^{-\frac{1}{2}\mathrm{y}.C^{-1}.\mathrm{y}^T}$$

$$\mathcal{P}[\phi|\mathrm{y}] \ \propto\ L(\mathrm{y}|\phi) \,.\, \mathcal{P}[\phi]$$

Taking the log from both sides will decrease computational load and increase speed:

$$\ln(L(\mathrm{y}|\phi)) = -\frac{1}{2}\ln(|C|) - \frac{1}{2}\mathrm{y}.C^{-1}.\mathrm{y}^T$$

$$\begin{aligned}
\ln(\mathcal{P}[\phi|\mathrm{y}]) \ &\propto \ln(L(\mathrm{y}|\phi)) + \ln(\mathcal{P}[\phi) \\
&= -\frac{1}{2}\ln(|C|) - \frac{1}{2}\mathrm{y}.C^{-1}.\mathrm{y}^T && \text{(log liklihood given full data: X, y)} \\
&+ \sum_{i=1}^{q} \mathcal{P}[\kappa_i] && \text{(priors for calibration parameters)} \\
&+ \sum_{i=1}^{p+q} \mathcal{P}[\theta_{si}] + \sum_{i=1}^{p+q} \mathcal{P}[\alpha_{si}] \ + \ \mathcal{P}[\sigma_s^2] && \text{(priors for } \eta(.) \text{ hyperparameters)} \\
&+ \sum_{i=1}^{p} \mathcal{P}[\theta_{bi}] + \sum_{i=1}^{p} \mathcal{P}[\alpha_{bi}] \ + \ \mathcal{P}[\sigma_b^2] && \text{(priors for } \delta_\kappa(.) \text{ hyperparameters)} \\
&+ \ \mathcal{P}[\sigma_\epsilon^2] && \text{(prior for measurement error variance)}
\end{aligned}$$

Above equation is intractable and thus a simulation-based method must be used to sample from posterior distribution. `FBC` implements a version Markov Chain Monte Carlo (MCMC) simulation.

Full Model

KOH model combines simulation and field data to form a joint model using joint dataset:

$$\mathbf{y} \ = \begin{bmatrix} \mathbf{y_f} \\ \mathbf{y_s} \end{bmatrix} = (y_1, \ \ldots \ , \ y_{n+m})^T \qquad \text{(joint vector of responses)}$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_\kappa \\ \mathbf{X_s} \end{bmatrix} = \begin{bmatrix} \mathbf{x_1} \ \mathbf{x_2} \ \ldots \ \mathbf{x_{p+q}} \end{bmatrix} \qquad \text{(joint input matrix)}$$

$$\mathbf{x_i} = (x_1, x_2, ..., x_{n+m}) \quad \forall i \in \{1, 2, ..., p+q\}$$

Since $\mathbf{X_f}$ is a sub-matrix of $\mathbf{X}$, we can represent the functional relationship between input and response for full model with $\zeta(.)$, which is considered to be realization of a random function and derived from $\eta(.)$ and $\delta_\kappa(.)$:

$$\mathbf{y} \ = \zeta(\mathbf{X})$$

Because both $\eta(.)$ and $\delta_\kappa(.)$ are GPs, $\zeta(.)$ can also be considered a zero mean GP:

$$\zeta(.) \sim GP \ (0, \ C(.,.))$$

Where covariance matrix C is dependent to full input matrix $\mathbf{X}$ and hyperparameters of $\eta(.)$ and $\delta_\kappa(.)$, which in turn are dependent to model hyperparameters.

Using matrix notation, input/output relationship of both experiments is presented below in matrix notation. This relations can be used to derive a relationship for joint data:

$$\mathrm{y} \ = \zeta(X) = \eta(X) + \begin{bmatrix} \delta_\kappa(X_f) + \mathcal{E} & 0 \\ 0 & 0 \end{bmatrix}$$

Since X_f is a subset of matrix X, the joint response y can be modeled as a random function $\zeta(X)$. In the ball example, the full input matrix X is a (163×2) matrix by stacking X_κ on X_s Note that since κ is unknown, the initial value `c0` is used internally to build X_κ.

Where, C_η and C_δ are covariance matrices of full input matrix X and original field input matrix X_f. And C is characterized as:

$$C(X, X) = C_\eta(X, X) + \begin{bmatrix} C_\delta(X_f, X_f) + \sigma_\epsilon^2.I_n & 0 \\ 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} C_\eta(X_f, X_f) + C_\delta + \sigma_\epsilon^2.I_n & C_\eta(X_s, X_f) \\ C_\eta(X_f, X_s) & C_\eta(X_s, X_s) \end{bmatrix}$$

Note that C_s covariance matrix of the full data X is further divided to components $C_\eta(X_f, X_f)$, $C_\eta(X_s, X_f)$, $C_\eta(X_f, X_s)$, and $C_\eta(X_s, X_s)$ to optimize the computation.

References