Objective calibration of climate models using multivariate quadratic emulation

Documentation and Example

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Chapter 1

Introduction

This document gives an introduction for an parameter estimation procedure for complex computer models with very large data output. The methodology relies on the publication "Bellprat, O., S. Kotlarski, D. Lüthi, and C. Schär (2012), Objective calibration of regional climate models, J. Geophys. Res., 117, D23115, doi:10.1029/2012JD018262. (Bellprat et al., 2012b)" and has originally been designed for an objective calibration of model parameters in physical parameterizations of regional climate models using a calibration theory published in (Neelin et al., 2010). In practice, the approach can be applied to any optimization problem, yet if the target model or function is computationally very efficient, flexible approaches provide more accurate solutions.

The number of required simulations using such alternative approaches is yet too large for high resolution climate models since typically only few tenths of simulations can be afforded. The present framework therefore aims at minimizing the computational costs to calibrate unconfined model parameters in climate models. Presently state-of-the-art atmospheric model are tuned using expert knowledge and hand-tuning without following a well defined strategy. This condition inhibits for instance model comparison using two different parameterizations as the model will always depend on how the tuning is performed. The proposed procedure therefore is not only an approach to improve model performance but also to compare model parameterizations which have undergone the same tuning efforts.

Nonetheless expert knowledge is still required in the proposed framework by the definition of model parameters which are calibrated and their uncertainty ranges. This selection is a choice of the user, as well as the definition of a cost-function which is optimized. The tool hence is a way to facilitate high-dimensional problem solving given certain definitions which allows for a transparent and re-producible calibration of climate models.

The following chapters will guide a user for application of the methodology. The first chapter gives the methodological background. The second chapter aims at providing an overview of the code package and the work flow for a potential application. This followed by an overview of all functions as part of the package are presented for more in-depth understanding.

Chapter 2

Method

Although methodology of the calibration framework is documented in the reference publication, a short summary of the important equations is summarized here. The basic idea of the framework is to build a computationally efficient statistical model that approximates the model output fields for an n-dimensional parameter space (often termed as model emulator, model surrogate, or *metamodel*). Using such a metamodel the high dimensional problem can be solved efficiently with common optimization procedures that require typically O^{5-9} simulations for parameter problems with 10 or less parameters. These number of simulations are not possible to perform with a climate model due to computational constraints of current high-performance computing centers.

There are numerous approaches how to approximate model parameter experiments (e.g. Neural Networks or Gaussian Processes) and several approaches have been applied to climate models as discussed in Annan and Hargreaves (2007). The present framework relies on a metamodel that approximates the parameter space using a multivariate quadratic regression. This choice has been made as the approach uses only the minimum number of model simulations that are required to account for non-linear behavior and parameter interactions in model parameter experiments. The use of a quadratic regression further inhibits over-fitting and allows for analytical solutions of the parameter space.

In order to estimate the multivariate quadratic metamodel only the boarders of the n-dimensional space have to be sampled (a design which is referred as a Koshal design in the literature). The Fig.2.1 illustrates such a design for two parameters (P1,P2) where in the center the default values (cross) and each dimension a minimum and maximum parameter value is sampled (circles). Additionally, in order to take parameter interactions into account, one corner point needs to be simulated (triangle) which corresponds to N*2+N(N-1)/2 simulations for N parameters.

Using the design points the following linear set of equations can be solved to estimate the linear term "a" and the non-linear term "B",

$$\Phi^* = \Phi_{ref} + \mu_*^T a + \mu_*^T B \mu_*. \tag{2.1}$$

where Φ corresponds to the data field which is approximated (Φ_{ref} is the reference field, Φ^* the predicted field by the metamodel) based on parameter vector $\mu*$ which describes the parameter values centered around the default value and normalized by the parameter range,

$$\mu_* = \frac{\mu_p - \mu_{def}}{max(\mu_p) - min(\mu_p)}. \tag{2.2}$$

Using centered parameter values has the advantage that the prediction of a parameter combination in one dimension is independent from the other parameter dimensions and therefore also their inaccuracies. The normalization avoids rounding errors in case the parameters vary in very different magnitudes.

The metamodel is by its definition quadratically smooth in space and only interaction between two parameters are allowed. This simplification is a good approximation of parameter experiments in climate models (Neelin et al., 2010, Bellprat et al., 2012b) but some inaccuracies because of this simplification

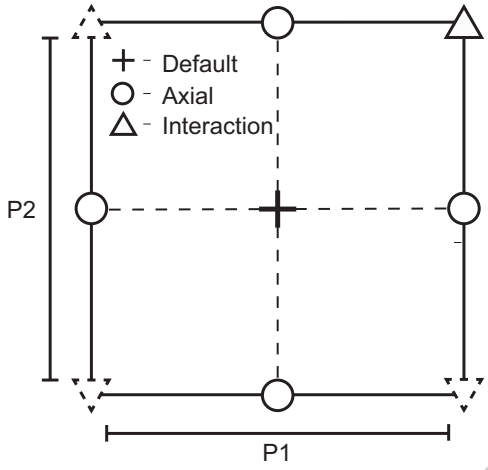

Figure 2.1: Koshal parameter experiment design required to estimate the parameters of the metamodel

can arise. In particular the estimation of the parameter interactions has proven to be mis-represented by this simplification. Possible reasons might be that three-way parameter are not determined even tough they seem to have important contributions in climate models (Rougier et al., 2009) or that the quadratic interaction term is not flexible enough to capture the true parameter interactions in the model. To constrain this uncertainty it is therefore advisable to use several simulation to estimate the interaction terms to achieve higher accuracy, yet typically the parameter interactions play only a minor role to determine the parameter space (Bellprat et al., 2012b, Bracco et al., 2013). Nevertheless, if higher metamodel accuracies are desired, a Gaussian Process (GP) approach is here advised (Rougier et al., 2009, a Matlab code for GP emulation is provided here http://www.gaussianprocess.org/).

Using the fitted metamodel the agreement of the model with the observations can be maximized using performance function. This function is a choice of the user and is independent of the calibration framework and thus different objective functions can be optimized. We here choose to use a multivariate least-square estimation (Performance Score PS) considering uncertainty sources of predictability and observations as defined in Bellprat et al. (2012a).

Using a definition of the model performance the parameter space can be sampled to identify optimal parameter configurations. Finding such optimal configurations is albeit the linearisation of the climate model using the metamodel a tedious task in very high dimensional parameter spaces. The most challenging problem of such optimization problems is that within the parameter space many local maxima may exist which need to be distinguished but also identified. Sampling the parameter space (with N number of parameters) using a grid design is very inefficient in this case as the number of parameter combinations required grows with the exponent of parameters (power N). A further key limitation of grid sampling is the "collapsing" property: multiple parameter configurations have the same parameter value projected on the parameter axis. This limits the sampling in space and thus the small scale non-linearities i.e. local maxima are misrepresented.

Again numerous approaches from optimization theory exist to efficiently find these maxima. Here we use a Latin hypercube sampling (LHS) approach to reduce the dimensionality of the parameter problem. The approach has been introduced by McKay et al. (2000) and is widely used for determination of computer experiments. To illustrate the concept a comparison between a grid sample and a Latin hypercube sample is shown in Fig.2.2 again for two parameters. The baseline of the LHS is the number of parameter combinations M which are sampled. In case of a grid design for two parameters using a minimum, a center and maximum parameter value the number of parameter combinations corresponds to $M = 3^2 = 9$ experiments. Instead of sampling each combination for a fix number of intervals (grid design) the number of intervals in a LHS corresponds to the number of experiments M. The sample is subsequently drawn as such that each parameter combination uses a different parameter value as any other combination. This approach avoids the "collapsing" property of a grid design and makes the

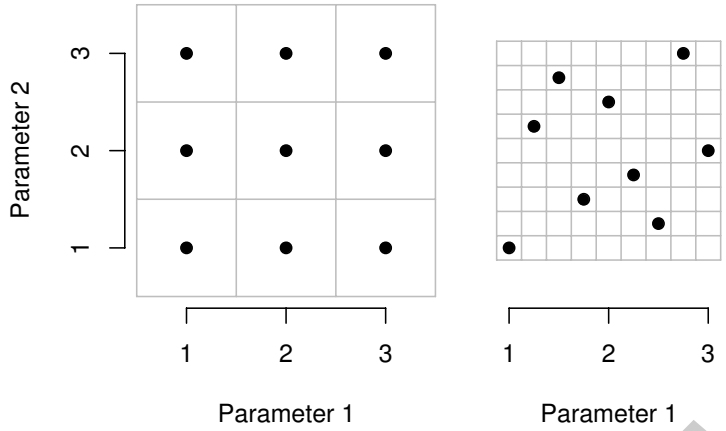

Figure 2.2: Comparison of grid-sampling and Latin hypercube sampling from Urban and Fricker (2010)

sampling independent of the number of parameters considered.

There are multiple samples which can be drawn for such a design corresponding to $(M!)^{N-1}$. The common approach to select one these samples is to use the sample with highest sum of Euclidean distances or to minimize the correlation structure between all parameter combinations. The LHS is used in the reference publication to find optimal parameter configurations using a 1 Million LHS for five parameters (i.e. 1 Million different values for each parameter sampled). Further a LHS sample is used to draw an independent parameter sample for a validation ensemble of the metamodel is used.

Alternative procedures for the calibration of the model parameters is possible using machine learning theory as Genetic Algorithms (Goldberg, 1989, toolbox integrated in Matlab as `gatool`) or Bayesian statistics as a Marcov Chain Monte Carlo (MCMC, Matlab code available here http://helios.fmi.fi/ lainema/mcmc/) integration. Generally these approaches are more efficient but require a multitude of additional assumptions. A further approach to constrain the parameter uncertainty without a calibration procedure is history matching, recently also applied in climate models (Williamson et al., 2013).

Chapter 3

Code structure and working flow

The structure of the program code is shown in Fig.3.1. Four main operation tasks are defined in square blocks, the definition of calibration suite, the estimation of the metamodel, the validation of the metamodel and the optimization of the model parameters. Relying on these main task, optional routines can be called which are shown in ellipsoid areas. The data of is stored and accessed by three matlab structures termed *parameters* (contains information on parameters and experiments), *datamatrix* (contains simulated data of parameter experiments and validation sets) and *metamodel* (contains parameters and information on the fitted metamodel). All matlab routines can be called using these data structures, which are described with more detail in the next sections.

3.1 Definitions and data

3.1.1 *Parameter*

Within the *parameter* structure all information about the model parameters are stored. The individual fields describe for each parameter in *name* a string of the parameter name, *name_tex* the same name string using LaTeX standards for plotting, in *range* a vector with the minimum and maximum parameter value, in *default* the reference parameter value, in *experiments* the parameter values of all experiments used to fit the metamodel, in *constrain* additional parameter experiments outside of the Koshal design to further constrain the metamodel, and in *validation* the parameter values of the independent experiments used to validate the metamodel.

```
parameters =

1xN struct array with fields:
    name
    name_tex
    range
    default
    experiments
    constrain
    validation
```

3.1.2 *Datamatrix*

The *datamatrix* contains all data from the simulations which is needed to estimate and validate the metamodel, and to compute model scores if they are not emulated directly. A function to read-in data must be built by the user, an example how to read NetCDF data is provided. The individual fields of this structure contain in *moddata* all model data of the parameter experiments used to fit the metamodel, in *refdata* the data of the reference simulation, in *valdata* the data of the independent simulations for the validation of the metamodel, in *obsdata* the observations which are used to compute a model score if specified any, in *score* the name of the function that computes the model score (an example using *ps* is provided), in *constrain* the data of the simulations needed to additionally constrain

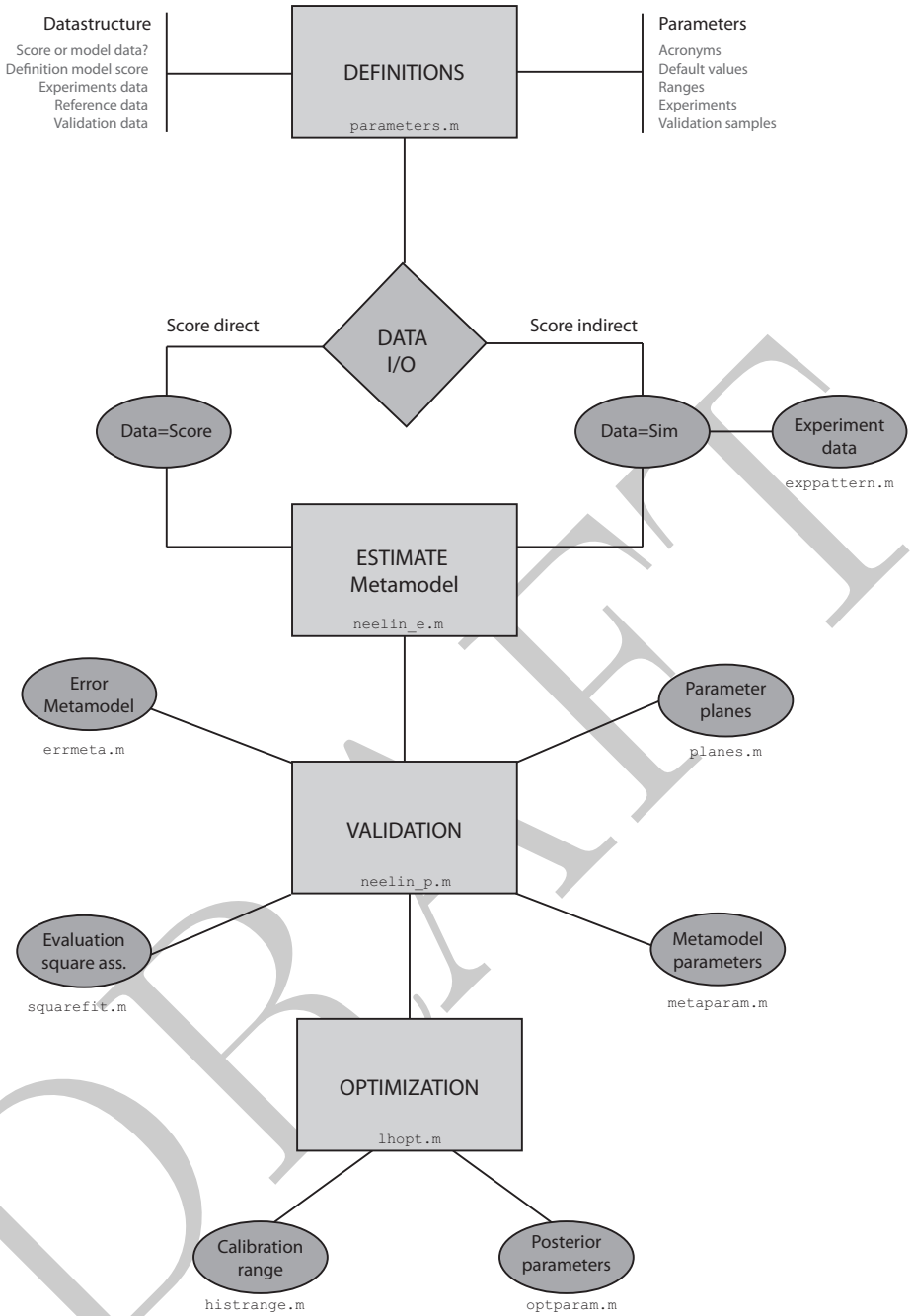

Figure 3.1: Schematic figure on the calibration framework. The framework is divided in four main tasks illustrated with square blocks: the definition of the calibration suite, the estimation of the metamodel, the validation of the metamodel and the optimization of the model parameters. For each task different functions are provided which are called using three data structures of the framework: the *datamatrix* (containing the data of the simulations and its definitions), the *parameters* (containing the information about the parameters and its values of the experiments), and *metamodel* (containing the estimated metamodel parameters). All functions need either all of these data structures or only two of them. More information about the functions are provided in the function alphabet of this document.

the metamodel. Further information of physical variables can be specified which are listed in the field *variables* that describes in the first term the index within the data structure that corresponds to different physical variables and in the continuation the strings of the variable names. Further physical limits for these variables can be set in *limits*, with a lower and upper bound for which each prediction with the metamodel is constrained.

```
datamatrix =

      moddata: [5-D double]
      refdata: [4-D double]
      valdata: [5-D double]
      obsdata: [4-D double]
        score: 'ps'
    constrain: [5-D double]
    variables: {[4]  'T2M'  'PR'  'CLCT'}
       limits: {[-Inf Inf]  [0 Inf]  [0 100]}
```

3.1.3 *Metamodel*

The estimated metamodel parameters are stored in the *metamodel* structure. For each data point a linear a and non-linear matrix B is estimated, the dimensions of field a and B therefore corresponds to the dimensions of the data plus a dimension for all parameters. In case additional simulations are used to constrain the metamodel a constant term c is used, otherwise only the data of the reference simulation is used as a constant term.

```
metamodel =
            a: [6-D double]
            B: [7-D double]
            c: [6-D double]
```

3.2 Metamodel estimation

The estimation solves the linear set of equations resulting from equation 2.1. The data matrix is for this purpose linearized such that the estimation is independent on the number of dimensions. This allows that the metamodel can be estimated on multivariate model data or integrated data of for instance a performance score directly (one value per experiment). The estimation of the metamodel is called using `neelin_e` which gives as an output the estimated metamodel.

```
metamodel = neelin_e(datamatrix,parameters)
```

The linear set of equation is solved by using the axial and default experiments (See Fig.2.1) for a quadratic regression in each parameter dimension, which can subsequently used to estimate the interaction term using the interaction experiments.

Depending on the number of experiments provided the function differs between different estimations. If the number of experiments is small than the number required for a Koshal design (2*N+N(N-1)) the estimation of the interaction terms is omitted and only the linear and quadratic term is estimated. If the number of experiments is larger than the linear set of equations the additional experiments are used to further estimate the interaction terms using a least square estimation. In case the number of experiments is small than 2*N the estimation can not be performed.
In case additional experiments are desired to use to further constrain the metamodel linear and square parameters the function `neelin_c` can be used, which uses the definitions of datamatrix.constrain and parameters.constrain to narrow the uncertainty of the metamodel. This function should be called after the initial estimation of the metamodel as the following:

```
metamodel = neelin_c(datamatrix,parameters,metamodel)
```

3.3 Metamodel validation

Once the metamodel is estimated the metamodel can be evaluated with a number different analysis functions. The base function for this purpose is metamodel prediction function `neelin_p` which predicts the data of a given parameter experiment using the three base structures (metamodel, parameters, datamatrix) and a vector of parameter values for which the data should be predicted.

```
datamatrix = neelin_p(metamodel,parameters,datamatrix,pvector)
```

Given the prediction function independent simulations not used to estimate the metamodel can be used to assess the accuracy of the metamodel. This error of the metamodel can be estimated using the function:

```
[errstd]=errmeta(metamodel,parameters,datamatrix)
```

The function estimates the standard error to predict a number of experiments defined in datamatrix.valdata with parameter values defined in parameters.validation. Further a scatter plot of the simulated and predicted data points is produced.

Further metamodel analysis tools are the `planes` function, that plots pair-wise parameter planes predicted by the metamodel, `metaparam` which plots the metamodel parameters normalized by the variability of the data, and `squarefit` which allows to visualize the quadratic regression averaged for all the data points. If datamatrix.variables is specified, referring to physically different variables in the data, all the aforementioned figures are separated for these variables.

3.4 Parameter optimization

If the accuracy of the metamodel satisfies the needs of the problem the parameter space can be sampled in order to determine optimal model parameters. The calibration package offers for this purpose a Latin hypercube sampling that can be called using:

```
[lhscore lhexp popt]=lhopt(metamodel,parameters,datamatrix,lhacc)
```

The number `lhacc` determines the number of samples drawn from the LHS. The optimization yields for each sample a performance score (`lhscore` depending on the definition of the score), the experiment of the parameters (`lhexp`) and the optimal model parameter setting (`popt`). The optimal parameter corresponds to the parameter sets which according to the metamodel yields the highest score. However, given that the metamodel is associated with an uncertainty it is more reasonable to determine a distribution of parameter combinations which yield best model performance.

This distribution of optimized model parameters can be computed using the following function:

```
optparam(parameters,lhscore,lhexp,popt,errstd)
```

Additionally to visualize the whole performance space captured by the metamodel, a empirical distribution of the performance score can be visualized using the following command:

```
histplot(lhscore,datamatrix)
```

Chapter 4

Function Alphabet

The available functions of the package are briefly described here with a short description of the functionality, an example of the produced figure (if any produced) and the description from the header of the code. The figures are based on an example of a calibration of the regional climate model COSMO-CLM for 8 parameters. The underlying description of the variables and observations selected are described in Bellprat et al. (n.d.). Additionally, to the functions of the calibration framework, a very simple toy model `calmo_toy` is provided which allows to test the effect of noise in the experiment data and effect of structural error of the quadratic assumption.

4.1 exppattern.m

In order to visualize the effect of the model parameters from the different experiments a plot procedure is provided which summarizes the the difference of the experiments with respect to the reference.

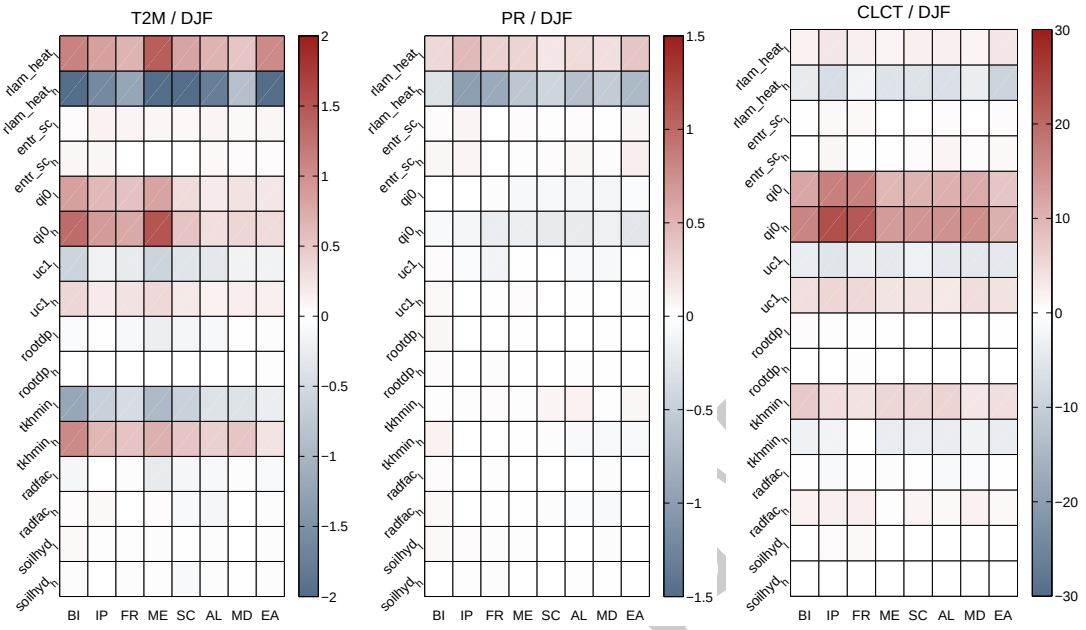

Figure 4.1: Sensitivity of parameter experiments divided in to variables, regions and seasons.

Header:

```
% Plot routine to visualize experiments for a Neelin fit
% NAME
%   exppattern
% PURPOSE
%   Create mosaic plots for dimesensions simulation, region, and varable
% INPUTS
%   From the structure datamatrix and paramters the
%   following fields are
%   processed (mind the same naming in the input)
%
%   datamatrix.moddata:
%
%           Model data for all experiments
%
%   parameters.name:
%
%           Name of parameter, parameter experiments
%
% OUTUTS
%   Pcolor plots given the number of model variables
% HISTORY
%   First version: 11.10.2013
```

4.2 errmeta.m

When using a validation set of simulations the function `errmeta.m` allows the user to estimate the prediction error of the metamodel. The error of the metamodel is further visualized using the scatter plots of the simulated and predicted data points as shown in Fig.4.2.

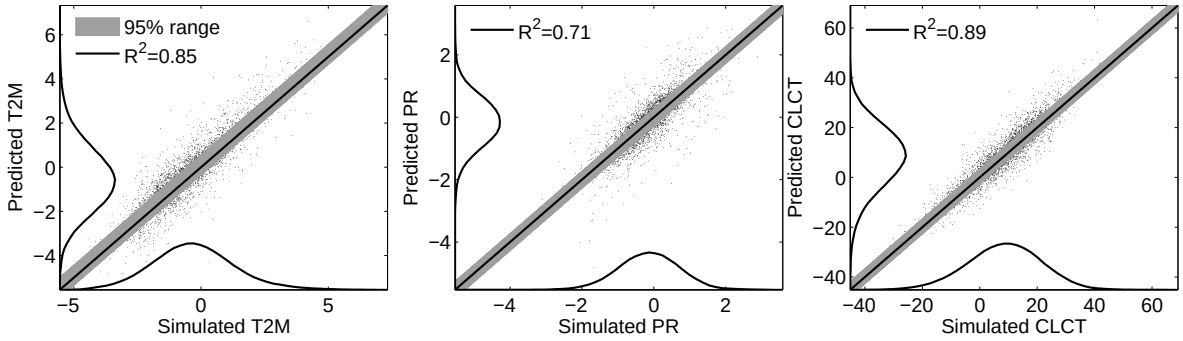

Figure 4.2: Simulated and predicted data points with the metamodel divided into different variables.

Header:

```
% Estimate the error of the metamodel to predict indpendent model information
% NAME
%   errmeta
% PURPOSE
%   Predict modeldata on of independt simulations and estimate the
%   standard error of the metamodel
%
% INPUTS
%   The structure metamodel, parameters and datamatrix
%   are used for the inpute of neelin_p. Addionally the parameter
%   matrix is read
%
%   parameters.experiments:
%
%           Parameter matrix of experiments on which metamodel is
%           estimated
%   phyd:
%
%           Index in the model data along which the prediction
%           error is physically seperated (ex: ind of different
%           model variabiles (temperature,precipitation,clouds))
% OUTUTS
%   Plot: Scatter plot for each defined variable of simulated and
%   predicted points
%   errstd: Standard error to predict the model data
%   errps: Standard error to predict the model score
% HISTORY
% First version: 11.10.2013
```

4.3 histplot.m

This functions allows to characterize the full calibration range of the parameter space in the for the specified performance function. Further the level of the reference function and the level of performance of the optimized configuration is plotted as shown in Fig.4.3.

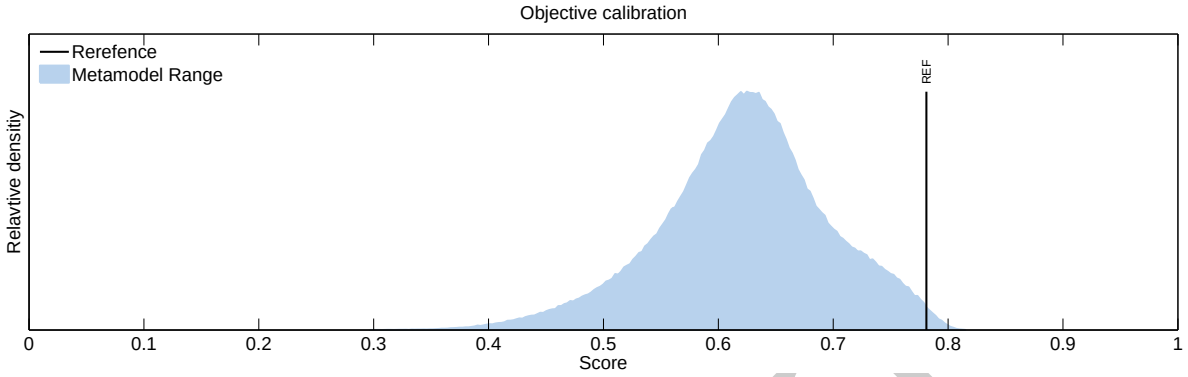

Figure 4.3: Calibration range of the Latin hypercube sample along the performance score (PS) in comparison to the reference (REF) simulation. The blue area above the reference simulation indicates the potential of the calibration to improve the model performance.

Header:

```
%   Plot full performance range sampled with the Latin hypercube
%   experiment as a histogramm
% NAME
%   neelin_p
% PURPOSE
%   Predict data using the metamodel for a parameter matrix
% INPUTS
%   From the structure metamodel, parameters and datamatrix the following fields are
%   processed (mind the same naming in the input)
%
%   datamatrix.reffdata:
%
%            Modeldata using default parameter settings to
%            determine/compute the model score of the reference
% OUTUTS
%   Plot: Histogram plot
% HISTORY
% First version: 11.10.2013
```

4.4 lhopt.m

The optimization of the optimal parameter configurations is done using a Latin hypercube sampling described in `lhopt.m`. For a given number of samples the function computes the predicted performance score of each sample and looks for the best combination. The output of the function is then further used to for `histplot.m` and `optparam.m`.

Header:

```
% Optimise model parameters using a Latin hypercube sampling
% NAME
%   neelin_p
% PURPOSE
%   Create a sample of parameters using a Latin hypercube design
%   and predict the model performance of the sample using the
%   metamodel.
% INPUTS
%   From the structure metamodel, parameters and datamatrix the following fields are
%   processed (mind the same naming in the input)
%
%   metamodel.a:
%
%          Vector of linear terms of the metamodel [...,N,1] additional
%          data dimensions possible (ex:a~[Regions,Variables,Time,N,1])
%
%   metamodel.B:
%
%           Matrix of quadratic and interactions terms [...,N,N] additional
%           data dimensions possible (ex:a~[Regions,Variables,Time,N,N])
%
%   parameters.range:
%
%            Range of values for each paramter to normalize the
%            scale.
%
%   parameters.default:
%
%            Default values of parameters to center the scale
%
%   datamatrix.reffdata:
%
%            Modeldata of when using default parameter values to
%            to center the datamatrix
%
%   pvector: Parameter values for one experiment with the
%            dimension of [N,1] N=Number parameters
% OUTUTS
%   dmatrix: Predicted data for parameter experiment
% HISTORY
% First version: 11.10.2013
```

4.5 metaparam.m

To assess the linear, quadratic and inter-action terms of the metamodel a function is provided which shows these terms when averaging for the whole data structure as shown in Fig.4.4.

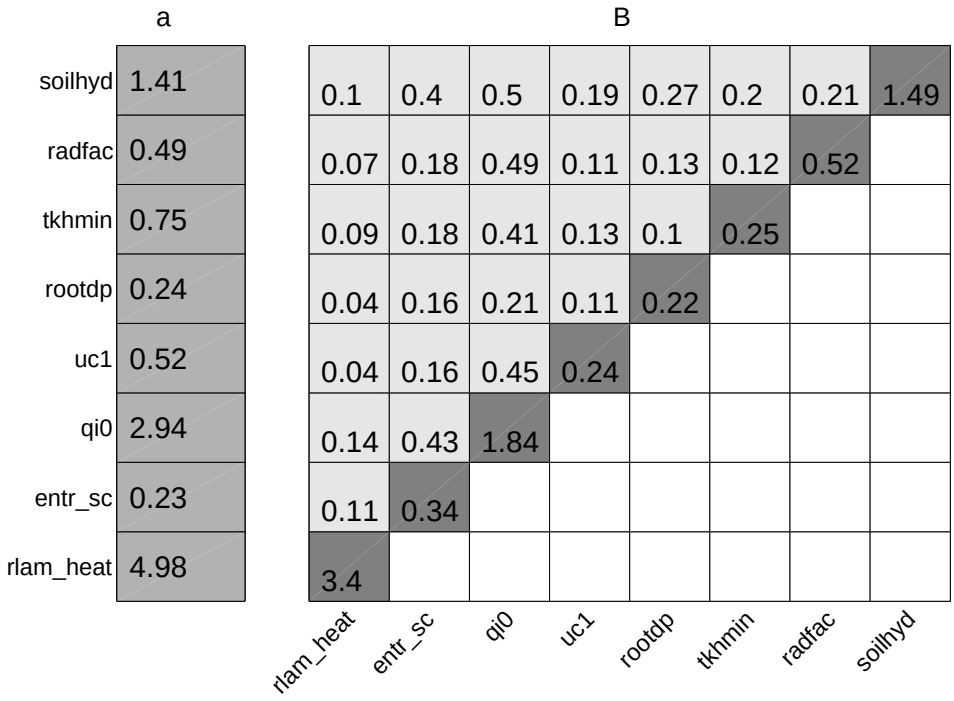

Figure 4.4: Parameter values of the metamodel divided into the linear contribution (first column on the left "a"), the quadratic contribution (diagonal values in the matrix "B"), and interaction values (off-diagonal values in the matrix "B"). The values are normalized by the range of the parameter values in order to compare the contribution of each term between the parameters.

Header:

```
% Visualize fitted metamodel parameters
% NAME
%   metaparam
% PURPOSE
%   Show normalized linear,quadratic and interaction terms for each
%   parameter and interaction
% INPUTS
%   The structure metamodel, parameters,datamatrix are used
% OUTUTS
%   Plot: Histogram of the difference between predicted and actual
%   model data
% HISTORY
% First version: 11.10.2013
```

4.6 neelin_e.m

Using the definitions in section 3.2 this function allows to estimate the metamodel creating a metamodel structure which contains all information to make a prediction of a given parameter set.

Header:

```
% Quadratic regression metamodel as described in Neelin et al. (2010) PNAS
% NAME
%   neelin_f
% PURPOSE
%   Estimate a mutlivariate quadratic metamodel which estimates quadratic
%   regressions in each parameter dimensions and computes interaction
%   terms for all pair of parameter experiments
% INPUTS
%   From the structure parameters and datamatrix the following fields are
%   processed (mind the same naming in the input)
%
%   parameters.experiments:
%
%            Parameter values for each experiment with the
%            dimension of [N, 2*N+N*(N-1)/2]
%            The structure NEEDS to be as follows
%            Example for 2 parameters (p1,p2)
%
%            [p1_l dp2 ] ! Low parameter value for p1 default dp2
%            [p1_h dp2 ] ! High parameter value for p1 default dp2
%            [dp1  p2_l] ! Low parameter value for p2 default dp1
%            [dp1  p2_h] ! Hihg parameter value for p2 default dp1
%            [p1_l p2_h] ! Experiments with interaction (no default)
%                        ! Additional experiments used to
%                        constrain interaction terms
%   parameters.range:
%
%            Range of values for each paramter to normalize the
%            scale.
%
%   parameters.default:
%
%            Default values of parameters to center the scale
%
%   datamatrix.moddata:
%
%            Modeldata corresponding to the dimenoins of
%            parameter.experiments
%
%   datamatrix.reffdata:
%
%            Modeldata of when using default parameter values to
%            to center the datamatrix
%            fitted. Not needed if metamodel fits score data directly
% OUTUTS
%   structure metamodel.
%   a: Metamodel parameter for linear terms [N,1]
%   B: Metamodel parameter for quadratic and interaction terms
%      [N,N]. Quadratic terms in the diagonal, interaction terms
%      in the off-diagonal. Matrix symetric, B(i,j)=B(j,i).
% HISTORY
% First version: 11.10.2013
```

4.7 neelin_p.m

Based on an estimated metamodel and a parameter set of chosen this function predicts the data that would result from a simulation with the specified parameter set.

Header:

```
1
2  % Forecast using regression metamodel as described in Neelin et al. (2010) PNAS
3  % NAME
4  %   neelin_p
5  % PURPOSE
6  %   Predict data using the metamodel for a parameter matrix
7  % INPUTS
8  %   From the structure metamodel, parameters and datamatrix the following fields are
9  %   processed (mind the same naming in the input)
10 %
11 %   metamodel.a:
12 %
13 %          Vector of linear terms of the metamodel [...,N,1] additional
14 %          data dimensions possible (ex:a~[Regions,Variables,Time,N,1])
15 %
16 %   metamodel.B:
17 %
18 %           Matrix of quadratic and interactions terms [...,N,N] additional
19 %           data dimensions possible (ex:a~[Regions,Variables,Time,N,N])
20 %
21 %   parameters.range:
22 %
23 %            Range of values for each paramter to normalize the
24 %            scale.
25 %
26 %   parameters.default:
27 %
28 %            Default values of parameters to center the scale
29 %
30 %   datamatrix.reffdata:
31 %
32 %            Modeldata of when using default parameter values to
33 %            to center the datamatrix
34 %
35 %   pvector: Parameter values for one experiment with the
36 %            dimension of [N,1] N=Number parameters
37 % OUTUTS
38 %   dmatrix: Predicted data for parameter experiment
39 % HISTORY
40 % First version: 11.10.2013
```

4.8 neelin_c.m

Additional simulations than needed to estimate the metamodel can be used to further constrain the linear and quadratic terms of the metamodel. By defining these parameter configuration and data in the structures `parameters` and `datamatrix` this function can be called as described in section 3.2

Header:

```
% Constrain linear and quadratic metamodel terms with additinal simulations
% NAME
%   neelin_c
% PURPOSE
%   Use additional simulations to narrow uncertainty of the
%   metamodel paramters, particulary if strong unequal distancies
%   between default and min/max values.
% INPUTS
%   From the structure parameters and datamatrix the following fields are
%   processed (mind the same naming in the input)
%
%   parameters.constrain:
%
%            Parameter values for each experiment for
%            additional parameter samplilng
%
%   parameters.range:
%
%            Range of values for each paramter to normalize the
%            scale.
%
%   parameters.default:
%
%            Default values of parameters to center the scale
%
%   datamatrix.moddata:
%
%            Modeldata corresponding to the dimenoins of
%            parameter.experiments
%
%   datamatrix.reffdata:
%
%            Modeldata of when using default parameter values to
%            to center the datamatrix
%            fitted. Not needed if metamodel fits score data
%            directly
%
%   datamatrix.constrain
%
%            Simulation data of experiments used to further sample
%            parameter ranges
%
% OUTUTS
%   Updatated metamodel structure
% HISTORY
% First version: 4.11.2013
```

4.9 optparam.m

To empirically estimate the posterior parameter distributions the current functions uses the uncertainty of the metamodel (one standard deviation from `errmeta.m`) and selects the best parameter combinations from `lhopt` which lie within this uncertainty. The following figure is then produced.

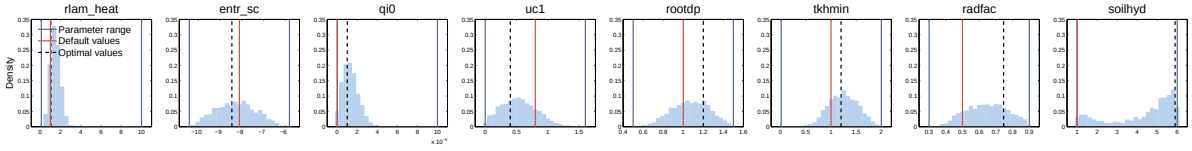

Figure 4.5: Distribution of the model parameters which lead to best model results. The distribution is computed from a sample of parameter combinations which, given the uncertainty of the metamodel (`errstd`), give the best model results. From this sub-sample of the Latin hypercube sample the empirical distribution of the values are plotted. This approach is an approximation of determination of a posterior parameter distribution without the definition of distribution priors.

Header:

```
1  %   Plot posterior parameter distributions given the uncertainty of
2  %   the metamodel prescribed in errm
3  % NAME
4  %   optparam
5  % PURPOSE
6  %   Plot parameter distributions which lead to best model results
7  %   given the uncertainty of the metamodel
8  % INPUTS
9  %   From the structure metamodel, parameters and datamatrix the following fields are
10 %   processed (mind the same naming in the input)
11 %
12 %   datamatrix.reffdata:
13 %
14 %            Modeldata using default parameter settings to
15 %            determine/compute the model score of the reference
16 % OUTUTS
17 %   Plot: Histogram plot
18 % HISTORY
19 % First version: 11.10.2013
```

4.10 planes.m

This routine allows to show the variations in the specified model performance along all planes of parameter pairs.

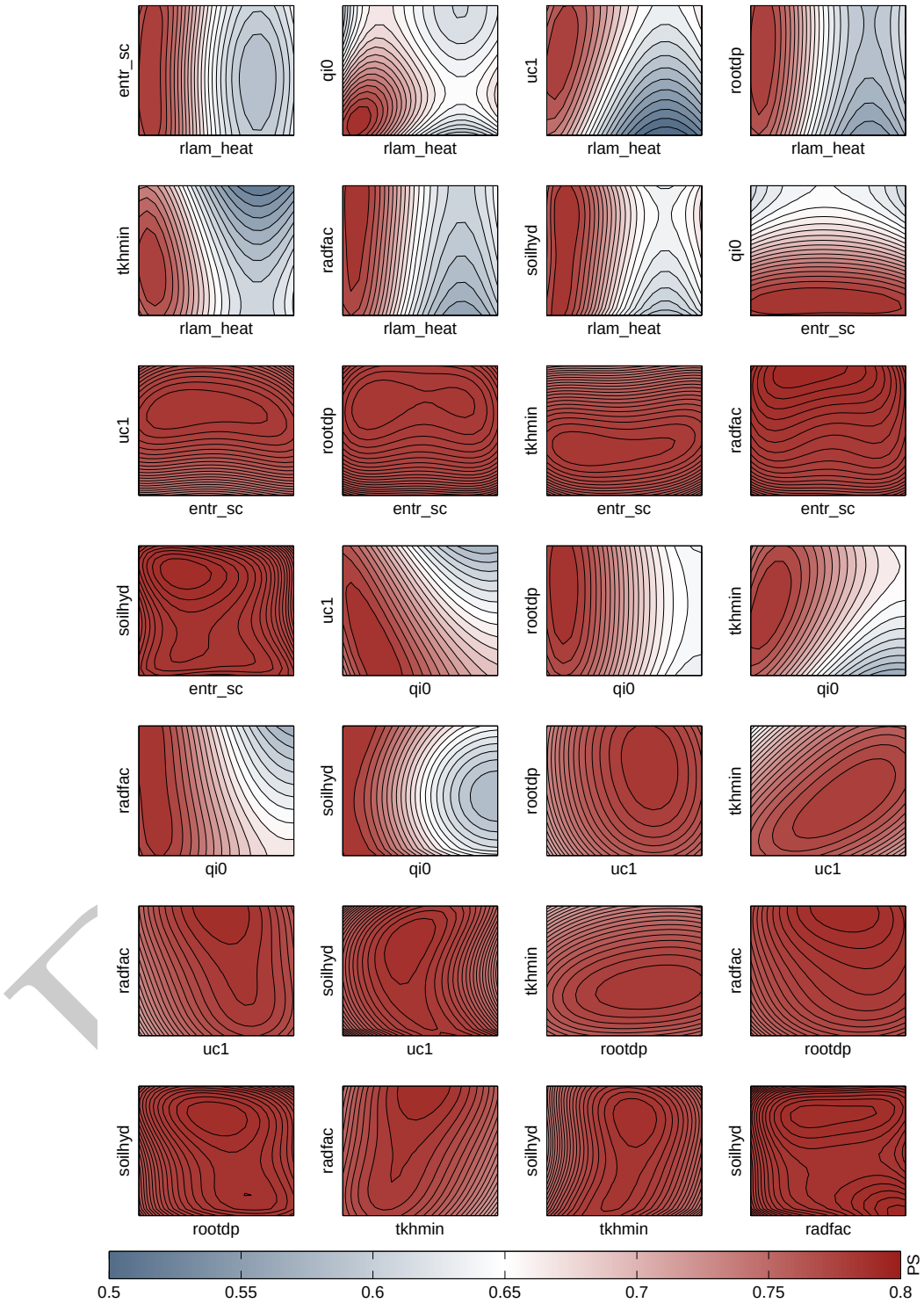

Figure 4.6: Contours of the model performance as predicted by the metamodel along planes of all possible parameter pairs.

Header:

```
% Plot performance planes for each parameter pair predicted
% by the metamodel
%
% NAME
%   planes
%
% PURPOSE
%
%   Predict performance surface for a parameter pairs between
%   the design points to visualize performance non-linearities.
%
% INPUTS
%
%   From the structure metamodel, parameters and datamatrix the following fields are
%   processed (mind the same naming in the input)
%
%   metamodel.a:
%
%          Vector of linear terms of the metamodel [...,N,1] additional
%          data dimensions possible (ex:a~[Regions,Variables,Time,N,1])
%
%   metamodel.B:
%
%           Matrix of quadratic and interactions terms [...,N,N] additional
%           data dimensions possible (ex:a~[Regions,Variables,Time,N,N])
%
%   parameters.range:
%
%            Range of values for each paramter to normalize the
%            scale.
%
%   parameters.default:
%
%            Default values of parameters to center the scale
%
%   datamatrix.reffdata:
%
%            Modeldata of when using default parameter values to
%            to center the datamatrix
%
%   pvector: Parameter values for one experiment with the
%            dimension of [N,1] N=Number parameters
% OUTUTS
%  pi:      Performance index for all data points
%  ps:      PS value for each simulation
% HISTORY
% First version: 11.10.2013
```

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