Using the emergent constraints app

Philip G Sansom[1], Daniel B Williamson[1,2]
[1]Department of Mathematical Sciences, University of Exeter, UK
[2]The Alan Turing Institute for Data Science and Artificial Intelligence

May 3, 2019

1 Getting Started

To run the Uncertainty quantification for emergent constraints app, you will need up to date versions of R and Stan. We recommend installing the latest version of RStudio, which you can install from here: `https://www.rstudio.com/products/rstudio/download/`. It will link you to the correct version of R to install and advise you to do that before installing RStudio.

We provide instructions for installing and running the app through RStudio as we believe this is easier, but it is not a requirement. Having installed RStudio, head to `https://mc-stan.org/users/interfaces/rstan` to install Stan and its implementation in R, rstan. Follow the instructions for your chosen platform carefully.

Having installed rstan and ensured it is working (certain platforms require giving R access to the c++ compiler through Rcpp, so do follow the instructions carefully).

You will also need to install the `shiny` R package. This can be installed directly from RStudio by typing

```
> install.packages("shiny")
```

Having completed these steps, download the zipped repository and place it in an appropriate directory. Navigate to that directory and inside of the folder with all of the app code itself within RStudio using the 'Files' tab and select the 'Set As Working Directory' option from the 'More' tab as shown in Figure 1

Having done so, click on `app.R` to open the App file and then click on the `Run App` button, highlighted in Figure 1. This should start the app, which will load in a new window.

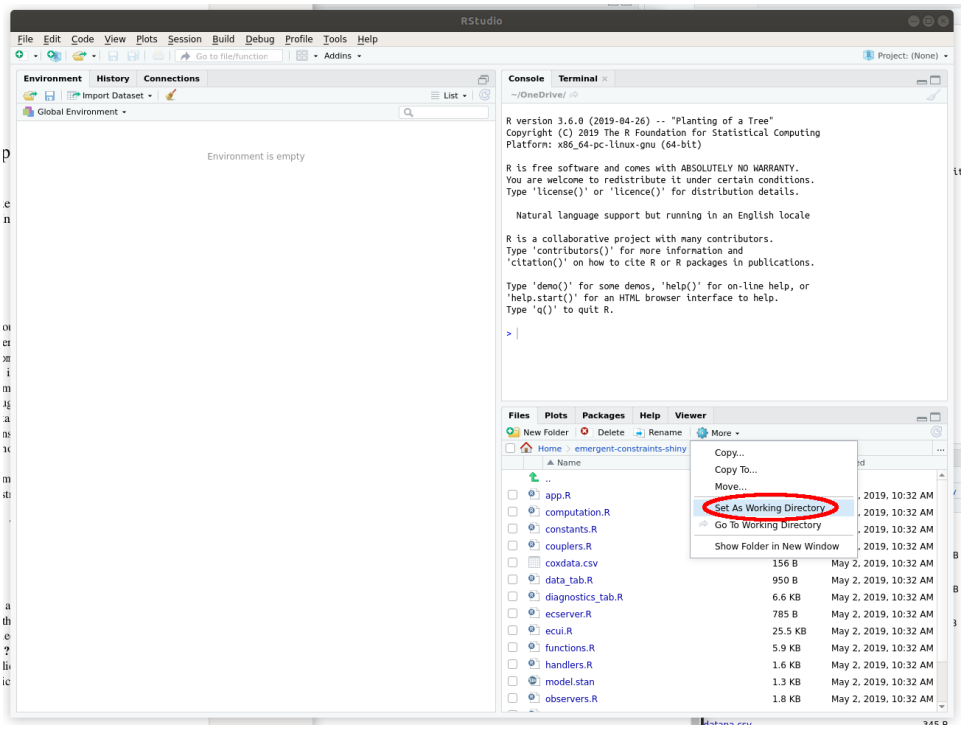

Figure 1: Set working directory.

2 Loading your own data

To load your own data, click on the `Data` tab in the navigation bar at the top of the screen. Once in the `Data` tab, click on the `Browse...` button highlighted in Figure 2, navigate to the directory containing your data, select the file containing your data and click the button marked `Open` to load it into the app.

Hint: By default, the app looks for files with the extension `.csv`. If the file containing your data does not appear in the `Browse...` dialogue, then click the drop-down menu marked `Customised Files` and select `All Files`.

Once you have loaded your data, the app will display the data in a table. The `Separator` and `Quote` radio boxes can be used to split the data into columns if the data are in a non-standard format.

Use the drop-down menus marked `Predictor` and `Response` to select the columns corresponding to the predictor variable and response variable to be analyzed. Your data should be plotted above the data table.

Finally, enter a values for the mean and standard deviation of your observations in the boxes marked `Observation` and `Observation uncertainty`.

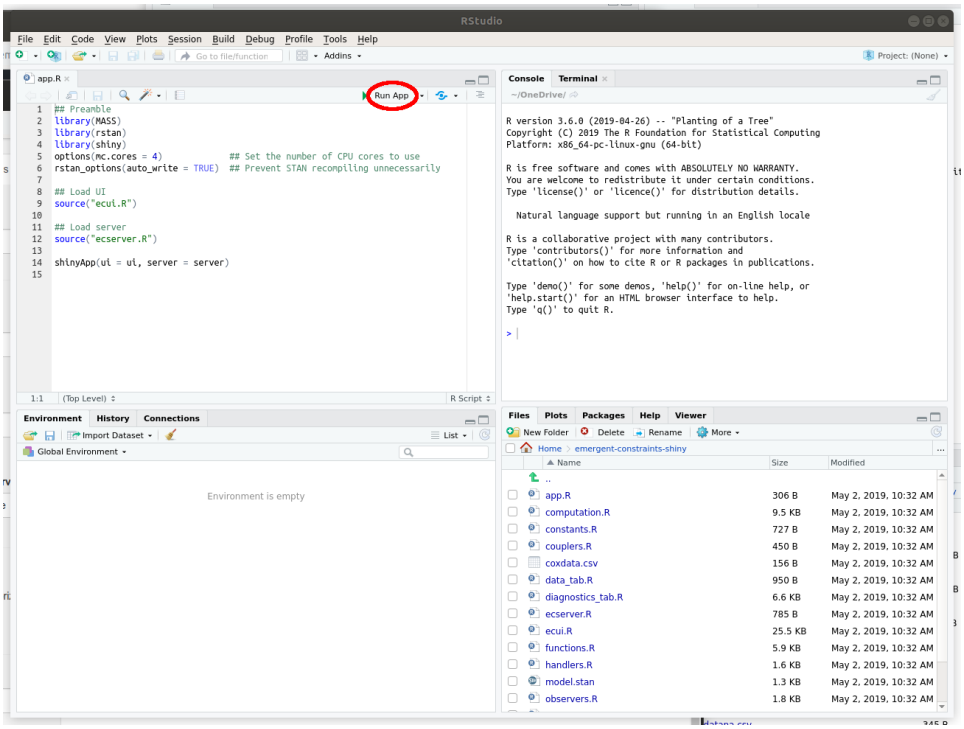

Figure 2: Run app.

The mean of your observations should appear in the plot as a dashed blue line.

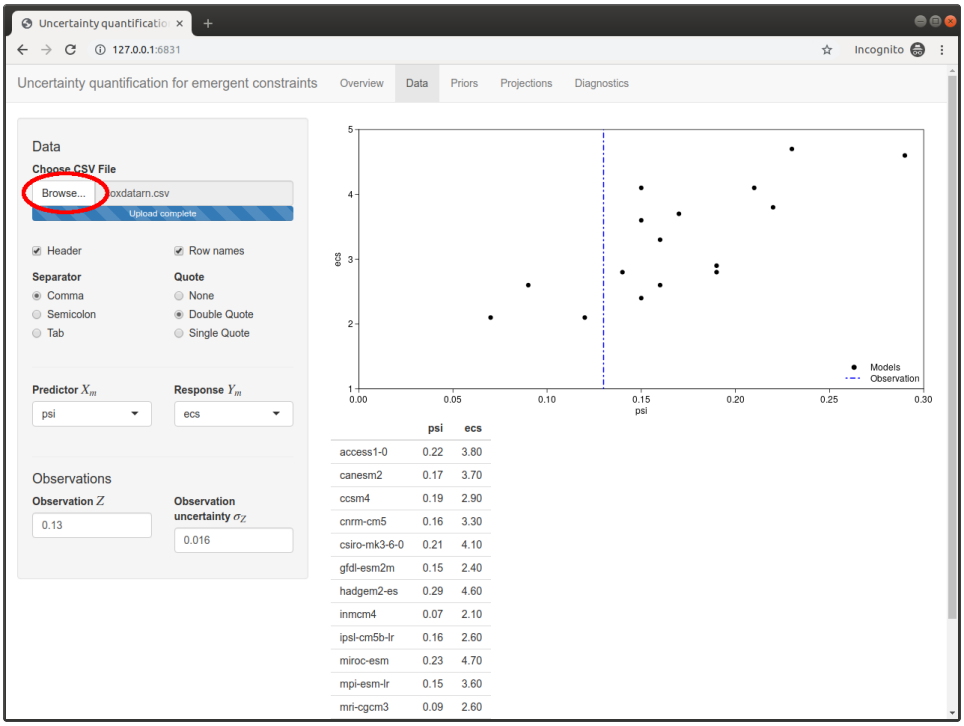

Figure 3: Loading your own data.

3 Setting the prior distributions

Once you have loaded your data into the app, click on the `Priors` button in the navigation bar to set the prior probability distributions. By default, reference priors are used for both the multi-model ensemble parameters and the real world parameters (See Williamson and Sansom [In submission] for details). If you wish to accept the reference parameters, then you can skip the rest of this section.

If you wish to set your own priors then select radio box marked `Informative` highlighted in Figure 3. By default, the app will attempt to determine sensible ranges for the hyper-parameters and offer you a series of sliders to select your own values from those ranges. The marginal priors for each parameter are plotted in the right-hand panel for reference. The prior predictive distribution of the model responses Y_m given the predictors X_m is also available to help guide your judgments.

If you wish to set a value outside of the range offered by the sliders, or simply require more precise control, then select the radio-box marked `Numerical` under the heading `Input style`. You will now be presented with a series of numeric input boxes where you can enter any value you

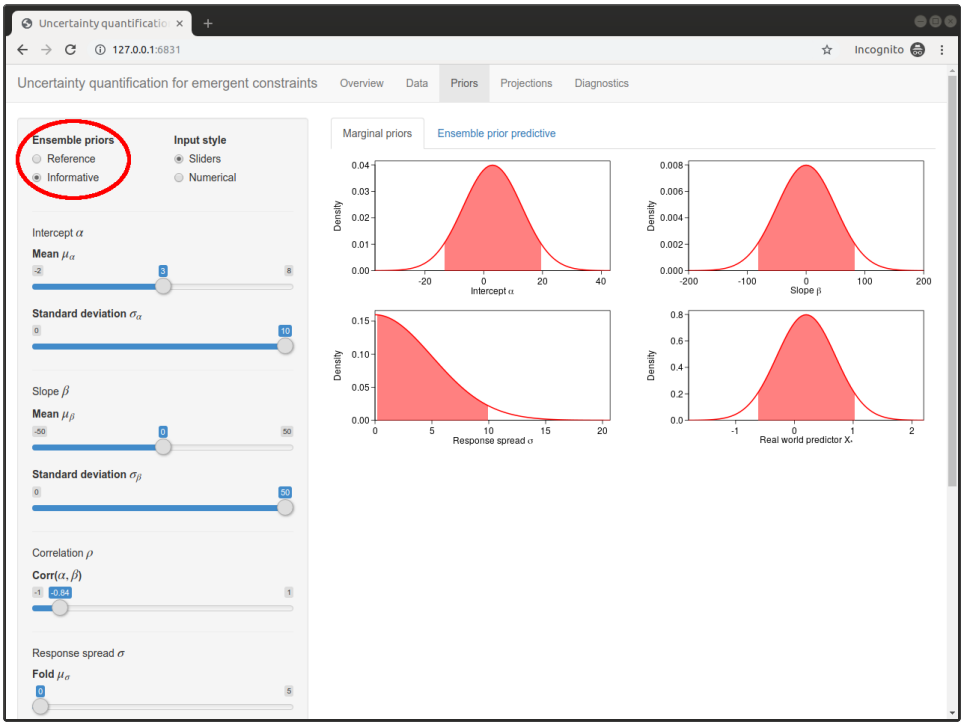

Figure 4: Specifying informative priors.

require. For an example of how to set your own priors, see Williamson and Sansom [In submission].

4 Making projections

Once you have set your priors, or accepted the reference priors, click on the tab marked `Projections` in the navigation bar. You will be presented with a plot of the marginal distribution of the real world response $Y^\star$ comparing the reference model to the conditionally exchangeable model with no added uncertainty (if you accepted the reference priors, the two distributions will be coincident). By default, the shading indicates 90 % credible intervals from each statistical model. The mean and quantiles of the intervals are printed in the table beneath the plot. From this screen, you can download the posterior samples for all model quantities under the conditionally exchangeable model by clicking the button marked `Download samples`. You can also download the marginal projection plot by clicking the button marked `Download plot`.

Various options to customize the plots are available by clicking on the tab marked `Plotting options` in the sidebar on the left and highlighted in Figure 4. In particular, you can change the width of the displayed credible intervals, by selecting the desired interval width from the dropdown marked `Interval width`, also highlighted in Figure 4. This will effect all plots throughout the app. The number of posterior samples can also be controlled from here.

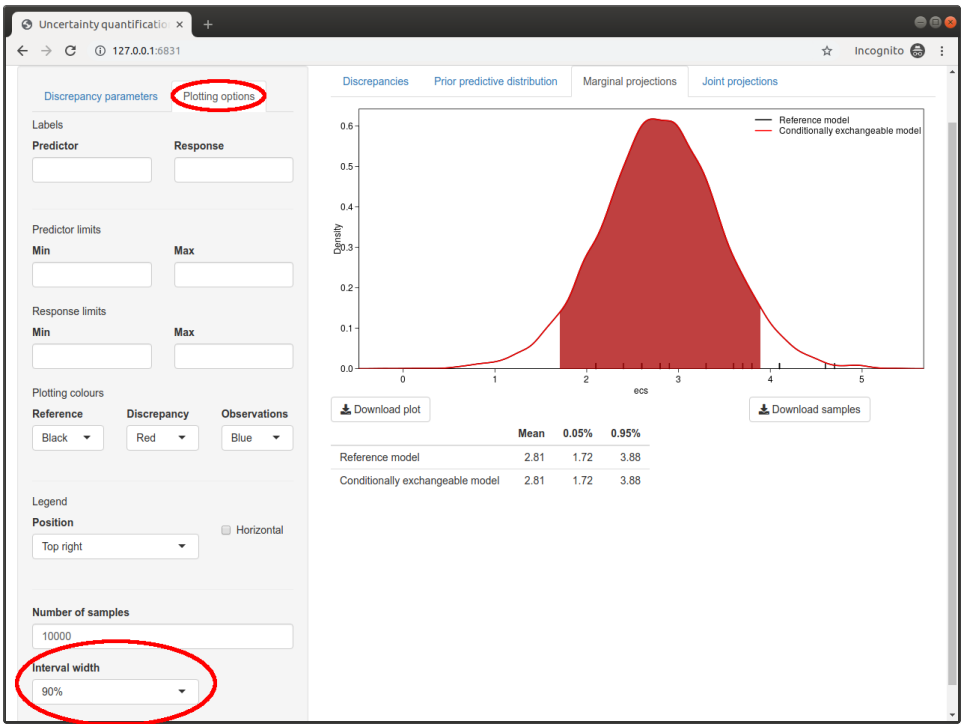

Figure 5: Plotting options.

The app provides three options for adding uncertainty about how the emergent relationship applies to the real world. These can be selected using the radio buttons in the tab marked `Discrepancy parameters` in the sidebar on the left, highlighted in Figure 4. The default `None` adds no uncertainty to the ensemble parameter, i.e., it assumes real world is exchangeable with the models! The `Guided` option allows you to perform the analysis suggested in Williamson and Sansom [In submission]. To perform this analysis, enter your current best estimate of the response mean in the box marked `Current response mean`, and your standard deviation for this estimate in the box marked `Current response SD`. Finally, use the drop-down marked `Likelihood of emergent relationship` to specify how confident you are that the linear relationship between the models should also exist in the real world. The `Manual` option functions similarly to setting your own priors and gives you complete flexibility to specify your uncertainty about the relationship between the models and the real world.

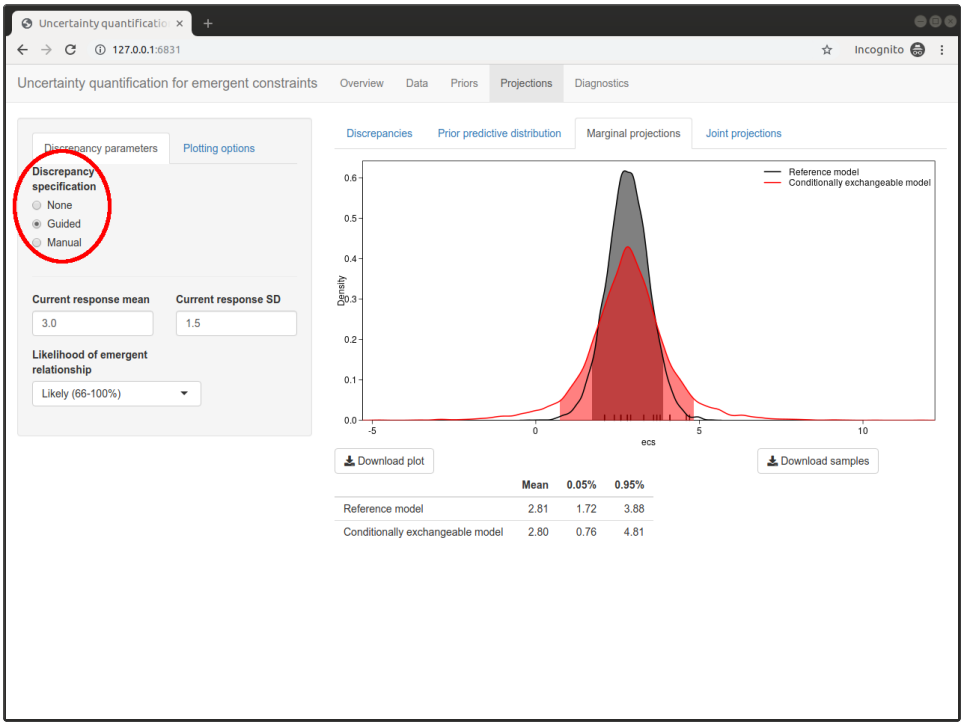

Figure 6: Guided uncertainty quantification.

Various additional tools are provided to help you specify your uncertainty about the relationship between the models and the real world. By clicking on the `Discrepancies` tab highlighted in Figure 4, you will be presented with plots comparing the marginal distributions of the climate model

parameters with the real world parameters. If you have selected the `Guided` uncertainty option, then you will also be presented with a table giving listing the additional uncertainty added to each model parameter. If you have specified your own prior for the real world predictor $X^\star$, then the prior predictive distribution of the real world response can also be viewed using the tabs in the right hand pane.

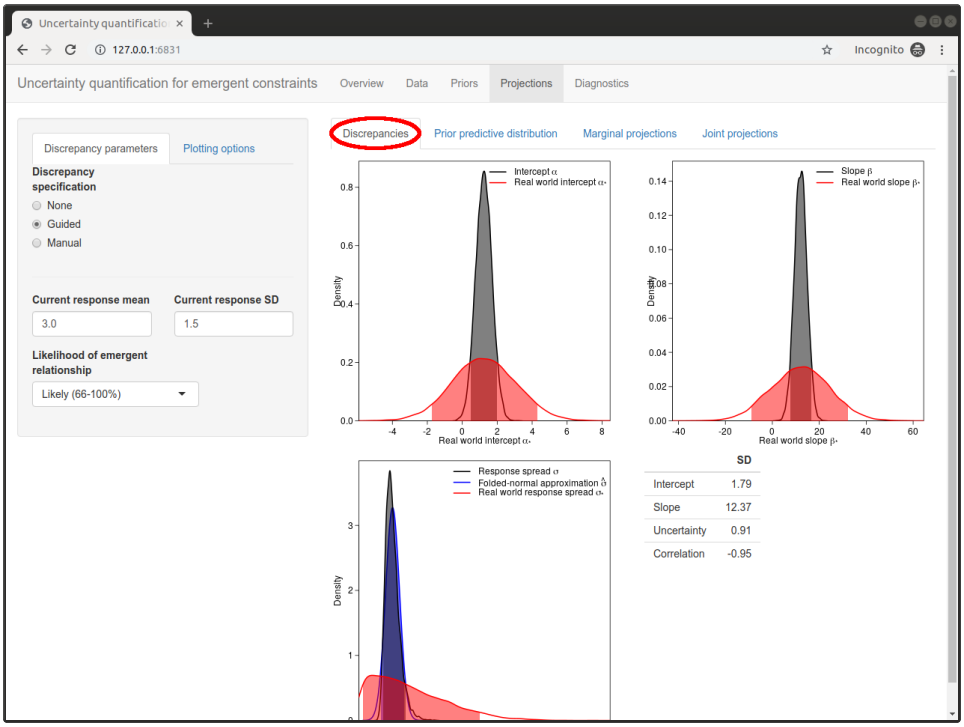

Figure 7: The marginal discrepancies.

The final tab in the right hand pane is marked `Joint projections` and highlighted in Figure 4. This gives access to the joint distribution plots shown in Williamson and Sansom [In submission]. The climate model data are plotted as together with with prediction intervals for $Y^\star$ given $X_\star$ from both the reference model and the conditionally exchangeable model. These are useful for visualizing the geometric effect of adding uncertainty to the climate model parameters. The cloud of grey points are a sample from the joint distribution of the real world $X^\star$ and $Y^\star$.

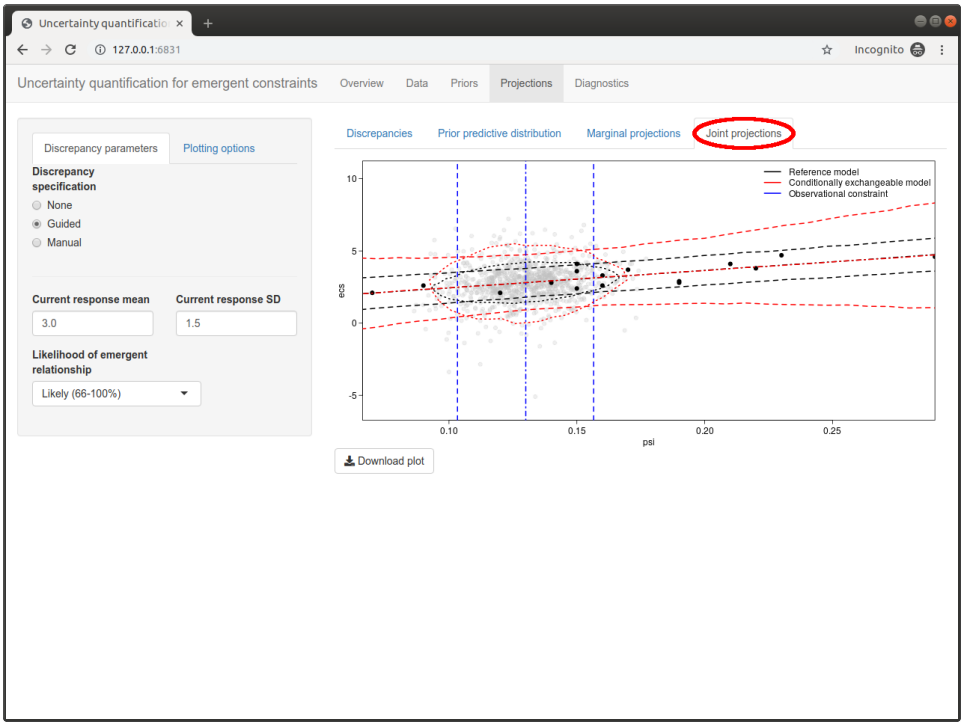

Figure 8: Joint distribution of the real world.

5 Diagnostics

The `Diagnostics` tab in the top navigation bar provides various tools for assessing the success of the posterior sampling. The section `Summary statistics` in the sidebar on the left provides a summary of the posterior samples. Particular attention should be payed to final two columns `n_eff` and `Rhat`, highlighted in Figure 5. The effective number of samples `n_eff` should be large, at least 1000. `Rhat` provides a summary of the convergence of the sampler chains and should closely approach 1, preferably < 1.01, but definitely < 1.10.

By default, the app runs four parallel sampling chains. The sidebar tabs `Model parameters` and `Sample information` highlighted in Figure 5 provide visual summaries of the outputs of each chain. The individual chains are plotted in different colors. Any systematic differences or deviations between chains may indicate that the chains have not properly converged, increasing the number of posterior samples or checking your prior specifications may help.

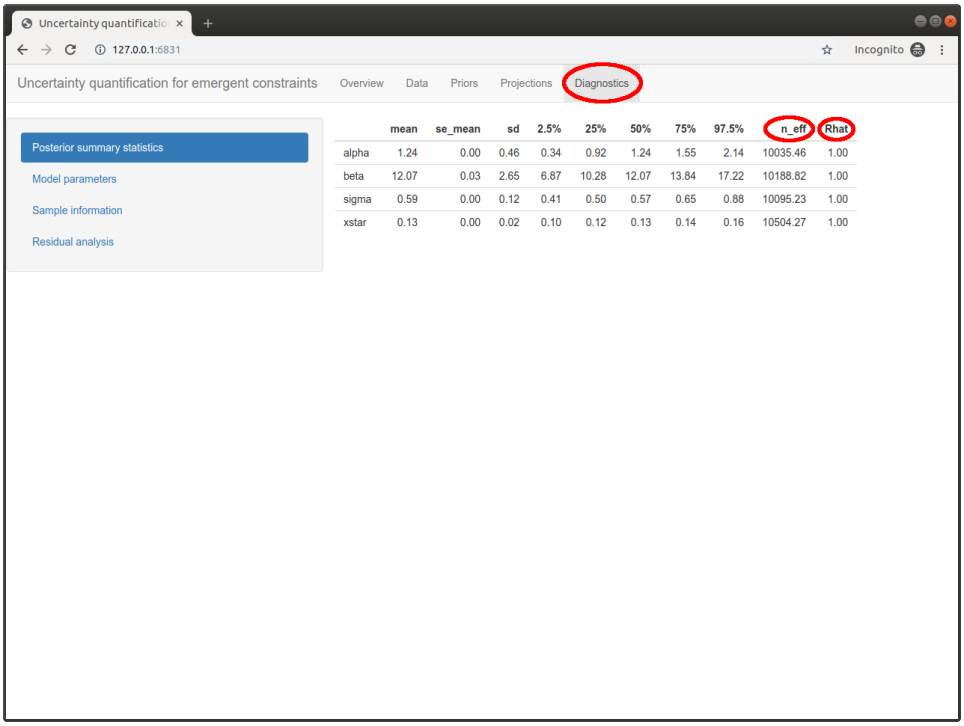

Figure 9: Summary statistics.

References

D. B. Williamson and P. G. Sansom. How are emergent constraints quantifying uncertainty and what do they leave behind? *Bulletin of the American Meteorological Association*, In submission.

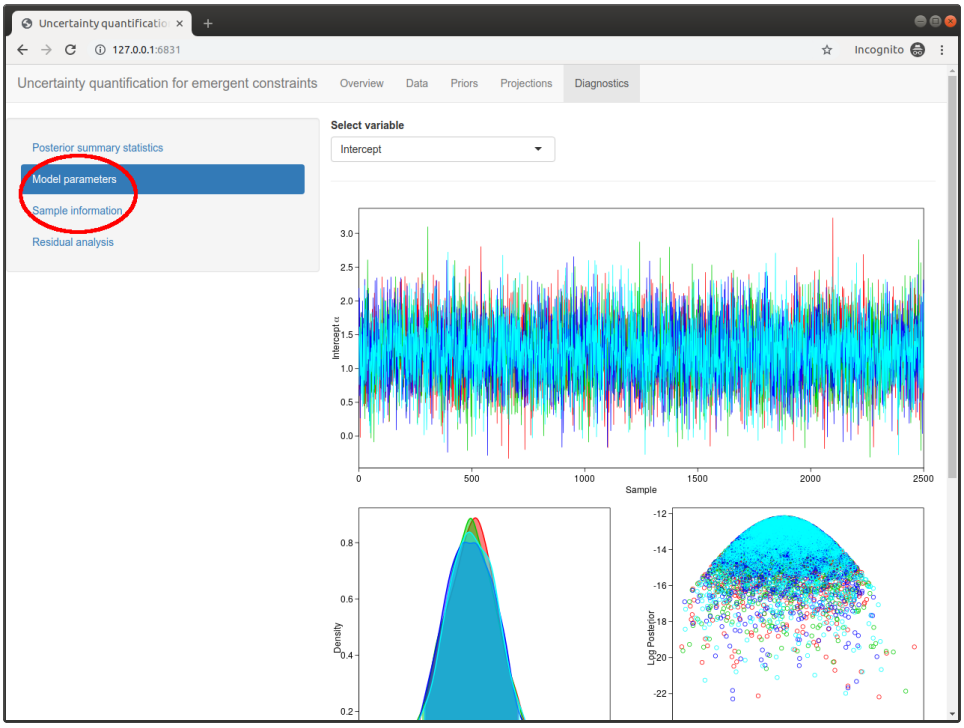

Figure 10: Graphical summaries of parameter samples for each chain.