A critical review of statistical calibration/prediction models handling data inconsistency and model inadequacy

Supporting Information

Pascal PERNOT & Fabien CAILLIEZ*

Laboratoire de Chimie Physique,

UMR8000, CNRS / Univ. Paris-Sud,

F-91405 Orsay, France

E-mail: pascal.pernot@u-psud.fr

Contents

The data and codes to reproduce the results of the article are provided:

• R scripts¹ and data for the analysis of temperature-dependent synthetic and Kr viscosity data.

How-to Run the codes

The main script is located in code. To run it, launch R CMD BATCH code/reprod.R in the base directory, or run interactively in RStudio.

The code might take some time to run. It takes advantage of multicore architectures to run (4) parallel Markov chains. The progress can be followed in the simulation/XXX/diagnostics directory, where XXX is the name of the dataset (SD-1, SD-2, SD-3 or Kr) Note that, due to the stochastic sampling method, the numerical results might be slightly different from the ones in the article.

The results are generated in simulation/XXX:

- files with extension .rda contain the outputs of the models and can be loaded to further processing. To rerun one of the models, delete the corresponding file. and rerun the reprod.R code
- directory diagnostics contains diagnostic plots and summaries to check the sample generation.
- directories figures and tables contain the data and plots from which the article's results are drawn.

Session Info

```
R version 3.3.1 (2016-06-21)
Platform: x86_64-redhat-linux-gnu (64-bit)
Running under: CentOS Linux 7 (Core)
locale:
[1] LC_CTYPE=fr_FR.UTF-8 LC_NUMERIC=C LC_TIME=fr_FR.UTF-8 LC_COLLATE=fr_FR.UTF-8
[5] LC_MONETARY=fr_FR.UTF-8 LC_MESSAGES=fr_FR.UTF-8 LC_PAPER=fr_FR.UTF-8 LC_NAME=C
[9] LC_ADDRESS=C LC_TELEPHONE=C LC_MEASUREMENT=fr_FR.UTF-8 LC_IDENTIFICATION=C
attached base packages:
[1] tcltk parallel stats graphics grDevices utils datasets methods base
other attached packages:
[1] aplpack_1.3.0 rstan_2.11.1 StanHeaders_2.11.0 ggplot2_2.1.0 knitr_1.14
loaded via a namespace (and not attached):
[1] Rcpp_0.12.6 codetools_0.2-14 digest_0.6.10 grid_3.3.1 plyr_1.8.4 gtable_0.2.0
[7] magrittr_1.5 stats4_3.3.1 evaluate_0.9 scales_0.4.0 KernSmooth_2.23-15 highr_0.6
[13] stringi_1.1.1 labeling_0.3 tools_3.3.1 stringr_1.1.0 munsell_0.4.3 rsconnect_0.4.3
[19] inline_0.3.14 colorspace_1.2-6 gridExtra_2.2.1
```

References

(1) R Core Team, R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing: Vienna, Austria, 2015.