References for "An Extensive and Reproducible Comparison of Computer Model Emulators"

Kellin Rumsey

August 4, 2025

Emulators

This study uses the `duqling` package [Rum23] for reproducible and transparent comparisons.

We compare 16 different computer model emulators, each representing a popular or innovative approach to surrogate modeling. Below, you'll find each emulator's short name (as used in the poster figures), its full descriptive name, and a primary reference or software source. For more information, see the the corresponding subsection or the cited literature.

The emulators are compared 60 different test functions, with 10 replications each. Training designs were generated with $n = 500$ points from a maximin Latin hypercube design with a noise-to-signal ratio of 0 (i.e. deterministic computer models). For more details on the functions, see the `duqling` documentation.

Short Name	Full Name	R Package	Reference
svecgp	Scaled Vecchia GP	`spareGParts`	[KGL22]
bppr	Bayesian Projection Pursuit Regression	`BayesPPR`†	[CFR24]
bass	Bayesian Multivariate Adaptive Regression Splines Surfaces	`BASS`	[FS20]
apce	Adaptive Bayesian Polynomial Chaos	`khaos`†	in prep
lagp	Local Approximate GP	`laGP`	[Gra16]
rffgp	Random Fourier Features GP	`gplite`	[RR07]
fitc	Inducing Point GP	`gplite`	[SG05]
spce	Sparse Bayesian Polynomial Chaos	`khaos`†	[SYFM17]
bart	Bayesian Additive Regression Trees	`BART`	[SSM19]
confrf	Conformal Random Forests	`conforest`†	[JBLL14]
mpgp	Subset of Data GP - Matching Pursuit	`spareGParts`†	[KC05]
blm	Bayesian linear model	base R	[GCSR95]
bnn	Bayesian Neural Network with STAN	`bnns`	[CC25]
btreelm	Bayesian Treed Linear Model	`tgp`	[Gra07]
bcart	Bayesian CART	`tgp`	[Gra07]
lasodgp	Subset of Data GP - alcopt	`laGP`	[Gra16]

Table 1: Emulator short names, full names, package, and primary references. Methods are sorted by performance (% of cases with top 5 smallest RMSE).

† Note on Github Packages

Some of these R packages are not on CRAN but can be found on Github:

```
# mpgp and svecgp
devtools::install_github("knrumsey/spareGParts")
?spareGParts::mpgp
?spareGParts::svecgp

# apce and spce
devtools::install_github("knrumsey/khaos")
?khaos::spce
?khaos::apce
```

```
# BayesPPR
devtools::install_github("gqcollins/BayesPPR")
?BayesPPR::bppr
```

References

[CC25] Swarnendu Chatterjee and Maintainer Swarnendu Chatterjee. Package 'bnns'. 2025.

[CFR24] Gavin Collins, Devin Francom, and Kellin Rumsey. Bayesian projection pursuit regression. *Statistics and Computing*, 34(1):29, 2024.

[FS20] Devin Francom and Bruno Sansó. Bass: An r package for fitting and performing sensitivity analysis of bayesian adaptive spline surfaces. *Journal of Statistical Software*, 94:1–36, 2020.

[GCSR95] Andrew Gelman, John B Carlin, Hal S Stern, and Donald B Rubin. *Bayesian data analysis*. Chapman and Hall/CRC, 1995.

[Gra07] Robert B Gramacy. tgp: an r package for bayesian nonstationary, semiparametric nonlinear regression and design by treed gaussian process models. *Journal of Statistical Software*, 19:1–46, 2007.

[Gra16] Robert B Gramacy. lagp: large-scale spatial modeling via local approximate gaussian processes in r. *Journal of Statistical Software*, 72:1–46, 2016.

[JBLL14] Ulf Johansson, Henrik Boström, Tuve Löfström, and Henrik Linusson. Regression conformal prediction with random forests. *Machine learning*, 97(1):155–176, 2014.

[KC05] Sathiya Keerthi and Wei Chu. A matching pursuit approach to sparse gaussian process regression. *Advances in neural information processing systems*, 18, 2005.

[KGL22] Matthias Katzfuss, Joseph Guinness, and Earl Lawrence. Scaled vecchia approximation for fast computer-model emulation. *SIAM/ASA Journal on Uncertainty Quantification*, 10(2):537–554, 2022.

[RR07] Ali Rahimi and Benjamin Recht. Random features for large-scale kernel machines. *Advances in neural information processing systems*, 20, 2007.

[Rum23] Kelin Rumsey. duqling. Technical report, Los Alamos National Laboratory (LANL), Los Alamos, NM (United States), 2023.

[SG05] Edward Snelson and Zoubin Ghahramani. Sparse gaussian processes using pseudo-inputs. *Advances in neural information processing systems*, 18, 2005.

[SSM19] Rodney Sparapani, Charles Spanbauer, and Robert McCulloch. The bart r package. *Accessed on Aug*, 21:2019, 2019.

[SYFM17] Qian Shao, Anis Younes, Marwan Fahs, and Thierry A Mara. Bayesian sparse polynomial chaos expansion for global sensitivity analysis. *Computer Methods in Applied Mechanics and Engineering*, 318:474–496, 2017.