

dimensions a zero will appear. I.e., the placement of 0/0.626 indicates the LLM is active in the 2nd dimension of the 2nd partition. 0.626 is the  $d$ - (range) parameter that would have been used if the LLM were inactive. Whenever all dimensions are under the LLM, the  $d$ -parameter print is simply [0]. This also happens when forcing the LLM (i.e., for `blm` and `btlm`), where [0] appears for each partition. These prints will look slightly different if the isotropic instead of separable correlation is used, since there are not as many range parameters.

### B.3 Collaboration with `predict.tgp`

In this section I revisit the motorcycle accident data in order to demonstrate how the `predict.tgp` function can be helpful in collaborative uses of `tgp`. Consider a fit of the motorcycle data, and suppose that we do inference for the model parameters only (obtaining no samples from the posterior predictive distribution). The "`tgp`"-class output object can be saved to a file using the R-internal `save` function.

```
> library(MASS)
> out <- btgpllm(X = mcycle[, 1], Z = mcycle[, 2],
+   bprior = "b0", mOr1 = TRUE, pred.n = FALSE, verb = 0)
> save(out, file = "out.Rsave")
> out <- NULL
```

Note that there is nothing to plot here because there is no predictive data. (`out <- NULL` is set for illustrative purposes.)

Now imagine e-mailing the "out.Rsave" file to a collaborator who wishes to use your fitted `tgp` model. S/he could first load in the "`tgp`"-class object we just saved, design a new set of predictive locations `XX` and obtain kriging estimates from the MAP model.

```
> load("out.Rsave")
> XX <- seq(2.4, 56.7, length = 200)
> out.kp <- predict(out, XX = XX, pred.n = FALSE)
```

Another option would be to sample from the posterior predictive distribution of the MAP model.

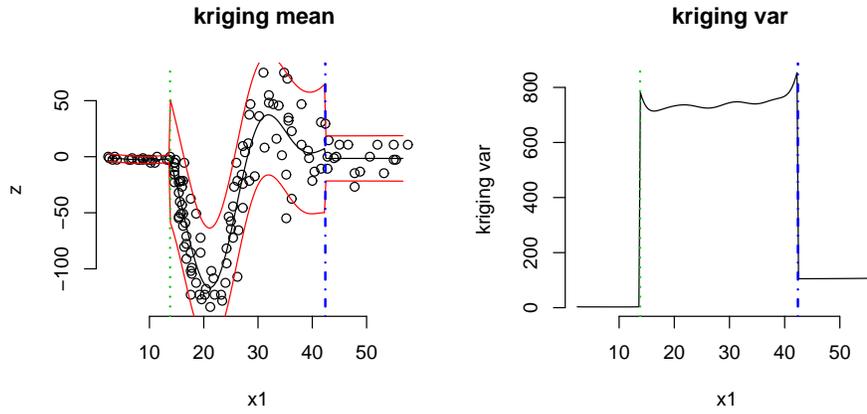
```
> out.p <- predict(out, XX = XX, pred.n = FALSE, BTE = c(0,
+   1000, 1))
```

This holds the parameterization of the `tgp` model *fixed* at the MAP, and samples from the GP or LM posterior predictive distributions at the leaves of the tree.

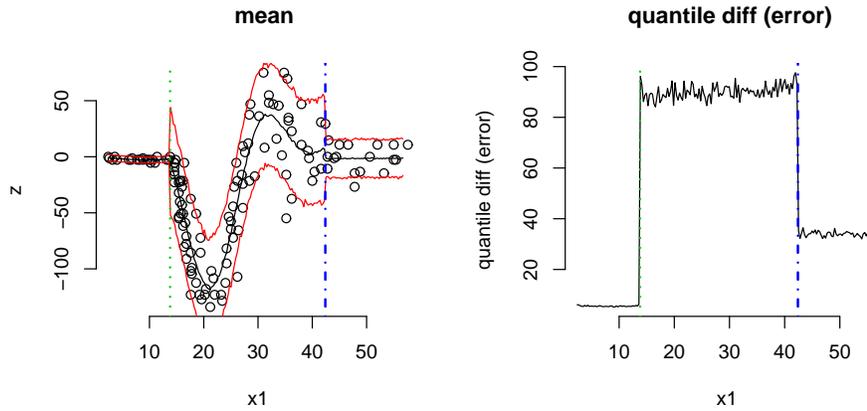
Finally, the MAP parameterization can be used as a jumping-off point for more sampling from the joint posterior and posterior predictive distribution.

```
> out2 <- predict(out, XX, pred.n = FALSE, BTE = c(0,
+   2000, 2), krige = FALSE)
```

```
> plot(out.kp, center = "km", as = "ks2")
```



```
> plot(out.p)
```



```
> plot(out2)
```

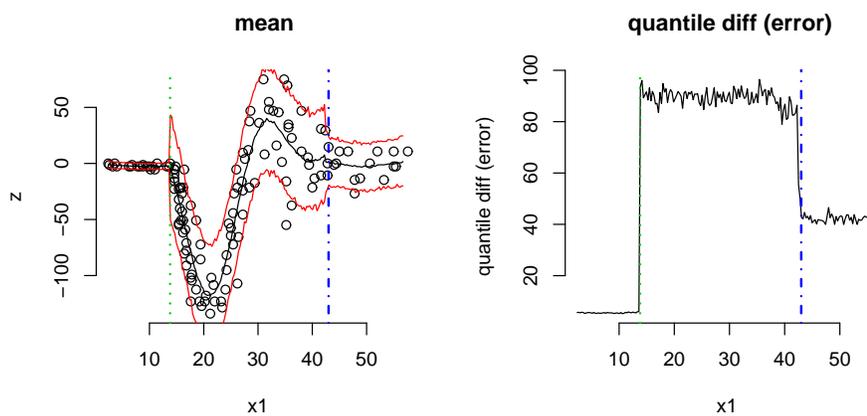


Figure 22: Predictive surfaces (*left*) and error/variance plots (*right*) resulting from three different uses of the `predict.tgp` function: MAP kriging (*top*), sampling from the MAP (*middle*), sampling from the joint posterior and posterior predictive starting from the MAP (*bottom*).

Since the return-value of a `predict.tgp` call is also a "tgp"-class object the process can be applied iteratively. That is, `out2` can also be passed to `predict.tgp`.

Figure 22 plots the posterior predictive surfaces for each of the three calls to `predict.tgp` above. The kriging surfaces are smooth within regions of the partition, but the process is discontinuous across partition boundaries. The middle surface is simply a Monte Carlo-sample summarization of the kriging one above it. The final surface summarizes samples from the posterior predictive distribution when obtained jointly with  $\mathcal{T}|\boldsymbol{\theta}$  and  $\boldsymbol{\theta}|\mathcal{T}$ . Though these summaries are still “noisy” they depict a process with smoother transitions across partition boundaries than ones conditioned only on the MAP.

The `predict.tgp` function can also sample from the ALC statistic and calculate expected improvements (EI) at the `XX` locations.

## C Configuration and performance optimization

In what follows I describe customizations and enhancements that can be made to `tgp` at compile time in order to take advantage of custom computing architectures. The compilation of `tgp` with a linear algebra library different from the one used to compile R (e.g., ATLAS), and the configuration and compilation of `tgp` with parallelization is described in detail.

### C.1 Linking to ATLAS

ATLAS [26] is supported as an alternative to standard BLAS and LAPACK for fast, automatically tuned, linear algebra routines. Compared to standard BLAS/Lapack, those automatically tuned by ATLAS are significantly faster. If you know that R has already been linked to tuned linear algebra libraries (e.g., on OSX), then compiling with ATLAS as described below, is unnecessary—just install `tgp` as usual. As an alternative to linking `tgp` to ATLAS directly, one could re-compile all of R linking it to ATLAS, or some other platform-specific BLAS/Lapack, i.e., Intel’s Math Kernel Library, or AMD’s Core Math Library, as described in:

```
http://cran.r-project.org/doc/manuals/R-admin.html
```

Look for the section titled “Linear Algebra”. While this is arguably best solution since all of R benefits, the task can prove challenging to accomplish and may require administrator (root) privileges. Linking `tgp` with ATLAS directly is described here.

Three easy steps (assuming, of course, you have already compiled and installed ATLAS – <http://math-atlas.sourceforge.net>) need to be performed before you install the `tgp` package from source.

1. Edit `src/Makevars`. Comment out the existing `PKG_LIBS` line, and replace it with:

```
PKG_LIBS = -L/path/to/ATLAS/lib -llapack -lcblas -latlas
```