```
Sampling @ nn=361 pred locs:
r=1000 d=0.0233355 0(0.0162573) 0(1.05867); mh=3 n=(50,10,20)
r=2000 d=0.0201525 0.0323228 0.735674; mh=3 n=(48,15,17)
r=3000 d=0.0212731 0.00712512 0.214455; mh=3 n=(48,14,18)
r=4000 d=0.0235209 0(0.696318) 0(0.0374696); mh=3 n=(50,10,20)
r=5000 d=0.019617 0(0.840593) 0.0798781; mh=3 n=(50,12,18)
Grow: 0.5882%, Prune: 0%, Change: 36.02%, Swap: 44.1%
finished repetition 1 of 2
removed 3 leaves from the tree
burn in:
**GROW** @depth 0: [1,0.5], n=(60,20)
**GROW** @depth 1: [0,0.45], n=(45,12)
**PRUNE** @depth 1: [0,0.45]
r=1000 d=0.0230657 1.17737; mh=3 n=(57,23)
r=2000 d=0.0171015 1.02635; mh=3 n=(57,23)
Sampling @ nn=361 pred locs:
r=1000 d=0.0194236 1.04473; mh=3 n=(60,20)
**GROW** @depth 1: [0,0.45], n=(45,12)
r=2000 d=0.0212965 0.0533747 0(0.998999); mh=3 n=(50,10,20)
r=3000 d=0.0192226 0(0.0149189) 0(1.15603); mh=3 n=(50,12,18)
r=4000 d=0.0234385 0.0988804 1.21228; mh=3 n=(48,14,18)
r=5000 d=0.0216443 0(1.4039) 0.133204; mh=3 n=(50,12,18)
Grow: 0.7072%, Prune: 0.1488%, Change: 31.02%, Swap: 46.31%
finished repetition 2 of 2
removed 3 leaves from the tree
```

Progress indicators show where the LLM  $(\mathtt{corr=0}(d))$  or the GP is active. Figure 10 shows how similar the resulting posterior predictive surfaces are compared to the treed GP (without LLM).

Finally, viewing 1-d projections of tgp-class output is possible by supplying a 1-vector proj argument to the plot.tgp. Figure 11 shows the two projections for exp.btgpllm. In the *left* surface plots the open circles indicate the mean of posterior predictive distribution. Red lines show the 90% intervals, the norm of which are shown on the *right*.

# 3.4 Motorcycle Accident Data

The Motorcycle Accident Dataset [24] is a classic nonstationary data set used in recent literature [21] to demonstrate the success of nonstationary models. The data consists of measurements of the acceleration of the head of a motorcycle rider as a function of time in the first moments after an impact. In addition to being nonstationary, the data has input—dependent noise (heteroskedasticity) which makes it useful for illustrating how the treed GP model handles this nu-

## > plot(exp.btgpllm, main = "treed GP LLM,")

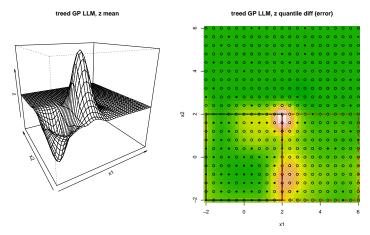


Figure 10: Left: posterior predictive mean using btgpllm on synthetic exponential data; right image plot of posterior predictive variance with data locations X (dots) and predictive locations XX (circles).

ance. There are at least two—perhaps three—three regions where the response exhibits different behavior both in terms of the correlation structure and noise level.

The data is included as part of the MASS library in R.

#### > library(MASS)

Figure 12 shows how a stationary GP is able to capture the nonlinearity in the response but fails to capture the input dependent noise and increased smoothness (perhaps linearity) in parts of the input space.

```
> moto.bgp <- bgp(X = mcycle[, 1], Z = mcycle[, 2],
+ m0r1 = TRUE, verb = 0)</pre>
```

Since the responses in this data have a wide range, it helps to translate and rescale them so that they have a mean of zero and a range of one. The m0r1 argument to b\* functions automates this procedure. Progress indicators are suppressed.

A Bayesian Linear CART model is able to capture the input dependent noise but fails to capture the waviness of the "whiplash"—center— segment of the response.

```
> moto.btlm <- btlm(X = mcycle[, 1], Z = mcycle[, 2],
+ m0r1 = TRUE, verb = 0)</pre>
```

Figure 13 shows the resulting piecewise linear predictive surface and MAP partition  $(\hat{T})$ .

A treed GP model seems appropriate because it can model input dependent smoothness and noise. A treed GP LLM is probably most appropriate since the

Figure 11: 1-d projections of the posterior predictive surface (*left*) and normed predictive intervals (*right*) of the 1-d tree GP LLM analysis of the synthetic exponential data. The *top* plots show projection onto the first input, and the *bottom* ones show the second.

left-hand part of the input space is likely linear. One might further hypothesize that the right-hand region is also linear, perhaps with the same mean as the left-hand region, only with higher noise. The b\* functions can force an i.i.d. hierarchical linear model by setting bprior="b0".

```
> moto.btgpllm <- btgpllm(X = mcycle[, 1], Z = mcycle[,
+ 2], bprior = "b0", m0r1 = TRUE, verb = 0)
> moto.btgpllm.p <- predict(moto.btgpllm)</pre>
```

The predict.tgp function obtains posterior predictive estimates from the MAP

> plot(moto.bgp, main = "GP,", layout = "surf")

GP, z mean

Figure 12: Posterior predictive distribution using  $\mathsf{bgp}$  on the motorcycle accident data: mean and 90% credible interval

30

х1

40

50

> plot(moto.btlm, main = "Bayesian CART,", layout = "surf")

20

10

### Bayesian CART, z mean

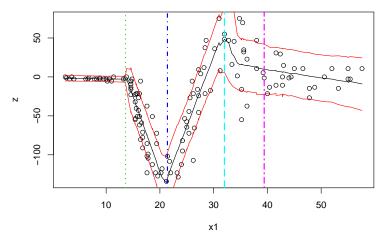


Figure 13: Posterior predictive distribution using btlm on the motorcycle accident data: mean and 90% credible interval

parameterization (a.k.a., *kriging*). The resulting posterior predictive surface is shown in the *top-left* of Figure 14. The *bottom-left* of the figure shows the norm (difference) in predictive quantiles, clearly illustrating the treed GP's ability to capture input-specific noise in the posterior predictive distribution. The *right*-hand side of the figure shows the MAP surfaces obtained from the output of the

```
> par(mfrow = c(1, 2))
 > plot(moto.btgpllm, main = "treed GP LLM,", layout = "surf")
 > plot(moto.btgpllm.p, center = "km", layout = "surf")
            treed GP LLM, z mean
                                                          z kriging mean
    20
                                               20
    0
                                               0
    -20
                                               -20
    -100
                                               -100
            10
                 20
                      30
                           40
                                50
                                                       10
                                                           20
                                                                30
                                                                     40
                                                                          50
                      х1
                                                                x1
> par(mfrow = c(1, 2))
 > plot(moto.btgpllm, main = "treed GP LLM,", layout = "as")
 > plot(moto.btgpllm.p, as = "ks2", layout = "as")
      treed GP LLM, quantile diff (error)
                                                            kriging var
    80
quantile diff (error)
                                               900
    9
                                           kriging var
                                               400
    40
                                               200
    20
                                               0
            10
                 20
                      30
                           40
                                50
                                                       10
                                                           20
                                                                30
                                                                     40
                                                                          50
```

Figure 14: top Posterior predictive distribution using treed GP LLM on the motorcycle accident data. The left-hand panes how mean and 90% credible interval; bottom Quantilenorm (90%-5%) showing input-dependent noise. The right-hand panes show similar kriging surfaces for the MAP parameterization.

## predict.tgp function.

The tgp-default bprior="bflat" implies an improper prior on the regression coefficients  $\boldsymbol{\beta}$ . It essentially forces  $\mathbf{W} = \infty$ , thus eliminating the need to specify priors on  $\boldsymbol{\beta}_0$  of  $\mathbf{W}^{-1}$  in (1). This was chosen as the default because it works well in many examples, and leads to a simpler overall model and a faster implementation. However, the Motorcycle data is an exception. More-

over, when the response data is very noisy (i.e., low signal-to-noise ratio), tgp can be expected to partition heavily under the bprior="bflat" prior. In such cases, one of the other proper priors like the full hierarchical bprior="b0" or bprior="bmzt" might be preferred.

## 3.5 Friedman data

This Friedman data set is the first one of a suite that was used to illustrate MARS (Multivariate Adaptive Regression Splines) [10]. There are 10 covariates in the data ( $\mathbf{x} = \{x_1, x_2, \dots, x_{10}\}$ ). The function that describes the responses (Z), observed with standard Normal noise, has mean

$$E(Z|\mathbf{x}) = \mu = 10\sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5,$$
 (18)

but depends only on  $\{x_1, \ldots, x_5\}$ , thus combining nonlinear, linear, and irrelevant effects. Comparisons are made on this data to results provided for several other models in recent literature. Chipman et al. [5] used this data to compare their treed LM algorithm to four other methods of varying parameterization: linear regression, greedy tree, MARS, and neural networks. The statistic they use for comparison is root mean-square error (RMSE)

$$MSE = \sum_{i=1}^{n} (\mu_i - \hat{z}_i)^2 / n \qquad RMSE = \sqrt{MSE}$$

where  $\hat{z}_i$  is the model–predicted response for input  $\mathbf{x}_i$ . The  $\mathbf{x}$ 's are randomly distributed on the unit interval.

Input data, responses, and predictive locations of size N = 200 and N' = 1000, respectively, can be obtained by a function included in the tgp package.

```
> f <- friedman.1.data(200)
> ff <- friedman.1.data(1000)
> X <- f[, 1:10]
> Z <- f$Y
> XX <- ff[, 1:10]</pre>
```

This example compares Bayesian treed LMs with Bayesian GP LLM (not treed), following the RMSE experiments of Chipman et al. It helps to scale the responses so that they have a mean of zero and a range of one. First, fit the Bayesian treed LM, and obtain the RMSE.

```
> fr.btlm \leftarrow btlm(X = X, Z = Z, XX = XX, tree = c(0.95, + 2), pred.n = FALSE, mOr1 = TRUE, verb = 0)
> fr.btlm.mse \leftarrow sqrt(mean((fr.btlm$ZZ.mean - ff$Ytrue)^2))
> fr.btlm.mse
```

[1] 1.939446

Next, fit the GP LLM, and obtain its RMSE.