Workshop Speech Prosody. Part III: Trees for Smoothing Splines, or GAM trees

Marjolein Fokkema

Context and challenges

It likely goes without saying that smoothing or penalized splines are a powerful tool. Many would argue that with parametric (or unpenalized) spline models, "choosing the optimal number and positions of knots is a complex task" (e.g., Eilers and Marx, 1996). Others argue that "simple unpenalized regression splines work as well as penalized splines that use more parameters" (Chen & Harrell, 2019).

In Part II, it was shown how *parametric* splines can be fitted with GLMM trees. Yet, correct specification of the spline bases for parametric estimation may be challenging, while it may also be critical for accurate recovery of the tree structure. Much of the popularity of smoothing splines may be due to their relatively low dependence on (correct) user specification of the spline bases, which may also be beneficial for subgroup detection. A current challenge is that smoothing splines have a heavy computational burden, which worsens if we want to perform subgroup detection.

The methods discussed this far employ model scores, which are partial derivatives of parameter estimates. For parametric models, these are often easy to compute. Yet, for semi-parametric models, and even mixed-effects models, these are difficult to compute. Often, these scores or partial derivatives arise as a by-product of model estimation and can simply be extracted from a fitting model and used to test for parameter stability. Yet, packages such as mgcv and lme4 use a penalized iteratively re-weighted least squares (PIRLS) algorithm. PIRLS indirectly maximizes the marginal likelihood, that conditions out the random effects (in lme4) and/or smoothing parameter (in lme4). This provides accurate and fast computation. But to obtain the scores, they have to be computed afterwards, which brings a very heavy computation load.

To make it possible to partition based on smoothing spline models, package **gamtree** critically uses packages **gamm4** for the spline fitting, **merDeriv** (Wang et al., 2018, 2022) for obtaining the scores and **partykit** for the partitioning. It is a slow but feasible procedure, and our initial results indicate it is the only currently possible way obtain valid subgroup detection from smoothing-spline models.

Fitting a smoothing-spline or GAM tree

Where splinetree fits an unpenalized or parametric spline model, gamtree fits a smoothing spline model. Functionality is currently limited; only 1 smoothing spline term can currently be specified, and no random effects or global part of the model can be specified (this will be supported in future versions). In order to account for the nested data structure, the cluster argument can be employed to account for the correlated nature of the data. For those familiar with multilevel models, this resembles a GEE-type approach, as compared to a mixed-effects modeling approach.

We use the same dataset from Wieling (2018) as in the previous example:

load("full2.rda")
summary(full)

```
##
          Speaker
                         Lang
                                          Word
                                                      Sound
                                                                     Loc
   VENI_EN_10: 4302
##
                         EN:71152
                                                      T:62428
                                                                  Final:62052
                                     thighs : 7199
    VENI EN 19:
##
                  3867
                         NL:55025
                                     tongs
                                            : 7127
                                                      TH:63749
                                                                  Init:64125
    VENI_EN_17:
                  3860
                                     fort
                                              7000
##
##
    VENI EN 21:
                  3739
                                     ties
                                             : 6840
    VENI EN 2 :
                                     forth : 6727
##
                 3717
    VENI EN 11:
                                     thongs: 6640
##
                 3714
                                     (Other):84644
##
    (Other)
               :102978
##
        Trial
                           Time
                                             Pos
                                                                Pos01
##
    355
                              :0.0000
           :
                922
                      Min.
                                        Min.
                                                :-6.7536
                                                           Min.
                                                                   :-0.9791
##
    317
           :
                887
                      1st Qu.:0.2466
                                        1st Qu.:-0.3441
                                                           1st Qu.: 0.4235
    300
               883
                      Median :0.5000
                                        Median : 0.3214
                                                           Median : 0.5582
##
           :
                                                : 0.3029
##
    305
                864
                      Mean
                              :0.5000
                                        Mean
                                                           Mean
                                                                   : 0.5555
           :
                      3rd Qu.:0.7534
                                                           3rd Qu.: 0.6983
    301
##
                843
                                        3rd Qu.: 1.0126
##
    137
                816
                              :1.0000
                                                : 5.5685
                                                           Max.
                                                                   : 1.6425
                      Max.
                                        Max.
##
    (Other):120962
##
          XS
                                хt
##
   Min.
           :-2.656455
                                 :-2.99309
                         Min.
    1st Qu.:-0.564698
                         1st Qu.:-0.72922
##
##
    Median :-0.094659
                         Median :-0.02276
##
   Mean
           : 0.009832
                         Mean
                                 :-0.03114
    3rd Qu.: 0.704837
                         3rd Qu.: 0.65035
##
   Max.
           : 2.286645
                                 : 2.96587
                         Max.
##
words <- c("tent","tenth")</pre>
dat <- droplevels(full[full$Word %in% words,])</pre>
library("gamtree")
```

We apply function gamtree to a subsample of the datatto a sample of data to reduce computation:

Note that for function gamtree, unlike functions (g)lmertree and splinetree, there are 2 instead of 3 vertical bars in the model formula. There is no 'global' part of the model, there is only the node-specific smoothing splines.

Note that for function gamtree, unlike functions (g)lmertree and splinetree, arguments passed to the tree fitting method (such as minsize) must be supplied indirectly, through the tree_ctrl argument. See ?gamtree for more information.

The fraction of data used can be increased by decreasing the value of 2. This will yield a smaller training sample, faster computation, but also lower power to detect splits.

I specified verbose = TRUE, so model-fitting progress is printed to the command line, which is helpful with computationally intensive procedures:

```
-- Node 1 -----
Number of observations: 6419
Parameter instability tests:
              Word
                     Lang xt
statistic 3.664566e+01 18.239390896 9.0737169 8.0189338
p.value 2.187296e-07 0.001570277 0.8075415 0.9132161
Best splitting variable: Word
Perform split? yes
Selected split: tent | tenth
-- Node 2 -----
Number of observations: 3171
Parameter instability tests:
     Word Lang xt
statistic 0 7.429725 5.716734 7.4429399
p.value NA 0.167803 0.982616 0.8755934
Best splitting variable: Lang
Perform split? no
-- Node 3 -----
Number of observations: 3248
Parameter instability tests:
      Word Lang xt xs
statistic 0 11.53103154 5.7293237 6.6883481
p.value NA 0.02727358 0.9830592 0.9395335
Best splitting variable: Lang
Perform split? yes
Selected split: EN | NL
-- Node 4 -----
Number of observations: 1895
Parameter instability tests:
   Word Lang xt
statistic 0 0 6.6126884 4.0047402
p.value NA NA 0.7569283 0.9822791
Best splitting variable: xt
Perform split? no
-- Node 5 -----
Number of observations: 1353
Parameter instability tests:
  Word Lang xt xs
statistic 0 0 2.2878959 5.7623263
p.value NA NA 0.9992052 0.7693788
```

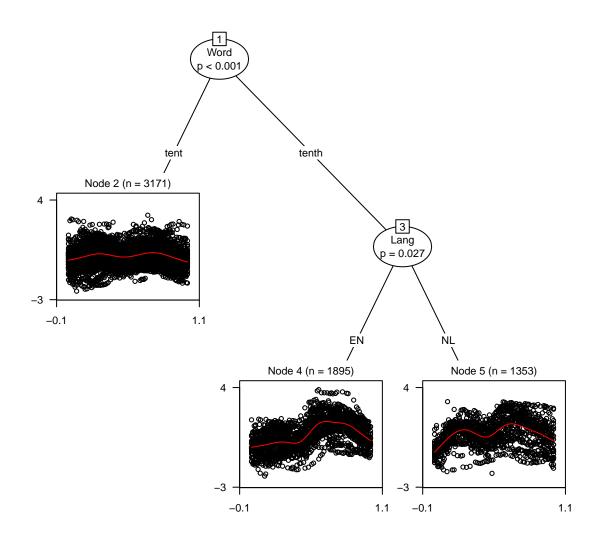
```
Best splitting variable: xs
Perform split? no
```

We see that the parameter stability tests for the noise variables are very well behaved. Significant p-values are only observed for the true predictors Word and Lang.

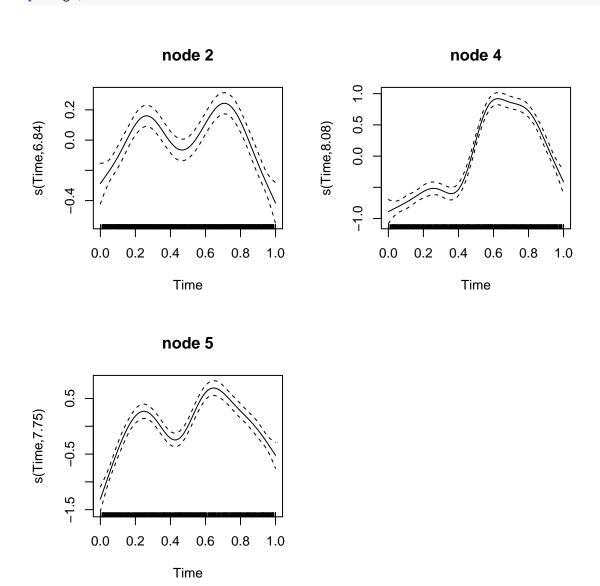
If you could not repeat the analyses, you can download the fitted tree from the GitHub repository and load it into ${\tt R}$ as follows:

```
load(file = "gamtree.rda")
```

We can plot the resulting tree, as well as the node-specific models. But beware that the confidence bands are overly optimistic, because they do *not* account for the searching of the tree structure!



```
par(mfrow = c(2, 2))
plot(gt, which = "terms")
```



From exploration to confirmation: Sample splitting can be beneficial!

Although reducing the number of training observations reduces the power to detect differences and subgroups, it brings a striking advantage: The part of the data (test data) that has not been used for fitting the tree can be used to refit a GAM with the subgroup structure found by the tree. This (re)fitted GAM will provide valid (a.k.a. 'honest') model estimates and hypothesis tests (e.g., Athey & Imbens, 2015). The idea is to estimate the unknown subgroup structure (i.e., exploration) on one part of the data, and to test the significance of effects (i.e., confirmation) on another part of the data.

We can extract node memberships for new data using the predict method (by specifying type = "response", we could obtain predicted values instead of predicted nodes):

```
test_dat <- dat[test, ]
test_dat$nodes <- factor(predict(gt, newdata = dat[test, ], type = "node"))</pre>
```

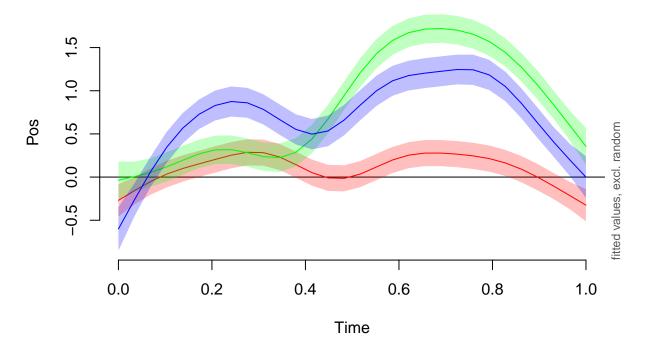
For the latter part, familiar techniques such as those described by Wieling (2018) and plotting methods such as implemented in package **itsadug** can be used. We could use the original indicators **Word** and **Lang**, but we can also incorporate the newly derived subgroups in the by argument of function s:

```
library("mgcv")
library("itsadug") ## for plot_smooth function
test_m <- bam(Pos ~ nodes + s(Time, by=nodes) + s(Speaker, bs="re"),
              data = test_dat)
summary(test_m)
##
## Family: gaussian
## Link function: identity
## Formula:
## Pos ~ nodes + s(Time, by = nodes) + s(Speaker, bs = "re")
## Parametric coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 0.10223
                          0.06969
                                    1.467
                                             0.142
## nodes4
               0.72349
                          0.02444
                                   29.603
                                            <2e-16 ***
## nodes5
               0.60786
                          0.02807
                                  21.654
                                            <2e-16 ***
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
## Approximate significance of smooth terms:
##
                     edf Ref.df
                                    F p-value
## s(Time):nodes2 7.481 8.429 18.63 <2e-16 ***
## s(Time):nodes4 7.843
                         8.653 151.71
                                       <2e-16 ***
## s(Time):nodes5 7.868 8.667
                                53.77
                                       <2e-16 ***
## s(Speaker)
                 40.197 41.000
                                44.97
                                       <2e-16 ***
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
##
## R-sq.(adj) = 0.445
                        Deviance explained = 45.1%
## fREML = 7254.4 Scale est. = 0.53813
plot_smooth(test_m, view = "Time", plot_all = "nodes", rug = FALSE,
           rm.ranef = TRUE)
```

```
## * nodes : factor; set to the value(s): 2, 4, 5.
## * Time : numeric predictor; with 30 values ranging from 0.000000 to 1.000000.
## * Speaker : factor; set to the value(s): VENI_NL_5. (Might be canceled as random effect, check below
## * NOTE : The following random effects columns are canceled: s(Speaker)
##
```

Summary:





Although we used a different set of observations, and we 'did not know' the truly relevant variables in advance, we obtained very similar results and identical conclusions as Wieling (2018): Native English speakers pronounce "Tent" and "Tenth" with clear differences, while Native Dutch speakers do not show such a clear difference. We can easily distinguish Native English speakers from Native Dutch speakers by their pronounciation of "Tenth", but not by their pronounciation of "Tent".

References

Athey, S., & Imbens, G. W. (2015). Machine learning methods for estimating heterogeneous causal effects. *Proceedings of the National Academy of Sciences*, 1050(5), 1-26. https://doi.org/10.1073/pnas.1510489113

Chen, Q., & Harrell Jr, F. E. (2019). Comment: Penalized spline of propensity methods for treatment comparison. *Journal of the American Statistical Association*, 114 (525), 28-30. https://doi.org/10.1080/01621459.2018.1537915

Eilers, P. H., & Marx, B. D. (1996). Flexible smoothing with B-splines and penalties. *Statistical Science*, 11(2), 89-121. https://doi.org/10.1214/ss/1038425655

Wang, T., & Merkle, E. C. (2018). merDeriv: derivative computations for linear mixed effects models with application to robust standard errors. *Journal of Statistical Software*, 87, 1-16. https://doi.org/10.18637/jss.v087.c01

Wang, T., Graves, B., Rosseel, Y., & Merkle, E. C. (2022). Computation and application of generalized linear mixed model derivatives using lme4. *Psychometrika*, 87(3), 1173-1193.