Morning session: computer lab exercises

Please make sure that the following packages are installed:

- 1. devtools (install.packages("devtools"));
- 2. qgam (library(devtools); install_github("mfasiolo/qgam"));
- 3. mgcViz (library(devtools); install_github("mfasiolo/mgcViz"));
- 4. gamair (install.packages("gamair")).

The exercises you could try in the first morning session are:

- 1. Ozone modelling (solution in "Ozone.html");
- 2. Bone mineral density modelling (sol: "bone_density.html");
- 3. Forecasting electricity demand on GEFCom2014 data (sol: "gefcom_small.html");

while in the second morning session you could try:

- 1. C0₂ modelling (sol: "CO2_modelling.html");
- 2. Individual electricity demand modelling (sol: "Ind_elect.html");
- 3. Big GAM modelling of GEFCom14 electricity demand data (sol: "gefcom_big.html");
- 4. Mackerel egg data (sol: "Mackerel.html");
- 5. Retinopathy among diabetics (sol: "Retinopath.html");
- 6. Larynx cancer in Germany (sol: "Larinx.html");

but feel free to try mgcv and mgcViz on your own data.

Questions 1, 4, 7 and 8 have been adapted from Simon Wood's notes.

1 Ozone modelling

Data frame ozone contains daily(ish) ozone measurements over Los Angeles (03, ppm), along with:

vh The height at which the atmospheric pressure is 500mb in metres.

wind the wind speed (reported as miles per hour, but this seems improbable).

humidity (usual % scale).

temp air temperature (Fahrenheit).

ibh the inversion layer base height in feet.

ibt the inversion base temperature (Fahrenheit).

dpg 'Dagget air pressure gradient' (mmhg).

vis visibility in miles.

doy Julian day, where 1 is Jan 1 1976.

The aim is to build a GAM model to explore the relationship between ozone and the other variables. Questions:

- 1. Load the data using ozone<-read.table("data/ozone.txt") and use something like pairs(ozone) to look at it.
- 2. Load mgcViz and use gamV to fit a Gaussian GAM with 03 as response, where log(E(03)) is given by a sum of smooth functions (e.g. s(wind)) of each of the predictors. You will need to use the log-link, which requires using the argument family=gaussian(link=log) in the call to gamV. Plot the fitted effects using plot.
- 3. Check the model residuals using the qq and check functions. Do you see any residual pattern when you plot the residuals against the fitted values or linear predictor?
- 4. Refit the model using a Gamma as response distribution (Gamma(link=log)), and re-check the residuals. Does the residual distribution look better?
- 5. Fit an alternative model where you are using the identity-link (Gamma(link=identity)). Does a model with an additive (i.e. identity-link) structure do better than that with a multiplicative (log-link) structure in terms of AIC?
- 6. Plot the smoothed effects again and use the **summary** function to see which effects are significant. Try simplifying the model.
- 7. Once you have converged on a model, plot it and interpret the fitted smooth effects: do they make sense?

2 Bone mineral density modelling

This dataset is taken from the package lava. It consists of 112 girls randomized to receive calcium or placebo. The response variable of interests consists of longitudinal measurements of bone mineral density (g/cm^2) measured approximately every 6th month for 3 years. All girls are approximately 11yo at the start of the trial. The main variables are:

- bmd bone mass density;
- group placebo or supplement;
- person factor indicating the id of each girl;
- age the age of each girl at the time of each measurement;

Questions:

- 1. Load mgcViz and the data with load("data/calcium.rda"). Then use gamV to fit a Gaussian GAM model with bmd as response and linear effects for age and group. In the call to gamV set the argument aViz=list(nsim = 50) to have some simulated responses for residuals checks. Use summary to print the model output. Is the placebo effect significant? (which is the same as asking whether the treatment effect is significant)
- 2. Use check1D with the l_gridCheck1D layer to check that the mean of the negative residuals does not depart too much from 0, for any of the subjects. If you see significant departures add a random effect for person to the models formula (s(person, bs="re")), then re-fit and re-check the residuals. Print the model output again using summary.

- 3. Now modify the model formula to use a smooth effect for age, and plot the fitted effects using plot. Use the function AIC to compare the model with a smooth effects for age with the model which uses a linear age effect.
- 4. Verify whether the smooth age effect is different between the placebo and the treatment group, by using a by-factor smooth. To do this substitute s(age) with s(age, by=group) in the model formula, refit and then plot the fitted effects. To see the difference between the two smooths more clearly, use the plotDiff function with the l_fitLine and l_ciLine layers.

3 Forecasting electricity demand on GEFCom2014 data

Here we consider the electricity demand dataset, taken from the GEFCom2014 challenge. The dataset covers the period January 2005 to December 2011 and it contains the following variables:

- NetDemand net electricity demand between 11am and 12am.
- wM instantaneous temperature.
- wM_s95 exponential smooth of wM, that is $wM_s95[i] = a*wM[i] + (1-a)*wM_s95[i]$ with a=0.95.
- Posan periodic index in [0, 1] indicating the position along the year.
- Dow factor variable indicating the day of the week (I think that 0=Saturday and 6=Sunday, but I am not sure).
- Trend progressive counter, useful for defining the long term trend.
- NetDemand. 24 lagged version of NetDemand, that is demand at the same time of the previous day.
- Year should be obvious.

Questions:

- 1. Load mgcViz and the data (load("data/gefcom_small.rda")). Use gamV to fit a Gaussian GAM where the model formula (e.g. y~s(x)) contains: smooth effects for wM, wM_s95, Posan (optionally use a cyclic basis for the latter by doing s(Posan, bs="cc")); parametric effects for Trend, Dow and NetDemand.24. In the call to gamV set the argument aViz=list(nsim = 50) to have some simulated responses for residuals checking. Plot all the fitted effects using plot.
- 2. Use check1D with the l_gridCheck1D layer to check that the mean of the negative residuals does not depart too much from 0, depending on the value of Trend. Do you see any systematic pattern? Use the function check to see whether you should increase k for any of the smooth effects.
- 3. Refit the model but now include a smooth effect for Trend (with k=6) and increase that basis dimension of the effects of wM, wM_s95, Posan to k = 20, 15 and 15 respectively. Compare this model to the old one in terms of AIC, re-check the residuals using check1D and recheck the bases dimension using check. Does everything look good? Increasing too much the basis dimension for Trend is not a good idea, why?
- 4. Use qq to produce a QQ-plot of the residuals, do you see any problem? Refit the same model, but now use a scaled Student-t distributions by setting family = scat. Any improvement in AIC? How do the residuals look now?

5. Check whether a scaled Student-t with log-link function scat(link=log) achieves lower AIC. The plot all the fitted effects of final model using plot (you can set allTerms=TRUE to plot also the parametric effects). Do the effects make sense?

4 CO_2 modelling

If you are new to R avoid this question¹, which is about modelling data with seasonality, and the need to be very careful if trying to extrapolate with QGAMs (or any statistical model). The data frame co2s contains monthly measurements of CO₂ at the south pole from January 1957 onwards. The columns are co2, the month of the year, month, and the cumulative number of months since January 1957, c.month. There are missing co2 observations in some months. Questions:

- 1. Load mgcv and the data with library(gamair); data(co2s)
- 2. Plot the CO₂ observations against cumulative months.
- 3. Fit a Gaussian additive model with a smooth effect for c.month, using the gam function. Use the cr basis, and a basis dimension of 100.
- 4. Obtain the predicted CO₂ for each month of the data, plus 36 months after the end of the data, as well as associated standard errors. Produce a plot of the predictions with twice standard error bands. Are the predictions in the last 36 months credible? NB: to produce the plot you have to write your own code, mgcv does not produce such plots.
- 5. Fit the model $\mathbb{E}(CO_2) = f_1(c.month_i) + f_2(month_i)$ where f_1 and f_2 are smooth functions. Use a basis of dimension 50 for f_1 and a cyclic basis for f_2 . In the gam call, you will need to set argument knots to list(month=c(1,13)) to make so that that the effect of January is the same as January, not that December and January are the same!
- 6. Repeat the prediction and plotting in question 4 for the new model. Are the predictions more credible now? Explain the differences between the new results and those from question 4.

5 Individual electricity demand modelling

Here we consider electricity demand from 28 commercial costumers. The dataset covers roughly three months and it contains the following variables:

- load power usage from an individual costumer (in KW, I guess);
- DateTime the date and the time of day;
- instant the time of day, where 1 corresponds to 00:00-00:30, 2 to 00:30-01:00 and so on;
- dow factor variable indicating the day of the week;
- temp instantaneous temperature;
- tempL exponential smooth of temp, that is tempL[i] = a*temp[i] + (1-a)*tempL[i] with a=0.95;
- ID the ID of each individual costumer;

¹From Simon Wood's notes

- load48SM lagged version of smoothed load, where the smoothing was performed as for tempL.
- day a counter depending on the day.

Questions:

- 1. Load mgcViz and the data (load("data/Ind_elect.rda")). Then use bamV to fit a Gaussian GAM model with smooth effects for instant, temp and day, and parametric effects for dow and ID. In the call to bamV set aViz = list(nsim = 50) to perform the response simulations needed for residuals checking. Look at the model output using plot and summary.
- 2. Now we start looking for interactions. Use the check2D function with the l_gridCheck2D layer to look for interactions between ID and instant, temp and day. Notice that the binned mean residuals should ideally fall in the range (-2, 2) if the model is correct. Do you see large deviation? If so for which costumer(s) in particular?
- 3. Modify the model formula to include by-factor smooths, that is s(instant, by = ID, id = 1) s(temp, by = ID, id = 2) and s(day, by = ID, id = 3). The id argument make so that each of the 3 by-factor smooths has its own smoothing parameter, but the same smoothing parameter is used across costumer. Refit the model using bamV, and set the argument aGam=list(discrete=TRUE) to speed up computation by discretisation. Compare this models to the previous one using AIC, and repeat the residuals checks. Any improvement?
- 4. Use check to verify whether the number of basis functions used for the smooth effects is sufficiently large. Double 'k' for any of the effects where the number of basis functions seems to small, and re-fit. After re-fitting, check whether AIC has improved.
- 5. Use the check2D function with the 1_gridCheck2D layer to look for interactions between ID and load48SM. If the effect of load48SM seems important, include the corresponding by-factor smooth by adding s(load48SM, by = ID, id = 4) to the model and re-fit.
- 6. Look at the model output using plot, using the select argument to plot any specific effect (you can't plot them all together, because the model includes tens of them). Compare the consumption of some of the individual costumers with the model predictions (which you can find in fittedModel\$fitted.values). Do some costumers look much harder to predict than others?

6 Big GAM modelling of GEFCom14 electricity demand data

Here we use again data from the GEFCom14 challenge, but this data set is 24 times larger than the one used in a previous exercise. This is because it contains data corresponding to all the 24 hourly slots. The variable Instant indicates the hourly window corresponding to each row of the data set. All remaining covariates have the same interpretation as before. Questions:

1. Load mgcViz and the data (load("data/gefcom_big.rda")). Create a model formula with smooth effects wM, wM_s95, Instant, Trend and Posan. Use regression splines bases (bs='cr') for all smooths apart from Posan, for which you should use an cyclic basis (bs='cc'). Use k = 6 for Trend and k = 20 for Posan. Leave k to its default for the other smooths. Use parametric fixed effects for Dow and NetDemand.24. Use this formula within a bamV call to fit a Gaussian GAM. When calling bamV set aGam=list(discrete=TRUE) to speed up computations (do this in all subsequent bamV calls) and aViz = list(nsim = 50) to perform the response simulations needed for residuals

- checking. Having fitted the model, look at the effects using plot (recall that you can use argument allTerms=TRUE to plot also the parametric effects).
- 2. Use check to verify whether the number of basis functions used for the smooth effects is sufficiently large. Also, use the check1D function with the l_gridCheck1D layer look for residual patterns across the variables.
- 3. Double 'k' for any of the effects where the number of basis functions seems to small, and re-fit. After re-fitting, check whether AIC has improved and repeat the residual checks.
- 4. We expect that several of the effects might depend on the time of day. Use the check2D function with the 1_gridCheck2D layer to look for interactions between Instant and NetDemand.24, wM, wM_s95 and Posan. Notice that the binned mean residuals should ideally fall in the range (-2, 2) if the model was correct. Do you see any residual pattern? If so, fit a model which includes the necessary tensor product interactions (e.g. ti(wM, Instant, k = c(10, 10))) and repeat the checks. Are the patterns still there?
- 5. Assuming that we are now satisfied with our model, we'll now have a detailed look at the fitted smooth effects. First, look at the marginal effects effects using the plot function. Use the expression print(plot(fit2, select = ???), pages = 1) to plot all the marginal effects on one page (substitute ??? with the indexes of the univariate effects in your model). Do the same to plot the 2D interactions. Think about whether each effect makes physical sense to you. As an alternative to plot, recall that you can extract any effect using the sm function and produce a plot with customized layers. You can use the listLayers function to get a list of the available layers. Then, use the plotRGL function to manipulate each bivariate effect interactively.
- 6. Extra question: the model could be improved further. For instance, use the check2D function with the l_gridCheck2D layer to look at how the standard deviation and skewness of the residuals vary across pairs of covariates (the e1071 package provides a skewness function, then you simply need to set gridFun = skewness in the call to l_gridCheck2D). Do you see any pattern? At this point we could consider a GAMLSS model with linear predictors for location, variance and skewness (e.g. the gaulss or shash family). However, bam methods does not yet support such models, so you'll need to use gam which can be much slower for large models.

7 Mackerel egg data

The following code loads and plots some data from a fish egg survey, for the purposes of spatial modelling.

```
library(mgcViz); load("data/mack.rda"); load("data/coast.rda")
## plot data....
with(mack,plot(lon,lat,cex=0.2+egg.dens/150,col="red"))
lines(coast)
ind <- c(1,3,4,5,10,11,16)
pairs(mack[,ind])</pre>
```

The main variables of interest in the mack data set are:

- egg.count number of eggs found in the net;
- c.dist distance from 200m seabed contour;

- b.depth depth of the ocean;
- temp.surf surface temperature of the ocean;
- temp. 20m water temperature at a depth of 20 meters
- lat latitude:
- lon longitude;
- salinity;
- net.area the area of the net used in m².

Questions:

- 1. Use the code above to load and plot the data;
- 2. Create a new variable mack\$log.net.area <- log(mack\$net.area), and use gamV to fit a Poisson GAM with 1D smooth effects for all the variables involved, with the exceptions of net.area and log.net.area. Instead include in the model formula the term offset(log.net.area), meant to take into account the fact that the number of eggs captured is proportional to the net area.
- 3. Look at the model residuals using qq. What kind of problem do you see? Re-fit the models using a negative binomial (family=nb) or Tweedie (family=tw) response distribution, and check which model is better in terms of residuals QQ-plots and AIC.
- 4. Let fit be the best of the three GAM models you just fitted. Use fit<-getViz(fit,nsim=50) to get some simulated residuals, and then use the check2D function with the l_gridCheck2D layer to look for residual patters across lon and lat. Then refit the model using a bivariate isotropic effect s(lon, lat, k=100), re-check the residuals and see whether AIC has improved.
- 5. Use check to verify whether the number of basis functions used for the smooth effects is sufficiently large. Then use the check1D function with the l_gridCheck1D layer look for residual patterns across some of the variables. If necessary, modify the model.
- 6. Plot the fitted effects using plot. Which effects look more important (look at the scales)? Use the plotRGL function to manipulate spatial effect interactively.

8 Retinopathy among diabetics

Data frame wesdr contains a subset of data from a Wisconsin study on development of retinopathy among diabetics. The following variables are provided:

- ret, a binary indicator of development of retinopathy by first follow up of study.
- bmi, the body mass index at entry to the study (between 18 and 25 is considered healthy).
- dur, the duration of diabetes, in years, at entry.
- gly, the percentage of glycosylated haemoglobin (HbA1C) in the blood (haemoglobin to which glucose has bound). 2.5-3.5% is normal for non-diabetics. 6.5% is generally considered good control for diabetics.

The aim is to model the probability of retinopathy as a function of the other variables. Questions:

- 1. Load mgcViz and the data (wesrd <- read.table("data/wesdr.txt")), and use pairs(wesdr) to look at it.
- 2. It is not immediately clear what model structure for the linear predictor is appropriate. So in the first instance try all smooth main effects plus two way interactions using ti terms. Use a logistic regression model (family = binomial). In the call to gamV set aViz = list(nsim = 50) to do some residual simulations, and aGam = list(select=TRUE) to do some variable selection. Use summary and plot to verify which effects seems important.
- 3. Simplify the model by removing non-significant effects and re-fit. Check the model residuals using QQ-plots of normally transformed residuals (qq(yourFit, type = "tnorm")) as well as the check1D function with the l_gridCheck1D layer look for residual patterns across the individual variables.
- 4. Use the plotRGL function to visualize and manipulate any bi-variate effect in your model interactively.

9 Larynx cancer in Germany

First load some data on cancer of the larynx by health reporting districts in Germany.

```
library(mgcViz)
load("data/german.polys.rda") ## load polygons defining German regions 'german.polys'
load("data/Larynx.rda") ## load Larynx cancer death data 'Larynx'
## Get regions "midpoints"....
X <- t(sapply(german.polys,colMeans,na.rm=TRUE))</pre>
```

The variables in the Larynx dataframe are:

region code identifying region;

E expected number of deaths (according to population and pan German total);

Y number of deaths from Larynx cancer 1986-1990;

x measure of smoking rate in region.

Questions:

1. Run the code above and then use gamV to fit a Poisson GAM with a smooth effects for x and the following Markov Random Field (MRF) effect for region:

```
s(region, k = 200, bs = "mrf", xt = list(polys=german.polys))
```

and the offset term offset(log(E)), meant to take into account the fact that the number of death is proportional to the population of each region. The latter is meant to take into account the fact that number of cancer cases is proportional to population in each region. In the call to gamV set aViz = list(nsim = 50) to do some residual simulations for later checking. Plot the fitted effects.

- 2. Now substitute the MRF smooth either with the isotropic smooth s(X[,1],X[,2],k=200) or with the tensor product smooth te(X[,1],X[,2],k=c(15, 15)). Plot the corresponding fitted effects and compare them. Which model does better in terms of AIC?
- 3. Use the plotRGL function to visualize and compare the fitted isotropic and tensor product smooth. You can use the code

```
mfrow3d(1, 2)
plotRGL(sm(fit2,1), residuals = TRUE)
next3d()
plotRGL(sm(fit3,1), residuals = TRUE)
to get two rgl plots side by side.
```