

Nonlinear Modelling in R with GAMS

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1 Introduction to Generalized Additive Models

Trade-offs in Model Building

- Linear models
- GAMs
- Black-Box ML

```
library(mgcv)
gamfit = gam(y ~ s(x), data = dat)
```

The flexible smooths in GAM are constructed of many smaller functions, which are called basis functions. Each smooth is a sum of a number of basis functions and each basis function is multiplied by a coefficient, each of which is a parameter in the model

1.1 Basis Functions and Smoothing

The flexibility of GAM makes it easy to overfit the data.

- Close to the data (avoiding under-fitting)
- Not fitting the noise (avoid overfitting)

1.1.1 Smoothing parameter

The complexity of likelihood, or how much the curve changes its shape is measured by **wigginess**

$$\text{Fit} = \text{Likelihood} - \lambda * \text{Wigginess}$$

The key is balance the trade-off between Likelihood and Wigginess. The smoothing parameter λ is used to control the balance.

Normally we let the package chooses the smoothing parameter.

```
# Setting a fixed smoothing parameter
gam(y ~ s(x), data = dat, sp = 0.1)
gam(y ~ s(x, sp = 0.1), data = dat)

# Smoothing via restricted maximum likelihood
gam(y ~ s(x), data = dat, method = "REML")
```

REML is recommended as the smoothing algorithm. It is most likely to give stable and reliable results.

1.1.2 Number of basis functions

Set the number of basis functions

```
gam(y ~ s(x, k = 3), data = dat, method = "REML")
gam(y ~ s(x, k = 10), data = dat, method = "REML")
```

Use the defaults

```
gam(y ~ s(x), data = dat, method = "REML")
```

We can test if the number of basis functions is adequate using statistical tests.

1.2 Multivariate GAMs

- The `mgcv` package does not use character variables
- Normally we give splines to continuous variables, while keep categorical variables as they are in GAMs.
- Set by parameter, we can specify different smoothing in different categories.

```
model4b <- gam(hw.mpg ~ s(weight, by = fuel) + fuel, data = mpg,
               method = "REML")
```

2 Interpreting GAMs

A good way to interpret significant smooth terms in GAMs is: **A significant smooth term is the one where you cannot draw a horizontal line through the 95% confidence interval.**

Note that a high EDF (effective degrees of freedom) doesn't mean significance or vice versa. In the example model, the price term is non-linear but non-significant, meaning that it has some complexity, but there isn't certainty to the shape or direction of its effect.

The plots generated by `mgcv`'s `plot()` function are partial effect plots. That is, they show the component effect of each of the smooth or linear terms in the model, which add up to the overall prediction.

```
plot(gam_model, select = c(2, 3))
plot(gam_model, pages = 1)
plot(gam_model, pages = 1, all.terms = TRUE)
```

The first option we have when making our plots is which partial effect to show.

- The `select` argument chooses which terms we plot, with the default being all of them.
- Normally, each plot gets its own page, but using the `pages` argument, you can decide how many total pages to spread plots across.
- Finally, by default we only see the smooth plots, but by setting `all.terms = TRUE`, we can display partial effects of linear or categorical terms as well.

```
plot(gam_model, rug = TRUE)
plot(gam_model, residuals = TRUE)
plot(gam_model, rug = TRUE, residuals = TRUE,
     pch = 1, cex = 1)
```

We often want to show data alongside model predictions.

- The `rug` argument puts X-values along the bottom of the plot.
- The `residuals` argument puts partial residuals on the plot.

Partial residuals are the difference between the partial effect and the data, after all other partial effects have been accounted for.

2.1 Showing standard errors

```
plot(gam_model, se = TRUE)
plot(gam_model, shade = TRUE)
```

By default, plot will put standard errors on your plots. These show the 95% confidence interval for the mean shape of the effect. It is often preferable to use shading rather than lines to show these intervals, which can be achieved using the `shade = TRUE` argument.

2.2 Transforming standard errors

```
plot(gam_model, seWithMean = TRUE)
plot(gam_model, seWithMean = TRUE, shift = coef(gam_model)[1])
```

It is often useful to plot the standard errors of a partial effect term combined with the standard errors of the model intercept. This is because the confidence intervals at the mean value of a variable can be very tiny, and don't reflect the overall uncertainty in our model. Using the `seWithMean` argument adds in this uncertainty.

To make the plot even more interpretable, it is useful to shift the scale so that the intercept is included. Using the `shift` argument, we can shift the scale by value of the intercept, which is the first coefficient of the model. Now, the partial effect plot has a more natural interpretation: it shows us the prediction of the output, assuming other variables are at their average values.

2.3 Model checking