Generalized Additive Models

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Generalized additive models

- The polynomial and spline regression models can be regarded as special cases of a more general type of regression model known as a *generalized additive model* (GAM).
- Given n observations of a set of L predictor variabes $x_1, x_2 \ldots x_l \ldots x_L$ and outcome variable y, where $y_i, x_{1i}, x_{2i} \ldots x_{li} \ldots x_{Li}$ are the values of the outcome and predictors on observation i, then a GAM regression model of this data is:

$$y_i \sim D(\mu_i, \psi), \quad \mu_i = f_1(x_{1i}) + f_2(x_{2i}) + \ldots + f_L(x_{Li}), \quad \text{for } i \in 1 \ldots n,$$

  where D is some probability distribution with parameters ψ, and each predictor variable f_l is a *smooth function* of the predictor variable's values. Usually each smooth function f_l is a weighted sum of basis functions such as spline basis functions or other common types, some of which we describe below.

Generalized additive models "smooths"

- The smooth functions f_l might be defined as follows:

$$f_l(x_{li}) = \beta_{l0} + \sum_{k=1}^{K} \beta_{lk}\phi_{lk}(x_{li}),$$

where ϕ_{lk} is a basis function of x_{li}.

More general GAMs

- Instead of the outcome variable being described by a probability distribution D where the value of μ_i is the sum of smooth functions of the values of predictor variable at observation i, just as in the case of generalized linear models, we could transform μ_i by a deterministic *link function* g as follows:

$$y_i \sim D(g(\mu_i), \psi), \quad \mu_i = f_1(x_{1i}) + f_2(x_{2i}) + \ldots + f_L(x_{Li}), \quad \text{for } i \in 1 \ldots n.$$

More general still GAMs

- More generally still, each smooth function may in fact be a multivariate function, i.e. a function of multiple predictor variables.
- Thus, for example, a more general GAM than above might be as follows:

$$
\begin{aligned}
&y_i \sim D(g(\mu_i)), \\
&\mu_i = f_1(x_{1i}) + f_2(x_{2i}, x_{3i}, x_{4i}) + \ldots + f_L(x_{Li}), \quad \text{for } i \in 1 \ldots n,
\end{aligned}
$$

where in this case, f_2 is a 3-dimensional smooth function.

Using `mgcv`

- The R package `mgcv` is a powerful and versatile toolbox for using GAMs in R.
- We will use a classic data-set often used to illustrate nonlinear regression

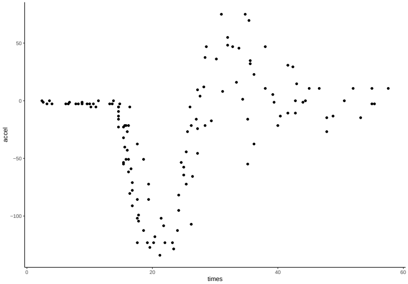


Figure 1: Head acceleration over time in a simulated motorcycle crash.

Using mgcv

- The main function we will use from `mgcv` is `gam`.
- By default, `gam` behaves just like `lm`.

```
library(mgcv)

M_0 <- gam(accel ~ times, data = mcycle)
```

- In other to use `gam` to do basis function regression, we must apply what `mgcv` calls *smooth terms*.
- There are many smooth terms to choose from in `mgcv` and there are many methods to specify them.
- Here, we will use the function simply named `s` to set up the basis functions.
- The default basis functions used with `s` are *thin plate splines*.

```
M_1 <- gam(accel ~ s(times), data = mcycle)
```

gam with *s* fit

- The plot of the fit of the above model can be accomplished using the base R `plot` function.

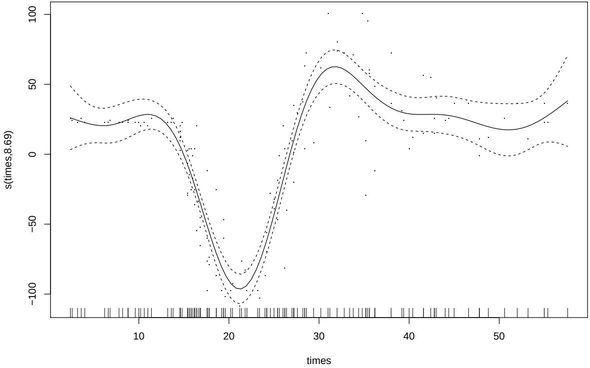


Figure 2: A thin plate spline basis function regression model applied to the `mycle` data set.

gam with s summary

```
summary(M_1)$s.table
#>                edf   Ref.df        F      p-value
#> s(times) 8.693314 8.971642 53.51503 2.957613e-71
```

- The `edf` is the effective degrees of freedom of the smooth term.
- We can interpret it values in terms of polynomial terms.
- In other words, a `edf` close to one means the smooth terms is effectively a linear function, while a `edf` close to 2 or close to 3, and so on, are effectively quadratic, cubic, and so on, models.
- The F statistic and p-value that accompanies this value tells us whether the function is significantly different to a horizontal line, which is a linear function with a zero slope.
- Even if the `edf` is greater than 1, the p-value may be not significant because there is too much uncertainty in the nature of the smooth function.

gam rank

- The number of basis functions used by `s` is reported by the `rank` attribute of the model.
- In our model, we see that it is 10.

```
M_1$rank
#> [1] 10
```

- In general, `mgcv` will use a number of different methods and constraints, which differ depending on the details of the model, in order to optimize the value of `k`.
- We can always, however, explicitly control the number of basis functions used by setting the value of `k` in the `s` function.

```
M_2 <- gam(accel ~ s(times, k = 5), data = mcycle)
M_2$rank
#> [1] 5
```

gam rank optimization

- How models with different numbers of bases differ in terms of AIC can be easily determined using the `AIC` function.
- To illustrate this, we will fit the same model with a range of value of `k` from 3 to 30.

```
M_k_seq <- map(seq(3, 20) %>% set_names(.,.),
               ~gam(accel ~ s(times, k = .), data = mcycle))
model_aic <- map_dbl(M_k_seq, AIC)
which.min(model_aic)
#> 9
#> 7
```

gam.check and k.check

- `gam.check` and `k.check` can be used for diagnosis and checking the number of basis functions

```
k.check(M_2)
#>          k'      edf   k-index p-value
#> s(times)  4 3.725477 0.3954199       0
M_3 <- gam(accel ~ s(times, k = 10), data = mcycle)
k.check(M_3)
#>          k'      edf  k-index p-value
#> s(times)  9 8.693314 1.148959   0.935
```

Smoothing penalty

- In addition to explicitly setting the number of basis functions, we can also explicitly set the *smoothing penalty* with the `sp` parameter used inside the `s` function.
- In general, the higher the smoothing penalty, the *less* flexibility in the nonlinear function.
- For example, very high values of the smoothing penalty effectively force the model to be a liner model.
- On the other hand, low values of the smoothing penalty may be overly flexible and overfit the data, as we saw above.

Smoothing penalty

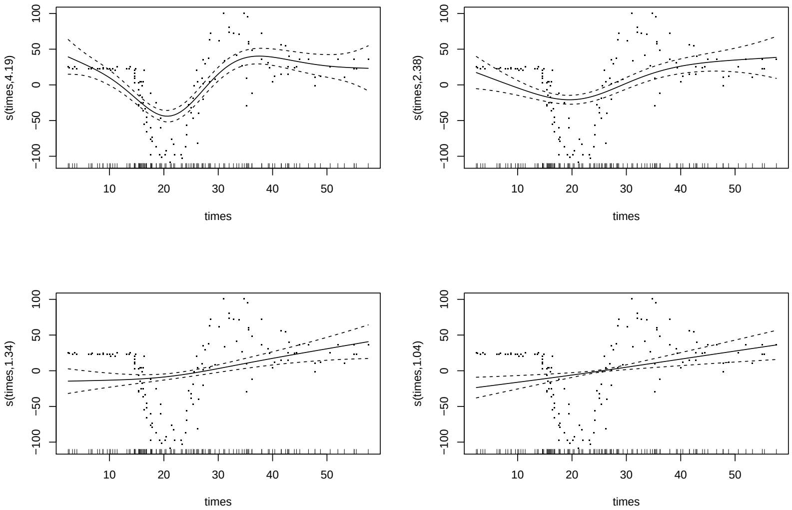


Figure 3: Plots of the fits of Gam models to the `mcycle` data with different

Optimizing smoothing penalty

- As with `k`, if `sp` is not explicitly set, `mgcv` uses a different methods, including cross-validation, to optimize the value of `sp` for any given model.

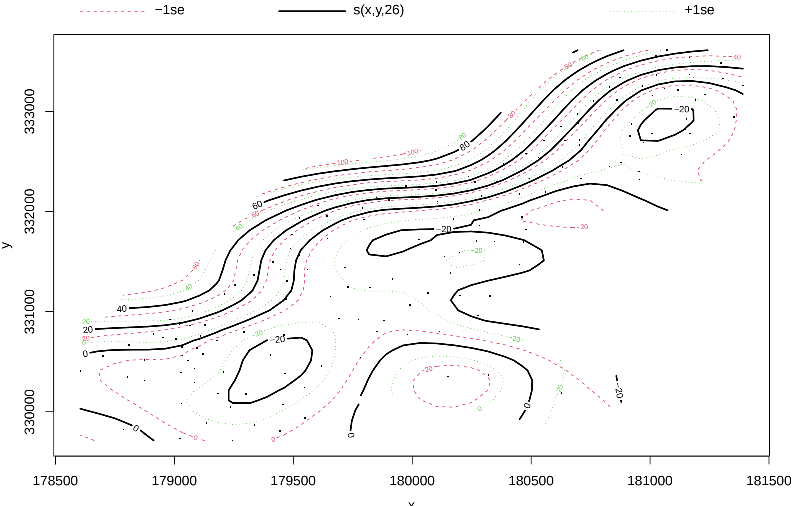
by factor smooth for interactions

- To model interactions with a categorical predictor variable, we must use *by factor* smooths.
- This effectively allows us to fit a separate smooth function for each value of the interacting categorical variable.

Multivariate basis functions for spatial etc models

```r
meuse <- read_csv('../data/meuse.csv')

M <- gam(copper ~ s(x, y), data = meuse)
```



Multivariate basis functions for continuous-continuous interactions

- Gams can handle continuous-continous interactions not possible otherwise.
- Let's say we have two predictors x_1, which is continuous, and x_2 which is binary, then a varying intercept linear model is

$$\mu_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2.$$

- When $x_2 = 0$, we have

$$\begin{aligned}\mu_i &= \beta_0 + \beta_1 x_1 + \underbrace{\beta_2 x_2}_{=0},\\ &= \beta_0 + \beta_1 x_1.\end{aligned}$$

- When $x_2 = 1$, we have

$$\begin{aligned}\mu_i &= \beta_0 + \beta_1 x_1 + \underbrace{\beta_2 x_2}_{=\beta_2},\\ &= (\beta_0 + \beta_2) + \beta_1 x_1.\end{aligned}$$

- In R, this `y ~ x_1 + x_2`.

Multivariate basis functions for continuous-continuous interactions

- A varying slope and varying intercept linear model is

$$\mu_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2.$$

- When $x_2 = 0$, we have

$$\begin{aligned}\mu_i &= \beta_0 + \beta_1 x_1 + \underbrace{\beta_2 x_2}_{=0} + \underbrace{\beta_3 x_1 x_2}_{=0},\\ &= \beta_0 + \beta_1 x_1.\end{aligned}$$

- When $x_2 = 1$, we have

$$\begin{aligned}\mu_i &= \beta_0 + \beta_1 x_1 + \underbrace{\beta_2 x_2}_{=\beta_2} + \underbrace{\beta_3 x_1 x_2}_{=\beta_3 x_1},\\ &= (\beta_0 + \beta_2) + (\beta_1 + \beta_3) x_1.\end{aligned}$$

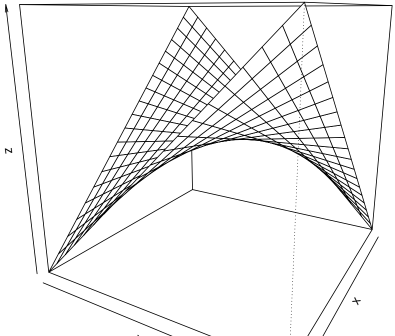
- In R, this `y \sim x_1 * x_2`.

Multivariate basis functions for continuous-continuous interactions

- What if x_1 and x_2 are both continous?
- What does `y ~ x_1 * x_2` do?
- It is still

$$\mu_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2,$$

which means that x_1 and x_2 are being multiplied. This means, our function from x_1 and x_2 to μ is essentially



Multivariate basis functions for continuous-continuous interactions

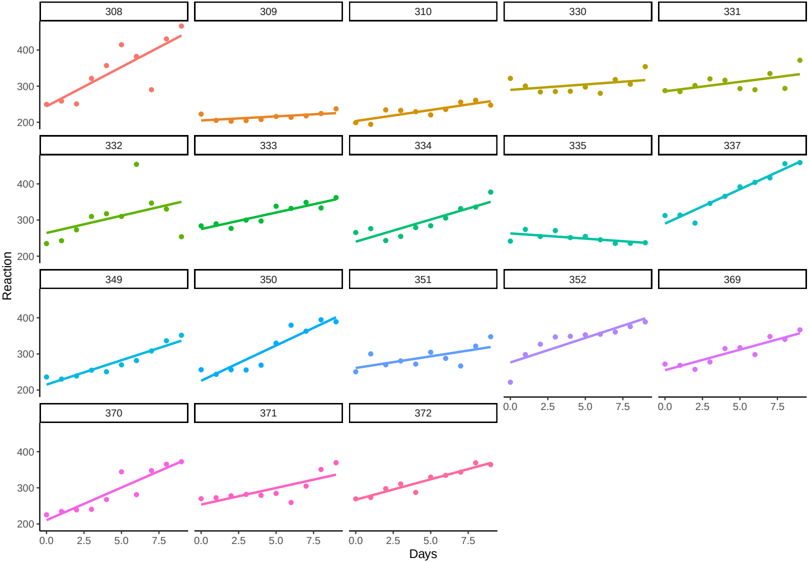
- We can instead model this surface as

```r
gam(y ~ te(x_1, x_2))
```

etc.

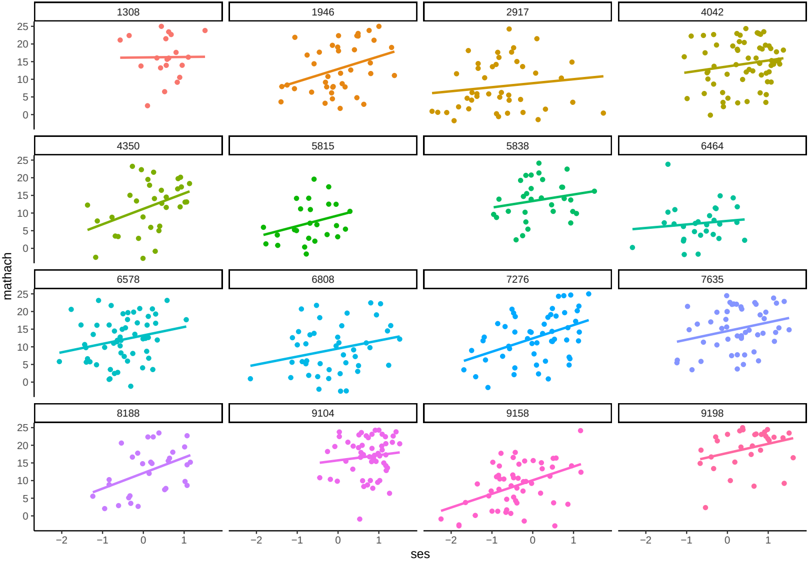
Multilevel data: Example 1

Reaction time as a function of sleep deprivation.



Multilevel data: Example 2

Mathematical achievement as function of socio-economic status.



Example: Reaction time and math achievement

- In this problem, we have J subject. For subject j, we have n_j data points.
- In observation i from subject j, their number of days without sleep is x_{ji} and the reaction time is y_{ji}.
- A multilevel model for this data is

$$\begin{aligned} y_{ji} &\sim N(\alpha_j + \beta_j x_{ji}, \sigma^2), \\ \alpha_j &\sim N(a, \tau_a^2), \\ \beta_j &\sim N(b, \tau_b^2). \end{aligned}$$

Example: Reaction time and math achievement

- The model

$$y_{ji} \sim N(\alpha_j + \beta_j x_{ji}, \sigma^2),$$
$$\alpha_j \sim N(a, \tau_a^2),$$
$$\beta_j \sim N(b, \tau_b^2),$$

can be re-written

$$y_{ji} = \underbrace{(a + \eta_j)}_{\alpha_j} + \underbrace{(b + \zeta_j)}_{\beta_j} x_{ji} + \epsilon_{ji},$$

or

$$y_{ji} = \underbrace{a + b x_{ji}}_{\text{Fixed effect}} + \underbrace{\eta_j + \zeta_j x_{ji}}_{\text{Random effect}} + \epsilon_{ji},$$

where

$$\eta_j \sim N(0, \tau_a^2),\ \zeta_j \sim N(0, \tau_b^2),\ \epsilon_j \sim N(0, \sigma^2).$$

Example: Reaction time and math achievement

- In the model just described, a and b are the general regression coefficients.
- The variance τ_a^2 tells us how much variation in the intercept term there is across schools. The variance τ_b^2 tells us how much variation in the slope term there is across schools.
- For example, 95% and 99% of the intercepts for individual schools will be in the ranges

  $$a \pm 1.96 \times \tau_a, \quad a \pm 2.56 \times \tau_a,$$

  respectively. Likewise, 95% and 99% of the slope terms for schools will be in the ranges

  $$b \pm 1.96 \times \tau_b, \quad b \pm 2.56 \times \tau_b.$$

Multilevel GAM

- Recall that an example of a simple multilevel normal linear model can be defined as follows:

$$
\begin{aligned}
y_{ji} \sim N(\mu_{ji}, \sigma^2), \quad \mu_{ji} = \alpha_j + \beta_j x_{ji}, \quad \text{for } i \in 1 \ldots n \\
\text{with} \quad \alpha_j \sim N(a, \tau^2_\alpha), \quad \beta_j \sim N(b, \tau^2_\beta) \quad \text{for } j \in 1 \ldots J.
\end{aligned}
$$

- This model can be rewritten as

$$
\begin{aligned}
& y_{ji} \sim N(\mu_{ji}, \sigma^2), \\
& \mu_{ji} = a + \nu_j + b x_{ji} + \xi_j x_{ji}, \quad \text{for } i \in 1 \ldots n, \quad j \in 1 \ldots J, \\
\text{with} \quad & \nu_j \sim N(0, \tau^2_\alpha), \quad \xi_j \sim N(0, \tau^2_\beta), \quad \text{for } j \in 1 \ldots J.
\end{aligned}
$$

Multilvel GAM

- A GAM version of this model might be as follows.

$$
\begin{aligned}
& y_{ji} \sim N(\mu_{ji}, \sigma^2), \\
& \mu_{ji} = a + \nu_j + f_1(x_{ji}) + f_{2j}(x_{ji}), \quad \text{for } i \in 1 \ldots n, \quad j \in 1 \ldots J, \\
\text{with} \quad & \nu_j \sim N(0, \tau_\alpha^2), \quad f_{2j} \sim F(\Omega), \quad \text{for } j \in 1 \ldots J.
\end{aligned}
$$

Here, $f_{21}, f_{22} \ldots f_{2j} \ldots f_{2J}$ are *random smooth functions*, sampled from some function space $F(\Omega)$, where Ω specifies the parameters of that function space.