Advanced Topics in Regression

Kernels, Smoothers, and Generalized Additive Models

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Kernels

In Statistical contexts: **a kernel is a symmetric PDF**

Examples:

- Normal distribution
- Uniform distribution

Kernel Regression

The classical kernel regression estimator is the **Nadaraya-Wetson** estimator:

$$\hat{y}_h(x) = \sum_{i=1}^{n} w_i(x) Y_i$$

where:

$$w_i(x) = \frac{K(\frac{x - X_i}{h})}{\sum_{j=1}^{n} K \frac{x - X_j}{h}}$$

Regression estimate is the average of all the weighted observed response values

- Farther x is from the observation, the less weight that observation has in determining the regression estimate at x.

Nadaraya-Wetson

- given training data with explanatory variable x and continuous response y
- bandwidth h > 0
- and a new point

Example of a linear smoother: class of models where predictions are weighted sums of the response variable.

Local Regression

We can fit a linear model **at each point** x_{new} with weights given by kernel function centered on x_{new}

Local regression of the kth order with kernel function K solves the following:

$$\hat{\beta}(x_{new}) = \arg\min_{\beta} \Big\{ \sum_{i} K_h(|x_{new} - x_i|) \cdot (y_i - \sum_{j=0}^{k} x_i^k \cdot \beta_k)^2 \Big\}$$

So, every single observation has its own set of coefficients

The predicted value is then:

$$\hat{y}_{new} = \sum_{j=0}^{k} x_{new}^k \cdot \hat{\beta}_k(x_{new})$$

This is a smoother prediction than with kernel regression but comes at a higher computational cost

- LOESS replaces kernel with k nearest neighbors (discrete average)

Smoothing Splines

Use a **smooth function** s(x) to predict y, control smoothness directly by minimizing the **spline objective function:**

$$\sum_{i=1}^{n} (y_i - s(x_i))^2 + \lambda \int (s''(x))^2 dx$$

$$= \text{fit data} + \text{impose smoothness}$$

$$\Rightarrow \text{model fit} = \text{likelihood} - \lambda \cdot \text{wiggliness}$$

Estimate the **smoothing spline** $\hat{s}(x)$ that **balances the tradeoff between the model fit and the wiggliness**

Basis Functions

Splines are piecewise cubic polynomials with **knots** (boundary points for functions) at every data point.

- Practical alternative: linear combination of a set of **basis functions**

Examples:

For a cubic polynomial:

- $B_1(x) = 1,\ B_2(x) = x,\ B_3(x) = x^2,\ B_4(x) = x^3$

$$r(x) = \sum_{j}^{4} \beta_j B_j(x)$$

* Linear in the transformed variables $B_1(x), B_2(x), B_3(x), B_4(x)$ but it is **nonlinear in x**

We extend this idea for splines *piecewise* using indicator functions so the spline is a weighted sum:

$$s(x) = \sum_{j}^{m} \beta_j B_j(x)$$

Generalized Additive Models (GAMS)

- relationships between individual explanatory variables and the response variable are smooth (either linear or nonlinear via basis functions)
- estimate the smooth relationships simultaneously to predict the response by just adding them up

generalized like GLMs where g() is the link function for the expected value of the response E(Y) and **additive** over the p variables.

$$g(E(Y)) = \beta_0 + s_1(x_1) + s_2(x_2) + \cdots + s_p(x_p)$$

* can be a convenient balance between flexibility and interpretability

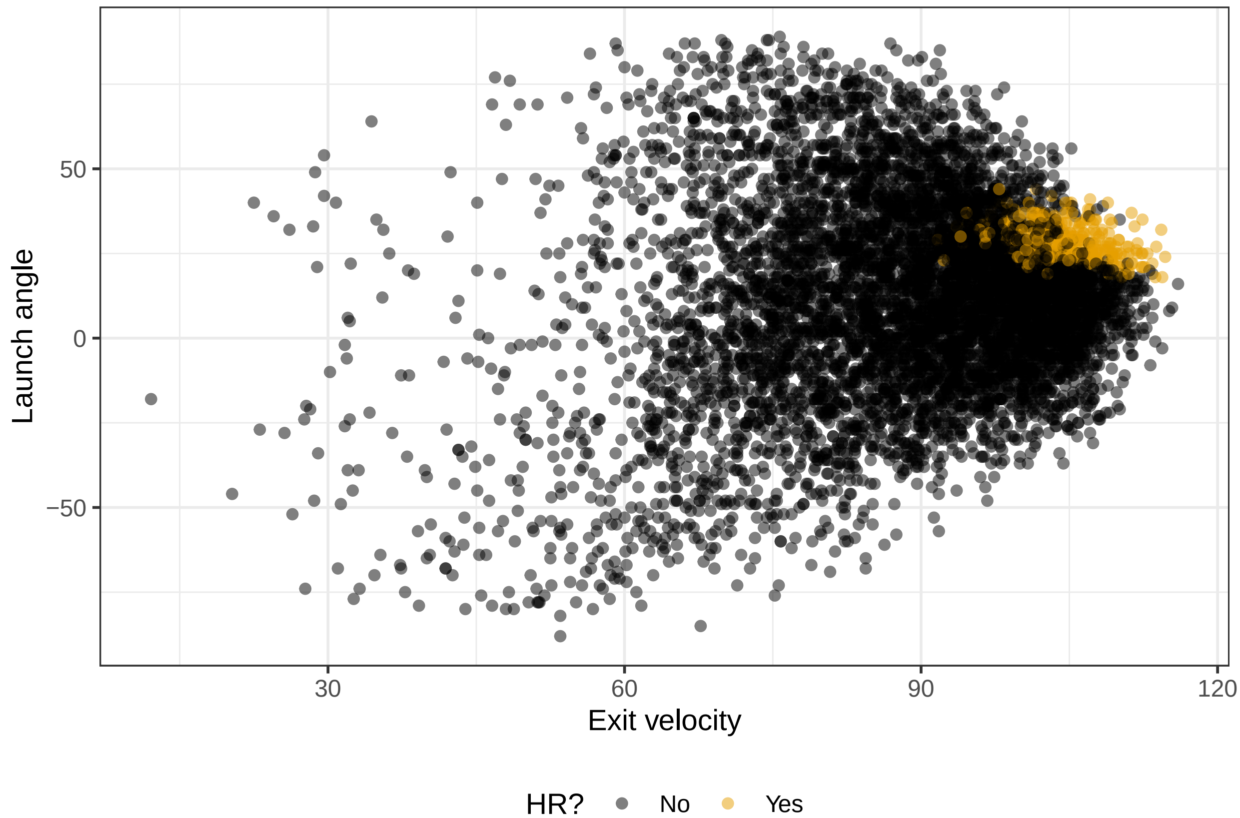
- you can combine linear and nonlinear terms!

Example

```
batted_ball_data <- read_csv("https://shorturl.at/moty2") %>%
  mutate(is_hr = as.numeric(events == "home_run")) %>%
  filter(!is.na(launch_angle), !is.na(launch_speed), !is.na(is_hr))

head(batted_ball_data)
```

```
## # A tibble: 6 x 32
##   player_name    batter stand events     hc_x  hc_y hit_distance_sc launch_speed
##   <chr>           <dbl> <chr> <chr>     <dbl> <dbl>           <dbl>        <dbl>
## 1 Daza, Yonathan 602074 R     force_out 103.  150.               18         97.4
## 2 Robles, Victor 645302 R     single     58.6 120.              158         80.2
## 3 Hoerner, Nico  663538 R     field_out  99.3 166.               20        101.
## 4 Clemens, Kody  665019 L     field_out 126.  191.              165         84
## 5 Rosario, Amed  642708 R     field_out  97.4 170.                9         94.3
## 6 Castro, Willi  650489 L     sac_fly   178.   58.9             369         96
## # i 24 more variables: launch_angle <dbl>, hit_location <dbl>, bb_type <chr>,
## #   barrel <dbl>, pitch_type <chr>, release_speed <dbl>, effective_speed <dbl>,
## #   if_fielding_alignment <chr>, of_fielding_alignment <chr>, game_date <date>,
## #   balls <dbl>, strikes <dbl>, outs_when_up <dbl>, on_1b <dbl>, on_2b <dbl>,
## #   on_3b <dbl>, inning <dbl>, inning_topbot <chr>, home_score <dbl>,
## #   away_score <dbl>, post_home_score <dbl>, post_away_score <dbl>, des <chr>,
## #   is_hr <dbl>
```

```
batted_ball_data %>%  ggplot(aes(x = launch_speed, y = launch_angle,
                                 color = as.factor(is_hr))) +
  geom_point(alpha = 0.5) +
  ggthemes::scale_color_colorblind(labels = c("No", "Yes")) +
  labs(x = "Exit velocity", y = "Launch angle", color = "HR?") +
  theme_bw() +
  theme(legend.position = "bottom")
```




```
# setting up the training data

set.seed(2004)

batted_ball_data <- batted_ball_data %>%
  mutate(is_train = sample(rep(0:1, length.out = nrow(batted_ball_data))))
```

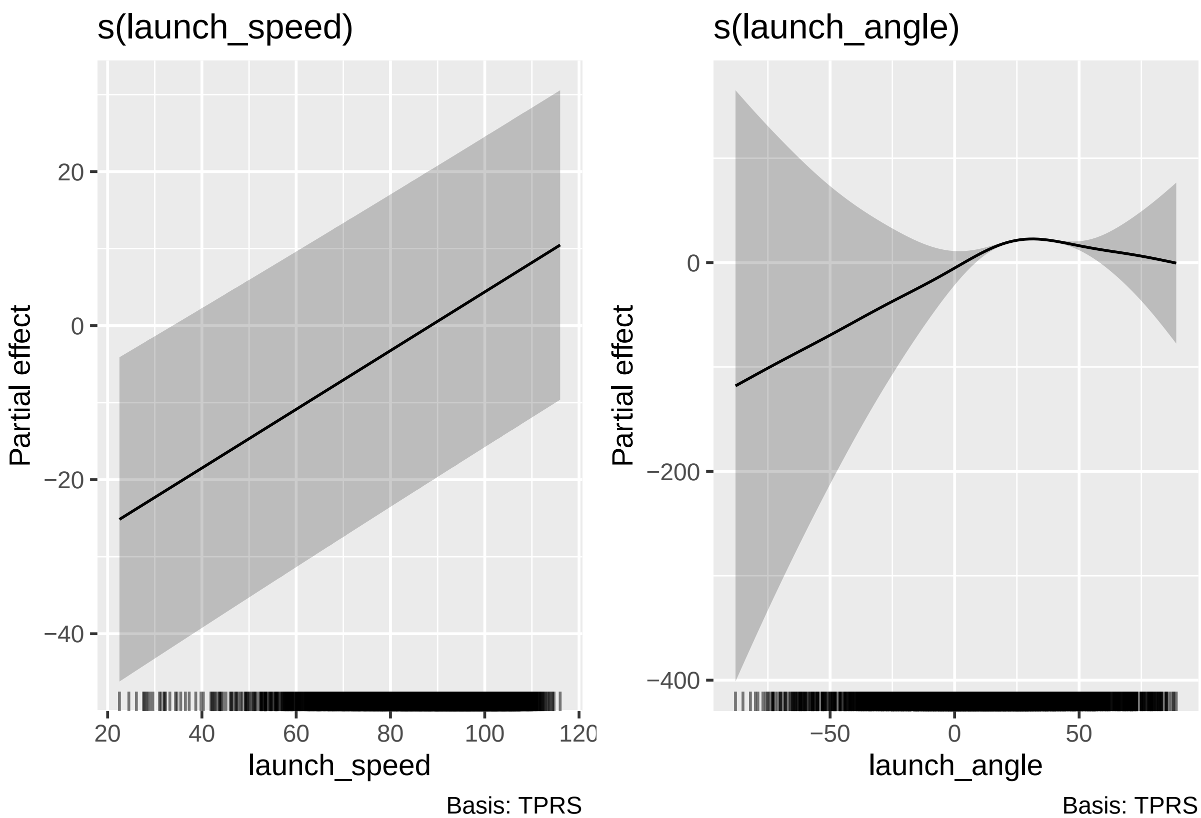
```
init_logit_gam <- gam(is_hr ~ s(launch_speed) + s(launch_angle),
     data = filter(batted_ball_data, is_train == 1), family = binomial, method = "REML")

# REML allows for a more stable solution
```

```
summary(init_logit_gam)
```

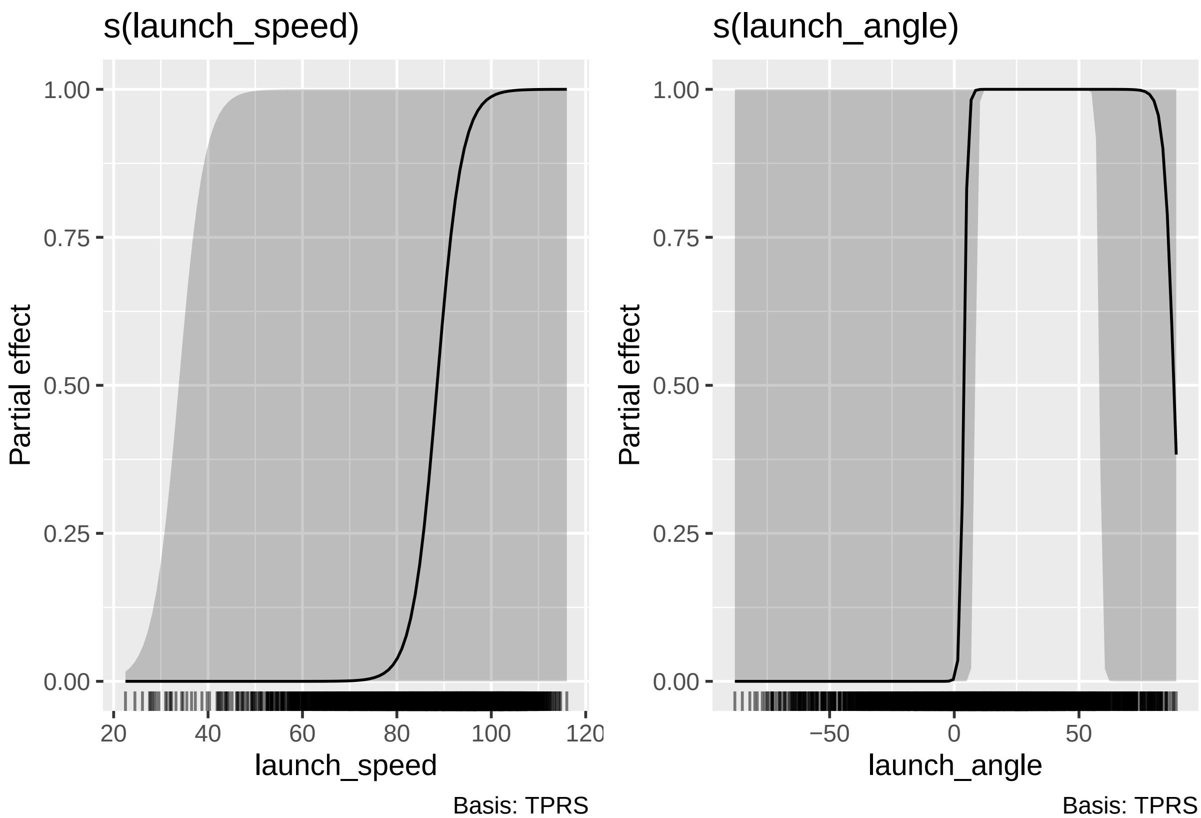
```
##
## Family: binomial
## Link function: logit
##
## Formula:
## is_hr ~ s(launch_speed) + s(launch_angle)
##
## Parametric coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)   -26.96      10.31  -2.614  0.00895 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##                   edf Ref.df Chi.sq p-value
```

```
## s(launch_speed) 1.000  1.000  151.5  <2e-16 ***
## s(launch_angle) 2.962  3.305  112.0  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.588   Deviance explained = 68.3%
## -REML = 231.49  Scale est. = 1         n = 3517
```

```
# displays the partial effect of each term in the model. Add up to the overall prediction
draw(init_logit_gam)
```

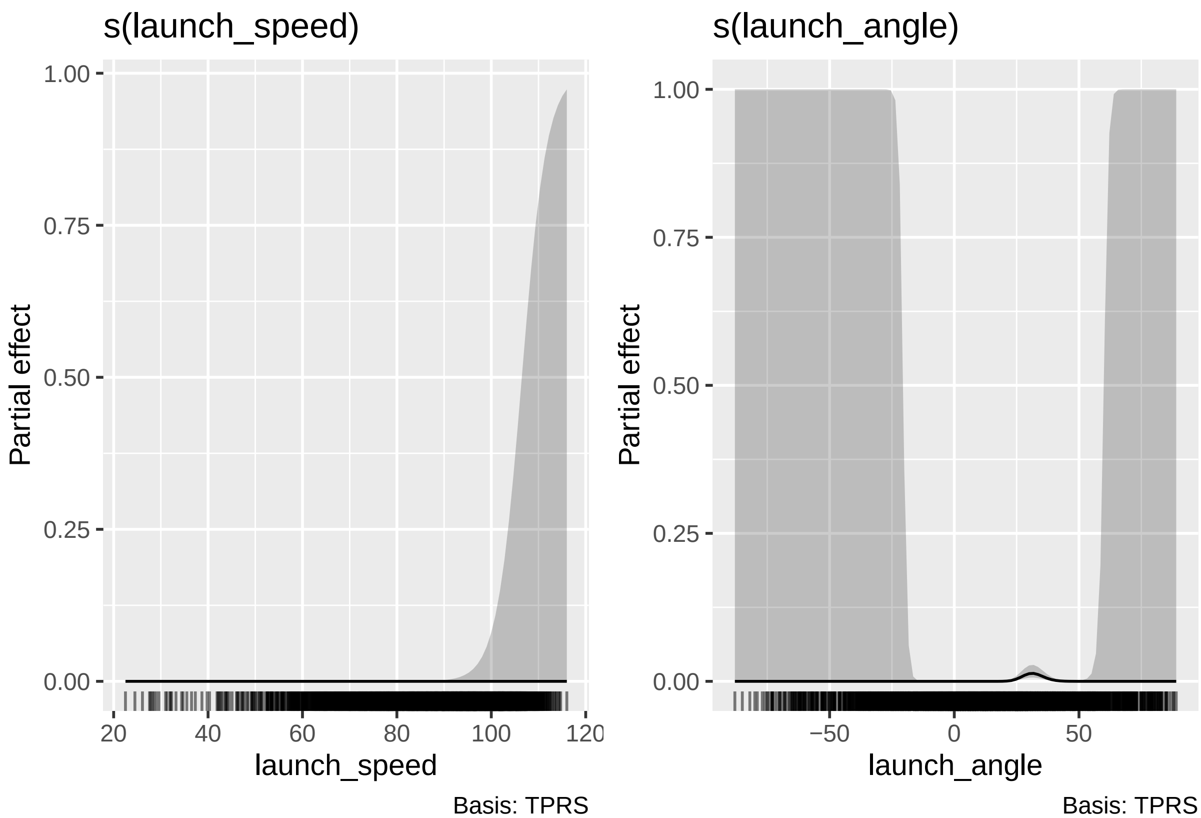



```
draw(init_logit_gam, fun = plogis)
```



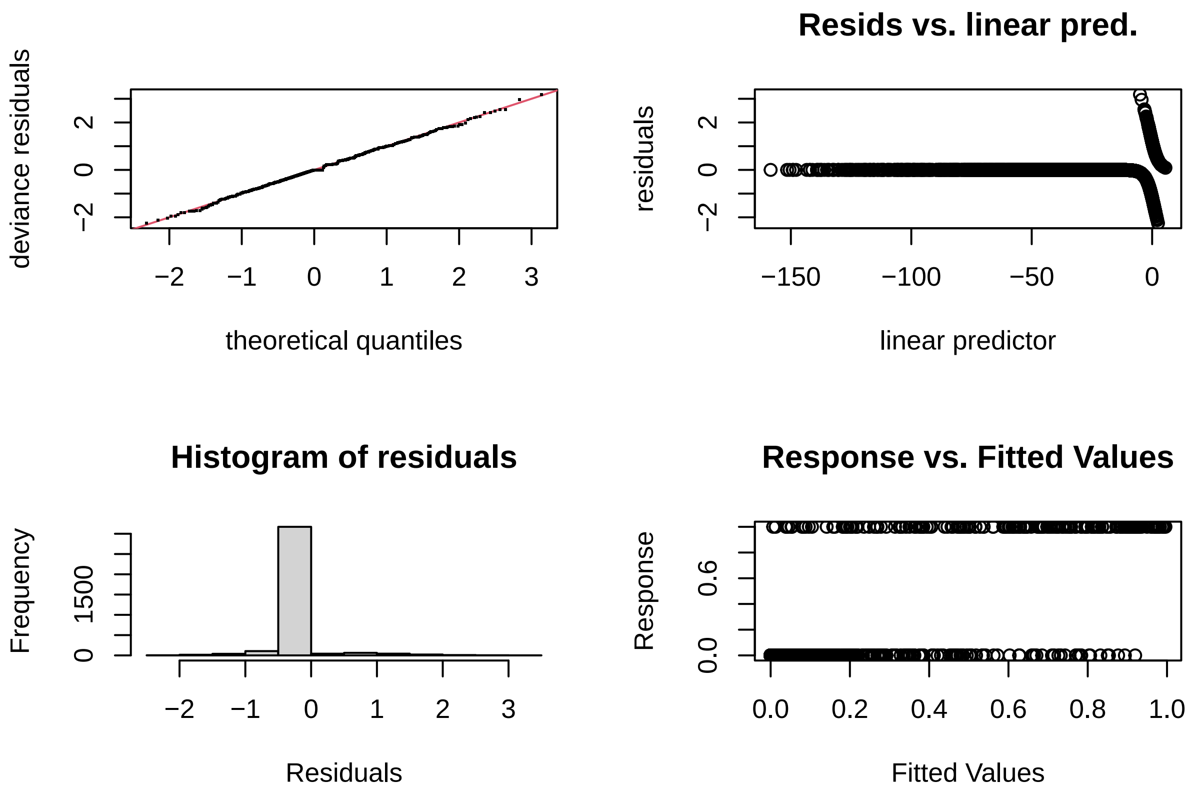

```
#centered on average value of 0.5 because it's the partial effect without the intercept
```

```
draw(init_logit_gam, fun = plogis, constant = coef(init_logit_gam)[1])
```




```
# intercept reflects relatively rare occurence of HRs!
```

```
# Use gam.check() to see if we need more basis functions based on an approximate test
gam.check(init_logit_gam)
```




```
##
## Method: REML   Optimizer: outer newton
## full convergence after 11 iterations.
## Gradient range [-5.632542e-05,-2.964163e-06]
## (score 231.4864 & scale 1).
## Hessian positive definite, eigenvalue range [5.631851e-05,0.8679399].
## Model rank =  19 / 19
##
## Basis dimension (k) checking results. Low p-value (k-index<1) may
## indicate that k is too low, especially if edf is close to k'.
##
##                     k'  edf k-index p-value
## s(launch_speed) 9.00 1.00    1.05    1.00
## s(launch_angle) 9.00 2.96    0.97    0.08 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
batted_ball_data <- batted_ball_data %>%
  mutate(init_gam_hr_prob = as.numeric(predict(init_logit_gam,
  newdata = batted_ball_data, type = "response")),
  init_gam_hr_class = as.numeric(init_gam_hr_prob >= 0.5))

batted_ball_data %>%
  group_by(is_train) %>%
  summarize(correct = mean(is_hr == init_gam_hr_class))
```

```
## # A tibble: 2 x 2
##   is_train correct
##      <int>   <dbl>
## 1        0   0.977
```

```
## 2        1   0.972
```

What about the linear model?

```
init_linear_logit <- glm(is_hr ~ launch_speed + launch_angle,
            data = filter(batted_ball_data, is_train == 1), family = binomial)

batted_ball_data <- batted_ball_data %>%
  mutate(init_glm_hr_prob = predict(init_linear_logit,
          newdata = batted_ball_data, type = "response"),
         init_glm_hr_class = as.numeric(init_glm_hr_prob >= 0.5))

batted_ball_data %>%
  group_by(is_train) %>%
  summarize(correct = mean(is_hr == init_glm_hr_class))
```

```
## # A tibble: 2 x 2
##   is_train correct
##      <int>   <dbl>
## 1        0   0.960
## 2        1   0.951
```

- there are very few situations in reality where linear regressions perform better than an additive model using smooth functions – especially since smooth functions can just capture the linear model