

Generalized Additive Models (GAMs)

CMDA 4654 Project 2

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Generalized Additive Models and why we use them

- Type of generalized linear model
- Response variable depends on smooth functions $f_i(x_i)$
- General structure of a GAM:

$$g(E(Y)) = \beta_0 + f_1(x_1) + f_2(x_2) + \cdots + f_n(x_n)$$

- Smooth functions can be many different things (polynomials, splines, weighted means, etc)

Summations

A Linear Model sums the linear terms

$$y_i = \beta_0 + \sum_j \beta_j x_{ji} + \epsilon_i$$

GAMs sums the *smooth functions*

$$y_i = \beta_0 + \sum_j s_j(x_{ji}) + \epsilon_i$$

Where

$$\epsilon_i \sim N(0, \sigma^2), y_i \sim \text{Normal}$$

Splines

A *Spline* is a function made of up basis functions (the smoothing functions)

These simpler functions form a set of functions called the *basis*

When using a spline for GAMs, each basis function has a coefficient

The spline is formed by weighing the basis function coefficients and summing them at each value of x

Wiggleness and Penalized fit

As in the same case with a polynomial regression of excess “wiggles” not constraining the “Wiggleness” in the way that we penalize the fit in order to prevent overfitting

W or wiggleness is defined by:

$$\int_{\mathbb{R}} [f'']^2 dx = \beta^T \mathbf{S} \beta = W$$

Constraining Wiggleness

We have to make wiggleness important by looking into the log-likelihood, or the measure of closeness to the data

The term **smoothing operator** λ defines the trade-off to find *spline* coefficients to maximize the penalized log-likelihood fit

$$\mathcal{L}_p(\beta) = \mathcal{L}(\beta) - \frac{1}{2}\lambda\beta^T\mathbf{S}\beta$$

or

$$\mathcal{L}_p = \log(\text{Likelihood}) - \lambda W$$

Selecting smooth

There are multiple methods to choose from the right amount of wiggle, some are: AIC, Mallows C_p , Maximum Likelihood(ML), and Restricted Maximum Likelihood(REML). The most commonly method is REML for it's numerical stability

There are two ways to optimize the given λ :

- Predictive: Reducing generalization error
- Bayesian: Using priors for basis coefficients

Maximizing Wiggleness

In a regular regression, the degree of freedom typically equal the predictors in the model. In the case for GAMs, we look at the smoothing *basis* of size k and consider that with **penalized** fitting, their parameters are limited. Thus, the models **effective** degrees of freedom (EDF) will not equal the size k

The models effective degrees of freedom are given by $\text{trace}(F)$ where F is the EDF matrix

$$F = (X^T W X + \sum_j \lambda_j S_j)^{-1} X^T W X$$

Generalized Additive Models in R

- Two options for packages, mgcv and gam
- mgcv is more commonly used and better supported

Smooth interactions in R

- 1 Bivariate smoothing
 - $s(x, z, bs = 'tp')$
- 2 Tensor products smoothing
 - $te(x, z)$

gam.check()

- A good way to check how well GAM model fits
- Usually Gaussian by default
- Creates 4 plots
 - Q-Q Plot of Residuals
 - Histogram of Residuals
 - Residual vs Linear Predictor Plot
 - Observed vs. fitted values

Simulated Dataset (Baby Example 1)

```
library(mgcv)
set.seed(0)
sim_data <- gamSim(1, n = 400, dist="normal", scale=2)
```

Gu & Wahba 4 term additive model

```
head(sim_data)
```

	y	x0	x1	x2	x3	f	f0
1	5.114211	0.8966972	0.1478457	0.34826473	0.04572472	7.962274	0.6377368
2	2.175828	0.2655087	0.6588776	0.85868745	0.36652658	5.514517	1.4814113
3	6.334878	0.3721239	0.1850700	0.03443876	0.74139303	3.576406	1.8407682
4	6.853276	0.5728534	0.9543781	0.97099715	0.93350625	8.692625	1.9478442
5	7.743879	0.9082078	0.8978485	0.74511014	0.67320995	8.752859	0.5687870
6	13.920886	0.2016819	0.9436971	0.27325524	0.70135711	16.190349	1.1841037
	f1	f2	f3				
1	1.344055	5.980482e+00	0				
2	3.735028	2.980780e-01	0				
3	1.447937	2.877006e-01	0				
4	6.744695	8.611364e-05	0				
5	6.023672	2.160400e+00	0				
6	6.602142	8.404104e+00	0				

Simulated Dataset using gam()

```
fit <- gam(y ~ s(x0) + s(x1) + s(x2) + s(x3), data = sim_data)
summary(fit)
```

Family: gaussian
Link function: identity

Formula:
y ~ s(x0) + s(x1) + s(x2) + s(x3)

Parametric coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	7.9150	0.1049	75.44	<2e-16 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:

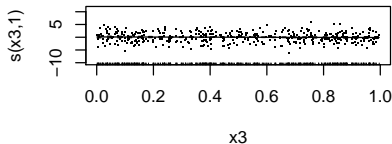
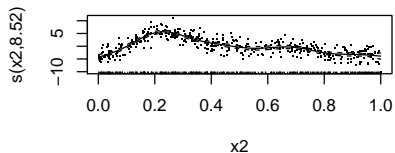
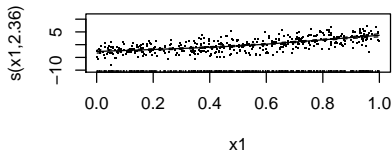
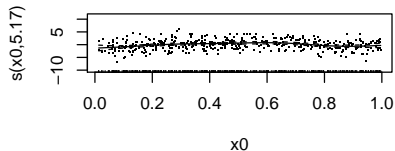
	edf	Ref.df	F	p-value
s(x0)	5.173	6.287	4.564	0.000134 ***
s(x1)	2.357	2.927	103.053	< 2e-16 ***
s(x2)	8.517	8.931	84.308	< 2e-16 ***
s(x3)	1.000	1.000	0.441	0.506929

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) = 0.726 Deviance explained = 73.7%
GCV = 4.611 Scale est. = 4.4029 n = 400

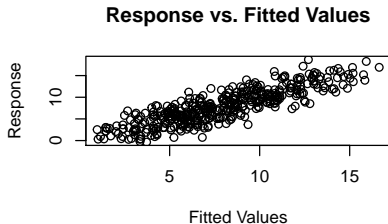
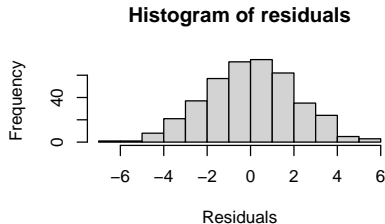
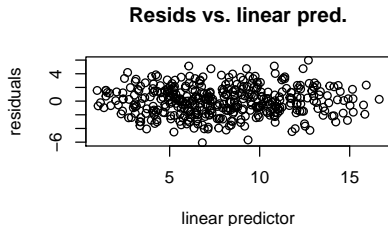
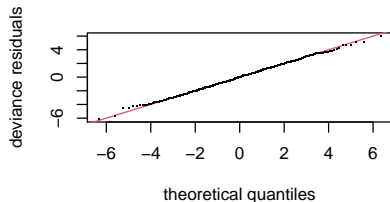
Simulated Dataset using plot() of GAM fit

```
plot(fit, pages=1, residuals=TRUE)
```



Simulated Dataset using gam.check()

```
gam.check(fit)
```



Mtcars Dataset (Baby Example 2)

```
data("mtcars")
mtcars_gam <-
  gam(mpg ~ s(displ), data = mtcars, method = "REML")
summary(mtcars_gam)
```

Family: gaussian
Link function: identity

Formula:
mpg ~ s(displ)

Parametric coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	20.0906	0.3788	53.04	<2e-16 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:

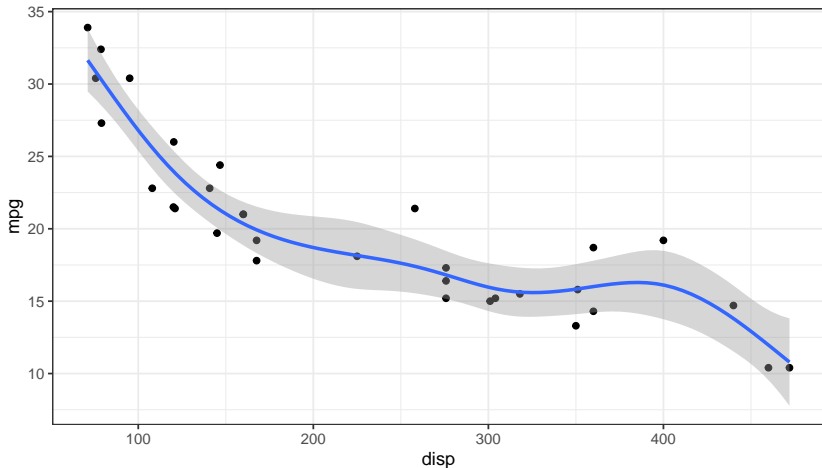
	edf	Ref.df	F	p-value
s(displ)	4.884	5.904	36.3	<2e-16 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) = 0.874 Deviance explained = 89.4%
-REML = 74.101 Scale est. = 4.5918 n = 32

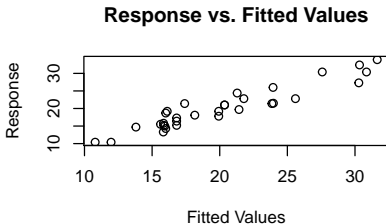
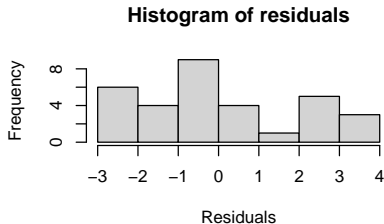
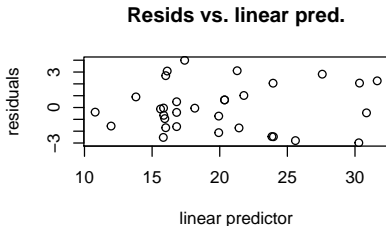
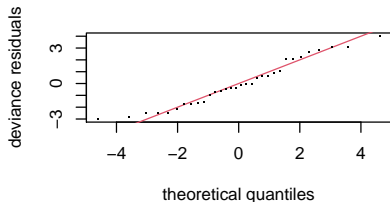
Mtcars Dataset using gam on ggplot

```
library(ggplot2)
ggplot(data = mtcars, aes(x = disp, y = mpg)) +
  theme_bw() + geom_point() +
  geom_smooth(method = "gam", formula = y ~ s(x))
```



Mtcars Dataset using gam.check()

```
gam.check(mtcars_gam)
```



Example - Health Data - Explaining Data Set

We will be demonstrating GAMs on heart-rate data from an Ironman Triathlete sleeping. The original study also examined the heart-rates of subjects practicing Yogi and Chi meditation techniques (taken from a paper titled “Heart Rate Oscillations during Meditation”). More info including the source material can be found here:

<https://physionet.org/content/meditation/1.0.0/>

We will focus on a small snippet of the non-linear material.

Example - Health Data - Data Cleaning

```
# Read dataset
i_df <- read.csv("./i9.csv", header = FALSE)
colnames(i_df) <- c("time", "hr")
# Re-index the time
i_df$time <- i_df$time - 42301.30
i_df <- i_df[ !(i_df$time > 425),]
# Remove outliers
i_df <- i_df[ !(i_df$hr > 80),]

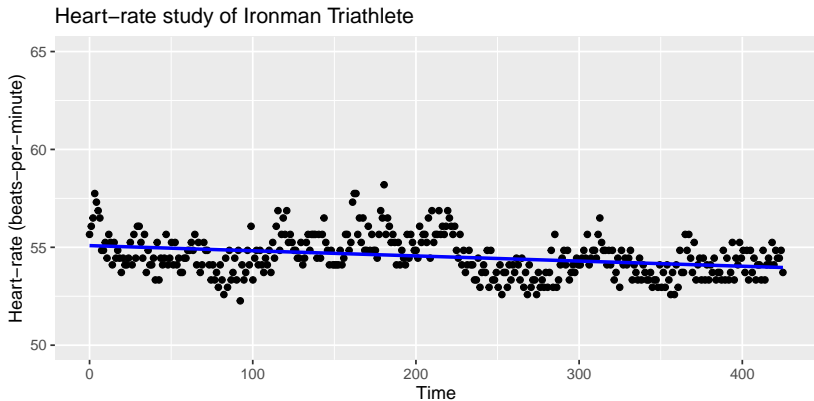
# Create scatter-plot
p <- ggplot(i_df, aes(x=time, y=hr)) +
  geom_point() +
  labs(title = 'Heart-rate study of Ironman Triathlete',
        x = "Time",
        y = "Heart-rate (beats-per-minute)") +
  ylim(50, 65)

head(i_df)
```

	time	hr
1	-0.003	55.6586
2	1.067	56.0748
3	2.130	56.4972
4	3.169	57.7478
5	4.216	57.3066
6	5.270	56.8720

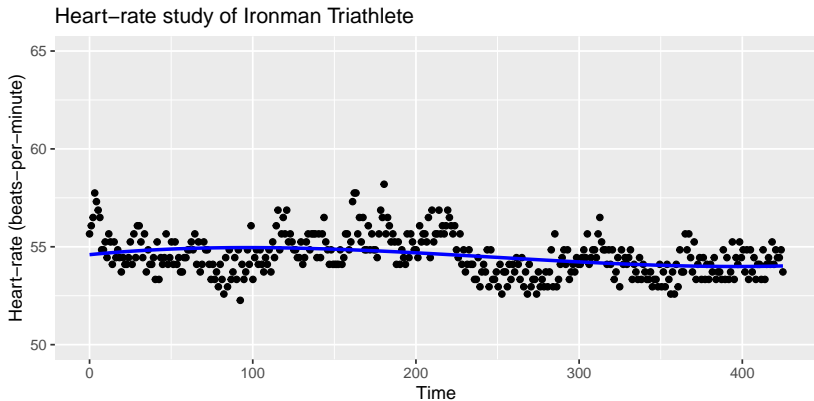
Example - Health Data - LM

```
# Linear Model Fit (uses formula = y~x)
p + geom_smooth(method = 'lm', se=FALSE, color = 'blue')
```



Example - Health Data - Splines

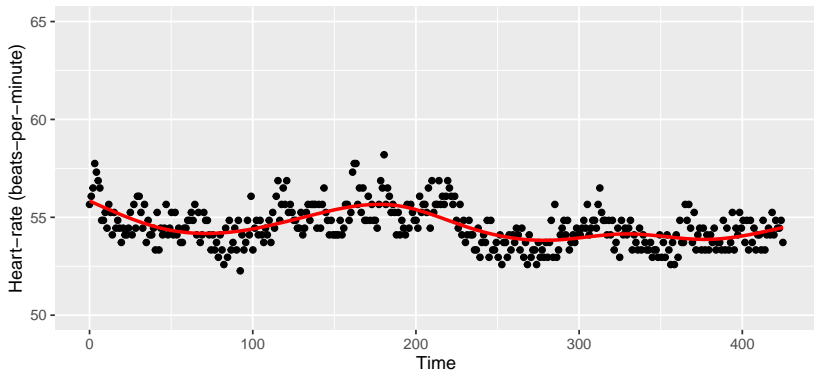
```
# Model Fit adjusting splines  
p + geom_smooth(method = 'lm', formula = y~splines::bs(x,3), se=FALSE, color = 'blue')
```



Example - Health Data - GAM

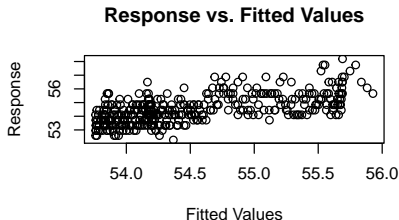
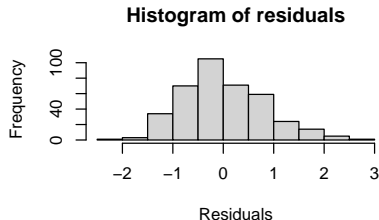
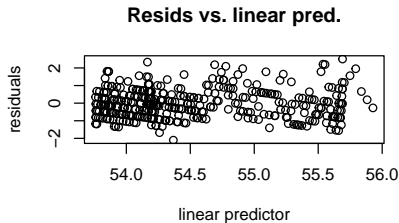
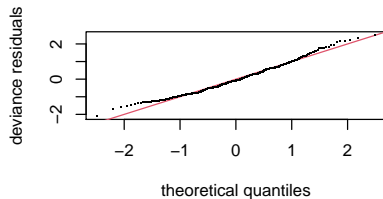
```
# GAM Model Fit (formula = y ~ s(x, bs = "cs"))  
p + geom_smooth(method = 'gam', se=FALSE, color = 'red')
```

Heart-rate study of Ironman Triathlete



Example - GAM diagnostics

```
gam_fit <- gam(hr ~ s(time), data = i_df, method = "REML")  
gam.check(gam_fit)
```



LOESS vs. GAM

While watching a presentation on GAMs and how they work with non-linear data, you might have asked yourself: why use GAMs? Why not just use LOESS (or LOWESS)? Some differences to consider:

- Memory efficiency: LOESS uses $O(n^2)$ memory
- Runtime efficiency: GAM can be slower
- Both are used by default in `geom_smooth`
 - Uses LOESS if $n < 1000$
 - Uses GAM otherwise

Conclusion

- The benefits of implementing GAMs provides a flexible framework to accurately model nonlinear relationships.
- It's formed from basis functions, which weigh regression functions to form larger functions known as smooths
- To control overfitting, we penalize the fit of the model by adjusting the goodness of fit

Fun Reminder



Dr Gavin Simpson 🙌🇪🇺

@ucfagls

Replying to @millerdl

140 char vrsn

- 1 GAMs are just GLMs
- 2 GAMs fit wiggly terms
- 3 use + s(foo) not foo in frmla
- 4 use method = "REML"
- 5 gam.check()

2:37 PM · Mar 16, 2017 · TweetDeck

References

- <https://m-clark.github.io/generalized-additive-models/introduction.html> - Clark GAMs Tutorial
- <https://fromthebottomoftheheap.net/slides/gam-intro-webinar-2020/gam-intro.html#1> - Simpson Intro to GAMs
- https://www.mrc-bsu.cam.ac.uk/wp-content/uploads/GAM_slides1.pdf - MRC BioStatistics AM & GAMs
- anson.ucdavis.edu/~jihao/handout5_w15.html - Difference between mgcv and gam packages

Further Reading

GAM itself can be a very wide and deep topic. The following resources might also be of interest to the reader:

- *Generalized Additive Models: An Introduction with R* (Simon N. Wood)
- *Generalized Additive Models* (T.J. Hastie, R.J. Tibshirani)
- *An Introduction to Statistical Learning: With Applications in R* (Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani)