

# Generalized Additive Models (GAMs)

## CMDA 4654 Project 2

Group 19: Brady Bolton, Eryk Jesse, Charles Lee, Dan Schlicht

# Generalized Additive Models



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

# Generalized Additive Models

- 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)

# Generalized Additive Models

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 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**  $\lambda$  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  $\lambda$ :

- 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

## Description

mgcv provides functions for generalized additive modelling ([gam](#) and [bam](#)) and generalized additive mixed modelling ([gamm](#), and [random.effects](#)). The term GAM is taken to include any model dependent on unknown smooth functions of predictors and estimated by quadratically penalized (possibly quasi-) likelihood maximization. Available distributions are covered in [family.mgcv](#) and available smooths in [smooth.terms](#).

Particular features of the package are facilities for automatic smoothness selection (Wood, 2004, 2011), and the provision of a variety of smooths of more than one variable. User defined smooths can be added. A Bayesian approach to confidence/credible interval calculation is provided. Linear functionals of smooths, penalization of parametric model terms and linkage of smoothing parameters are all supported. Lower level routines for generalized ridge regression and penalized linearly constrained least squares are also available. In addition to the main modelling functions, [jagam](#) provided facilities to ease the set up of models for use with JAGS, while [ginla](#) provides marginal inference via a version of Integrated Nested Laplace Approximation.

# Example - Simulated Data

```
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				

# Example - Simulated Data

```
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

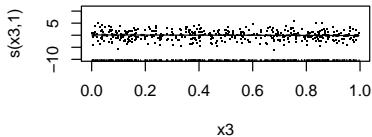
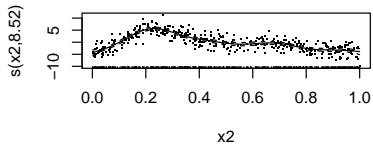
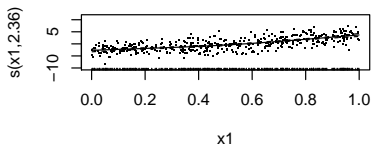
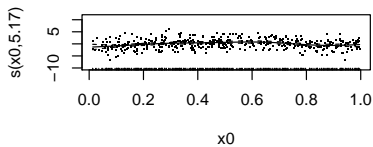
---

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

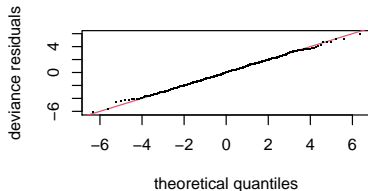
# Example - Simulated Data

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

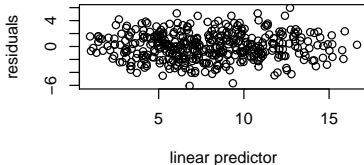


# Example - Simulated Data

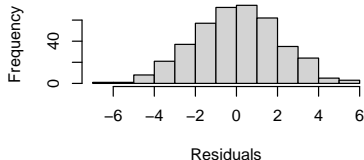
```
gam.check(fit)
```



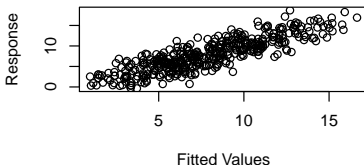
**Resids vs. linear pred.**



**Histogram of residuals**



**Response vs. Fitted Values**



# Example - mtcars

```
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 ***

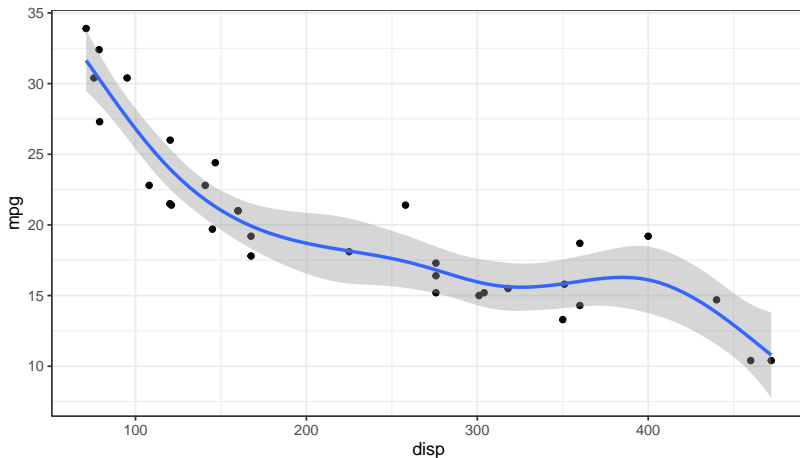
---

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

# Example - mtcars

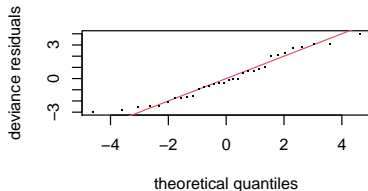
```
library(ggplot2)
ggplot(data = mtcars, aes(x = disp, y = mpg)) +
  theme_bw() + geom_point() +
  geom_smooth(method = "gam", formula = y ~ s(x))
```



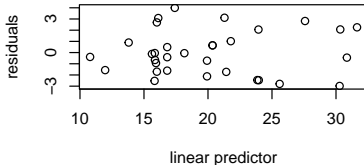


# Example - mtcars

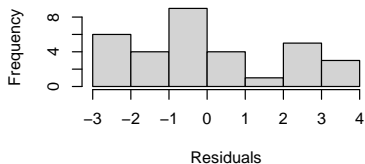
```
gam.check(mtcars_gam)
```



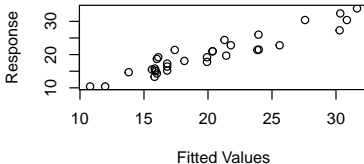
**Resids vs. linear pred.**



**Histogram of residuals**



**Response vs. Fitted Values**



## Example - mtcars

## Example - iris

```
data("iris")
```

## Example - iris

## Example - iris

## Example - iris

## Example - Health Data

```
df <- read.csv("estimated_inpatient.csv")
```

## Example - Health Data



## Example - Health Data

## Example - Health Data

## Example - Health Data

## Example - Health Data

# 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

# Conclusion

# Conclusion

# 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](https://www.mrc-bsu.cam.ac.uk/wp-content/uploads/GAM_slides1.pdf) - MRC BioStatistics AM & GAMs