Generalized Additive Models (GAMs)

CMDA 4654 Project 2

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Generalized Additive Models

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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:
  $g(\mathrm{E}(Y)) = \beta_0 + f_1(x_1) + f_2(x_2) + \cdots + f_n(x_n)$
- 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

Wiggliness and Penalized fit

As in the same case with a polynomial regression of excess "wiggles" not constraining the "Wiggliness" in the way that we penalize the fit in to prevent overfitting

W or wiggliness is defined by:

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

Constraining Wiggliness

We have to make wiggliness 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

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

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, Mallow $\mathcal{C}_p$, 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 Wiggliness

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 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
```

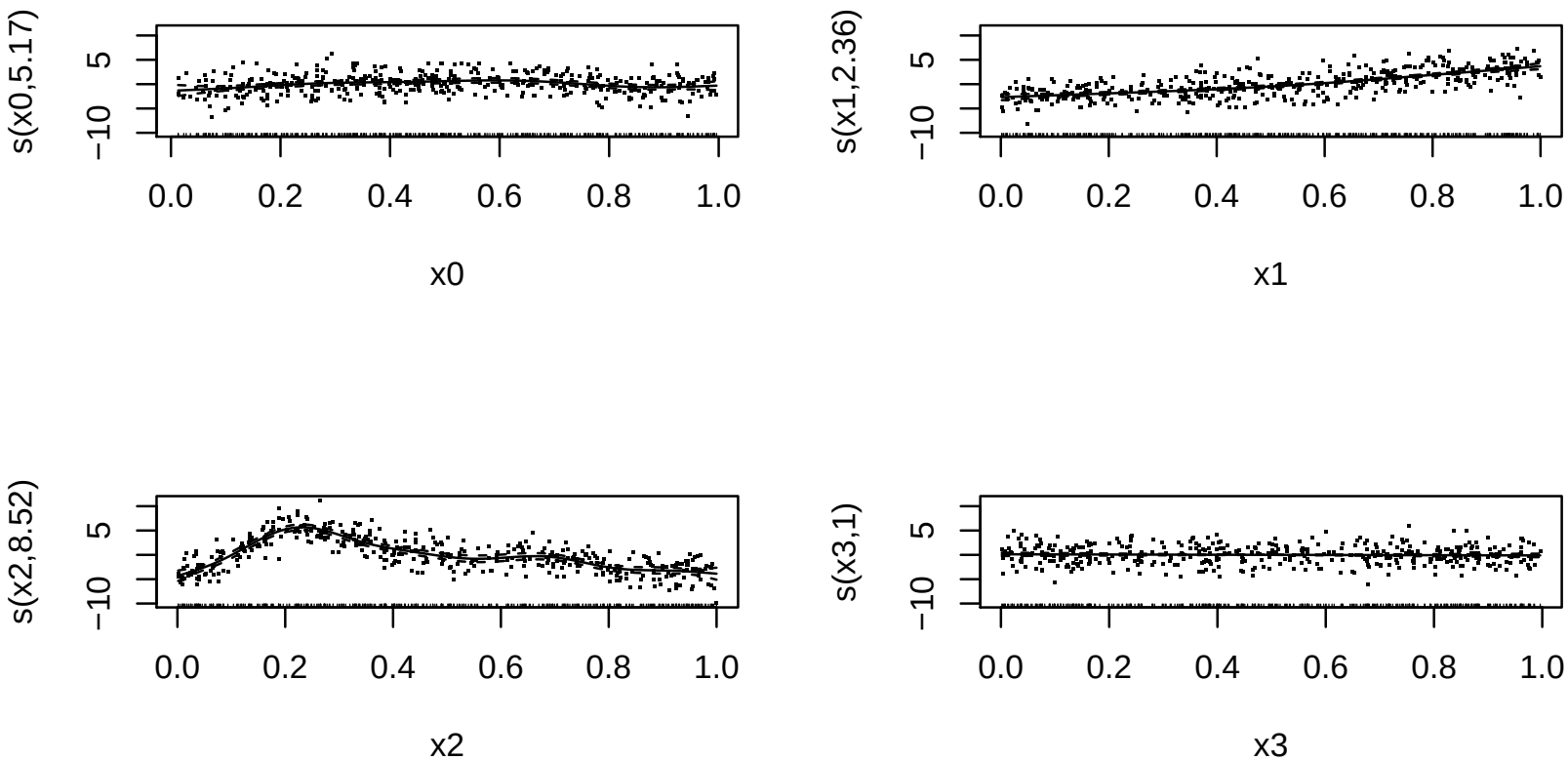
Example - Simulated Data

```r
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
```

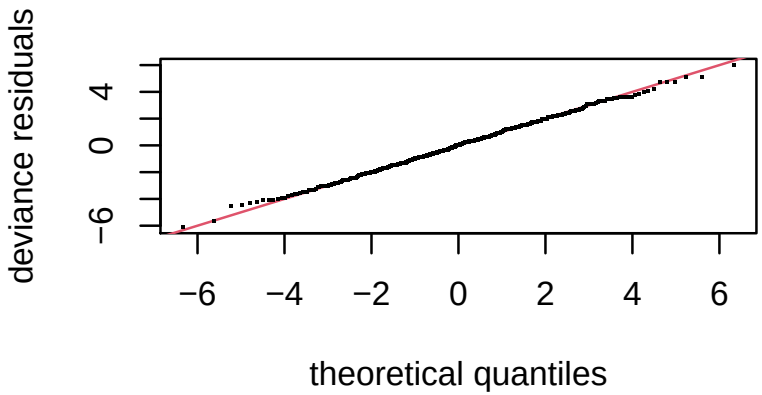
Example - Simulated Data

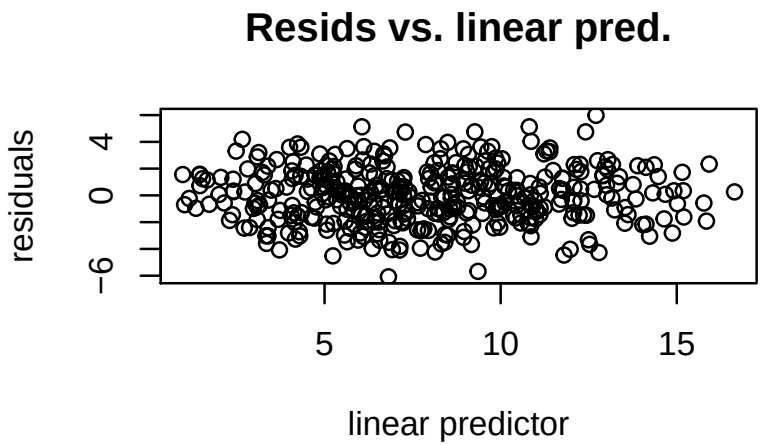
```
plot(fit, pages=1, residuals=TRUE)
```

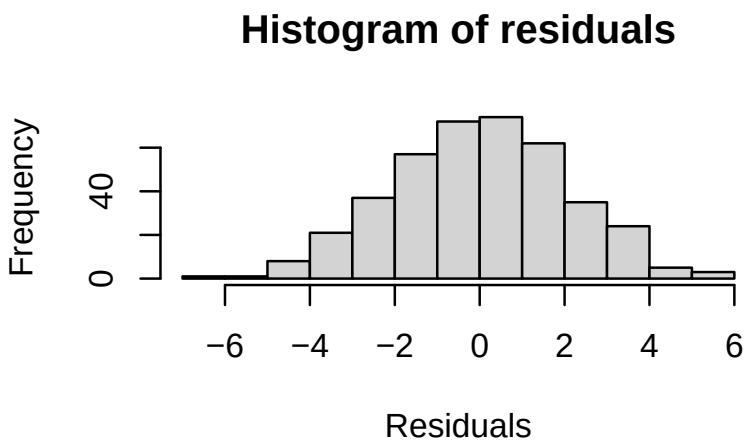


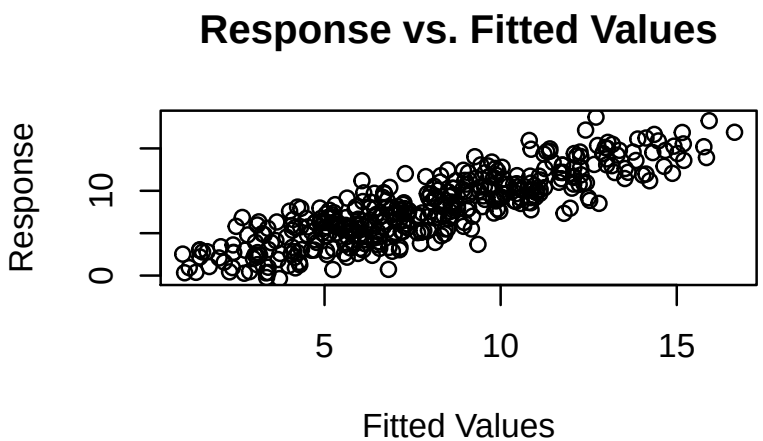
Example - Simulated Data

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









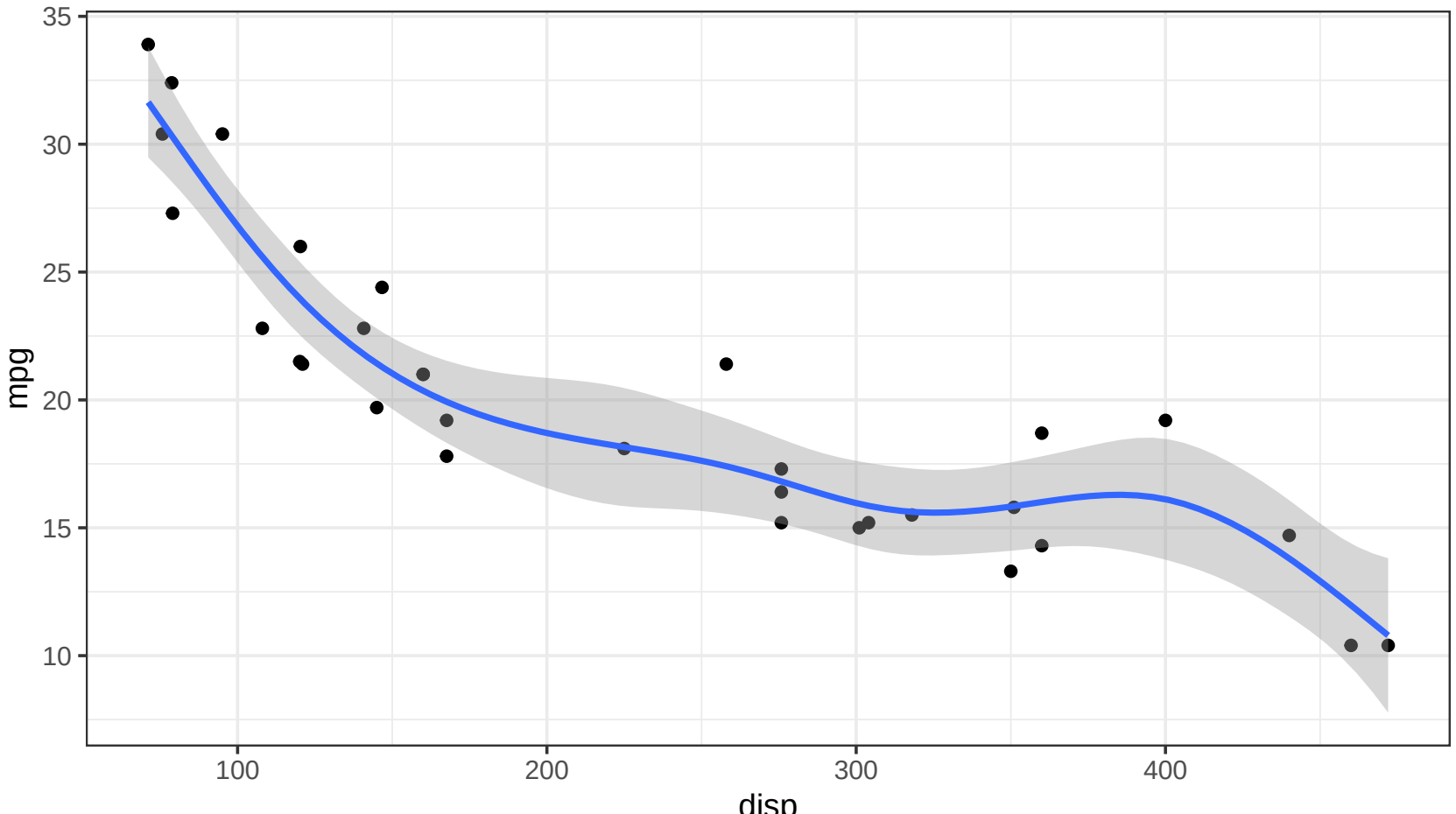
Example - mtcars

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

```
Family: gaussian
Link function: identity

Formula:
mpg ~ s(disp)

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(disp) 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
```

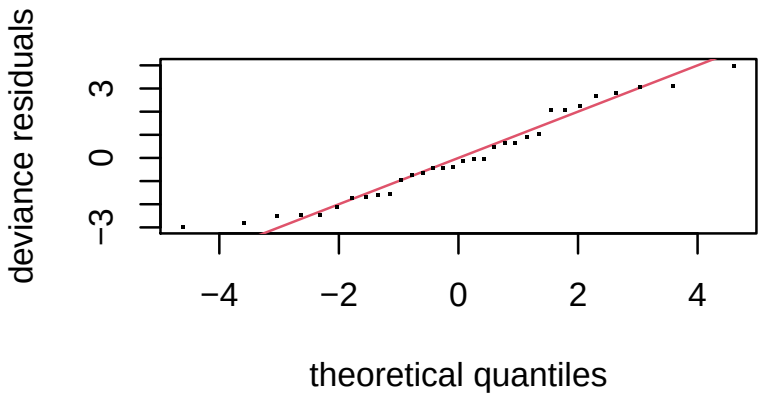
Example - mtcars

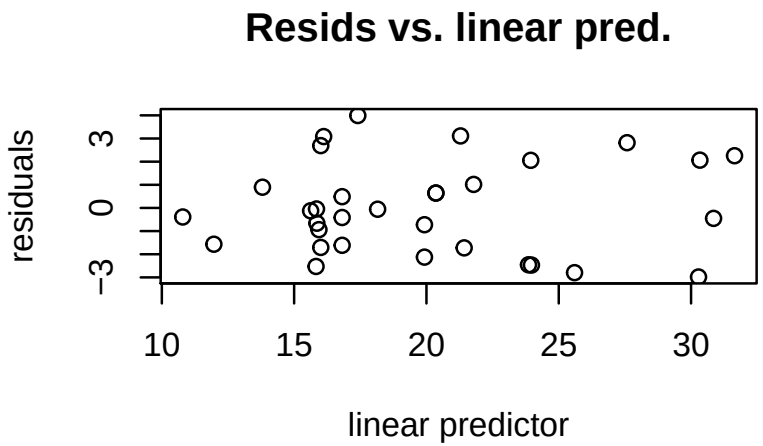
```
library(ggplot2)
ggplot(data = mtcars, aes(x = disp, y = mpg)) +
  theme_bw() + geom_point() +
  geom_smooth(method = "gam", formula = y ~ s(x))
```

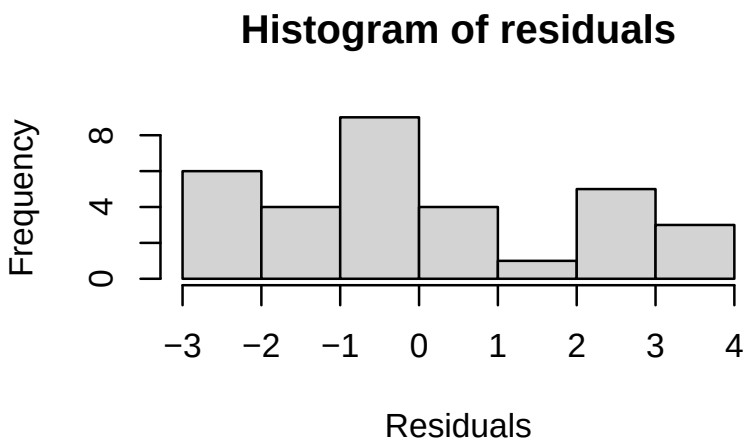


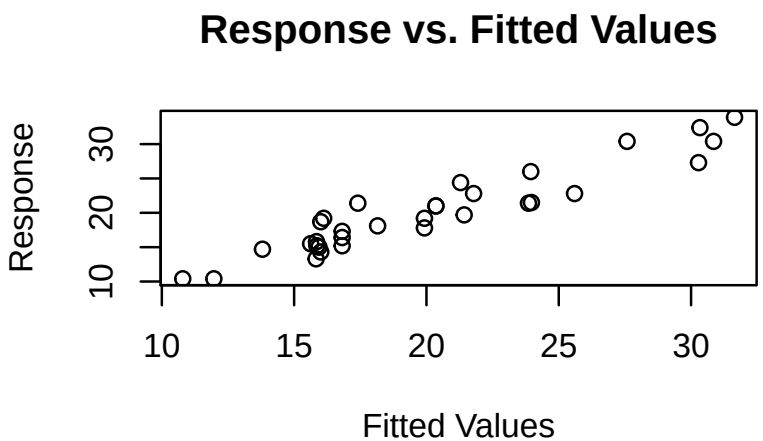
Example - mtcars

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









Example - mtcars

Example - Health Data - Explaining Data Set

Dataset pulled from the Department of Health & Human Services (HHS) which is a a cabinet-level department of the U.S. federal government. The Dataset provides state-aggregated data for estimated patient impact and hospital utilization by COVID-19 Patients by a State Timeseries.

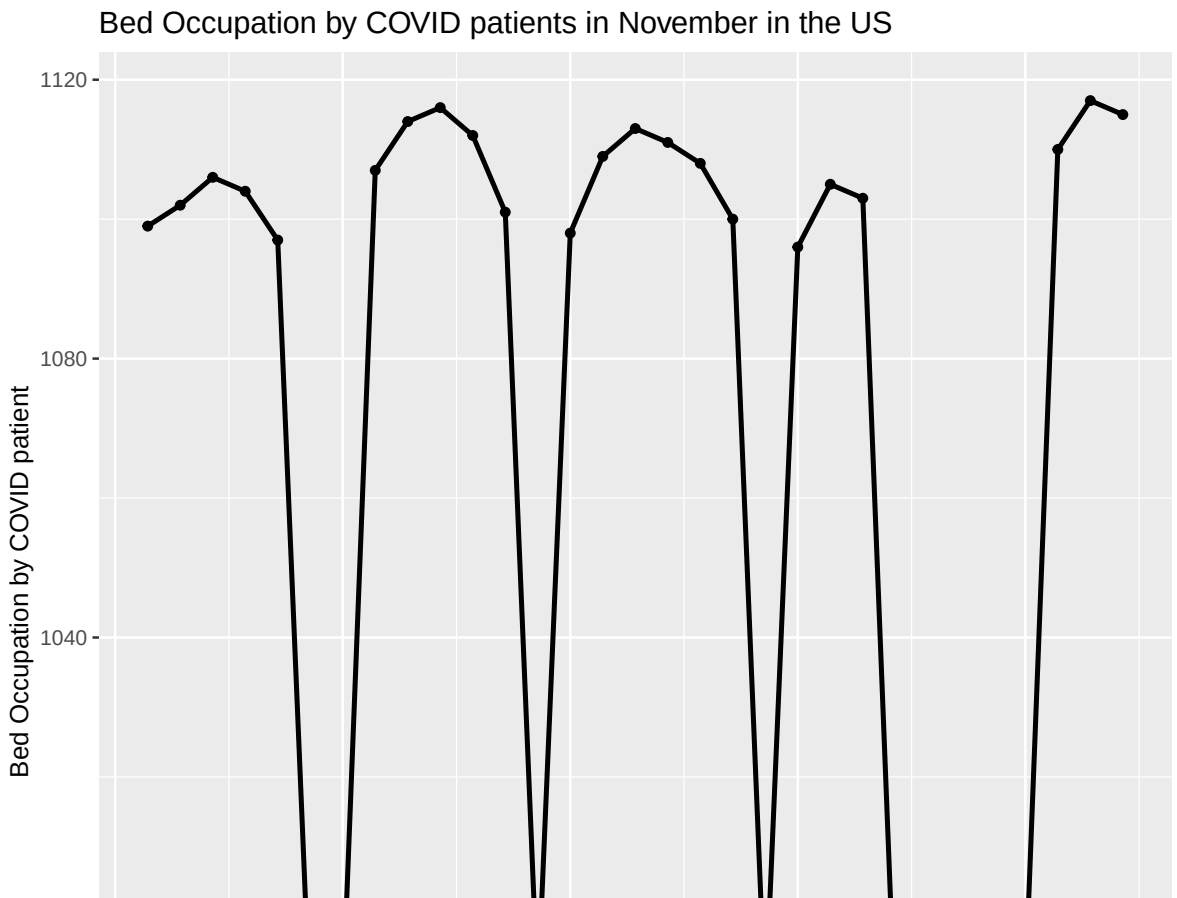
https://healthdata.gov/dataset/covid-19-estimated-patient-impact-and-hospital-capacity-state

Example - Health Data - Data Cleaning

```r
bedOcc <- read.csv("estimated_inpatient.csv", header = TRUE)
library(ggplot2)
library(tidyverse)

# Read dataset
bedOcc <- bedOcc %>%
          select(state, collection_date, Inpatient.Beds.Occupied.Estimated, Total.Inpatient.Beds) %>%
          drop_na()

# Convert from Character to Numeric and Date variable type
bedOcc$Inpatient.Beds.Occupied.Estimated <- as.factor(bedOcc$Inpatient.Beds.Occupied.Estimated)
bedOcc$Inpatient.Beds.Occupied.Estimated <- as.numeric(bedOcc$Inpatient.Beds.Occupied.Estimated)
bedOcc$Total.Inpatient.Beds <- as.factor(bedOcc$Total.Inpatient.Beds)
bedOcc$Total.Inpatient.Beds <- as.numeric(bedOcc$Total.Inpatient.Beds)
bedOcc$collection_date <- as.Date(bedOcc$collection_date)
```

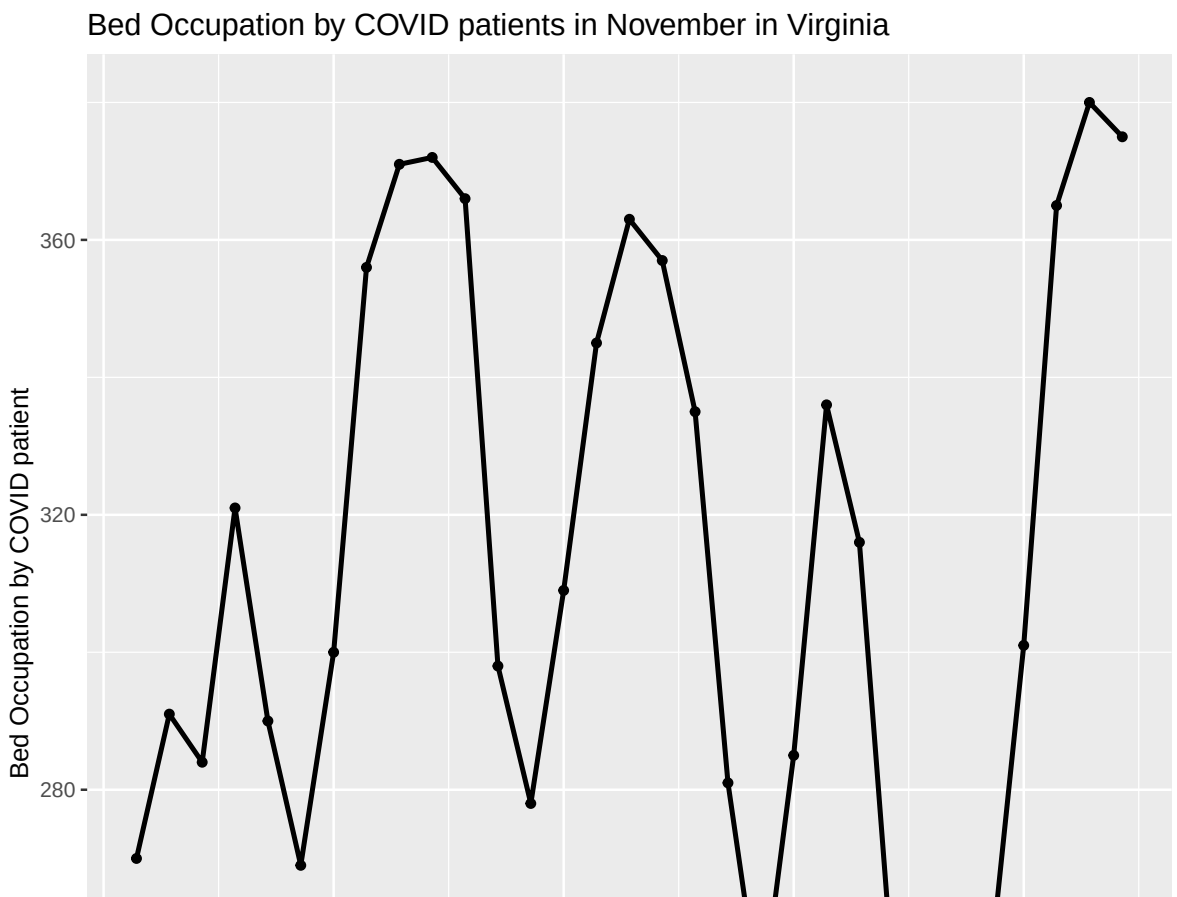
Example - Health Data - Country Wide

```
# Bed Occupation for COVID-19 patients Country Wide
bedOccCW <- bedOcc %>%
            filter(state == 'CW')
ggplot(data = bedOccCW, aes(x = collection_date, y = Inpatient.Beds.Occupied.Estimated)) + geom_point() +
  geom_line(color = "black", size = 1) +
  labs(title = 'Bed Occupation by COVID patients in November in the US', x = "Date", y = "Bed Occupation b
```



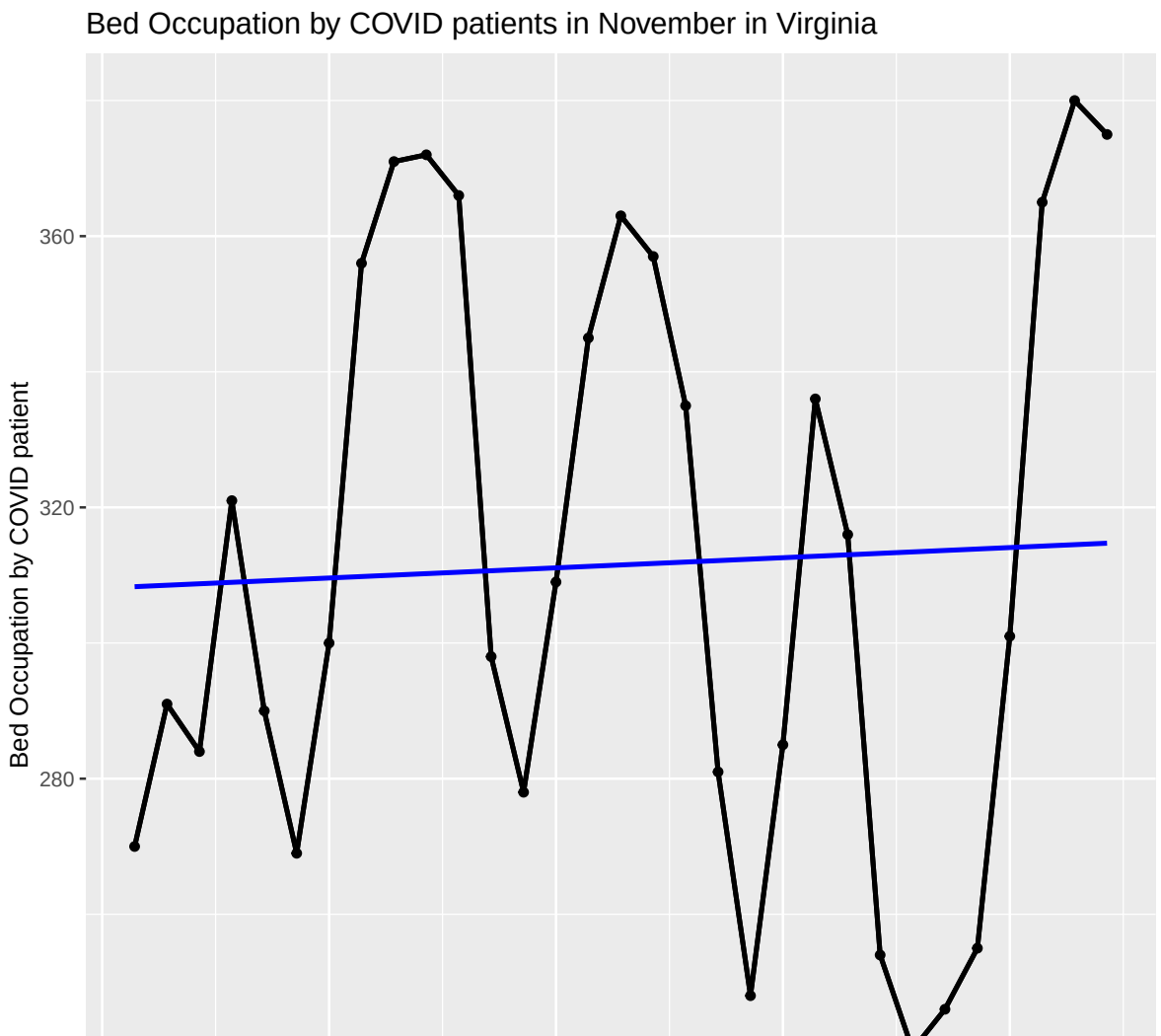
Example - Health Data - VA

```
bedOccVA <- bedOcc %>%
            filter(state == 'VA')
p <- ggplot(data = bedOccVA, aes(x = collection_date, y = Inpatient.Beds.Occupied.Estimated)) + geom_point
  geom_line(color = "black", size = 1) +
  labs(title = 'Bed Occupation by COVID patients in November in Virginia', x = "Date", y = "Bed Occupatio
p
```



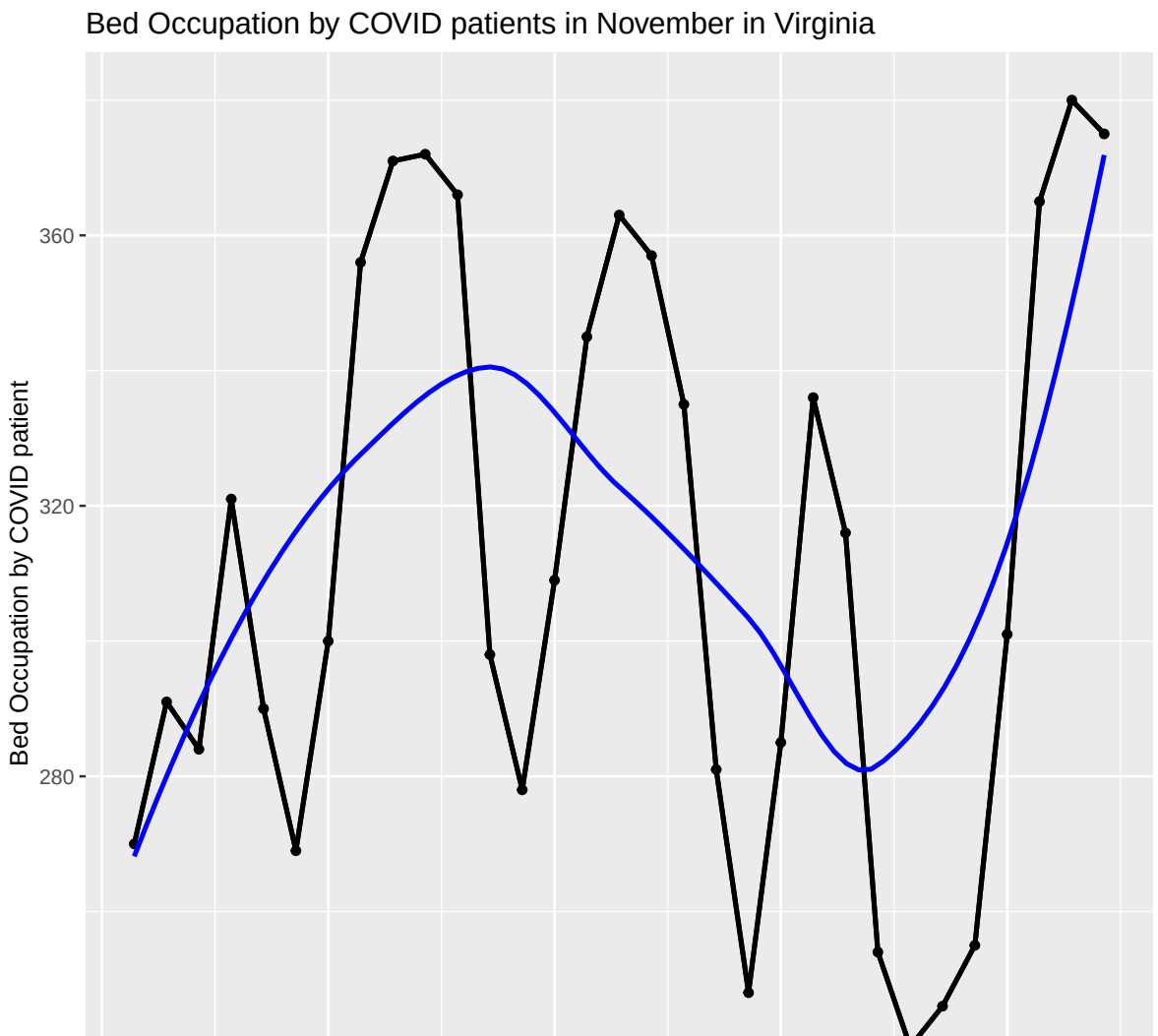
Example - Health Data - LM

```
# Linear Model Fit (uses formula = y~x)
p + geom_line(color = "black", size = 1) + geom_smooth(method = 'lm', se=FALSE, color = 'blue')
```



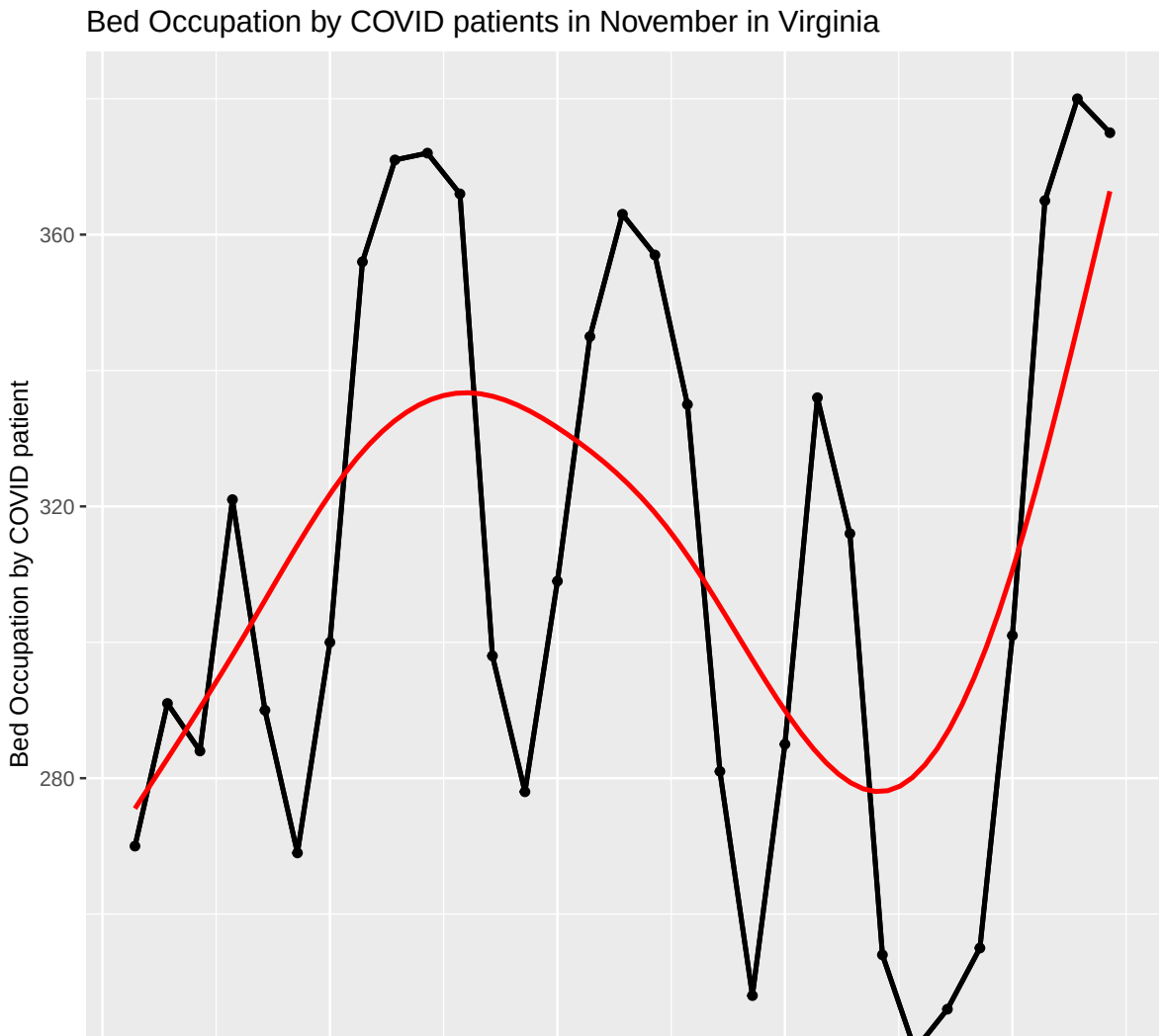
Example - Health Data - Loess

```
# Loess Model Fit
p + geom_line(color = "black", size = 1) + geom_smooth(method = 'loess', se=FALSE, color = 'blue')
```



Example - Health Data - GAM

```
# GAM Model Fit (formula = y ~ s(x, bs = "cs"))
p + geom_line(color = "black", size = 1) + geom_smooth(method = 'gam', se=FALSE, color = 'red')
```



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 - MRC BioStatistics AM & GAMs