

QCB 508 – Week 10

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Contents

Logistic Regression	2
Goal	2
Bernoulli as EFD	2
Model	3
Maximum Likelihood Estimation	3
Iteratively Reweighted Least Squares	3
GLMs	4
glm() Function in R	4
Example: Grad School Admissions	4
Explore the Data	4
Logistic Regression in R	6
Summary of Fit	7
ANOVA of Fit	7
Example: Contraceptive Use	8
A Different Format	8
Fitting the Model	8
Summary of Fit	9
ANOVA of Fit	9
More on this Data Set	10
Generalized Linear Models	10
Review: Multiparameter Fisher Info Matrix	10
Review: Multiparameter Asymptotic MVN	10
GLM Definition	10
Exponential Family Distributions	10
Natural Single Parameter EFD	11
Dispersion EFDs	11
Example: Normal	11
EFD for GLMs	11
Components of a GLM	12
Link Functions	12
Calculating MLEs	12
Iteratively Reweighted Least Squares	13
Estimating Dispersion	13
CLT Applied to the MLE	13
Approximately Pivotal Statistics	13
Deviance	14
Generalized LRT	14
Example: Grad School Admissions	14

glm() Function	18
Nonparametric Regression	18
Simple Linear Regression	18
Simple Nonparametric Regression	19
Smooth Functions	19
Smoothness Parameter λ	19
The Solution	19
Natural Cubic Splines	19
Basis Functions	20
Calculating the Solution	20
Linear Operator	20
Degrees of Freedom	20
Bayesian Interpretation	21
Bias and Variance Trade-off	21
Choosing λ	21
Smoothers and Spline Models	22
Smoothers in R	22
Example	22
Generalized Additive Models	23
Ordinary Least Squares	23
Additive Models	24
Backfitting	24
GAM Definition	24
Overview of Fitting GAMs	24
GAMs in R	24
Example	25
Bootstrap for Statistical Models	32
Homoskedastic Models	32
Residuals	32
Studentized Residuals	33
Confidence Intervals	33
Hypothesis Testing	33
Parametric Bootstrap	34
Extras	34
Source	34
Session Information	34

Logistic Regression

Goal

Logistic regression models a Bernoulli distributed response variable in terms of linear combinations of explanatory variables.

This extends least squares regression to the case where the response variable captures a dichotomous outcome (e.g., “success” vs “failure”).

Bernoulli as EFD

If $Y \sim \text{Bernoulli}(p)$, then its pmf is:

$$\begin{aligned}
f(y; p) &= p^y (1 - p)^{1-y} \\
&= \exp \left\{ \log \left(\frac{p}{1-p} \right) y + \log(1-p) \right\}
\end{aligned}$$

In exponential family distribution (EFD) notation,

$$\eta(p) = \log \left(\frac{p}{1-p} \right) \equiv \text{logit}(p),$$

$A(\eta(p)) = \log(1 + \exp(\eta)) = \log(1 - p)$, and y is the sufficient statistic.

Model

$(\mathbf{X}_1, Y_1), (\mathbf{X}_2, Y_2), \dots, (\mathbf{X}_n, Y_n)$ are distributed so that $Y_i | \mathbf{X}_i \sim \text{Bernoulli}(p_i)$, where $\{Y_i | \mathbf{X}_i\}_{i=1}^n$ are jointly independent and

$$\text{logit}(E[Y_i | \mathbf{X}_i]) = \log \left(\frac{\Pr(Y_i = 1 | \mathbf{X}_i)}{\Pr(Y_i = 0 | \mathbf{X}_i)} \right) = \mathbf{X}_i \boldsymbol{\beta}.$$

From this it follows that

$$p_i = \frac{\exp(\mathbf{X}_i \boldsymbol{\beta})}{1 + \exp(\mathbf{X}_i \boldsymbol{\beta})}.$$

Maximum Likelihood Estimation

The $\boldsymbol{\beta}$ are estimated from the MLE calculated from:

$$\begin{aligned}
\ell(\boldsymbol{\beta}; \mathbf{y}, \mathbf{X}) &= \sum_{i=1}^n \log \left(\frac{p_i}{1-p_i} \right) y_i + \log(1-p_i) \\
&= \sum_{i=1}^n (\mathbf{x}_i \boldsymbol{\beta}) y_i - \log(1 + \exp(\mathbf{x}_i \boldsymbol{\beta}))
\end{aligned}$$

Iteratively Reweighted Least Squares

1. Initialize $\boldsymbol{\beta}^{(1)}$.
2. For each iteration $t = 1, 2, \dots$, set

$$p_i^{(t)} = \text{logit}^{-1}(\mathbf{x}_i \boldsymbol{\beta}^{(t)}), \quad z_i^{(t)} = \text{logit}(p_i^{(t)}) + \frac{y_i - p_i^{(t)}}{p_i^{(t)}(1 - p_i^{(t)})}$$

and let $\mathbf{z}^{(t)} = \left\{ z_i^{(t)} \right\}_{i=1}^n$.

3. Form $n \times n$ diagonal matrix $\mathbf{W}^{(t)}$ with (i, i) entry equal to $p_i^{(t)}(1 - p_i^{(t)})$.
4. Obtain $\boldsymbol{\beta}^{(t+1)}$ by performing the weighted least squares regression (see GLS from earlier)

$$\boldsymbol{\beta}^{(t+1)} = \left(\mathbf{X}^T \mathbf{W}^{(t)} \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{W}^{(t)} \mathbf{z}^{(t)}.$$

5. Iterate Steps 2-4 over $t = 1, 2, 3, \dots$ until convergence, setting $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}^{(\infty)}$.

GLMs

For exponential family distribution response variables, the **generalized linear model** is

$$\eta(E[Y|\mathbf{X}]) = \mathbf{X}\boldsymbol{\beta}$$

where $\eta(\theta)$ is function of the expected value θ into the natural parameter. This is called the **canonical link function** in the GLM setting.

The **iteratively reweighted least squares** algorithm presented above for calculating (local) maximum likelihood estimates of $\boldsymbol{\beta}$ has a generalization to a large class of exponential family distribution response variables.

glm() Function in R

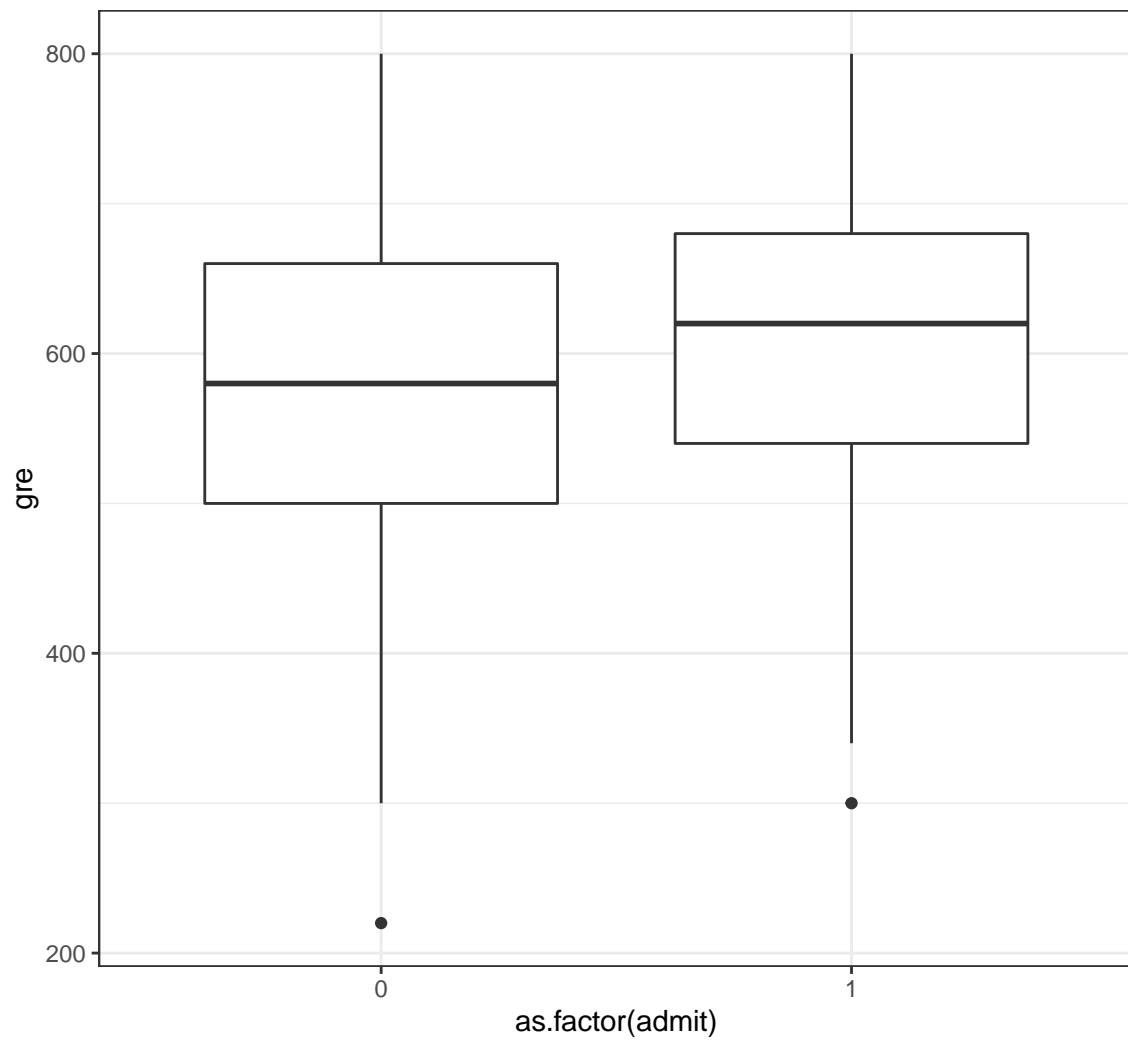
Example: Grad School Admissions

```
> mydata <-  
+   read.csv("https://stats.idre.ucla.edu/stat/data/binary.csv")  
> dim(mydata)  
[1] 400  4  
> head(mydata)  
  admit gre  gpa rank  
1     0 380 3.61   3  
2     1 660 3.67   3  
3     1 800 4.00   1  
4     1 640 3.19   4  
5     0 520 2.93   4  
6     1 760 3.00   2
```

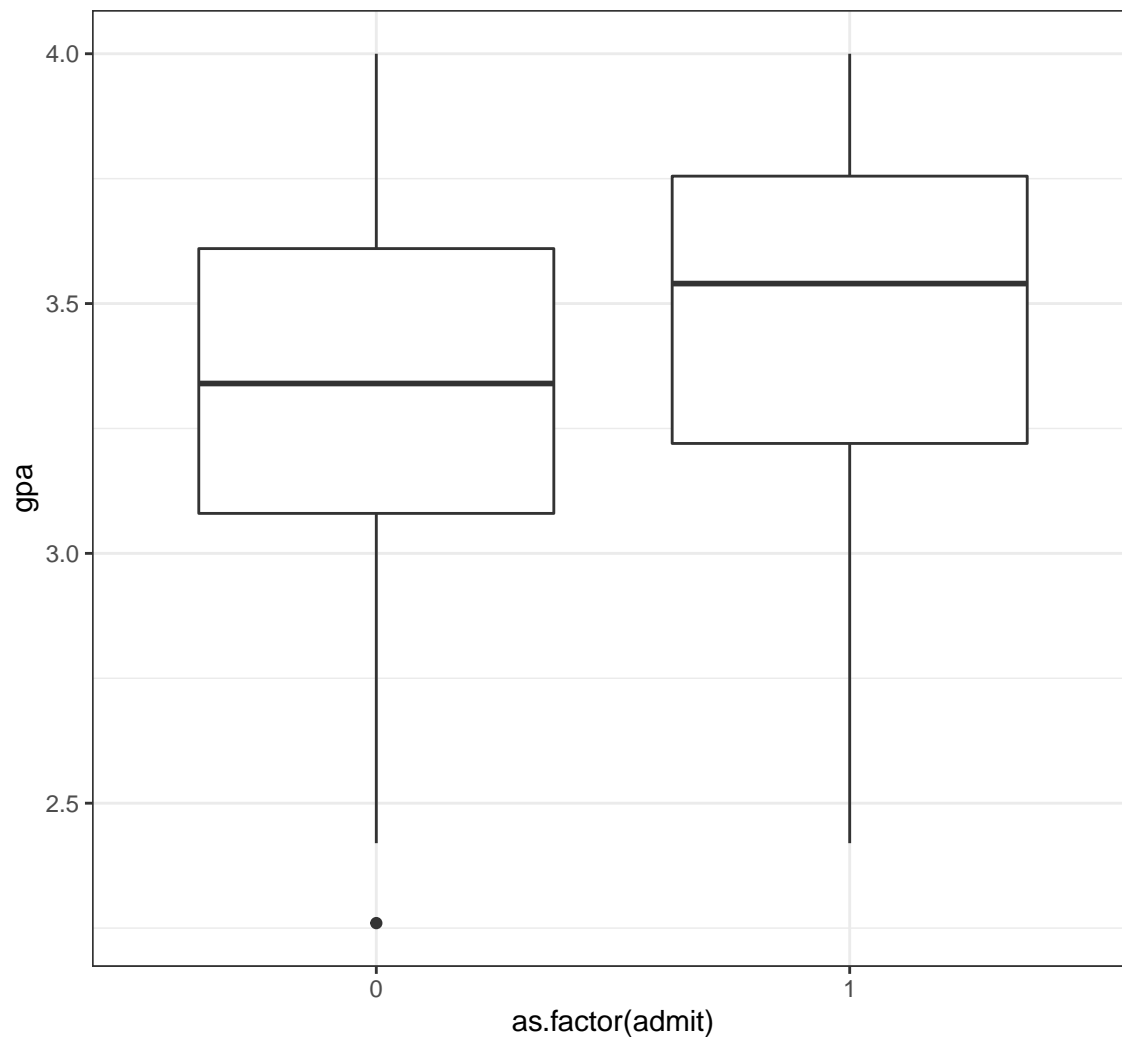
Data and analysis courtesy of <http://www.ats.ucla.edu/stat/r/dae/logit.htm>.

Explore the Data

```
> apply(mydata, 2, mean)  
  admit      gre      gpa      rank  
0.3175 587.7000  3.3899  2.4850  
> apply(mydata, 2, sd)  
  admit      gre      gpa      rank  
0.4660867 115.5165364  0.3805668  0.9444602  
>  
> table(mydata$admit, mydata$rank)  
  
      1  2  3  4  
0  28  97  93  55  
1  33  54  28  12  
  
> ggplot(data=mydata) +  
+   geom_boxplot(aes(x=as.factor(admit), y=gre))
```



```
> ggplot(data=mydata) +  
+   geom_boxplot(aes(x=as.factor(admit), y=gpa))
```



Logistic Regression in R

```
> mydata$rank <- factor(mydata$rank, levels=c(1, 2, 3, 4))
> myfit <- glm(admit ~ gre + gpa + rank,
+             data = mydata, family = "binomial")
> myfit
```

```
Call: glm(formula = admit ~ gre + gpa + rank, family = "binomial",
data = mydata)
```

Coefficients:

(Intercept)	gre	gpa	rank2
-3.989979	0.002264	0.804038	-0.675443
rank3	rank4		
-1.340204	-1.551464		

Degrees of Freedom: 399 Total (i.e. Null); 394 Residual

Null Deviance: 500

Residual Deviance: 458.5 AIC: 470.5

Summary of Fit

```
> summary(myfit)

Call:
glm(formula = admit ~ gre + gpa + rank, family = "binomial",
    data = mydata)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.6268  -0.8662  -0.6388   1.1490   2.0790

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -3.989979   1.139951  -3.500  0.000465 ***
gre           0.002264   0.001094   2.070  0.038465 *
gpa           0.804038   0.331819   2.423  0.015388 *
rank2        -0.675443   0.316490  -2.134  0.032829 *
rank3        -1.340204   0.345306  -3.881  0.000104 ***
rank4        -1.551464   0.417832  -3.713  0.000205 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 499.98  on 399  degrees of freedom
Residual deviance: 458.52  on 394  degrees of freedom
AIC: 470.52

Number of Fisher Scoring iterations: 4
```

ANOVA of Fit

```
> anova(myfit, test="Chisq")
Analysis of Deviance Table

Model: binomial, link: logit

Response: admit

Terms added sequentially (first to last)

      Df Deviance Resid. Df Resid. Dev  Pr(>Chi)
NULL                                399      499.98
gre    1  13.9204         398      486.06 0.0001907 ***
gpa    1   5.7122         397      480.34 0.0168478 *
rank   3  21.8265         394      458.52 7.088e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> anova(myfit, test="LRT")
Analysis of Deviance Table

Model: binomial, link: logit
```

Response: admit

Terms added sequentially (first to last)

	Df	Deviance	Resid. Df	Resid. Dev	Pr(>Chi)
NULL			399	499.98	
gre	1	13.9204	398	486.06	0.0001907 ***
gpa	1	5.7122	397	480.34	0.0168478 *
rank	3	21.8265	394	458.52	7.088e-05 ***

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

Example: Contraceptive Use

```
> cuse <-  
+ read.table("http://data.princeton.edu/wws509/datasets/cuse.dat",  
+           header=TRUE)  
> dim(cuse)  
[1] 16 5  
> head(cuse)  
  age education wantsMore notUsing using  
1  <25      low      yes      53      6  
2  <25      low      no       10      4  
3  <25     high     yes     212     52  
4  <25     high     no      50     10  
5 25-29     low     yes      60     14  
6 25-29     low     no      19     10
```

Data and analysis courtesy of <http://data.princeton.edu/R/glms.html>.

A Different Format

Note that in this data set there are multiple observations per explanatory variable configuration.

The last two columns of the data frame count the successes and failures per configuration.

```
> head(cuse)  
  age education wantsMore notUsing using  
1  <25      low      yes      53      6  
2  <25      low      no       10      4  
3  <25     high     yes     212     52  
4  <25     high     no      50     10  
5 25-29     low     yes      60     14  
6 25-29     low     no      19     10
```

Fitting the Model

When this is the case, we call the `glm()` function slightly differently.

```
> myfit <- glm(cbind(using, notUsing) ~ age + education + wantsMore,  
+             data=cuse, family = binomial)  
> myfit
```

```
Call: glm(formula = cbind(using, notUsing) ~ age + education + wantsMore,  
          family = binomial, data = cuse)
```



```

Coefficients:
(Intercept)      age25-29      age30-39      age40-49
      -0.8082       0.3894       0.9086       1.1892
educationlow  wantsMoreyes
      -0.3250      -0.8330

Degrees of Freedom: 15 Total (i.e. Null); 10 Residual
Null Deviance:      165.8
Residual Deviance: 29.92    AIC: 113.4

```

Summary of Fit

```

> summary(myfit)

Call:
glm(formula = cbind(using, notUsing) ~ age + education + wantsMore,
    family = binomial, data = cuse)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.5148  -0.9376   0.2408   0.9822   1.7333

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept)   -0.8082     0.1590  -5.083 3.71e-07 ***
age25-29       0.3894     0.1759   2.214 0.02681 *
age30-39       0.9086     0.1646   5.519 3.40e-08 ***
age40-49       1.1892     0.2144   5.546 2.92e-08 ***
educationlow  -0.3250     0.1240  -2.620 0.00879 **
wantsMoreyes  -0.8330     0.1175  -7.091 1.33e-12 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 165.772  on 15  degrees of freedom
Residual deviance: 29.917  on 10  degrees of freedom
AIC: 113.43

Number of Fisher Scoring iterations: 4

```

ANOVA of Fit

```

> anova(myfit)
Analysis of Deviance Table

Model: binomial, link: logit

Response: cbind(using, notUsing)

Terms added sequentially (first to last)

```

	Df	Deviance	Resid. Df	Resid. Dev
NULL			15	165.772
age	3	79.192	12	86.581
education	1	6.162	11	80.418
wantsMore	1	50.501	10	29.917

More on this Data Set

See <http://data.princeton.edu/R/glms.html> for more on fitting logistic regression to this data set.

A number of interesting choices are made that reveal more about the data.

Generalized Linear Models

Review: Multiparameter Fisher Info Matrix

Suppose that $X_1, X_2, \dots, X_n \stackrel{\text{iid}}{\sim} F_{\boldsymbol{\theta}}$ where $\boldsymbol{\theta} = (\theta_1, \theta_2, \dots, \theta_d)^T$ has MLE $\hat{\boldsymbol{\theta}}_n$.

The Fisher Information Matrix $I_n(\boldsymbol{\theta})$ is the $d \times d$ matrix with (i, j) entry

$$-\sum_{k=1}^n \mathbb{E} \left(\frac{\partial^2}{\partial \theta_i \partial \theta_j} \log f(X_k; \boldsymbol{\theta}) \right).$$

Review: Multiparameter Asymptotic MVN

Under appropriate regularity conditions, as $n \rightarrow \infty$,

$$\left(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta} \right) \xrightarrow{D} \text{MVN}_d(\mathbf{0}, I_n(\boldsymbol{\theta})^{-1}) \text{ and}$$

$$\left(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta} \right)^T I_n(\hat{\boldsymbol{\theta}}_n) \left(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta} \right) \xrightarrow{D} \text{MVN}_d(\mathbf{0}, \mathbf{I}).$$

GLM Definition

The **generalized linear model** (GLM) builds from OLS and GLS to allow for the case where $Y|\mathbf{X}$ is distributed according to an exponential family distribution. The estimated model is

$$g(\mathbb{E}[Y|\mathbf{X}]) = \mathbf{X}\boldsymbol{\beta}$$

where $g(\cdot)$ is called the **link function**. This model is typically fit by numerical methods to calculate the maximum likelihood estimate of $\boldsymbol{\beta}$.

Exponential Family Distributions

Recall that if Y follows an EFD then it has pdf of the form

$$f(y; \boldsymbol{\theta}) = h(y) \exp \left\{ \sum_{k=1}^d \eta_k(\boldsymbol{\theta}) T_k(y) - A(\boldsymbol{\eta}) \right\}$$

where $\boldsymbol{\theta}$ is a vector of parameters, $\{T_k(y)\}$ are sufficient statistics, $A(\boldsymbol{\eta})$ is the cumulant generating function. The functions $\eta_k(\boldsymbol{\theta})$ for $k = 1, \dots, d$ map the usual parameters $\boldsymbol{\theta}$ (often moments of the rv Y) to the *natural parameters* or *canonical parameters*.

$\{T_k(y)\}$ are sufficient statistics for $\{\eta_k\}$ due to the factorization theorem.

$A(\boldsymbol{\eta})$ is sometimes called the *log normalizer* because

$$A(\boldsymbol{\eta}) = \log \int h(y) \exp \left\{ \sum_{k=1}^d \eta_k(\boldsymbol{\theta}) T_k(y) \right\}.$$

Natural Single Parameter EFD

A natural single parameter EFD simplifies to the scenario where $d = 1$ and $T(y) = y$

$$f(y; \eta) = h(y) \exp \{ \eta(\theta)y - A(\eta(\theta)) \}$$

where without loss of generality we can write $E[Y] = \theta$.

Dispersion EFDs

The family of distributions for which GLMs are most typically developed are dispersion EFDs. An example of a dispersion EFD that extends the natural single parameter EFD is

$$f(y; \eta) = h(y, \phi) \exp \left\{ \frac{\eta(\theta)y - A(\eta(\theta))}{\phi} \right\}$$

where ϕ is the dispersion parameter.

Example: Normal

Let $Y \sim \text{Normal}(\mu, \sigma^2)$. Then:

$$\theta = \mu, \eta(\mu) = \mu$$

$$\phi = \sigma^2$$

$$A(\mu) = \frac{\mu^2}{2}$$

$$h(y, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{y^2}{\sigma^2}}$$

EFD for GLMs

There has been a very broad development of GLMs and extensions. A common setting for introducing GLMs is the dispersion EFD with a general link function $g(\cdot)$.

See the classic text *Generalized Linear Models*, by McCullagh and Nelder, for such a development.

Components of a GLM

1. *Random*: The particular exponential family distribution.

$$Y \sim f(y; \eta, \phi)$$

2. *Systematic*: The determination of each η_i from \mathbf{X}_i and $\boldsymbol{\beta}$.

$$\eta_i = \mathbf{X}_i \boldsymbol{\beta}$$

3. *Parametric Link*: The connection between $E[Y_i | \mathbf{X}_i]$ and $\mathbf{X}_i \boldsymbol{\beta}$.

$$g(E[Y_i | \mathbf{X}_i]) = \mathbf{X}_i \boldsymbol{\beta}$$

Link Functions

Even though the link function $g(\cdot)$ can be considered in a fairly general framework, the **canonical link function** $\eta(\cdot)$ is often utilized.

The canonical link function is the function that maps the expected value into the natural parameter.

In this case, $Y | \mathbf{X}$ is distributed according to an exponential family distribution with

$$\eta(E[Y | \mathbf{X}]) = \mathbf{X} \boldsymbol{\beta}.$$

Calculating MLEs

Given the model $g(E[Y | \mathbf{X}]) = \mathbf{X} \boldsymbol{\beta}$, the EFD should be fully parameterized. The Newton-Raphson method or Fisher's scoring method can be utilized to find the MLE of $\boldsymbol{\beta}$.

Newton-Raphson

1. Initialize $\boldsymbol{\beta}^{(0)}$. For $t = 1, 2, \dots$
2. Calculate the score $s(\boldsymbol{\beta}^{(t)}) = \nabla \ell(\boldsymbol{\beta}; \mathbf{X}, \mathbf{Y}) |_{\boldsymbol{\beta}=\boldsymbol{\beta}^{(t)}}$ and observed Fisher information

$$H(\boldsymbol{\beta}^{(t)}) = -\nabla \nabla^T \ell(\boldsymbol{\beta}; \mathbf{X}, \mathbf{Y}) |_{\boldsymbol{\beta}=\boldsymbol{\beta}^{(t)}}.$$

Note that the observed Fisher information is also the negative Hessian matrix.

3. Update $\boldsymbol{\beta}^{(t+1)} = \boldsymbol{\beta}^{(t)} + H(\boldsymbol{\beta}^{(t)})^{-1} s(\boldsymbol{\beta}^{(t)})$.
4. Iterate until convergence, and set $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}^{(\infty)}$.

Fisher's scoring

1. Initialize $\boldsymbol{\beta}^{(0)}$. For $t = 1, 2, \dots$
2. Calculate the score $s(\boldsymbol{\beta}^{(t)}) = \nabla \ell(\boldsymbol{\beta}; \mathbf{X}, \mathbf{Y}) |_{\boldsymbol{\beta}=\boldsymbol{\beta}^{(t)}}$ and expected Fisher information

$$I(\boldsymbol{\beta}^{(t)}) = -E[\nabla \nabla^T \ell(\boldsymbol{\beta}; \mathbf{X}, \mathbf{Y}) |_{\boldsymbol{\beta}=\boldsymbol{\beta}^{(t)}}].$$

3. Update $\boldsymbol{\beta}^{(t+1)} = \boldsymbol{\beta}^{(t)} + I(\boldsymbol{\beta}^{(t)})^{-1} s(\boldsymbol{\beta}^{(t)})$.
4. Iterate until convergence, and set $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}^{(\infty)}$.

When the canonical link function is used, the Newton-Raphson algorithm and Fisher's scoring algorithm are equivalent.

Exercise: Prove this.

Iteratively Reweighted Least Squares

For the canonical link, Fisher's scoring method can be written as an iteratively reweighted least squares algorithm, as shown earlier for logistic regression. Note that the Fisher information is

$$I(\boldsymbol{\beta}^{(t)}) = \mathbf{X}^T \mathbf{W} \mathbf{X}$$

where \mathbf{W} is an $n \times n$ diagonal matrix with (i, i) entry equal to $\text{Var}(Y_i | \mathbf{X}; \boldsymbol{\beta}^{(t)})$.

The score function is

$$s(\boldsymbol{\beta}^{(t)}) = \mathbf{X}^T (\mathbf{Y} - \mathbf{X} \boldsymbol{\beta}^{(t)})$$

and the current coefficient value $\boldsymbol{\beta}^{(t)}$ can be written as

$$\boldsymbol{\beta}^{(t)} = (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} \mathbf{X} \boldsymbol{\beta}^{(t)}.$$

Putting this together we get

$$\boldsymbol{\beta}^{(t)} + I(\boldsymbol{\beta}^{(t)})^{-1} s(\boldsymbol{\beta}^{(t)}) = (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} \mathbf{z}^{(t)}$$

where

$$\mathbf{z}^{(t)} = \mathbf{X} \boldsymbol{\beta}^{(t)} + \mathbf{W}^{-1} (\mathbf{Y} - \mathbf{X} \boldsymbol{\beta}^{(t)}).$$

This is a generalization of the iteratively reweighted least squares algorithm we showed earlier for logistic regression.

Estimating Dispersion

For the simple dispersion model above, it is typically straightforward to calculate the MLE $\hat{\phi}$ once $\hat{\boldsymbol{\beta}}$ has been calculated.

CLT Applied to the MLE

Given that $\hat{\boldsymbol{\beta}}$ is a maximum likelihood estimate, we have the following CLT result on its distribution as $n \rightarrow \infty$:

$$\sqrt{n}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \xrightarrow{D} \text{MVN}_p(\mathbf{0}, \phi(\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1})$$

Approximately Pivotal Statistics

The previous CLT gives us the following two approximations for pivotal statistics. The first statistic facilitates getting overall measures of uncertainty on the estimate $\hat{\boldsymbol{\beta}}$.

$$\hat{\phi}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T (\mathbf{X}^T \hat{\mathbf{W}} \mathbf{X}) (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \sim \chi_1^2$$

This second pivotal statistic allows for performing a Wald test or forming a confidence interval on each coefficient, β_j , for $j = 1, \dots, p$.

$$\frac{\hat{\beta}_j - \beta_j}{\sqrt{\hat{\phi}[(\mathbf{X}^T \hat{\mathbf{W}} \mathbf{X})^{-1}]_{jj}}} \sim \text{Normal}(0, 1)$$

Deviance

Let $\hat{\eta}$ be the estimated natural parameters from a GLM. For example, $\hat{\eta} = \mathbf{X}\hat{\beta}$ when the canonical link function is used.

Let $\hat{\eta}_n$ be the **saturated model** where Y_i is directly used to estimate η_i without model constraints. For example, in the Bernoulli logistic regression model $\hat{\eta}_n = \mathbf{Y}$, the observed outcomes.

The **deviance** for the model is defined to be

$$D(\hat{\eta}) = 2\ell(\hat{\eta}_n; \mathbf{X}, \mathbf{Y}) - 2\ell(\hat{\eta}; \mathbf{X}, \mathbf{Y})$$

Generalized LRT

Let \mathbf{X}_0 be a subset of p_0 columns of \mathbf{X} and let \mathbf{X}_1 be a subset of p_1 columns, where $1 \leq p_0 < p_1 \leq p$. Also, assume that the columns of \mathbf{X}_0 are a subset of \mathbf{X}_1 .

Without loss of generality, suppose that $\beta_0 = (\beta_1, \beta_2, \dots, \beta_{p_0})^T$ and $\beta_1 = (\beta_1, \beta_2, \dots, \beta_{p_1})^T$.

Suppose we wish to test $H_0 : (\beta_{p_0+1}, \beta_{p_0+2}, \dots, \beta_{p_1}) = \mathbf{0}$ vs $H_1 : (\beta_{p_0+1}, \beta_{p_0+2}, \dots, \beta_{p_1}) \neq \mathbf{0}$

We can form $\hat{\eta}_0 = \mathbf{X}\hat{\beta}_0$ from the GLM model $g(E[Y|\mathbf{X}_0]) = \mathbf{X}_0\beta_0$. We can analogously form $\hat{\eta}_1 = \mathbf{X}\hat{\beta}_1$ from the GLM model $g(E[Y|\mathbf{X}_1]) = \mathbf{X}_1\beta_1$.

The 2 log generalized LRT can then be formed from the two deviance statistics

$$2 \log \lambda(\mathbf{X}, \mathbf{Y}) = 2 \log \frac{L(\hat{\eta}_1; \mathbf{X}, \mathbf{Y})}{L(\hat{\eta}_0; \mathbf{X}, \mathbf{Y})} = D(\hat{\eta}_0) - D(\hat{\eta}_1)$$

where the null distribution is $\chi^2_{p_1-p_0}$.

Example: Grad School Admissions

Let's revisit a logistic regression example now that we know how the various statistics are calculated.

```
> mydata <-  
+ read.csv("http://www.ats.ucla.edu/stat/data/binary.csv")  
> dim(mydata)  
> head(mydata)
```

Fit the model with basic output. Note the argument `family = "binomial"`.

```
> mydata$rank <- factor(mydata$rank, levels=c(1, 2, 3, 4))  
> myfit <- glm(admit ~ gre + gpa + rank,  
+ data = mydata, family = "binomial")  
> myfit
```

```
Call: glm(formula = admit ~ gre + gpa + rank, family = "binomial",  
data = mydata)
```

Coefficients:

(Intercept)	gre	gpa	rank2
-3.989979	0.002264	0.804038	-0.675443
rank3	rank4		
-1.340204	-1.551464		

```
Degrees of Freedom: 399 Total (i.e. Null); 394 Residual
```

```
Null Deviance:      500
Residual Deviance: 458.5    AIC: 470.5
```

This shows the fitted coefficient values, which is on the link function scale – logit aka log odds here. Also, a Wald test is performed for each coefficient.

```
> summary(myfit)

Call:
glm(formula = admit ~ gre + gpa + rank, family = "binomial",
    data = mydata)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.6268  -0.8662  -0.6388   1.1490   2.0790

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -3.989979   1.139951  -3.500  0.000465 ***
gre           0.002264   0.001094   2.070  0.038465 *
gpa           0.804038   0.331819   2.423  0.015388 *
rank2        -0.675443   0.316490  -2.134  0.032829 *
rank3        -1.340204   0.345306  -3.881  0.000104 ***
rank4        -1.551464   0.417832  -3.713  0.000205 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 499.98  on 399  degrees of freedom
Residual deviance: 458.52  on 394  degrees of freedom
AIC: 470.52

Number of Fisher Scoring iterations: 4
```

Here we perform a generalized LRT on each variable. Note the `rank` variable is now tested as a single factor variable as opposed to each dummy variable.

```
> anova(myfit, test="LRT")
Analysis of Deviance Table

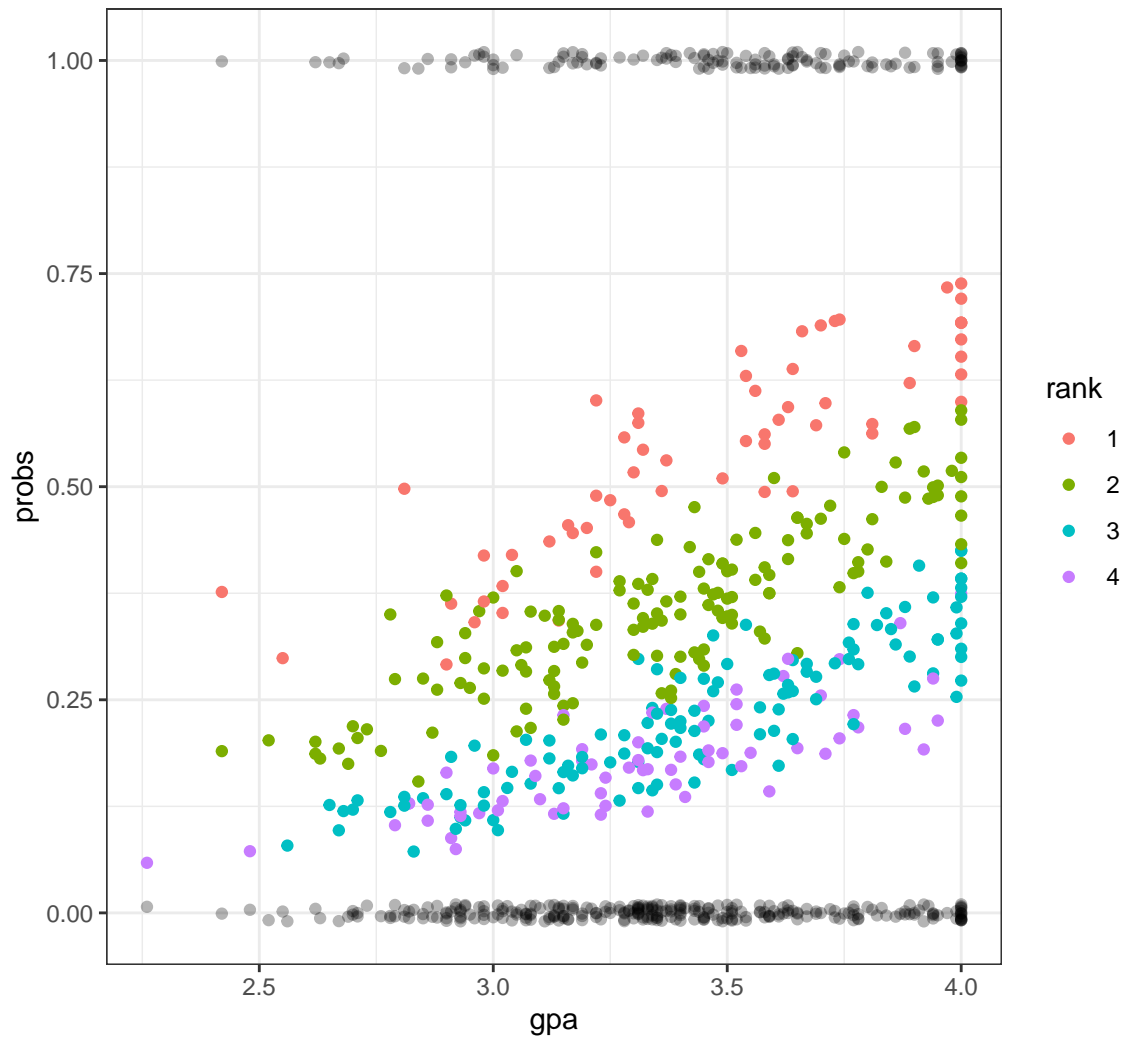
Model: binomial, link: logit

Response: admit

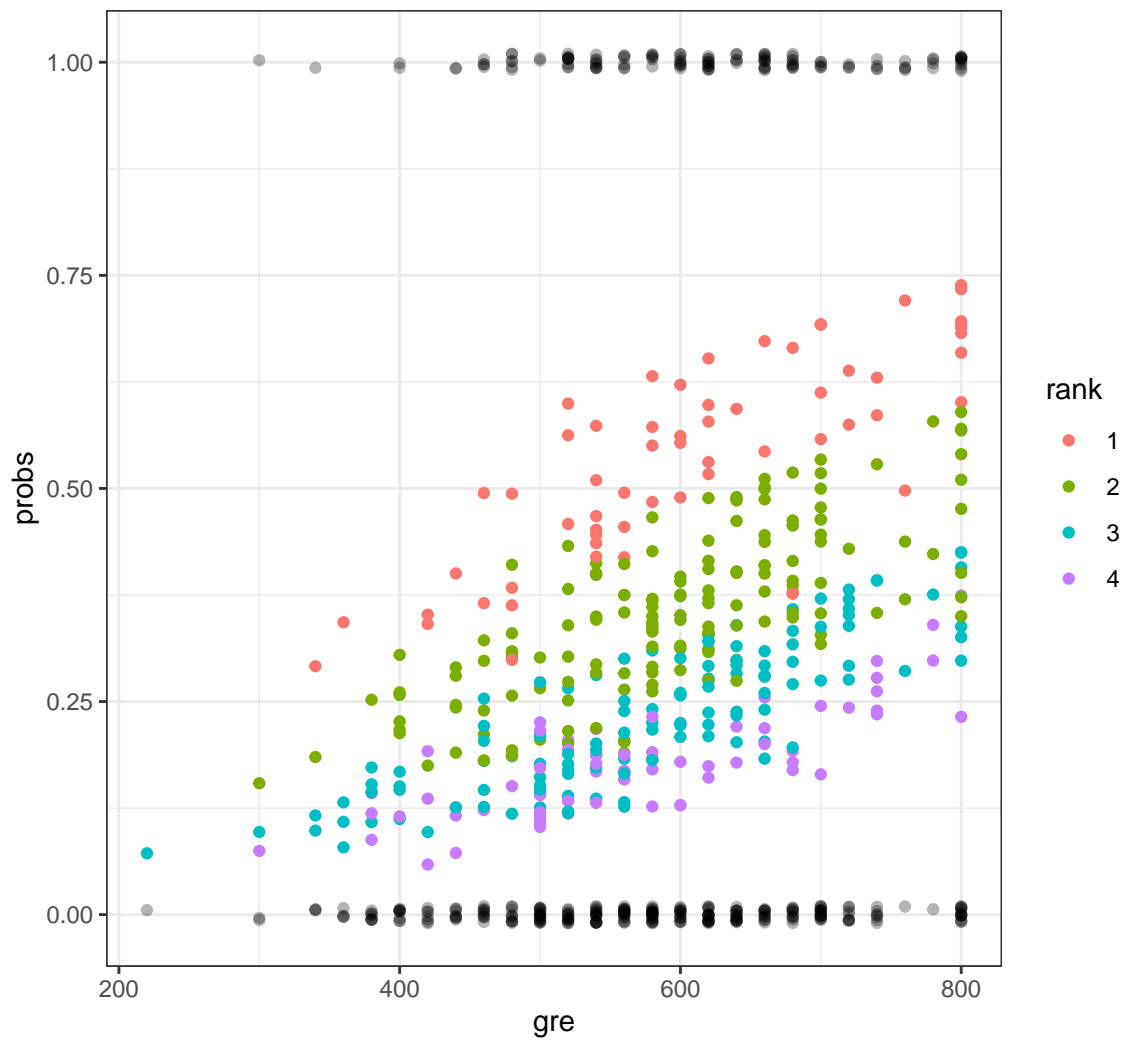
Terms added sequentially (first to last)

      Df Deviance Resid. Df Resid. Dev  Pr(>Chi)
NULL                                399      499.98
gre   1  13.9204      398      486.06 0.0001907 ***
gpa   1   5.7122      397      480.34 0.0168478 *
rank  3  21.8265      394      458.52 7.088e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

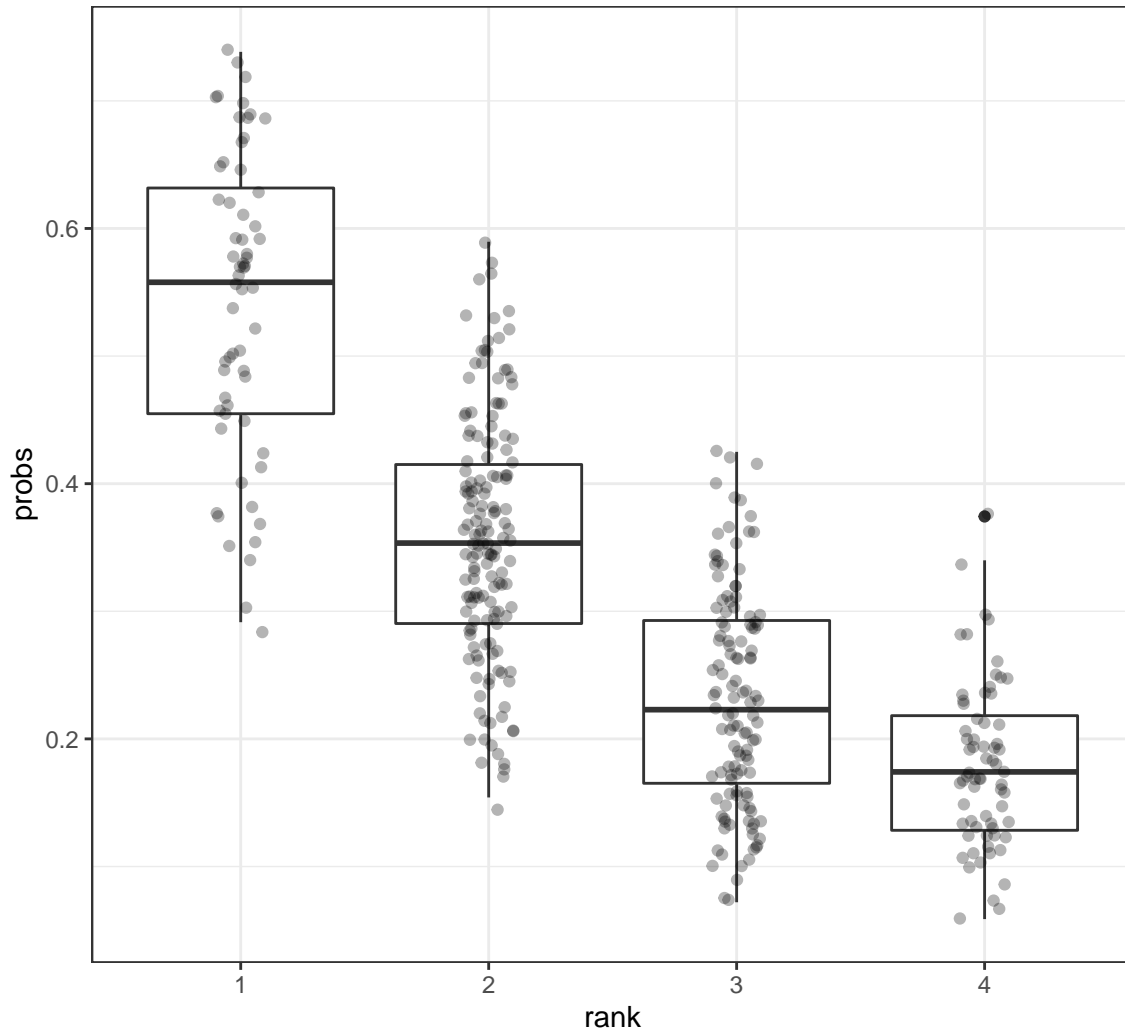
```
> mydata <- data.frame(mydata, probs = myfit$fitted.values)
> ggplot(mydata) + geom_point(aes(x=gpa, y=probs, color=rank)) +
+   geom_jitter(aes(x=gpa, y=admit), width=0, height=0.01, alpha=0.3)
```



```
> ggplot(mydata) + geom_point(aes(x=gre, y=probs, color=rank)) +
+   geom_jitter(aes(x=gre, y=admit), width=0, height=0.01, alpha=0.3)
```

```
> ggplot(mydata) + geom_boxplot(aes(x=rank, y=probs)) +
+   geom_jitter(aes(x=rank, y=probs), width=0.1, height=0.01, alpha=0.3)
```



glm() Function

The `glm()` function has many different options available to the user.

```
glm(formula, family = gaussian, data, weights, subset,
    na.action, start = NULL, etastart, mustart, offset,
    control = list(...), model = TRUE, method = "glm.fit",
    x = FALSE, y = TRUE, contrasts = NULL, ...)
```

To see the different link functions available, type:

```
help(family)
```

Nonparametric Regression

Simple Linear Regression

Recall the set up for simple linear regression. For random variables $(X_1, Y_1), (X_2, Y_2), \dots, (X_n, Y_n)$, **simple linear regression** estimates the model

$$Y_i = \beta_1 + \beta_2 X_i + E_i$$

where $E[E_i|X_i] = 0$, $\text{Var}(E_i|X_i) = \sigma^2$, and $\text{Cov}(E_i, E_j|X_i, X_j) = 0$ for all $1 \leq i, j \leq n$ and $i \neq j$. Note that in this model $E[Y|X] = \beta_1 + \beta_2 X$.

Simple Nonparametric Regression

In **simple nonparametric regression**, we define a similar model while eliminating the linear assumption:

$$Y_i = s(X_i) + E_i$$

for some function $s(\cdot)$ with the same assumptions on the distribution of $\mathbf{E}|\mathbf{X}$. In this model, we also have

$$E[Y|X] = s(X).$$

Smooth Functions

Suppose we consider fitting the model $Y_i = s(X_i) + E_i$ with the restriction that $s \in C^2$, the class of functions with continuous second derivatives. We can set up an objective function that regularizes how smooth vs wiggly s is.

Specifically, suppose for a given set of observed data $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ we wish to identify a function $s \in C^2$ that minimizes for some λ

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

Smoothness Parameter λ

When minimizing

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

it follows that if $\lambda = 0$ then any function $s \in C^2$ that interpolates the data is a solution.

As $\lambda \rightarrow \infty$, then the minimizing function is the simple linear regression solution.

The Solution

For an observed data set $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ where $n \geq 4$ and a fixed value λ , there is an exact solution to minimizing

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

The solution is called a **natural cubic spline**, which is constructed to have knots at x_1, x_2, \dots, x_n .

Natural Cubic Splines

Suppose without loss of generality that we have ordered $x_1 < x_2 < \dots < x_n$. We assume all x_i are unique to simplify the explanation here, but ties can be dealt with.

A **natural cubic spline** (NCS) is a function constructed from a set of piecewise cubic functions over the range $[x_1, x_n]$ joined at the knots so that the second derivative is continuous at the knots. Outside of the range ($< x_1$ or $> x_n$), the spline is linear and it has continuous second derivatives at the endpoint knots.

Basis Functions

Depending on the value λ , a different ncs will be constructed, but the entire family of ncs solutions over $0 < \lambda < \infty$ can be constructed from a common set of basis functions.

We construct n basis functions $N_1(x), N_2(x), \dots, N_n(x)$ with coefficients $\theta_1(\lambda), \theta_2(\lambda), \dots, \theta_n(\lambda)$. The NCS takes the form

$$s(x) = \sum_{i=1}^n \theta_i(\lambda) N_i(x).$$

Define $N_1(x) = 1$ and $N_2(x) = x$. For $i = 3, \dots, n$, define $N_i(x) = d_{i-1}(x) - d_{i-2}(x)$ where

$$d_i(x) = \frac{(x - x_i)^3 - (x - x_n)^3}{x_n - x_i}.$$

Recall that we've labeled indices so that $x_1 < x_2 < \dots < x_n$.

Calculating the Solution

Let $\boldsymbol{\theta}_\lambda = (\theta_1(\lambda), \theta_2(\lambda), \dots, \theta_n(\lambda))^T$ and let \mathbf{N} be the $n \times n$ matrix with (i, j) entry equal to $N_j(x_i)$. Finally, let $\boldsymbol{\Omega}$ be the $n \times n$ matrix with (i, j) entry equal to $\int N_i''(x) N_j''(x) dx$.

The solution to $\boldsymbol{\theta}_\lambda$ are the values that minimize

$$(\mathbf{y} - \mathbf{N}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{N}\boldsymbol{\theta}) + \lambda \boldsymbol{\theta}^T \boldsymbol{\Omega} \boldsymbol{\theta}.$$

which results in

$$\hat{\boldsymbol{\theta}}_\lambda = (\mathbf{N}^T \mathbf{N} + \lambda \boldsymbol{\Omega})^{-1} \mathbf{N}^T \mathbf{y}.$$

Linear Operator

Letting

$$\mathbf{S}_\lambda = \mathbf{N}(\mathbf{N}^T \mathbf{N} + \lambda \boldsymbol{\Omega})^{-1} \mathbf{N}^T$$

it follows that the fitted values are

$$\hat{\mathbf{y}} = \mathbf{S}_\lambda \mathbf{y}.$$

Thus, the fitted values from a NCS are constructed by taking linear combination of the response variable values y_1, y_2, \dots, y_n .

Degrees of Freedom

Recall that in OLS, we formed projection matrix $\mathbf{P} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$ and noted that the number of columns p of \mathbf{X} is also found in the trace of \mathbf{P} where $\text{tr}(\mathbf{P}) = p$.

The effective degrees of freedom for a model fit by a linear operator is calculated as the trace of the operator.

Therefore, for a given λ , the effective degrees of freedom is

$$\text{df}_\lambda = \text{tr}(\mathbf{S}_\lambda).$$

Bayesian Interpretation

Minimizing

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

is equivalent to maximizing

$$\exp \left\{ -\frac{\sum_{i=1}^n (y_i - s(x_i))^2}{2\sigma^2} \right\} \exp \left\{ -\frac{\lambda}{2\sigma^2} \int |s''(x)|^2 dx \right\}.$$

Therefore, the NCS solution can be interpreted as calculating the MAP where $Y|X$ is Normal and there's an Exponential prior on the smoothness of s .

Bias and Variance Trade-off

Typically we will choose some $0 < \lambda < \infty$ in an effort to balance the bias and variance. Let $\hat{Y} = \hat{s}(X; \lambda)$ where $\hat{s}(\cdot; \lambda)$ minimizes the above for some chosen λ on an independent data set. Then

$$\begin{aligned} \mathbb{E} \left[\left(Y - \hat{Y} \right)^2 \right] &= \mathbb{E} \left[(s(x) + E - \hat{s}(x; \lambda))^2 \right] \\ &= \mathbb{E} \left[(s(x) - \hat{s}(x; \lambda))^2 \right] + \text{Var}(E) \\ &= (s(x) - \mathbb{E}[\hat{s}(x; \lambda)])^2 + \text{Var}(\hat{s}(x; \lambda)) + \text{Var}(E) \\ &= \text{bias}_\lambda^2 + \text{variance}_\lambda + \text{Var}(E) \end{aligned}$$

where all of the above calculations are conditioned on $X = x$.

In minimizing

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

the relationship is such that:

$$\uparrow \lambda \implies \text{bias}^2 \uparrow, \text{variance} \downarrow$$

$$\downarrow \lambda \implies \text{bias}^2 \downarrow, \text{variance} \uparrow$$

Choosing λ

There are several approaches that are commonly used to identify a value of λ , including:

- Scientific knowledge that guides the acceptable value of df_λ
- Cross-validation or some other prediction quality measure
- Model selection measures, such as Akaike information criterion (AIC) or Mallows C_p

Smoothers and Spline Models

We investigated one type of nonparametric regression model here, the NCS. However, in general there are many such “smoother” methods available in the simple nonparametric regression scenario.

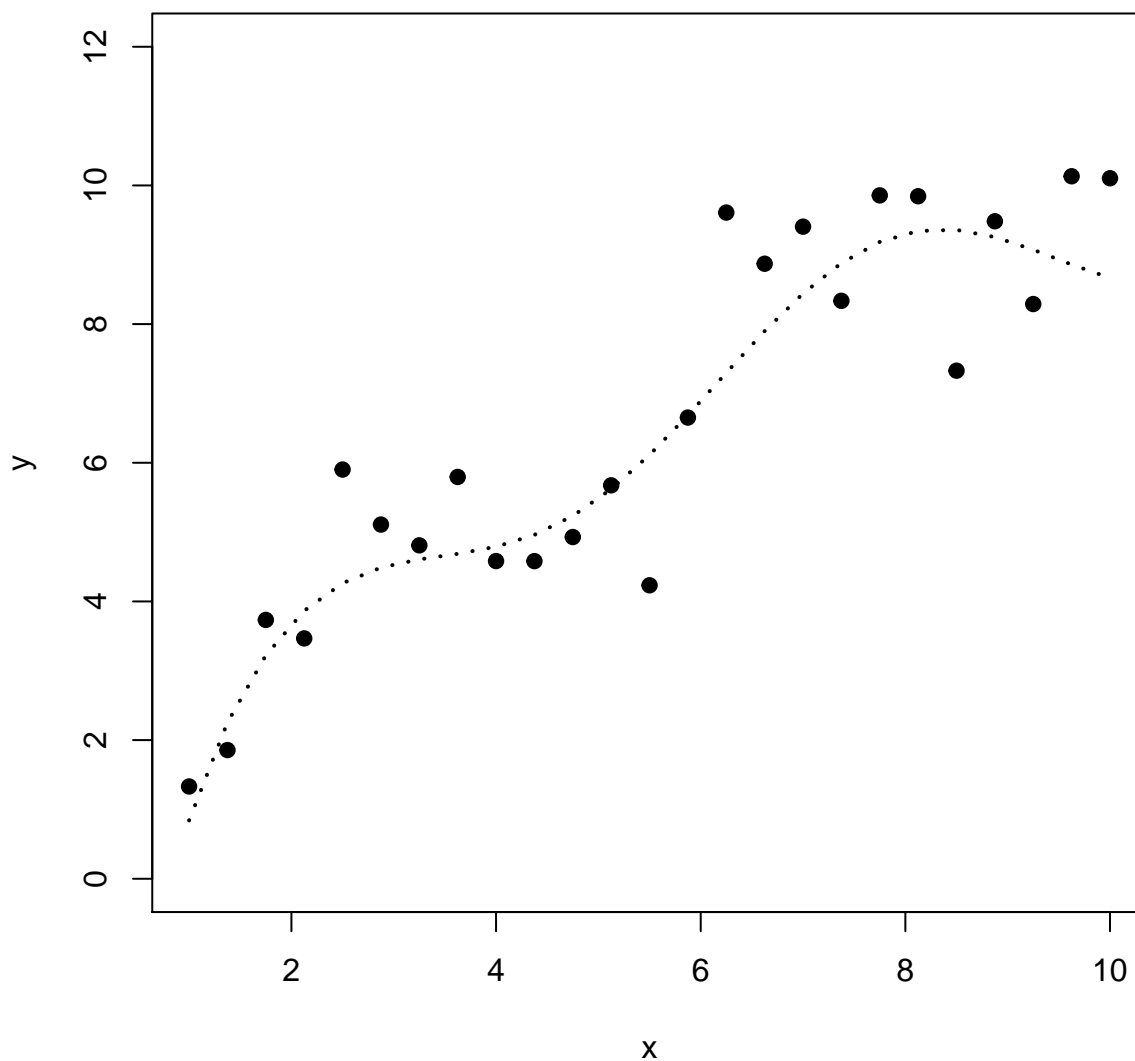
Splines are particularly popular since splines are constructed from putting together polynomials and are therefore usually tractable to compute and analyze.

Smoothers in R

There are several functions and packages available in R for computing smoothers and tuning smoothness parameters. Examples include:

- `splines` library
- `smooth.spline()`
- `loess()`
- `lowess()`

Example



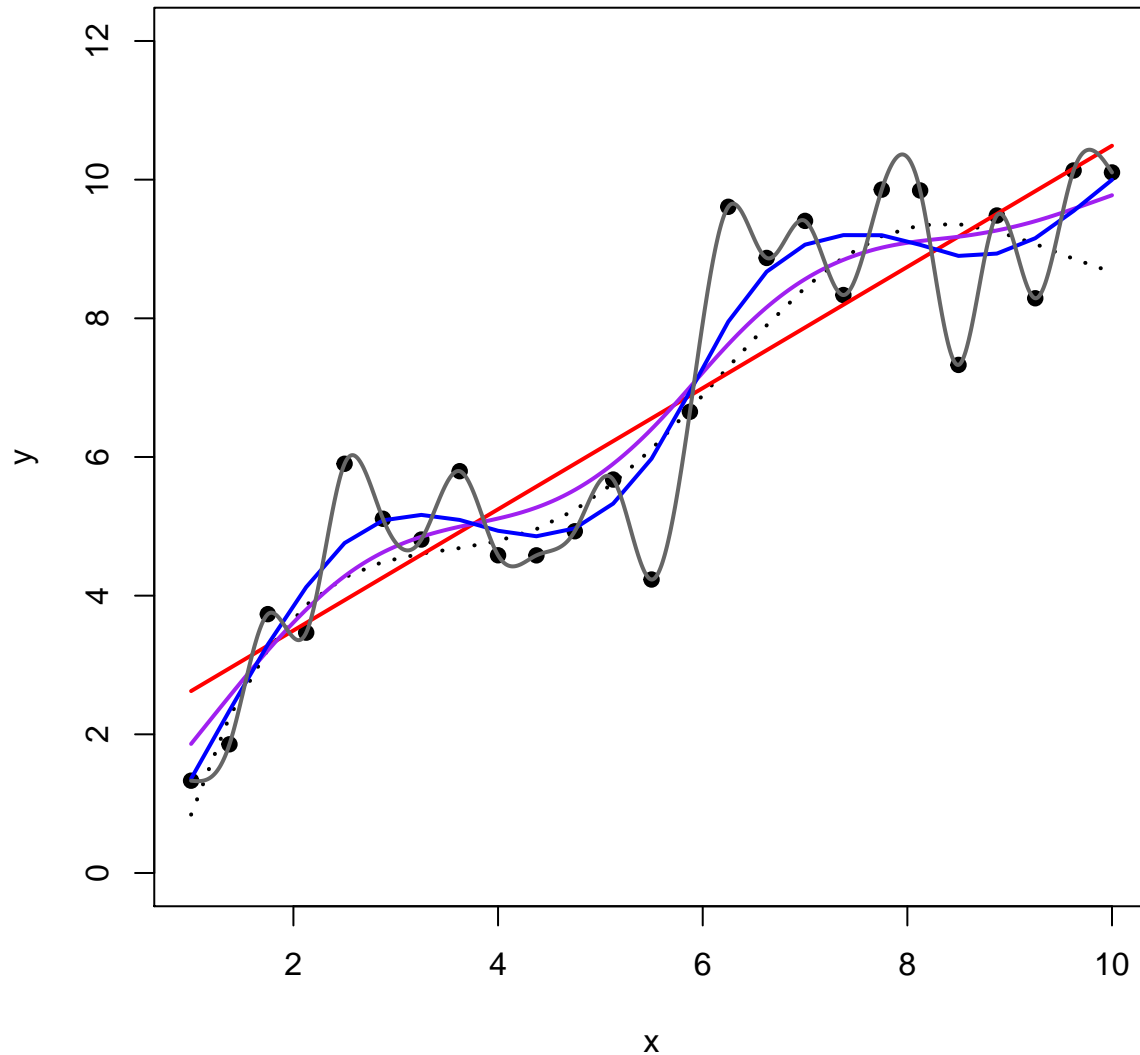
```
> y2 <- smooth.spline(x=x, y=y, df=2)
> y5 <- smooth.spline(x=x, y=y, df=5)
```

```

> y25 <- smooth.spline(x=x, y=y, df=25)
> ycv <- smooth.spline(x=x, y=y)
> ycv
Call:
smooth.spline(x = x, y = y)

Smoothing Parameter spar= 0.5162045 lambda= 0.0002730906 (11 iterations)
Equivalent Degrees of Freedom (Df): 7.293673
Penalized Criterion (RSS): 14.80602
GCV: 1.180651

```



Generalized Additive Models

Ordinary Least Squares

Recall that OLS estimates the model

$$\begin{aligned}
 Y_i &= \beta_1 X_{i1} + \beta_2 X_{i2} + \dots + \beta_p X_{ip} + E_i \\
 &= \mathbf{X}_i \boldsymbol{\beta} + E_i
 \end{aligned}$$

where $E[\mathbf{E}|\mathbf{X}] = \mathbf{0}$ and $\text{Cov}(\mathbf{E}|\mathbf{X}) = \sigma^2 \mathbf{I}$.

Additive Models

The **additive model** (which could also be called “ordinary nonparametric additive regression”) is of the form

$$\begin{aligned} Y_i &= s_1(X_{i1}) + s_2(X_{i2}) + \dots + s_p(X_{ip}) + E_i \\ &= \sum_{j=1}^p s_j(X_{ij}) + E_i \end{aligned}$$

where the $s_j(\cdot)$ for $j = 1, \dots, p$ are a set of nonparametric (or flexible) functions. Again, we assume that $E[\mathbf{E}|\mathbf{X}] = \mathbf{0}$ and $\text{Cov}(\mathbf{E}|\mathbf{X}) = \sigma^2 \mathbf{I}$.

Backfitting

The additive model can be fit through a technique called **backfitting**.

1. Initialize $s_j^{(0)}(x)$ for $j = 1, \dots, p$.
2. For $t = 1, 2, \dots$, fit $s_j^{(t)}(x)$ on response variable

$$y_i - \sum_{k \neq j} s_k^{(t-1)}(x_{ik}).$$

3. Repeat until convergence.

Note that some extra steps have to be taken to deal with the intercept.

GAM Definition

$Y|\mathbf{X}$ is distributed according to an exponential family distribution. The extension of additive models to this family of response variable is called **generalized additive models** (GAMs). The model is of the form

$$g(E[Y_i|\mathbf{X}_i]) = \sum_{j=1}^p s_j(X_{ij})$$

where $g(\cdot)$ is the link function and the $s_j(\cdot)$ are flexible and/or nonparametric functions.

Overview of Fitting GAMs

Fitting GAMs involves putting together the following three tools:

1. We know how to fit a GLM via IRLS
2. We know how to fit a smoother of a single explanatory variable via a least squares solution, as seen for the NCS
3. We know how to combine additive smoothers by backfitting

GAMs in R

Three common ways to fit GAMs in R:

1. Utilize `glm()` on explanatory variables constructed from `ns()` or `bs()`
2. The `gam` library
3. The `mgcv` library

Example

```
> set.seed(508)
> x1 <- seq(1, 10, length.out=50)
> n <- length(x1)
> x2 <- rnorm(n)
> f <- 4*log(x1) + sin(x1) - 7 + 0.5*x2
> p <- exp(f)/(1+exp(f))
> summary(p)
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
0.001842 0.074171 0.310674 0.436162 0.860387 0.944761
> y <- rbinom(n, size=1, prob=p)
> mean(y)
[1] 0.42
> df <- data.frame(x1=x1, x2=x2, y=y)
```

Here, we use the `gam()` function from the `mgcv` library. It automates choosing the smoothness of the splines.

```
> library(mgcv)
> mygam <- gam(y ~ s(x1) + s(x2), family = binomial(), data=df)
> library(broom)
> tidy(mygam)
# A tibble: 2 x 5
  term      edf ref.df statistic p.value
<chr> <dbl> <dbl>      <dbl> <dbl>
1 s(x1)  1.87   2.37      12.7  0.00531
2 s(x2)  1.00   1.00       1.16  0.281
```

```
> summary(mygam)

Family: binomial
Link function: logit

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

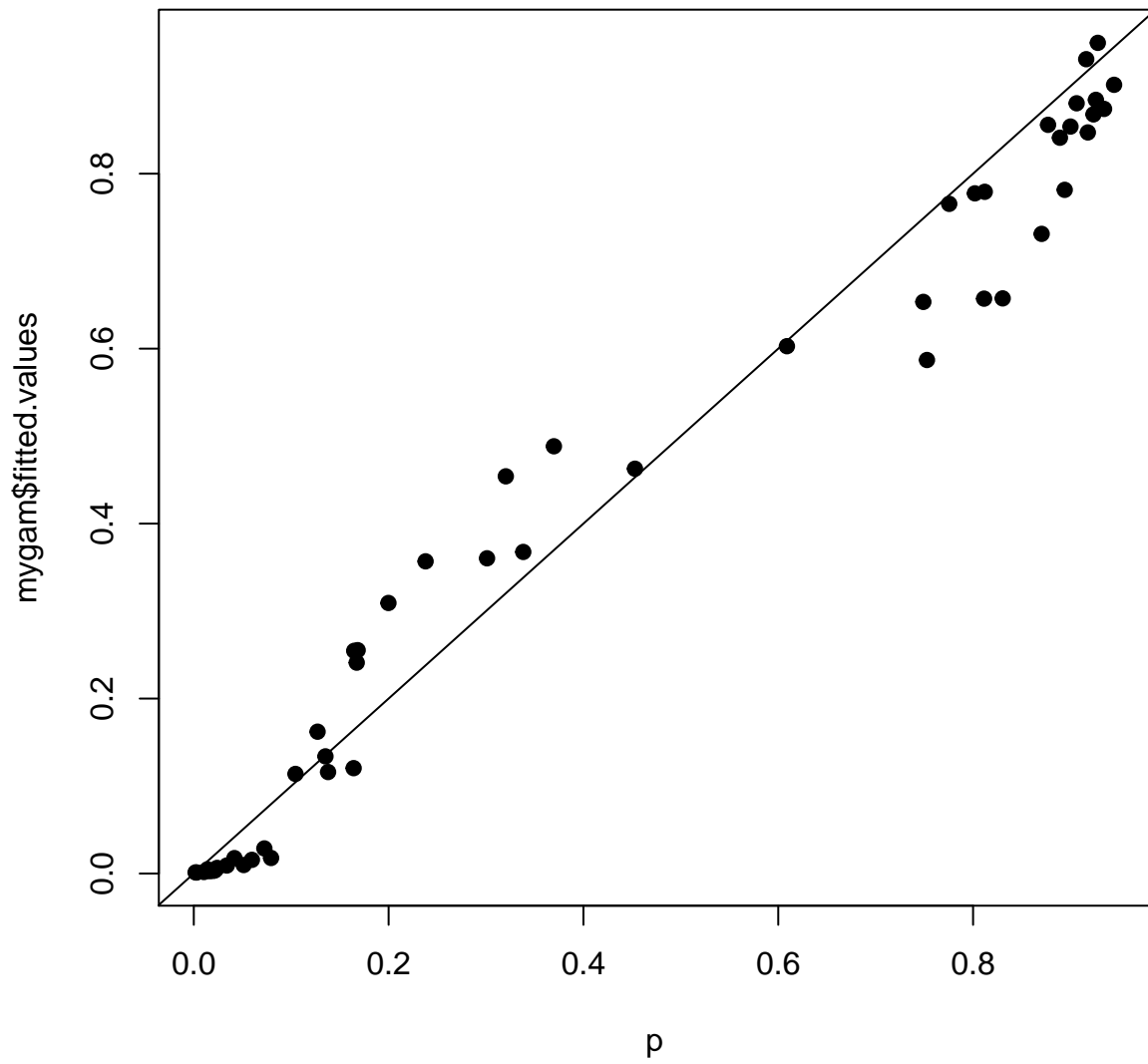
Parametric coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept)  -1.1380     0.6723  -1.693   0.0905 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
              edf Ref.df Chi.sq p-value
s(x1)  1.87   2.375 12.743 0.00531 **
s(x2)  1.00   1.000   1.163 0.28084
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.488   Deviance explained =  47%
UBRE = -0.12392  Scale est. = 1          n = 50
```

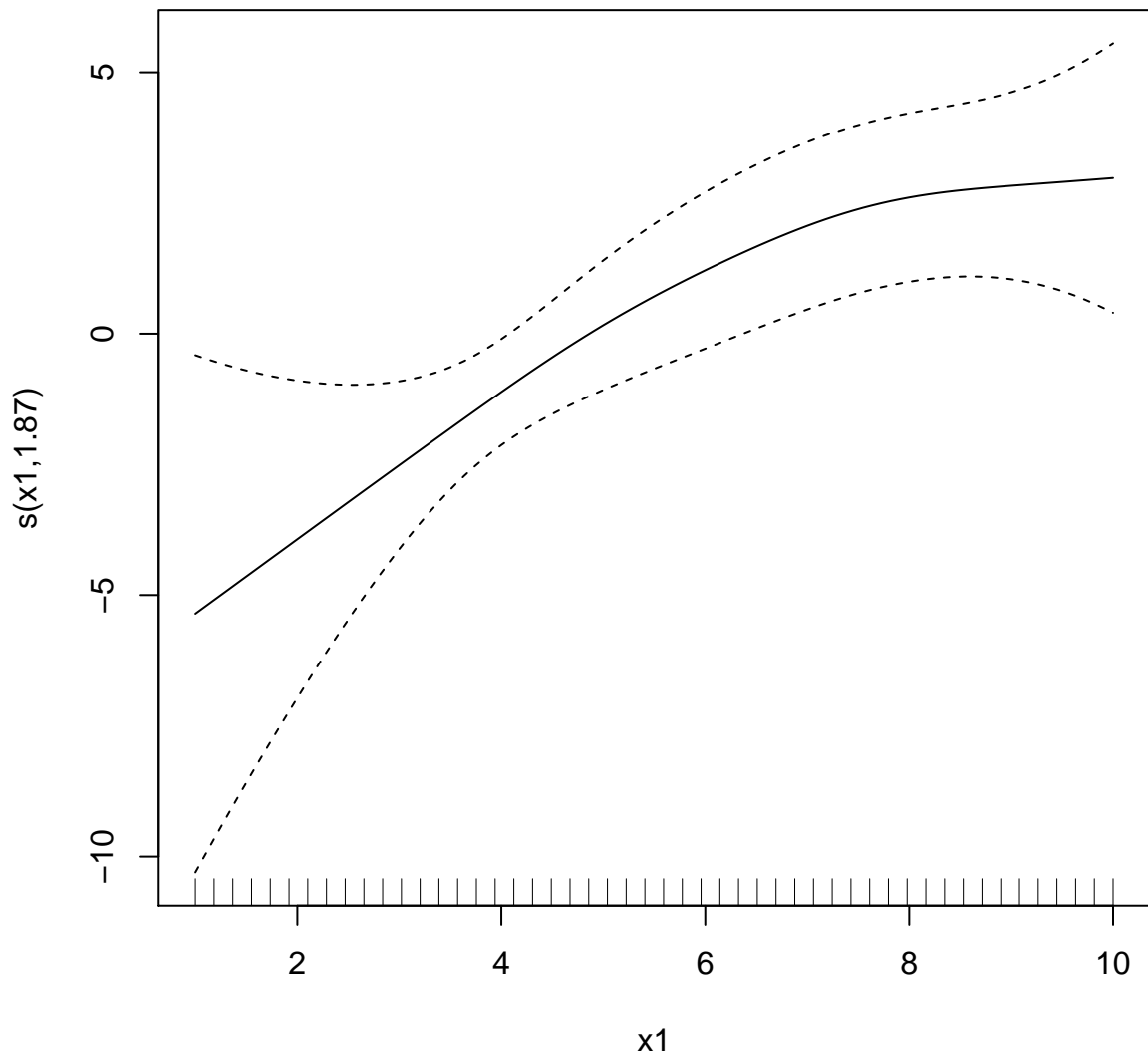
True probabilities vs. estimated probabilities.

```
> plot(p, mygam$fitted.values, pch=19); abline(0,1)
```



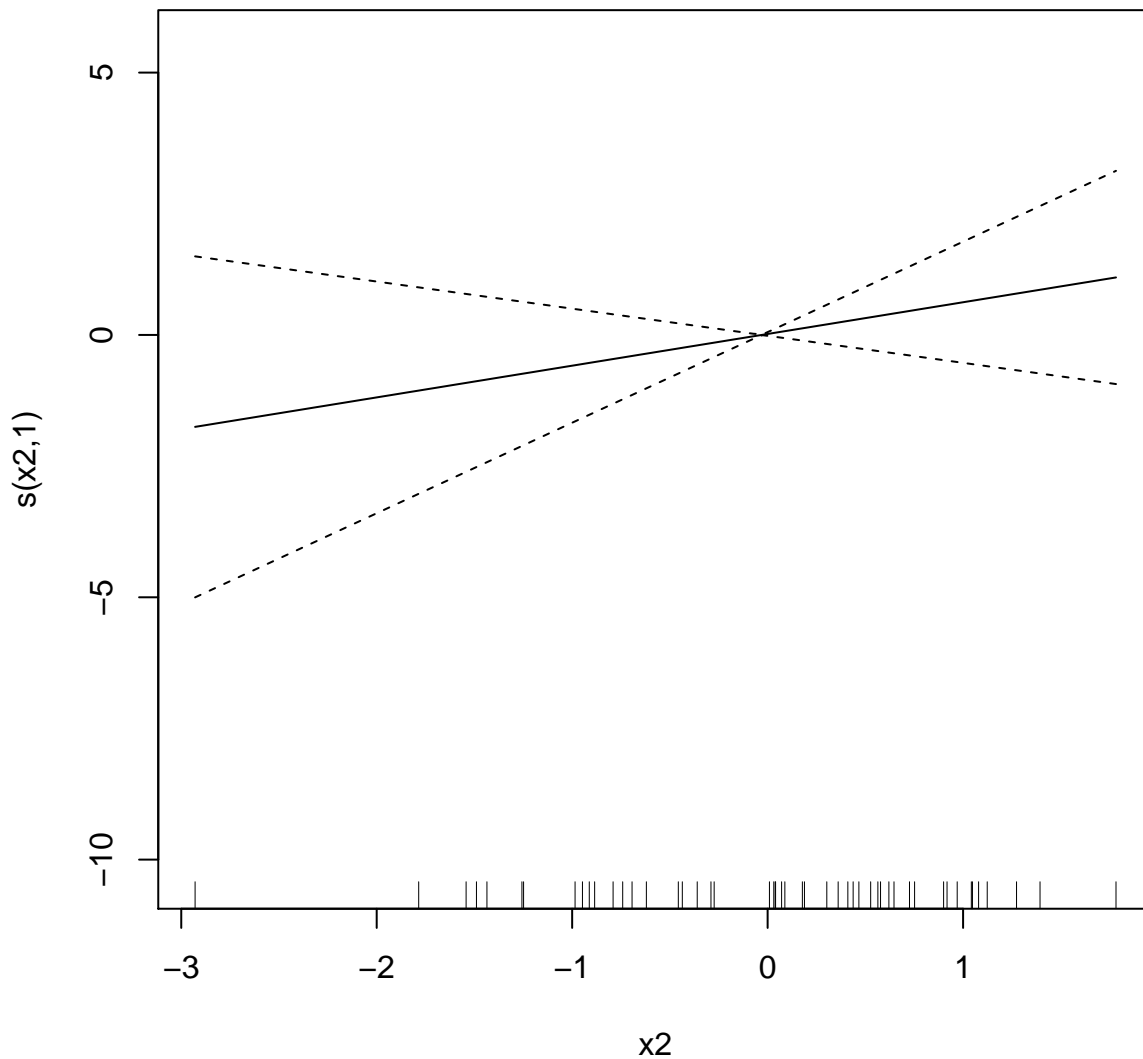
Smoother estimated for $x1$.

```
> plot(mygam, select=1)
```



Smoother estimated for x_2 .

```
> plot(mygam, select=2)
```



Here, we use the `glm()` function and include as an explanatory variable a NCS built from the `ns()` function from the `splines` library. We include a `df` argument in the `ns()` call.

```
> library(splines)
> myglm <- glm(y ~ ns(x1, df=2) + x2, family = binomial(), data=df)
> tidy(myglm)
# A tibble: 4 x 5
  term          estimate std.error statistic p.value
<chr>          <dbl>    <dbl>    <dbl>   <dbl>
1 (Intercept)   -10.9      5.31     -2.06  0.0396
2 ns(x1, df = 2)1  21.4     10.1      2.11  0.0348
3 ns(x1, df = 2)2   6.33      2.11      3.00  0.00272
4 x2             0.734     0.609     1.21  0.228
```

The spline basis evaluated at `x1` values.

```
> ns(x1, df=2)
      1      2
[1,] 0.0000000 0.0000000
[2,] 0.03114456 -0.02075171
[3,] 0.06220870 -0.04138180
[4,] 0.09311200 -0.06176867
```

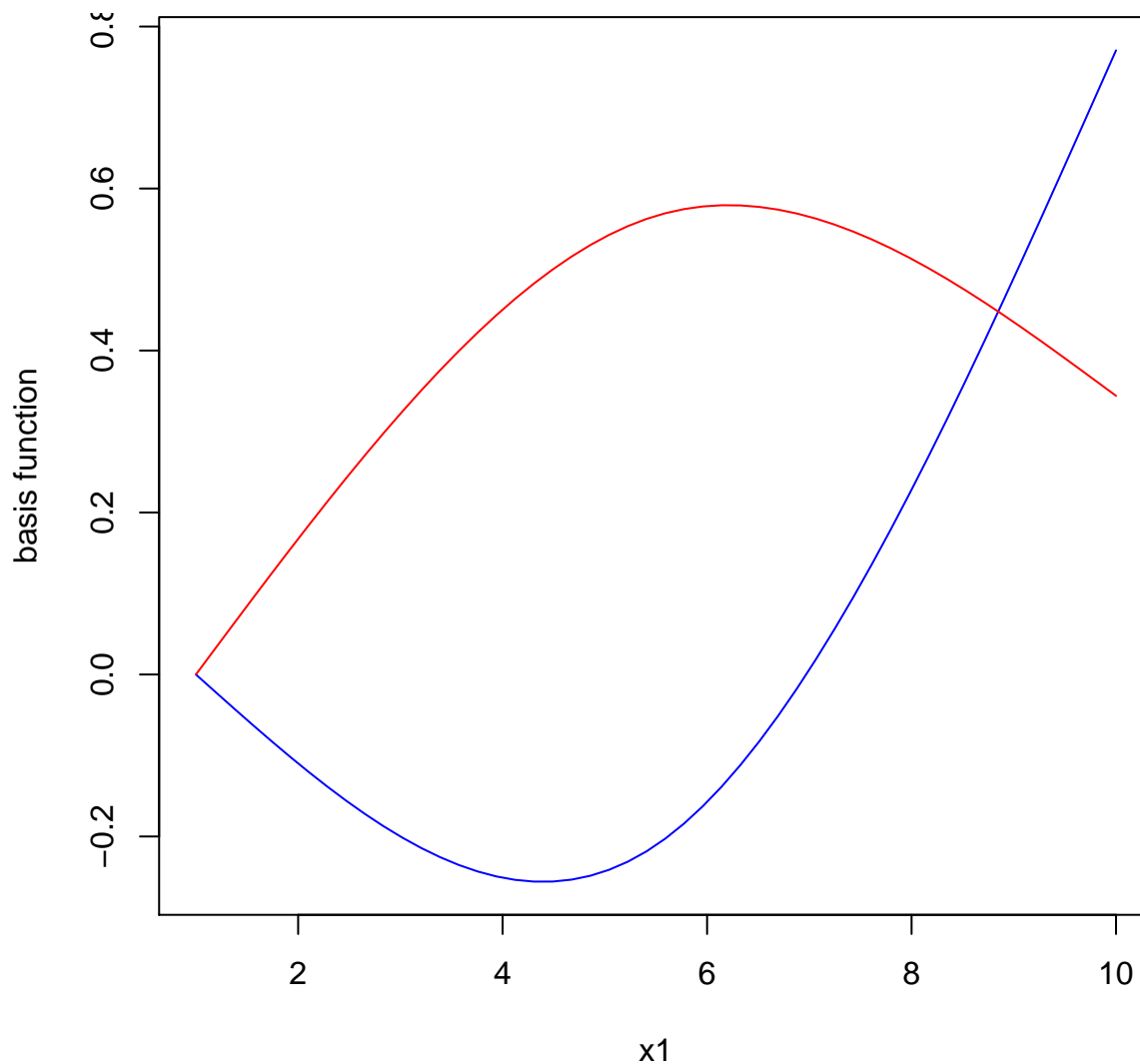
```

[5,] 0.12377405 -0.08179071
[6,] 0.15411442 -0.10132630
[7,] 0.18405270 -0.12025384
[8,] 0.21350847 -0.13845171
[9,] 0.24240131 -0.15579831
[10,] 0.27065081 -0.17217201
[11,] 0.29817654 -0.18745121
[12,] 0.32489808 -0.20151430
[13,] 0.35073503 -0.21423967
[14,] 0.37560695 -0.22550571
[15,] 0.39943343 -0.23519080
[16,] 0.42213406 -0.24317334
[17,] 0.44362840 -0.24933170
[18,] 0.46383606 -0.25354429
[19,] 0.48267660 -0.25568949
[20,] 0.50006961 -0.25564569
[21,] 0.51593467 -0.25329128
[22,] 0.53019136 -0.24850464
[23,] 0.54275927 -0.24116417
[24,] 0.55355797 -0.23114825
[25,] 0.56250705 -0.21833528
[26,] 0.56952943 -0.20260871
[27,] 0.57462513 -0.18396854
[28,] 0.57787120 -0.16253131
[29,] 0.57934806 -0.13841863
[30,] 0.57913614 -0.11175212
[31,] 0.57731586 -0.08265339
[32,] 0.57396762 -0.05124405
[33,] 0.56917185 -0.01764570
[34,] 0.56300897 0.01802003
[35,] 0.55555939 0.05563154
[36,] 0.54690354 0.09506722
[37,] 0.53712183 0.13620546
[38,] 0.52629468 0.17892464
[39,] 0.51450251 0.22310315
[40,] 0.50182573 0.26861939
[41,] 0.48834478 0.31535174
[42,] 0.47414005 0.36317859
[43,] 0.45929198 0.41197833
[44,] 0.44388099 0.46162934
[45,] 0.42798748 0.51201003
[46,] 0.41169188 0.56299877
[47,] 0.39507460 0.61447395
[48,] 0.37821607 0.66631397
[49,] 0.36119670 0.71839720
[50,] 0.34409692 0.77060206
attr(,"degree")
[1] 3
attr(,"knots")
50%
5.5
attr(,"Boundary.knots")
[1] 1 10

```

```
attr("intercept")
[1] FALSE
attr("class")
[1] "ns"      "basis"   "matrix"
```

Plot of basis function values vs x1.



```
> summary(myglm)
```

Call:

```
glm(formula = y ~ ns(x1, df = 2) + x2, family = binomial(), data = df)
```

Deviance Residuals:

Min	1Q	Median	3Q	Max
-2.0214	-0.3730	-0.0162	0.5762	1.7616

Coefficients:

	Estimate	Std. Error	z value	Pr(> z)
(Intercept)	-10.9229	5.3079	-2.058	0.03960 *
ns(x1, df = 2)1	21.3848	10.1318	2.111	0.03480 *
ns(x1, df = 2)2	6.3266	2.1103	2.998	0.00272 **

```

x2                0.7342    0.6089    1.206    0.22795
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```

(Dispersion parameter for binomial family taken to be 1)

```

Null deviance: 68.029 on 49 degrees of freedom
Residual deviance: 35.682 on 46 degrees of freedom
AIC: 43.682

```

Number of Fisher Scoring iterations: 7

```
> anova(myglm, test="LRT")
```

Analysis of Deviance Table

Model: binomial, link: logit

Response: y

Terms added sequentially (first to last)

	Df	Deviance	Resid.	Df	Resid. Dev	Pr(>Chi)
NULL				49	68.029	
ns(x1, df = 2)	2	30.755		47	37.274	2.097e-07 ***
x2	1	1.592		46	35.682	0.207

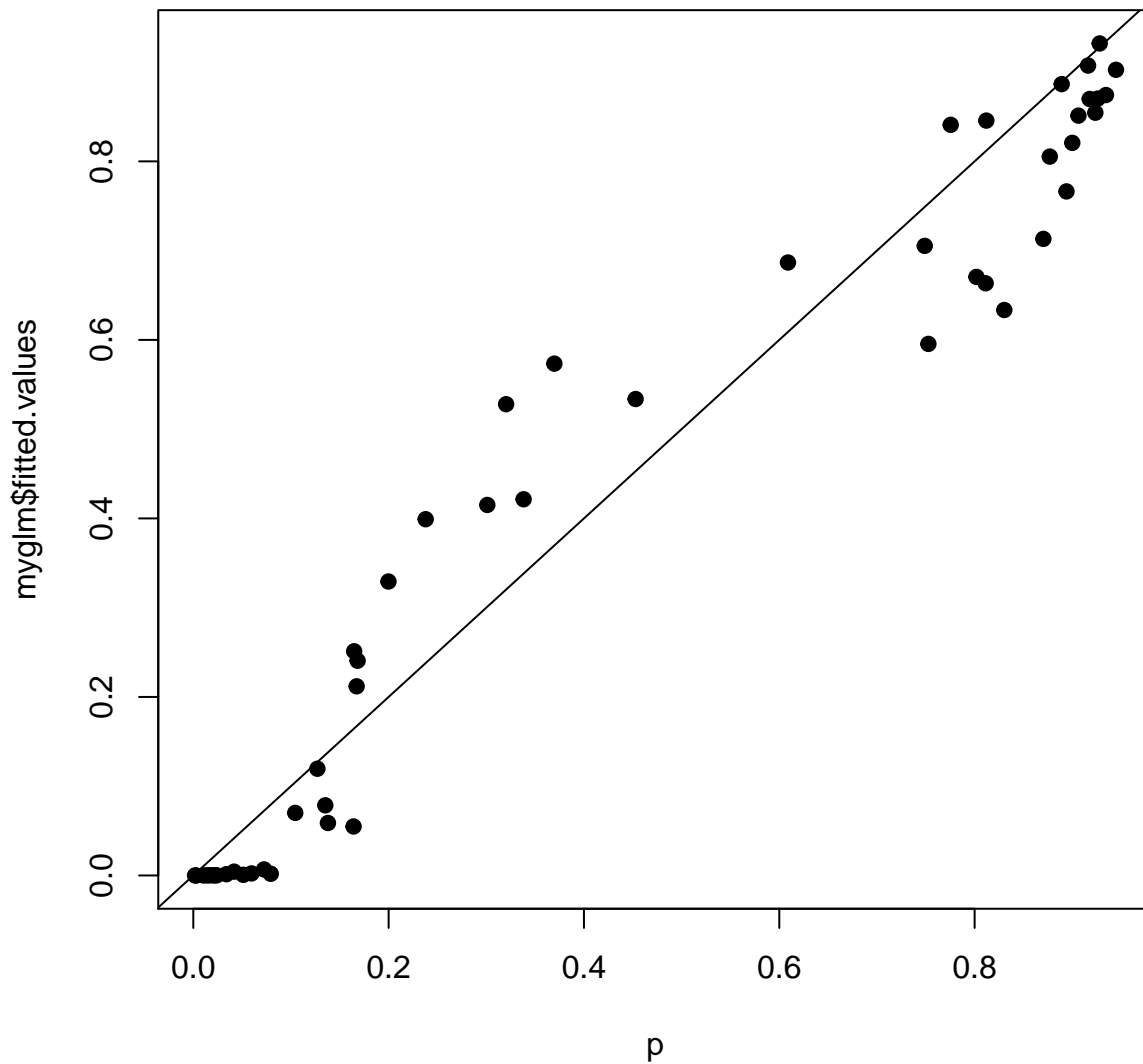
```

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

```

True probabilities vs. estimated probabilities.

```
> plot(p, myglm$fitted.values, pch=19); abline(0,1)
```



Bootstrap for Statistical Models

Homoskedastic Models

Let's first discuss how one can utilize the bootstrap on any of the three homoskedastic models:

- Simple linear regression
- Ordinary least squares
- Additive models

Residuals

In each of these scenarios we sample data $(\mathbf{X}_1, Y_1), (\mathbf{X}_2, Y_2), \dots, (\mathbf{X}_n, Y_n)$. Let suppose we calculate fitted values \hat{Y}_i and they are unbiased:

$$E[\hat{Y}_i | \mathbf{X}] = E[Y_i | \mathbf{X}].$$

We can calculate residuals $\hat{E}_i = Y_i - \hat{Y}_i$ for $i = 1, 2, \dots, n$.

Studentized Residuals

One complication is that the residuals have a covariance. For example, in OLS we showed that

$$\text{Cov}(\hat{\mathbf{E}}) = \sigma^2(\mathbf{I} - \mathbf{P})$$

where $\mathbf{P} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$.

To correct for this induced heteroskedasticity, we studentize the residuals by calculating

$$R_i = \frac{\hat{E}_i}{\sqrt{1 - P_{ii}}}$$

which gives $\text{Cov}(\mathbf{R}) = \sigma^2 \mathbf{I}$.

Confidence Intervals

The following is a bootstrap procedure for calculating a confidence interval on some statistic $\hat{\theta}$ calculated from a homoskedastic model fit. An example is $\hat{\beta}_j$ in an OLS.

1. Fit the model to obtain fitted values \hat{Y}_i , studentized residuals R_i , and the statistic of interest $\hat{\theta}$.
For $b = 1, 2, \dots, B$.
2. Sample n observations with replacement from $\{R_i\}_{i=1}^n$ to obtain bootstrap residuals $R_1^*, R_2^*, \dots, R_n^*$.
3. Form new response variables $Y_i^* = \hat{Y}_i + R_i^*$.
4. Fit the model to obtain \hat{Y}_i^* and all other fitted parameters.
5. Calculate statistic of interest $\hat{\theta}^{*(b)}$.

The bootstrap statistics $\hat{\theta}^{*(1)}, \hat{\theta}^{*(2)}, \dots, \hat{\theta}^{*(B)}$ are then utilized through one of the techniques discussed earlier (percentile, pivotal, studentized pivotal) to calculate a bootstrap CI.

Hypothesis Testing

Suppose we are testing the hypothesis $H_0 : E[Y|\mathbf{X}] = f_0(\mathbf{X})$ vs $H_1 : E[Y|\mathbf{X}] = f_1(\mathbf{X})$. Suppose it is possible to form unbiased estimates $f_0(\mathbf{X})$ and $f_1(\mathbf{X})$ given \mathbf{X} , and f_0 is a restricted version of f_1 .

Suppose also we have a statistic $T(\hat{f}_0, \hat{f}_1)$ for performing this test so that the larger the statistic, the more evidence there is against the null hypothesis in favor of the alternative.

The big picture strategy is to bootstrap studentized residuals from the unconstrained (alternative hypothesis) fitted model and then add those to the constrained (null hypothesis) fitted model to generate bootstrap null data sets.

1. Fit the models to obtain fitted values $\hat{f}_0(\mathbf{X}_i)$ and $\hat{f}_1(\mathbf{X}_i)$, studentized residuals R_i from the fit $\hat{f}_1(\mathbf{X}_i)$, and the observed statistic $T(\hat{f}_0, \hat{f}_1)$.
For $b = 1, 2, \dots, B$.
2. Sample n observations with replacement from $\{R_i\}_{i=1}^n$ to obtain bootstrap residuals $R_1^*, R_2^*, \dots, R_n^*$.
3. Form new response variables $Y_i^* = \hat{f}_0(\mathbf{X}_i) + R_i^*$.
4. Fit the models on the response variables Y_i^* to obtain \hat{f}_0^* and \hat{f}_1^* .
5. Calculate statistic $T(\hat{f}_0^{*(b)}, \hat{f}_1^{*(b)})$.

The p-value is then calculated as

$$\frac{\sum_{b=1}^B 1 \left(T(\hat{f}_0^{*(b)}, \hat{f}_1^{*(b)}) \geq T(\hat{f}_0, \hat{f}_1) \right)}{B}$$

Parametric Bootstrap

For more complex scenarios, such as GLMs, GAMs, and heteroskedastic models, it is typically more straightforward to utilize a parametric bootstrap.

Extras

Source

License

Source Code

Session Information

```
> sessionInfo()
R version 3.6.0 (2019-04-26)
Platform: x86_64-apple-darwin15.6.0 (64-bit)
Running under: macOS 10.15.3

Matrix products: default
BLAS: /Library/Frameworks/R.framework/Versions/3.6/Resources/lib/libRblas.0.dylib
LAPACK: /Library/Frameworks/R.framework/Versions/3.6/Resources/lib/libRlapack.dylib

locale:
[1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8

attached base packages:
[1] splines      stats      graphics  grDevices  utils      datasets
[7] methods     base

other attached packages:
[1] mgcv_1.8-31      nlme_3.1-144     broom_0.5.2
[4] forcats_0.5.0   stringr_1.4.0    dplyr_0.8.4
[7] purrr_0.3.3     readr_1.3.1      tidyr_1.0.2
[10] tibble_2.1.3    ggplot2_3.2.1    tidyverse_1.3.0
[13] knitr_1.28

loaded via a namespace (and not attached):
[1] tidyselect_1.0.0 xfun_0.12        haven_2.2.0
[4] lattice_0.20-40  colorspace_1.4-1 vctrs_0.2.3
[7] generics_0.0.2  htmltools_0.4.0  yaml_2.2.1
[10] utf8_1.1.4      rlang_0.4.5      pillar_1.4.3
[13] withr_2.1.2     glue_1.3.1       DBI_1.1.0
[16] dbplyr_1.4.2    modelr_0.1.6     readxl_1.3.1
[19] plyr_1.8.5      lifecycle_0.1.0  munsell_0.5.0
[22] gtable_0.3.0    cellranger_1.1.0 rvest_0.3.5
[25] codetools_0.2-16 evaluate_0.14     labeling_0.3
[28] fansi_0.4.1     highr_0.8        Rcpp_1.0.3
[31] scales_1.1.0    backports_1.1.5  jsonlite_1.6.1
[34] farver_2.0.3    fs_1.3.1         hms_0.5.3
[37] digest_0.6.25   stringi_1.4.6    grid_3.6.0
[40] cli_2.0.2       tools_3.6.0      magrittr_1.5
[43] lazyeval_0.2.2  crayon_1.3.4     pkgconfig_2.0.3
```

```
[46] Matrix_1.2-18      xml2_1.2.2      reprex_0.3.0
[49] lubridate_1.7.4    assertthat_0.2.1 rmarkdown_2.1
[52] httr_1.4.1         rstudioapi_0.11  R6_2.4.1
[55] compiler_3.6.0
```