Logistic Regression Diagnostics

Fundamental Techniques in Data Science

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Outline

Assumptions & Diagnostics

- Statistical Assumptions
- Residuals
- Diagnostics
- Computational Considerations
- Influential Cases

Recap: Model Definition

We define the logistic regression model as:

$$Y \sim \text{Bin}(\pi, 1)$$

$$\text{logit}(\pi) = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$$

We denote the untransformed linear predictor as η:

$$\eta = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$$

The logit link represents the natural log of the odds of success:

$$\text{logit}(\pi) = \ln\left(\frac{\pi}{1-\pi}\right)$$

Recap: Inverse Link Function

In logistic regression, the inverse link function, $g^{-1}(\cdot)$, is the *logistic function*:

$$\text{logistic}(X) = \frac{e^X}{1 + e^X}$$

So, we convert η to π by:

$$\pi = \frac{e^\eta}{1 + e^\eta} = \frac{\exp\left(\beta_0 + \sum_{p=1}^{P} \beta_p X_p\right)}{1 + \exp\left(\beta_0 + \sum_{p=1}^{P} \beta_p X_p\right)}$$

ASSUMPTIONS & DIAGNOSTICS

Assumptions of Logistic Regression

The first two assumptions of logistic regression are shared with linear regression.

1. The model is linear in the parameters.
   - This is OK: $logit(\pi) = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ + \beta_4 X^2 + \beta_5 X^3$
   - This is not: $logit(\pi) = \beta_0 X^{\beta_1}$
2. The predictor matrix is *full rank*.
   - $N > P$
   - No X_p can be a linear combination of other predictors.

Assumptions of Logistic Regression

The distributional assumptions of logistic regression are not framed in terms of residuals.

- Linear regression

$$Y \sim \mathrm{N}\left(\hat{Y}, \hat{\sigma}^2\right)$$

$$Y = \hat{Y} + \hat{\varepsilon}$$

$$\varepsilon \sim \mathrm{N}\left(0, \sigma^2\right)$$

- Logistic regression

$$Y \sim \text{Bin}\left(\hat{\pi}, 1\right)$$

Assumptions of Logistic Regression

The variance of the binomial distribution is a function of its mean.

- Linear regression

$$\bar{Y} = \hat{Y},\ \text{var}(Y) = \hat{\sigma}^2$$

- Logistic regression

$$\bar{Y} = \hat{\pi},\ \text{var}(Y) = \hat{\pi}\left(1 - \hat{\pi}\right)$$

So, we consider the entire outcome distribution in logistic regression.

- We can succinctly summarize the distributional assumptions of logistic regression as:

$$Y_i \overset{iid}{\sim} \text{Bin}\left(\hat{\pi}_i, 1\right)$$

Assumptions of Logistic Regression

We end up with three assumptions where the third assumption fills the role played by all residual-related assumptions in linear regression.

1. The model is linear in the parameters.
2. The predictor matrix is *full rank*.
3. The outcome is independently and identically binomially distributed.

$$
\begin{aligned}
Y_n &\overset{iid}{\sim} \text{Bin}\left(\hat{\pi}_n, 1\right) \\
\hat{\pi}_n &= \text{logistic}\left(\hat{\beta}_0 + \sum_{p=1}^{P} \hat{\beta}_p X_{np}\right)
\end{aligned}
$$

Example

To demonstrate these ideas, we'll fit a logistic regression model that predicts the chances of Titanic passengers surviving based on their age, sex, and ticket price

```r
## Read the data:
titanic <- titanic0 <- readRDS(here::here("data", "titanic.rds"))

## Estimate the logistic regression model:
glmFit <- glm(survived ~ age + sex + fare,
              data = titanic,
              family = "binomial")

## Save the linear predictor estimates:
titanic$etaHat <- predict(glmFit, type = "link")
```

Example

```
partSummary(glmFit, -1)

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  0.837621   0.215121   3.894 9.87e-05
age         -0.007404   0.006040  -1.226     0.22
sexmale     -2.392422   0.171288 -13.967  < 2e-16
fare         0.011586   0.002338   4.955 7.23e-07

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 1182.8  on 886  degrees of freedom
Residual deviance:  881.4  on 883  degrees of freedom
AIC: 889.4

Number of Fisher Scoring iterations: 5
```

Raw Residuals

In logistic regression the outcome is binary, $Y \in \{0, 1\}$, but the parameter that we're trying to model is continuous, $\pi \in (0, 1)$.

- Due to this mismatch in measurement levels, we don't have a natural definition of a ”residual” in logistic regression.
- We have a few potential operationalizations.

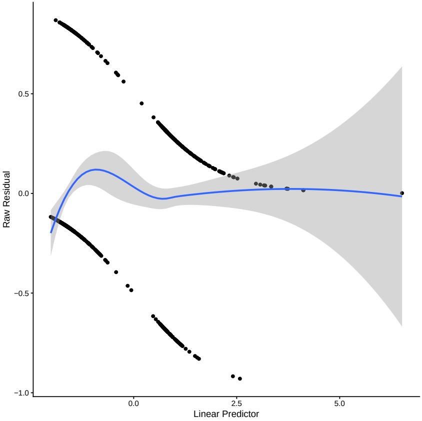
The most basic residual is the *raw residual*, e_n.

- The difference between the observed outcome value and the predicted probability.

$$e_n = Y_n - \hat{\pi}_n$$

Raw Residuals

```r
library(ggplot)

## Calculate the raw residuals:
titanic$e <-
  resid(glmFit, type = "response")

## Plot raw residuals vs. fitted
## linear predictor values:
ggplot(titanic, aes(etaHat, e)) +
  geom_point() +
  geom_smooth() +
  theme_classic() +
  xlab("Linear Predictor") +
  ylab("Raw Residual")
```

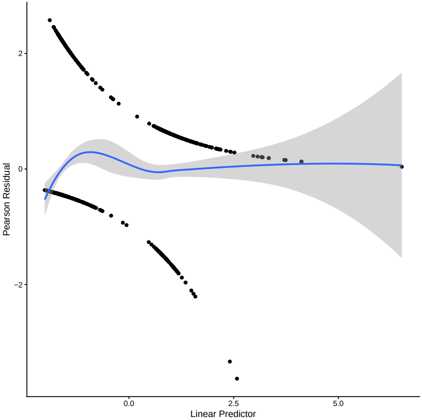


Pearson Residuals

Pearson residuals, r_n, are scaled raw residuals.

$$r_n = \frac{e_n}{\sqrt{\hat{\pi}_n(1 - \hat{\pi}_n)}}$$

```r
## Calculate the Pearson residuals:
titanic$r <-
  resid(glmFit, type = "pearson")
```



Deviance Residuals

Deviance residuals, d_n, are derived directly from the objective function used to estimate the model.

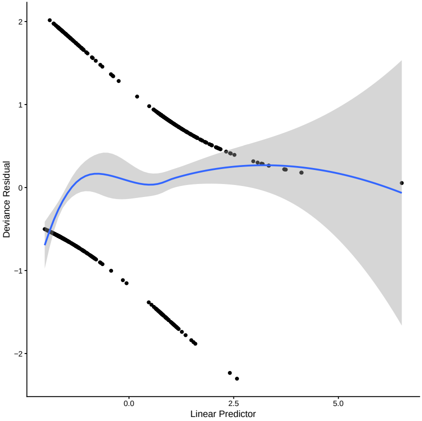
$$d_n = \text{sign}(e_n)\sqrt{-2\left[Y_n \ln\left(\hat{\pi}_n\right) + (1 - Y_n)\ln\left(1 - \hat{\pi}_n\right)\right]}$$

The *residual deviance*, D, is the sum of squared deviance residuals.

$$D = \sum_{n=1}^{N} d_n^2$$

Deviance Residuals

```
## Calculate the deviance residuals:
titanic$d <-
  resid(glmFit, type = "deviance")

## Calculate the residual deviance:
titanic$d^2 |> sum()

[1] 881.4048

summary(glmFit)$deviance

[1] 881.4048
```



Residual Deviance

The residual deviance quantifies how well the model fits the data.

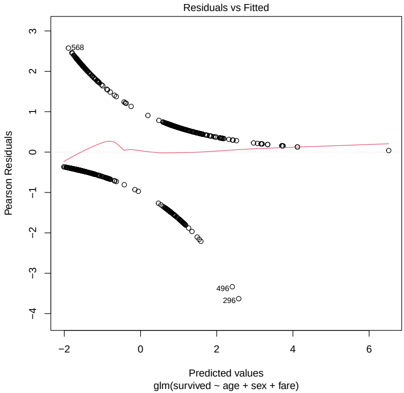
```
## Estimate a null model:
nullFit <- glm(survived ~ 1, family = binomial, data = titanic)

## Test the fit of our example model:
anova(nullFit, glmFit, test = "Chisq")

Analysis of Deviance Table

Model 1: survived ~ 1
Model 2: survived ~ age + sex + fare
  Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
1       886     1182.8
2       883      881.4  3   301.37 < 2.2e-16 ***
---
Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

A1: Linearity

```
plot(glmFit, 1)
```

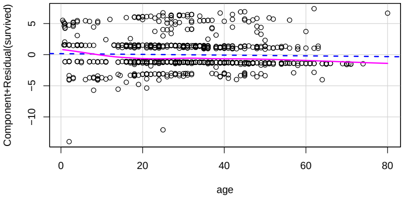
Assumption 1 implies a linear relation between continuous predictors and the *logit of the success probability*.

- We can basically evaluate the linearity assumption using the same methods we applied with linear regression.
- $\hat{Y} \rightarrow \hat{\eta} = \text{logit}\left(\hat{\pi}\right)$

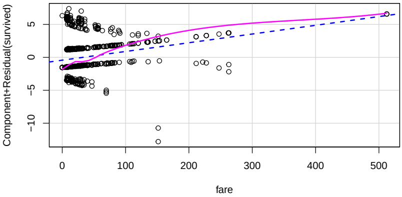


A1: Linearity

```
car::crPlot(glmFit, "age")
```



```
car::crPlot(glmFit, "fare")
```



A2: Predictor Matrix Rank

Assumption 2 implies two conditions:

1. $P < N$
2. No severe (multi)collinearity among the predictors

We can quantify multicollinearity with the *variance inflation factor* (VIF).

```
car::vif(glmFit)

     age      sex     fare
1.031829 1.007699 1.026373
```

VIF $>$ 10 indicates severe multicollinearity.

A3: IID Binomial

Assumption 3 implies several conditions.

1. The outcome, Y, is binary.
2. The linear predictor, η, can explain all the systematic trends in π.
   - No residual clustering after accounting for $\mathbf{X}$.
   - No important variables omitted from $\mathbf{X}$.

We can easily check the first condition with summary statistics.

```
levels(titanic$survived)

[1] "no"  "yes"

table(titanic$survived)


 no yes
545 342
```

Alternative Modeling Schemes

If we have a non-binary, categorical outcome, we can use a different type of model.

- Multiclass nominal variables: Multinomial logistic regression
  - `nnet::multinom()`
- Ordinal variables: Proportional odds logistic regression
  - `MASS::polr()`
- Counts: Poisson regression
  - `glm()` with `family = ’poisson’`

The binomial distribution (and logistic regression) is also appropriate for modeling the proportion of successes in N trials.

A3: Clustering

We can check for residual clustering by calculating the ICC using deviance residuals.

```r
## Check for residual dependence induced by 'class':
ICC::ICCbare(x = titanic$class, y = resid(glmFit, type = "deviance"))

[1] 0.1054665
```

Computational Considerations

In addition to the preceding statistical assumptions, we must satisfy three computational requirements that were not necessary in linear regression.

1. The sample size is large enough to support the necessary numerical estimation.
2. The outcome classes are sufficiently balanced.
3. There is no perfect prediction.

Sufficient Sample Size

Logistic regression models are estimated with numerical methods, so we need larger samples than we would for linear regression models.

- The sample size requirements increase with model complexity.

Some suggested rules of thumb:

- 10 cases for each predictor (Agresti, 2018)
- $N = 10P/\pi_0$ (Peduzzi, Concato, Kemper, Holford, & Feinstein, 1996)
    - P: Number of predictors
    - π_0: Proportion of the minority class
- $N = 100 + 50P$ (Bujang, Omar, & Baharum, 2018)

Balanced Outcomes

The logistic regression may not perform well when the outcome classes are severely imbalanced.

```r
with(titanic, table(survived) / length(survived))

survived
       no       yes
0.6144307 0.3855693
```

We have a few possible solutions for problematic imbalance:

- Down-sampling the majority class
- Up-sampling the minority class
- Use weights when estimating the logistic regression model
  - `weights` argument in `glm()`

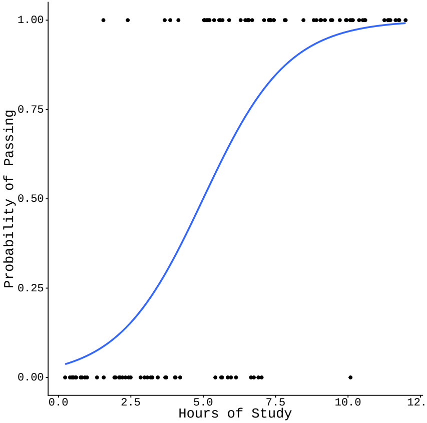
Perfect Prediction

We don't actually want to perfectly predict class membership.

- The model cannot estimate with perfectly separable classes.

Model regularization (e.g., ridge or LASSO penalty) may help.

- `glmnet::glmnet()`



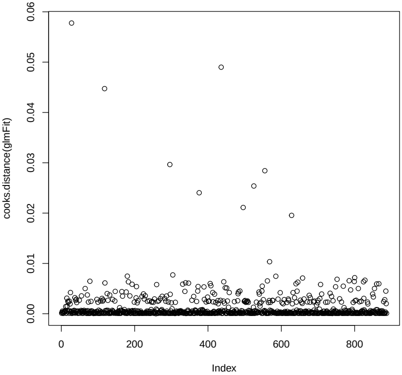
Influential Cases

As with linear regression, we need to deal with any overly influential cases.

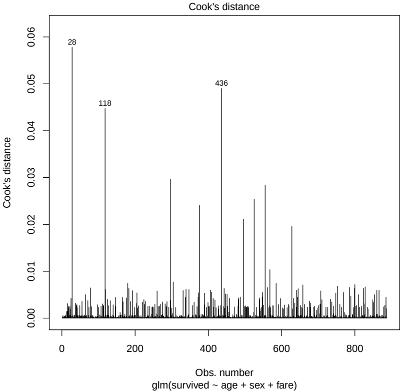
- We can use the linear predictor values to calculate Cook’s Distances.
- Any cases that exerts undue influence on the linear predictor will have the same effect of the predicted success probabilities.

Influential Cases

```
cooks.distance(glmFit) |> plot()
```

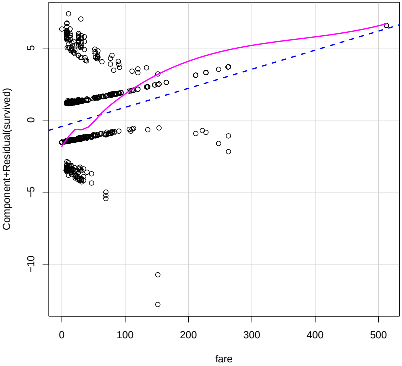


```
plot(glmFit, 4)
```

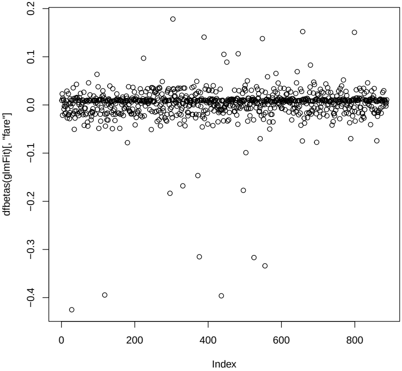


Influential Cases

```r
car::crPlots(glmFit, "fare")
```



```r
dfbetas(glmFit)[ , "fare"] |> plot()
```



Influential Cases

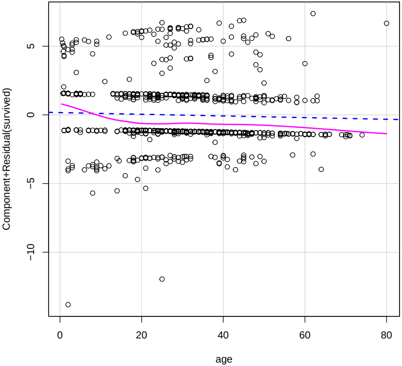
```
(maxCD  <- cooks.distance(glmFit) |> which.max())

28
28

(maxDFB <- dfbetas(glmFit)[ , "fare"] |> abs() |> which.max())

28
28

titanic0[maxDFB, ]

   survived class                          name  sex age
28       no   1st Mr. Charles Alexander Fortune male  19
   siblings_spouses parents_children fare
28                3                2  263
```

Influential Cases

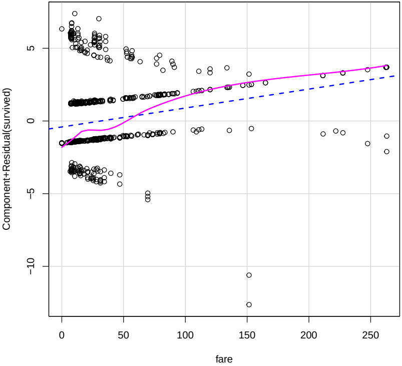
```r
# View the largest 12 fares:
sortFare <- titanic$fare |> sort(decreasing = TRUE)
head(sortFare, 12)

 [1] 512.3292 512.3292 512.3292 263.0000 263.0000 263.0000
 [7] 263.0000 262.3750 262.3750 247.5208 247.5208 227.5250

# Find the observation number for the three largest fares:
moneyBags <- which(titanic$fare %in% sortFare[1:3])

# Refit the model excluding the cases with the three largest fares:
titanic2 <- titanic[-moneyBags, ]
glmFit2 <- update(glmFit, data = titanic2)
```

Influential Cases

```
car::crPlots(glmFit2, "age")
```



```
car::crPlots(glmFit2, "fare")
```



Influential Cases

```
summary(glmFit)$coef |> round(3)

            Estimate Std. Error z value Pr(>|z|)
(Intercept)    0.838      0.215   3.894     0.00
age           -0.007      0.006  -1.226     0.22
sexmale       -2.392      0.171 -13.967     0.00
fare           0.012      0.002   4.955     0.00

summary(glmFit2)$coef |> round(3)

            Estimate Std. Error z value Pr(>|z|)
(Intercept)    0.840      0.215   3.899    0.000
age           -0.007      0.006  -1.221    0.222
sexmale       -2.393      0.171 -13.970    0.000
fare           0.011      0.002   4.824    0.000
```

Influential Cases

```
partSummary(glmFit, 4)

    Null deviance: 1182.8  on 886  degrees of freedom
Residual deviance:  881.4  on 883  degrees of freedom
AIC: 889.4

partSummary(glmFit2, 4)

    Null deviance: 1177.04  on 883  degrees of freedom
Residual deviance:  881.34  on 880  degrees of freedom
AIC: 889.34
```

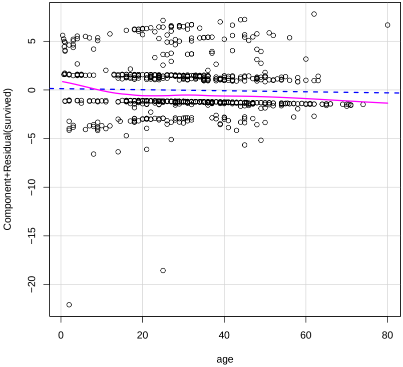
Influential Cases

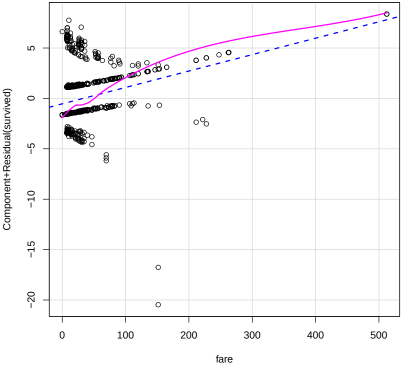
```
# Find the three most influential cases:
mostInf <- which(cooks.distance(glmFit) > 0.04)

# View the three most influential cases:
titanic0[mostInf, ]

    survived class                          name  sex age
28        no   1st Mr. Charles Alexander Fortune male  19
118       no   1st       Mr. Quigg Edmond Baxter male  24
436       no   1st              Mr. Mark Fortune male  64
    siblings_spouses parents_children     fare
28                 3                2 263.0000
118                0                1 247.5208
436                1                4 263.0000

# Refit the model excluding the three most influential cases:
titanic3 <- titanic[-mostInf, ]
glmFit3 <- update(glmFit, data = titanic3)
```

Influential Cases

```
car::crPlots(glmFit3, "age")
```

```
car::crPlots(glmFit3, "fare")
```





Influential Cases

```
summary(glmFit)$coef |> round(3)

            Estimate Std. Error z value Pr(>|z|)
(Intercept)    0.838      0.215   3.894     0.00
age           -0.007      0.006  -1.226     0.22
sexmale       -2.392      0.171 -13.967     0.00
fare           0.012      0.002   4.955     0.00

summary(glmFit3)$coef |> round(3)

            Estimate Std. Error z value Pr(>|z|)
(Intercept)    0.753      0.217   3.465    0.001
age           -0.008      0.006  -1.367    0.172
sexmale       -2.355      0.172 -13.668    0.000
fare           0.015      0.003   5.460    0.000
```

Influential Cases

```
partSummary(glmFit, 4)

    Null deviance: 1182.8  on 886  degrees of freedom
Residual deviance:  881.4  on 883  degrees of freedom
AIC: 889.4

partSummary(glmFit3, 4)

    Null deviance: 1179.8  on 883  degrees of freedom
Residual deviance:  870.8  on 880  degrees of freedom
AIC: 878.8
```

References

Agresti, A. (2018). *An introduction to categorical data analysis*. Hoboken, NJ: John Wiley & Sons.

Bujang, M. A., Omar, E. D., & Baharum, N. A. (2018). A review on sample size determination for cronbach's alpha test: a simple guide for researchers. *The Malaysian Journal of Medical Sciences*, *25*(6), 85.

Peduzzi, P., Concato, J., Kemper, E., Holford, T. R., & Feinstein, A. R. (1996). A simulation study of the number of events per variable in logistic regression analysis. *Journal of Clinical Epidemiology*, *49*(12), 1373–1379.