Logistic regression

Fundamental Techniques in Data Science

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Outline

Recap
Model assumptions
Residuals
Model selection
Confusion matrix

Generalized linear models (GLMs)

- The mean $E(Y|X) = g^{-1}(\eta) = g^{-1}(\beta_0 + \sum_{p=1}^{P} \beta_p X_p)$
  - A linear function η
  - The link function g
- The variance $V(g^{-1}(\eta))$

Logistic regression

The link function of logistic regression is logit link:

$$ln(\frac{p(Y=1)}{p(Y=0)}) = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$$

The interpretation of the coefficients is on log odds units.

Titanic data

```r
titanic <- read.csv(file = "data/titanic.csv", header = TRUE,
                    stringsAsFactors = TRUE)
```

The titanic data describes the survival status of passengers on the Titanic. For the heuristic, We only include four variables.

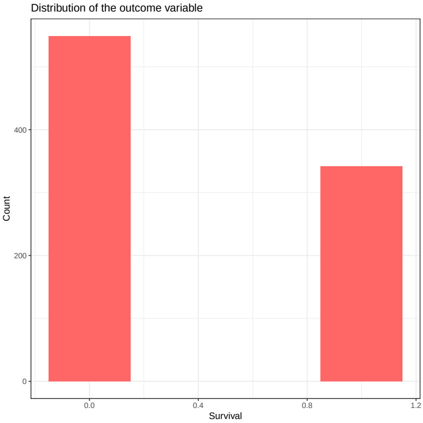
```r
titanic %>% head()

  Survived Pclass      Age    Sex
1        0      3 22.00000   male
2        1      1 38.00000 female
3        1      3 26.00000 female
4        1      1 35.00000 female
5        0      3 35.00000   male
6        0      3 29.69912   male
```

Binary response variable

Logistic regression assumes that the response variable only has two possible outcomes.

For example, “survived” describes the passenger’s survival status where 0 indicates did not survive and 1 indicates survived.



Binary response variable

We can also check the levels of the response variable.

```
titanic$Survived %>% unique()

[1] 0 1

titanic$Survived %>% factor() %>% levels()

[1] "0" "1"
```

The assumption is violated when the outcome is

- a multiclass categorical variable. (multinomial logistic regression `mnet::mutinom()`)
- an ordinal categorical variable. (ordered logistic regression `MASS::polr()`)

Balanced outomes

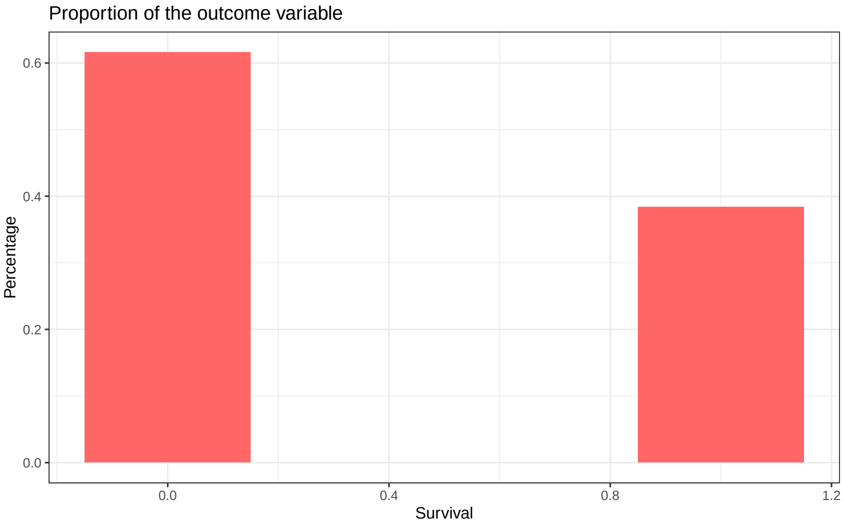
The logistic regression may not perform well when there is an imbalance in the classes of the binary response. A possible consequence is the inaccurate classification.

A certain amount of imbalance is normal and can be handled well by the logistic model in most cases. However, we should care about the severe imbalance, for instance, 1000 cases in the majority class and 1 case in the minority class.

```r
titanic$Survived %>% factor() %>% table() %>%
  prop.table() %>% round(digits = 3)
```

```
.
    0     1 
0.616 0.384 
```

Balanced outomes



Balanced outomes

Some solutions:

- down-sampling the majority class
- up-sampling the minority class
- adding weights to logistic regression (`weights` argument in `glm()`)

Sufficiently large sample size

Sample size in logistic regression is a complex issue. It depends on:

- the number of predictors
- the sample space of predictors
- the distribution of the binary response variable
- the scientific interests

Some suggestions for the sample size

- 10 cases for each predictor in the model (Agresti, 2018)
- $N = \frac{10 * k}{p}$, where
  - k is the number of predictors
  - p is the proportion of the minority class (Peduzzi, Concato, Kemper, Holford, & Feinstein, 1996)
- $N = 100 + 50 * k$, where k is the number of predictors (Bujang, Omar, & Baharum, 2018)

Issue : perfect prediction

Imbalanced outcomes and a small sample size may cause perfect prediction. The `glm()` may show warnings messages:

- glm.fit: algorithm did not converge
- fitted probabilities numerically 0 or 1 occurred

One possible solution is to fit the logistic regression with regularization (`glmnet::glmnet`).

No multicollinearity

The same assumption as in linear regression is that is no multicollinearity among the linear predictors.

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
    data = titanic) %>%
   VIF()

       Age        Sex     Pclass Sex:Pclass
  1.187231  22.400248   7.749858  20.200886
```

A VIF value larger than 10 indicates high multicollinearity.

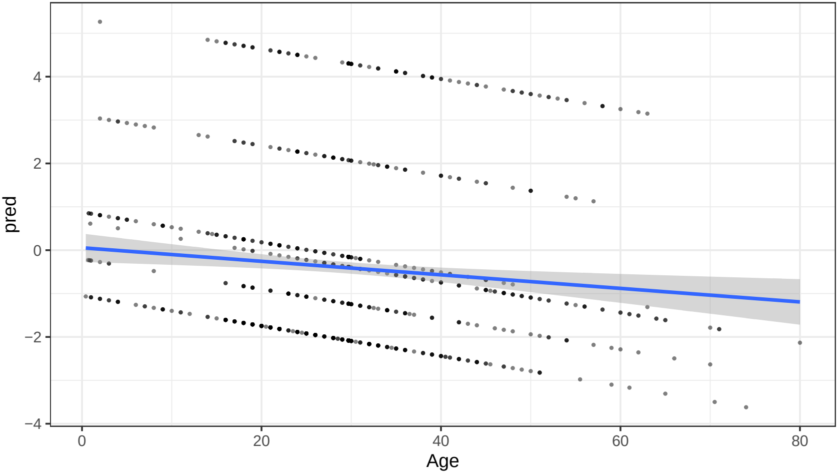
Linearity

Logistic regression assumes a linear relationship between continuous predictors and *the logit of the response variable*.

```r
pred <- glm(Survived ~ Age + Sex*Pclass, family = binomial,
            data = titanic) %>%
        predict(., type = "link")

ggplot(data = data.frame(Age = titanic$Age, pred = pred),
       aes(Age, pred)) +
  geom_point(size = 0.5, alpha = 0.5) +
  geom_smooth(method = "glm") + theme_bw()
```

Linearity



Linearity

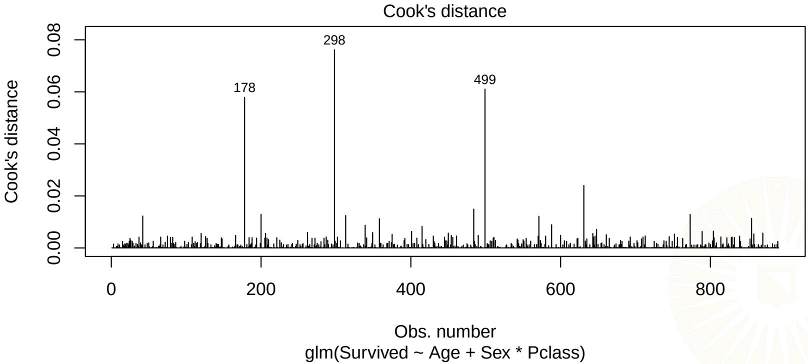
Some solutions for the violation of linearity:

- transform predictors (log transformation)
- add interaction terms or higher-order terms

No influential values or outliers

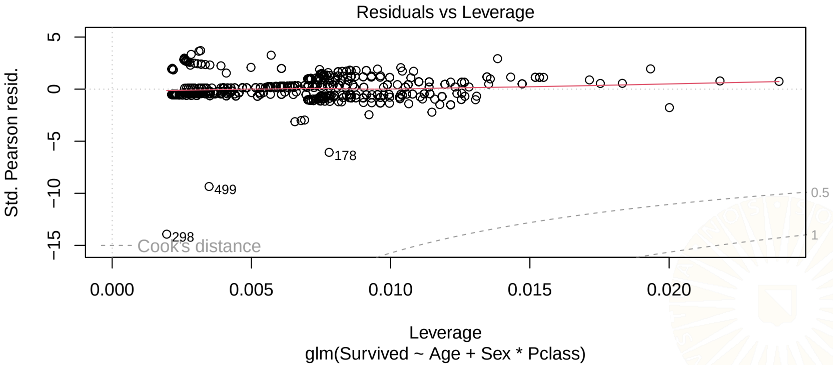
Influential values or outliers can seriously influence the fit of the logistic regression.

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
            data = titanic) %>% plot(., which = 4)
```



No influential values or outliers

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
    data = titanic) %>% plot(., which = 5)
```



No influential values or outliers

Some solutions for influential values or outliers:

- remove them
- keep them but mention them in the result
- robust logistic regression (`robust::glmrob`)

No influential values or outliers

```
glmRob(Survived ~ Age + Sex + Pclass, family = binomial(),
       data = titanic, method = "cubif") %>%
       summary() %>% .$coefficients

                Estimate  Std. Error    z value     Pr(>|z|)
(Intercept)  4.76878301 0.452599082  10.536440 5.867834e-26
Age         -0.03433009 0.007412619  -4.631304 3.633694e-06
Sexmale     -2.60924207 0.187095480 -13.946045 3.325391e-44
Pclass      -1.17625580 0.119412375  -9.850368 6.829363e-23

glm(Survived ~ Age + Sex + Pclass, family = binomial, data = titanic) %>%
  summary() %>% .$coefficients

                Estimate  Std. Error    z value     Pr(>|z|)
(Intercept)  4.73195642 0.449819406  10.519680 7.011095e-26
Age         -0.03342722 0.007347635  -4.549385 5.380296e-06
Sexmale     -2.61196394 0.186608818 -13.997002 1.625866e-44
Pclass      -1.16846287 0.118940571  -9.823922 8.881931e-23
```

Raw residual

The most basic residual is the *raw residual*, which is the difference between the observed value and the predicted probability:

$$e_i = y_i - \hat{p}_i$$

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
            data = titanic) %>% residuals(., type = "response") %>%
  head()

          1           2           3           4           5
-0.14000292  0.01770869  0.50655145  0.01598547 -0.09393664
          6
-0.11080960
```

Pearson residual

The Pearson residual is a scaled version of the raw residual.

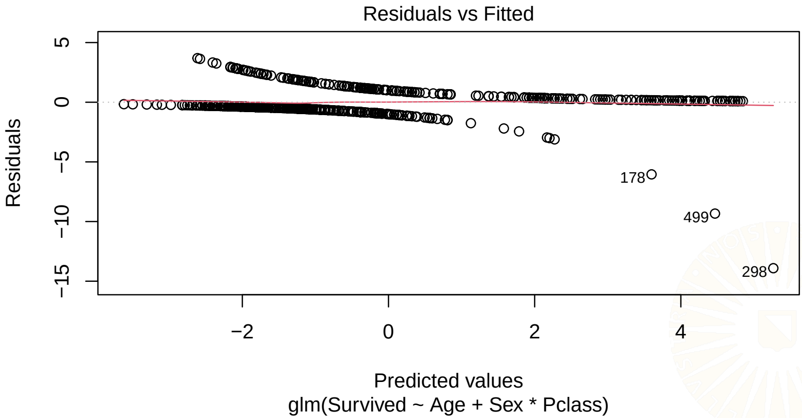
$$r_i = \frac{e_i}{\sqrt{\hat{p}_i(1-\hat{p}_i)}}$$

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
            data = titanic) %>% residuals(., type = "pearson") %>%
  head()

         1          2          3          4          5
-0.4034782  0.1342682  1.0131899  0.1274565 -0.3219869
         6
-0.3530135
```

Pearson residual

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
            data = titanic) %>% plot(., which = 1)
```



Deviance residual

Deviance residuals can be approximated with a standard normal distribution if the model fits well.

$$d_i = sign(e_i)[-2(y_i ln\hat{p}_i + (1 - y_i)ln(1 - \hat{p}_i))]^{1/2}$$

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
    data = titanic) %T>%
  {residuals(., type = "deviance") %>%
      head(., n = 6) %>%
      print()} %>%
  summary() %>% .$deviance.resid %>%
  head(., n = 6)

         1          2          3          4          5
-0.5492291  0.1890363  1.1885594  0.1795250 -0.4441757
         6
-0.4846522
         1          2          3          4          5
-0.5492291  0.1890363  1.1885594  0.1795250 -0.4441757
         6
-0.4846522
```

Residual deviance

The residual deviance is the sum of squared deviance residuals.

$$D = \sum_{i=1}^{N} d_i^2$$

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
            data = titanic) %>%
  summary() %>% .$deviance

[1] 781.1453
```

Residual deviance

The residual deviance is used to measure how well the model fits the data. It is similar to the sum of squared errors in linear regression.

```
result <- glm(Survived ~ Age + Sex*Pclass, family = binomial,
            data = titanic) %>% summary()
1 - pchisq(result$null.deviance - result $deviance,
           result$df.null - result$df.residual)

[1] 0
```

$$
\begin{aligned}
\texttt{null :}&\beta_1 = \beta_2 = \cdots = \beta_p = \texttt{ 0}\\
\texttt{alt :}&\texttt{at least one of the } \beta_i \texttt{ is different from 0}
\end{aligned}
$$

Generally, if the value is less than 0.05, the logistic regression is overall significant.

Model selection

Because including irrelevant variables leads to a needlessly complex model, we need to make the model selection among a large set of candidate models. I will introduce two techniques:

- forward selection
- backward selection

Forward selection

- Start with the null model (a model contains no variables)
- Include the most important variable in the model from the remaining predictors
- repeat step 2 until a stopping rule is reached

The selection criterion defines the most important variable. For example, If the criterion is AIC, the added variable should make the model has the lowest AIC.

Backward selection

- Start with the full model (a model contains all possible variables)
- Remove the least important variable from the model
- repeat step 2 until a stopping rule is reached

Model selection

Here, I show the backward selection by minimizing AIC. The stopping rule is that removal of the least important variable results in the increase of AIC.

```
glm(Survived ~ .^2, family = binomial, data = titanic) %>%
  step(trace = 0)


Call:  glm(formula = Survived ~ Pclass + Age + Sex + Pclass:Sex + Age:Sex,
    family = binomial, data = titanic)

Coefficients:
   (Intercept)          Pclass             Age
       6.73391        -2.09689        -0.01681
       Sexmale  Pclass:Sexmale     Age:Sexmale
      -4.86677         1.19508        -0.02689

Degrees of Freedom: 890 Total (i.e. Null);  885 Residual
Null Deviance:      1187
Residual Deviance: 778.4  AIC: 790.4
```

Confusion matrix

One of the most direct ways to evaluate classification performance is the *Confusion matrix*.

	True	
Predicted	Not survived	Survived
Not survived	507	144
Survived	42	198

Confusion Matrix of passengers’ survival on the Titanic

Confusion matrix

In the titanic example,

- **TP**: correctly predict people that survived
- **TN**: correctly predict people that did not survive
- **FP**: predict people survived, when they did not
- **FN**: predict people did not survive, but they did

Confusion matrix

- **true positive(TP)**: A test result that correctly indicates the presence of a condition.
- **true negative(TN)**: A test result that correctly indicates the absence of a condition.
- **false positive(FP)**: A test result which wrongly indicates that a particular condition is present.
- **false negative(FN)**: A test result which wrongly indicates that a particular condition is absent.

Confusion matrix

		Predicted condition	
		Positive(PP)	Negative(PN)
Actual condition	Positive(P)	True positive(TP)	False negative(FN)
	Negative(N)	Flase positive(FP)	True negative(TN)

Confusion matrix

```
Confusion.matrix<- glm(Survived ~ Age + Sex*Pclass, family = binomial,
    data = titanic) %>% predict(., type = "response") %>%
  {ifelse(. > 0.5, 1, 0)} %>% as.factor() %>%
  confusionMatrix(., reference = as.factor(titanic$Survived),
                  positive = "1")
Confusion.matrix$table

          Reference
Prediction   0   1
         0 507 144
         1  42 198

Confusion.matrix$overall

      Accuracy          Kappa  AccuracyLower  AccuracyUpper
  7.912458e-01   5.323785e-01   7.630562e-01   8.174942e-01
  AccuracyNull AccuracyPValue  McnemarPValue
  6.161616e-01   2.391263e-29   1.304808e-13
```

Confusion matrix

```
Confusion.matrix$byClass

         Sensitivity          Specificity
           0.5789474            0.9234973
      Pos Pred Value       Neg Pred Value
           0.8250000            0.7788018
           Precision               Recall
           0.8250000            0.5789474
                  F1           Prevalence
           0.6804124            0.3838384
      Detection Rate Detection Prevalence
           0.2222222            0.2693603
   Balanced Accuracy
           0.7512223
```

Summary of the confusion matrix

Accuracy:

- accuracy = (TP + TN) / (P + N)
- In titanic example, accuracy = 0.79, meaning that 79% are correctly classified.

Error rate:

- error rate = (FP + FN) / (P + N) = 1 - accuracy
- In titanic example, error rate = 0.21, meaning that 21% are not correctly classified.

Summary of the confusion matrix

Sensitivity:

- sensitivity = TP / (TP + FN)
- In titanic example, sensitivity = 0.58, meaning that if the passenger did survive, there is a 58% chance the model will detect this.

Specificity:

- specificity = TN / (TN + FP)
- In titanic example, specificity = 0.92, meaning that if the passenger did not survive, there is a 92% chance the model will detect this.

Summary of the confusion matrix

False positive rate:

- false positive rate (FPR) = FP / (TN + FP) = 1 - specificity
- In titanic example, FPR = 0.08, meaning that if a passenger did not survive, there is an 8% chance that the model predicts this passenger as surviving.

Summary of the confusion matrix

Positive predictive value:

- positive predictive value (PPV) = TP / (TP + FP)
- In titanic example, PPV = 0.83, meaning that if the passenger is predicted as surviving, there is an 83% chance that this passenger indeed survived.

Negative predictive value:

- negative predictive value (NPV) = TN / (TN + FN)
- In titanic example, NPV = 0.78, meaning that if a passenger is predicted as not surviving, there is a 78% chance that this passenger indeed does not survive.

ROC curve

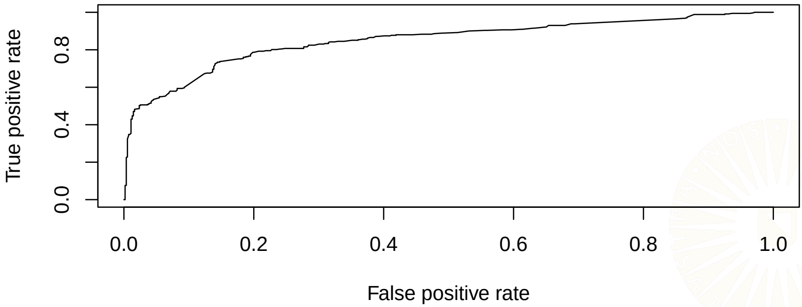
A receiver operating characteristic curve (ROC curve) is a graphical plot that illustrates the diagnostic ability of a binary classifier system as its discrimination threshold is varied. The ROC curve is created by plotting sensitivity against FPR (1 - specificity) at various threshold values.

ROC curve is mainly used for:

- evaluating the classification performance
- selecting discrimination threshold

ROC curve

```r
glm(Survived ~ Age + Sex*Pclass, family = binomial,
    data = titanic) %>% predict(., type = "response") %>%
  ROCR::prediction(., as.factor(titanic$Survived)) %>%
  ROCR::performance(., "tpr", "fpr") %>%
  plot()
```



Sensitivity versus specificity trade-off

Since sensitivity has a positive correlation with the false positive rate, there is a trade-off between sensitivity and specificity.

ROC curve

The Area Under the ROC Curve (AUC) summarizes the performance of the classification.

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
    data = titanic) %>% predict(., type = "response") %>%
  pROC::roc(as.factor(titanic$Survived), .) %>%
  auc()

Area under the curve: 0.8497
```

- AUC value from 0.7-0.8: acceptable
- AUC value from 0.8-0.9: excellent
- AUC value over 0.9: outstanding (Mandrekar, 2010)

Threshold selection

Sometimes, we do not want to use 0.5 as the threshold.

```
glm(Survived ~ Age + Sex*Pclass, family = binomial,
    data = titanic) %>% predict(., type = "response") %>%
  mutate(titanic, pred = .) %>%
  OptimalCutpoints::optimal.cutpoints(X = pred  ~ Survived,
                                      tag.healthy = 0,
                        control = control.cutpoints(),
                        methods = "ROC01",
                        data = ., ci.fit = FALSE,
                        conf.level = 0.95,
                        trace = FALSE) %>%
      .$ROC01 %>% .$Global %>% .$optimal.cutoff %>% .$cutoff

[1] 0.3530982
```

This threshold minimizes the distance between the selected point on the ROC plot and point (0, 1).

Weight sensitivity or specificity?

Selecting a point with the smallest distance to the point (0, 1) is to maximize $sensitivity^2 + specificity^2$. This optimized function has equal weights to sensitivity and specificity. However, in some scenarios, we care more about sensitivity or specificity.

Weight sensitivity or specificity?

- *When sensitivity is more important*
  - Predict whether a patient has a specific disease.
- *When specificity is more important*
  - Predict whether a person has committed a crime.

References

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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: MJMS*, *25*(6), 85.

Mandrekar, J. N. (2010). Receiver operating characteristic curve in diagnostic test assessment. *Journal of Thoracic Oncology*, *5*(9), 1315–1316.

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.