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Binary Response and Logistic Regression

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Binary Response Data

- **General setting:** $x_i \in \mathbb{R}^n, y_i \in \{0, 1\}$
- **Examples:**
  - Stimulus discrimination tasks
    - Shooter paradigm
    - Just noticeable difference in color perception
  - Mortality
    - *Is regular physical exercise life extending?*
    - *What are risk factors for severe COVID-19 symptoms?*
  - Performance assessment
    - Student assessment tests
    - Exam design: modeling task difficulty

Estimation

Basic idea: predict probability for class 1 as

$P(Y = 1) = \dfrac{\exp(\eta)}{1 + \exp(\eta)}$ with $\eta = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k$

- Underlying linear model $\eta_i = \beta_0 + \sum\limits_{j=1}^{k} \beta_j x_j$ that is plugged into the logistic function to obtain $P(Y = 1) \in [0, 1]$ and $P(Y = 1) + P(Y \neq 1) = 1$.

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Likelihood

Likelihood $\mathcal{L}(\beta|x_1, \ldots, x_n) = \prod_{i=1}^{n} \mathcal{L}_i(\beta|x_i)$

$$
\begin{aligned}
l(\beta|x_1, \ldots, x_n) &= \sum_{i=1}^{n} l_i(\beta|x_i) \\
&= \sum (1 - y_i) \log(1 - p(x_i; \beta)) + y_i \log p(x_i; \beta) \\
&= \sum y_i \log \frac{p(x_i; \beta)}{1 - p(x_i; \beta)} + \log(1 - p(x_i; \beta)) \\
&= \sum y_i x_i \beta - \log(1 + \exp(x_i \beta)) \\
&= \sum_{i=1}^{n} y_i \eta_i - \log(1 + \exp(\eta))
\end{aligned}
$$

- Maximize log-likelihood $l = \sum_{i=1}^{n} y_i \eta_i - \log(1 + \exp(\eta)) =: \mathtt{LL}$

Inference

- **Data format**
  - The criterion must be coded as 0/1 or as `factor`.
  - Predictors must be metric or dummy-coded
- **Interpretation**
  - Odds ratio for predictor x_j is equal to $\exp(\beta_j)$
  - Odds ratio OR_j quantifies how the odds $\frac{P(Y=1)}{P(Y=0)}$ change when x_j increases by 1 unit.

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Syntax

General syntax

- Command glm() (generalized linear model)
- Formula syntax:
    - y~x1+x2+x3 (no interactions)
    - y~x1*x2 (interactions)
    - y~x1+x2+x3+x1:x2 (selected interactions)
- Must provide a link function to glm() through the family parameter (cf. section Other link functions)
    - For logistic regression, we use family=binomial('logit').

Examples

```
m1 = glm(correct_response ~ iq + math_skill, data=df, family=binomial('logit'))
m2 = glm(fatal_accident ~ bmi + risk_seeking + gender, family=binomial('logit'))
m3 = glm(vaccination_skeptic ~ iq * income, family=binomial('logit'))
```

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Toy Example

The dataset $\texttt{df}$[1] contains the yearly sick leave hours, number of tweets on Twitter, IQ, and hair length of $N = 100$ employees along with their gender (binary: male/female) and whether they have ever suffered from depression (binary: yes/no):

```r
df %>% slice(sample(nrow(df))) %>% head(5)
```

```
##    ID depr gender avg_sickhours n_tweets iq hairlength
## 1 75   no   male          13.0        3 90       19.5
## 2 91   no   male          12.7        3 84        4.8
## 3 23  yes female          11.5       12 90       46.3
## 4 33   no female           5.4        3 97       40.4
## 5 86   no   male           8.6        1 83        4.4
```

```r
table(df$gender)
```

```
##
## female   male
##     50     50
```

---

[1]www.github.com/marvinschmitt/talk-binary-response

We define gender as criterion and avg_sickhours as predictor.
The logit link function leads to a logistic regression. The output's
coefficients correspond to $\beta_0, \ldots, \beta_k$.

```r
m = glm(gender ~ avg_sickhours, data = df, family = binomial('logit'))
m$coefficients
```

```
##  (Intercept) avg_sickhours
##   -4.2693393     0.4440937
```

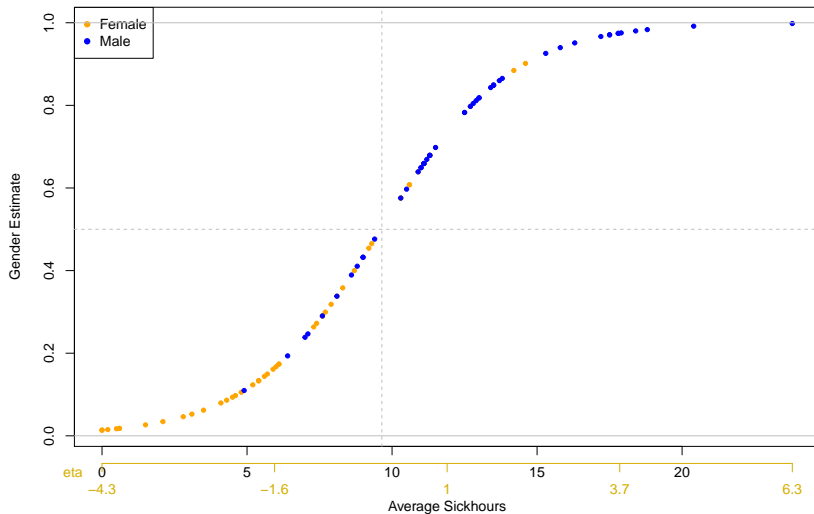- We can calculate η from the underlying linear model:
  $\eta = -4.27 + 0.44x_1$
- Thus, the criterion estimate is:

$$\hat{P}(Y = \text{male}) = \frac{\exp(\overbrace{-4.27 + 0.44x_1}^{\eta})}{1 + \exp(\underbrace{-4.27 + 0.44x_1}_{\eta})}$$

- The odds for gender=m are increased by the factor
  $\exp(0.44) = 1.55$ per additional sick leave hour.

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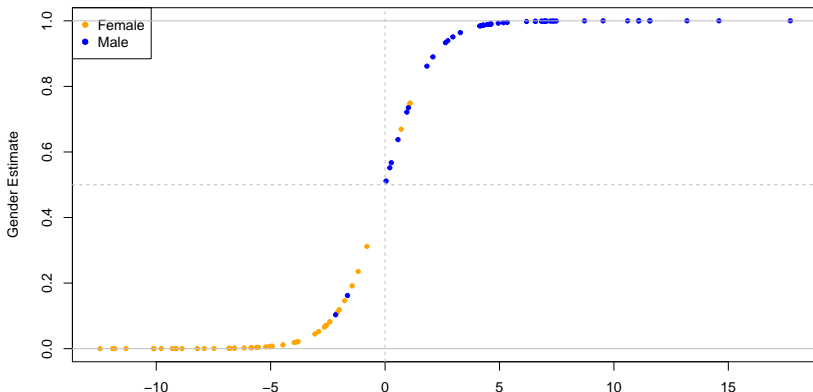Gender Estimate by Average Sickhours

Predictors: Avg. sick hours (x_1), Number of tweets (x_2)

```
m = glm(gender ~ avg_sickhours + n_tweets, data = df, family = binomial('logit'))
m$coefficients
```

```
##  (Intercept) avg_sickhours      n_tweets
##   -10.109104      1.621815     -1.197958
```

- $\eta = -10.11 + 1.62x_1 + -1.2x_2$

Gender Estimate by Average Sickhours and number of tweets

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Predictors: Avg. sick hours (x_1), Number of tweets (x_2), IQ (x_3)

```
m = glm(gender ~ avg_sickhours + n_tweets + iq, data = df, family = binomial('logit'))
```

```
## Warning: glm.fit: algorithm did not converge
```

```
## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
m$coefficients
```

```
##  (Intercept) avg_sickhours      n_tweets            iq
##   1998.03388     150.38876     -79.29431     -33.13080
```

- $\eta = 1998.03 + 150.39x_1 + -79.29x_2 + -33.13x_3$

- Note the output `Warning: glm.fit: algorithm did not converge`

    - Issue: Data is linearly separable (cf. section Issue: Linear Separability)
    - See the plot (next slide)

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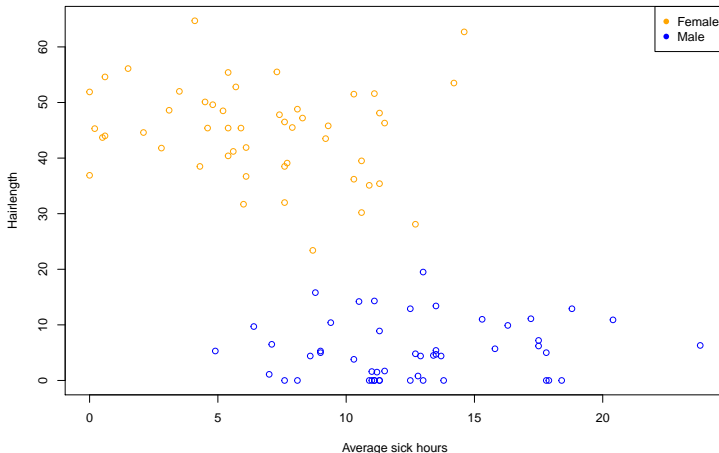Gender Estimate by Average Sickhours, number of tweets, and IQ
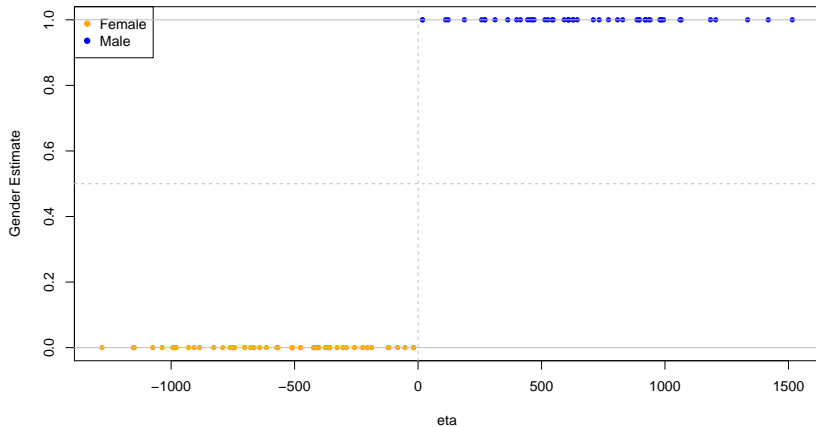
Predictors: Avg. sick hours (x_1), Hairlength (x_2)

```r
m = glm(gender ~ avg_sickhours + hairlength, data = df, family = binomial('logit'))
```

```
## Warning: glm.fit: algorithm did not converge
```

```
## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
```

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Model Evaluation

Logarithmic Scoring

- Basic evaluation of predicted probabilities:
    - For $Y_{true} = 1$, the predicted probability $\hat{P}(Y = 1)$ should be close to 1.
    - For $Y_{true} = 0$, the predicted probability $\hat{P}(Y = 1)$ should be close to 0.
- Compute $\texttt{logScore} = Y_i \ln(\hat{Y}_i) + (1 - Y_i) \ln(1 - \hat{Y}_i)$
    - $= \ln(\hat{Y}_i)$ if $Y_i = 1$
    - $= \ln(1 - \hat{Y}_i)$ if $Y_i = 0$

Model Selection

- Model selection aims at selecting a model M_i from a set of candidate models $M_1, \ldots, M_m$.
- The choice depends on the selection criterion and the
- For a model M with k parameters, the **Akaike-Information-Criterion** is defined as

$$AIC_M = -2 \log L_M + 2k$$

- R provides the step() function for stepwise selection from a set of models[2]. - The step() function uses the *AIC* as selection criterion for logistic regression models.

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[2]stepwise selection is not an ideal selection technique. Contemporary alternative: regularized methods

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```
m0 = glm(chd~1, data=chd_data, family=binomial('logit'))
m1 = step(m0, direction='both', trace=0,
          scope='~cigs+chol+weight+age')
summary(m1)
```

```
##
## Call:
## glm(formula = chd ~ chol + age + cigs, family = binomial("logit"),
##     data = chd_data)
##
## Deviance Residuals:
##     Min      1Q   Median      3Q      Max
## -1.1307  -0.4596  -0.3550  -0.2587   2.6391
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -8.655131   1.660169  -5.213 1.85e-07 ***
## chol         0.014092   0.003422   4.118 3.82e-05 ***
## age          0.056783   0.029257   1.941   0.0523 .
## cigs         0.017611   0.010368   1.699   0.0894 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 302.35  on 498  degrees of freedom
## Residual deviance: 276.65  on 495  degrees of freedom
## AIC: 284.65
##
## Number of Fisher Scoring iterations: 5
```

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Likelihood Ratio Test

- We can test competing nested models with the **Likelihood Ratio (LR) Test**
- Small model M_1 with k_1 parameters, Large model M_2 with k_2 parameters
- The difference of log-likelihoods is χ^2 distributed:
    - Test statistic $G^2 = -2LL_{M_1} - (-2LL_{M_2}) \sim \chi^2(df = k_2 - k_1)$
    - If $p < .05$, the larger model improves model fit.
- Implementation in R for example with `anova([models], test='Chisq')`

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```r
anova(m0, m1, m2, m3, m4, test="Chisq")
```

```
## Analysis of Deviance Table
##
## Model 1: chd ~ 1
## Model 2: chd ~ age
## Model 3: chd ~ age + cigs
## Model 4: chd ~ age + cigs + chol
## Model 5: chd ~ age + cigs + chol + height
##   Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
## 1       498     302.35
## 2       497     296.76  1   5.5866   0.01810 *
## 3       496     293.78  1   2.9815   0.08422 .
## 4       495     276.65  1  17.1342 3.483e-05 ***
## 5       494     275.52  1   1.1310   0.28755
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Hosmer and Lemeshow Goodness-of-fit test

- Approach of the HL test:
  - Partition the model population space into bins (*risk decentiles*)
  - Compare observed relative bin counts with predicted relative bin counts
  - Test statistic follows a χ^2 distribution
- Interpretation
  - $p < .05$ indicates a systematic deviance between observed and predicted bin counts.
- Reasons for a bad fit
  - Nonlinear influence of predictors on η
    - Solution: Polynomial logistic regression
    - e.g. $\eta = \beta_0 + \beta_{11}x_1 + \beta_{12}x_1^2 + \ldots + \beta_{1p}x_1^p + \beta_{21}x_2 + \ldots + \beta_{kp}x_k^p$
  - Interaction between predictors
    - Solution: Allow and analyze interactions (y~x1*x2).

```
df$gender01 = as.numeric(df$gender)-1  # recode to 0/1 for HL-test
m = glm(gender01 ~ avg_sickhours, data=df, family=binomial('logit'))
y_hat = predict(m, type="response")
hoslem.test(df$gender01, y_hat)  # default: g=10 bins
```

```
##
##  Hosmer and Lemeshow goodness of fit (GOF) test
##
## data:  df$gender01, y_hat
## X-squared = 3.6825, df = 8, p-value = 0.8846
```

```
hoslem.test(df$gender01, y_hat, g=5)  # g=5 bins
```

```
##
##  Hosmer and Lemeshow goodness of fit (GOF) test
##
## data:  df$gender01, y_hat
## X-squared = 0.57315, df = 3, p-value = 0.9026
```

Effect size

McFadden's ρ^2

- **Problem:** We cannot calculate the explained variance R^2
- **Approach:** Calculate McFadden's ρ^2 with the log-likelihood of the full model `m1` and the log-likelihood of the null model `m0` without predictors.
- **Optional:** Include a correction for the number of predictors k.
- **Formula:** $\rho^2 = 1 - \dfrac{\ln(L_1) \overbrace{-k}^{\text{correction}}}{\ln(L_0)}$

```
m0 = glm(gender ~ 1,               data=df, family=binomial('logit'))
m1 = glm(gender ~ avg_sickhours, data=df, family=binomial('logit'))
K = length(m1$coefficients) - 1 # number of predictors
as.numeric(1 -  logLik(m1)   /logLik(m0)) %>% round(3)
```

```
## [1] 0.36
as.numeric(1 - (logLik(m1)-K)/logLik(m0)) %>% round(3)
```
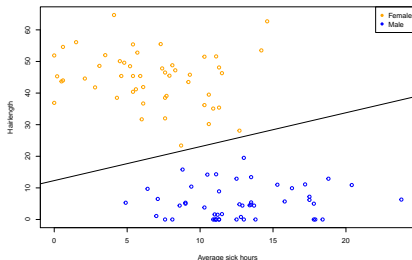
```
## [1] 0.346
```

Nagelkerke's R^2

- Another approach to compute an analogon to R^2 is
  Nagelkerke's (pseudo-) R^2:

```
m = glm(gender ~ avg_sickhours, data=df, family=binomial('logit'))
N = nrow(df)
(1-exp((m$dev-m$null)/N))/(1-exp(-m$null/N))
```

```
## [1] 0.5238511
```

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Issue: Linear Separability

- Linear separability of the data causes convergence issues.

- Unstable estimates of the parameters and their standard errors.
- Alternative: *Exact logistic regression*

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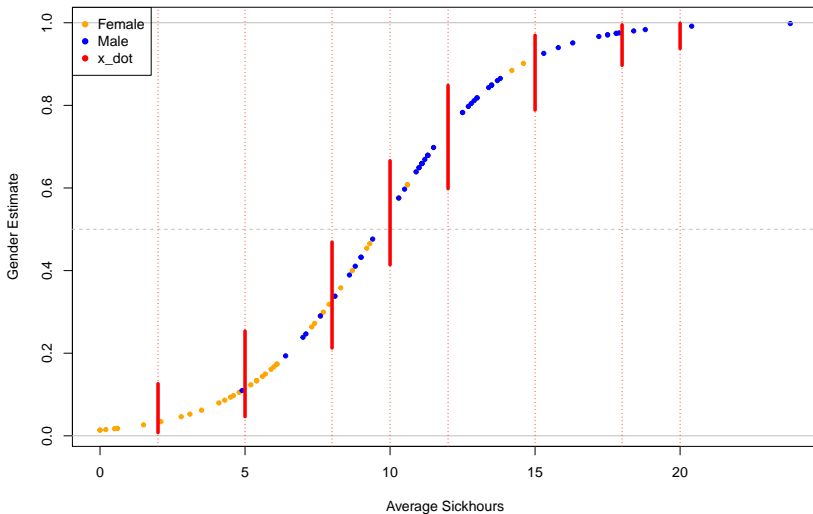Model Evaluation
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Predictions

- Given a new input $\dot{x}$, the prediction on the linear predictor is $\hat{\eta} = \dot{x}\hat{\beta}$.
- This prediction η can be equipped with a confidence interval.
- To obtain a probability confidence interval, $\hat{\eta}$ can be transformed with the well-known inverse link function:
$$\hat{p} = \frac{\exp(\eta)}{1 + \exp(\eta)}$$

```
m = glm(gender~avg_sickhours, data=df, family=binomial('logit'))
pred = predict(m,newdata=data.frame(avg_sickhours=10),se=T)
(pred_ci = c(pred$fit-1.96*pred$se.fit, pred$fit+1.96*pred$se.fit) %>% ilogit())
```

```
##         1         1
## 0.4141107 0.6660099
```

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Gender Estimate by Average Sickhours

- **Alternative:** Equip the odds ratio of β with a confidence interval:
  - 95% CI: $[\exp(\hat{\beta} - 1.96\hat{\sigma}_\beta), \exp(\hat{\beta} + 1.96\hat{\sigma}_\beta)]$
  - Invariant to the value of $\dot{x}$
  - Typically reported in clinical research papers.

```
m = glm(gender~avg_sickhours, data=df, family=binomial('logit'))
pred = predict(m,newdata=data.frame(avg_sickhours=10),se=T)
c(exp(pred$fit-1.96*pred$se.fit), exp(pred$fit+1.96*pred$se.fit))
```

```
##         1         1
## 0.7068071 1.9941010
```

Other link functions

```
mlogit    = glm(gender ~ avg_sickhours, data = df, family = binomial(link='logit'))
mprobit   = glm(gender ~ avg_sickhours, data = df, family = binomial(link='probit'))
mcloglog  = glm(gender ~ avg_sickhours, data = df, family = binomial(link='cloglog'))
mcauchit  = glm(gender ~ avg_sickhours, data = df, family = binomial(link='cauchit'))
```

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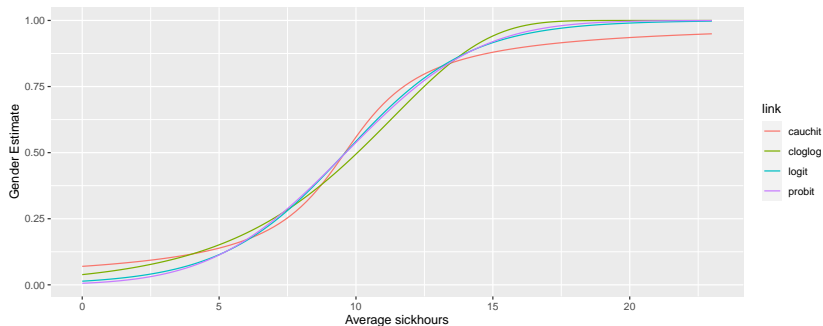
How to choose an appropriate link function?

- Usually, most observed data lies in the center of the distribution.
- Different link functions are typically similar in the center but differ in the **tails**.
- **Approach:** Select the link function based on *theoretical assumptions*, *experience*, and *domain expertise*.

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Questions?