Lecture 29: Logistic Regression

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- ▶ What is a regression model?
- Descriptive statistics graphical
- Descriptive statistics numerical
- Inference about a population mean
- Difference between two population means
- Some tips on R
- Simple linear regression (covariance, correlation, estimation, geometry of least squares)
 - ► Inference on simple linear regression model
 - ► Goodness of fit of regression: analysis of variance.
 - F-statistics.
 - Residuals.
 - Diagnostic plots for simple linear regression (graphical methods).

- Multiple linear regression
 - Specifying the model.
 - Fitting the model: least squares.
 - Interpretation of the coefficients.
 - Matrix formulation of multiple linear regression
 - Inference for multiple linear regression
 - T-statistics revisited.
 - More F statistics.
 - ▶ Tests involving more than one β .
- Diagnostics more on graphical methods and numerical methods
 - Different types of residuals
 - Influence
 - Outlier detection
 - Multiple comparison (Bonferroni correction)
 - Residual plots:
 - partial regression (added variable) plot,
 - partial residual (residual plus component) plot.

- Adding qualitative predictors
 - Qualitative variables as predictors to the regression model.
 - Adding interactions to the linear regression model.
 - Testing for equality of regression relationship in various subsets of a population
- ANOVA
 - All qualitative predictors.
 - One-way layout
 - Two-way layout
- Transformation
 - Achieving linearity
 - Stabilize variance
 - Weighted least squares
- Correlated Errors
 - Generalized least squares
- ► Bootstrapping linear regression
- Selection

- Colliniarity
 - ► Bias-variance tradeoff
 - Penalized Regression
 - Ridge
 - LASSO
 - ► Elastic net

Outline (Logistic regression)

- ▶ Most models so far have had response Y as continuous.
- Binary outcomes
 - Many responses in practice fall into the YES/NO framework.
 - **Examples**:
 - 1. medical: presence or absence of cancer
 - 2. financial: bankrupt or solvent
 - 3. industrial: passes a quality control test or not

Modelling probabilities

▶ For 0-1 responses we need to model

$$\pi(x_1,\ldots,x_p) = P(Y=1|X_1=x_1,\ldots,X_p=x_p)$$

- ► That is, Y is Bernoulli with a probability that depends on covariates $\{X_1, \ldots, X_p\}$.
- ▶ **Note:** $Var(Y) = \pi(1 \pi) = E(Y) \cdot (1 E(Y))$
- ▶ Or, the binary nature forces a relation between mean and variance of Y.
- ▶ This makes logistic regression a Generalized Linear Model.

- ▶ A local health clinic sent fliers to its clients to encourage everyone, but especially older persons at high risk of complications, to get a flu shot in time for protection against an expected flu epidemic.
- In a pilot follow-up study, 50 clients were randomly selected and asked whether they actually received a flu shot. Y = Shot
- ▶ In addition, data were collected on their age X_1 = Age and their health awareness X_2 = Health.Aware

A possible model

- Simplest model $\pi(X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$
- ► Problems / issues:
 - ▶ We must have $0 \le E(Y) = \pi(X_1, X_2) \le 1$. OLS will not force this.
 - Ordinary least squares will not work because of relation between mean and variance.

Logistic model

- ► Logistic model $\pi(X_1, X_2) = \frac{\exp(\beta_0 + \beta_1 X_1 + \beta_2 X_2)}{1 + \exp(\beta_0 + \beta_1 X_1 + \beta_2 X_2)}$
- ► This automatically fixes $0 \le E(Y) = \pi(X_1, X_2) \le 1$.
- ▶ **Define:** $\log \operatorname{it}(\pi(X_1, X_2)) = \log \left(\frac{\pi(X_1, X_2)}{1 \pi(X_1, X_2)}\right) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$

Logistic distribution

```
logit.inv = function(x) {
  return(exp(x) / (1 + exp(x)))
x = seq(-4, 4, length=200)
plot(x, logit.inv(x), lwd=2, type='l',
      col='red', cex.lab=1.2)
logit.inv(x)
   9.0
    0.2
    0.0
```

Х

Logistic transform: logit

0.0

0.2

```
logit = function(p) {
  return(log(p / (1 - p)))
p = seq(0.01, 0.99, length=200)
plot(p, logit(p), lwd=2, type='l',
     col='red', cex.lab=1.2)
    ^{\circ}
logit(p)
    7
```

0.4

p

0.6

0.8

1.0

Binary regression models

- ▶ Models E(Y) as $F(\beta_0 + \beta_1 X_1 + \beta_2 X_2)$ for some increasing function F (usually a distribution function).
- ➤ The logistic model uses the function (we called logit.inv above)

$$F(x) = \frac{e^x}{1 + e^x}.$$

- Can be fit using Maximum Likelihood / Iteratively Reweighted Least Squares.
- For logistic regression, coefficients have nice interpretation in terms of odds ratios (to be defined shortly).
- What about inference?

Criterion used to fit model

- Instead of sum of squares, logistic regression uses deviance:
- Let L be the likelihood function.
- ▶ $DEV(\mu|Y) = -2 \log L(\mu|Y) + 2 \log L(Y|Y)$ where μ is a location estimator for Y.
 - L(Y|Y)=1
 - deviance is always larger or equal than zero
 - deviance is zero only if the fit is perfect
- ▶ If Y is Gaussian with independent $N(\mu_i, \sigma^2)$ entries then $DEV(\mu|Y) = \frac{1}{\sigma^2} \sum_{i=1}^{n} (Y_i \mu_i)^2$
- If Y is a binary vector, with mean vector π then $DEV(\pi|Y) = -2\sum_{i=1}^{n} (Y_i \log(\pi_i) + (1 Y_i) \log(1 \pi_i))$

Minimizing deviance \iff Maximum Likelihood

Deviance for logistic regression

- For any binary regression model, $\pi = \pi(\beta)$.
- ► The deviance is:

$$DEV(\beta|Y) = -2\sum_{i=1}^{n} (Y_i \operatorname{logit}(\pi_i(\beta)) + \log(1 - \pi_i(\beta)))$$

For the logistic model, the RHS is:

$$-2\left[(X\beta)^T y + \sum_{i=1}^n \log \left(1 + \exp \left(\sum_{j=1}^p X_{ij} \beta_j \right) \right) \right]$$

- ▶ The logistic model is special in that $logit(\pi(\beta)) = X\beta$. If we used a different transformation, the first part would not be linear in $X\beta$.
- ▶ For ease of notation, we assume that X[,1]=1 corresponding to β_0

##

- Response: Flu shot is taken or not.
- Predictors: Age, Health awareness

Shot Age Health.Aware

```
## 1 0 38 40

## 2 1 52 60

## 3 0 41 36

## 4 1 46 59

## 5 1 41 70

## 6 0 43 49

flu.glm = glm(Shot ~ Age + Health.Aware,

data=flu.table,
```

family=binomial())

```
Call:
alm(formula = Shot ~ Age + Health.Aware, family = binomial(),
    data = flu.table)
Deviance Residuals:
             10 Median
-1 5522 -0 2962 -0 1124 0 4208 2 3244
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -21.58458
                         6.41824 -3.363 0.000771 ***
Age
              0.22178
                         0.07436 2.983 0.002858 **
Health.Aware 0.20351
                         0.06273 3.244 0.001178 **
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: 32.416 on 47 degrees of freedom
AIC: 38.416
Number of Fisher Scoring iterations: 6
```

- null deviance: how well the reponse is predicted when there is no predictors
- residual deviance: how well the reponse is predicted when there predictors
- in this example, residual deviance is smaller than the null deviance.

Odds Ratios

 One reason logistic models are popular is that the parameters have simple interpretations in terms of odds

$$ODDS(A) = \frac{P(A)}{1 - P(A)}.$$

Logistic model:

$$OR_{X_j} = \frac{ODDS(Y = 1 | \dots, X_j = x_j + h, \dots)}{ODDS(Y = 1 | \dots, X_j = x_j, \dots)} = e^{h\beta_j}$$

▶ If $X_j \in 0, 1$ is dichotomous, then odds for group with $X_j = 1$ are e^{β_j} higher, other parameters being equal.

Rare disease hypothesis

- ▶ When incidence is rare, $P(Y = 0) \approx 1$ no matter what the covariates X_i 's are.
- ▶ In this case, odds ratios are almost ratios of probabilities:

$$OR_{X_j} \approx \frac{\mathbb{P}(Y=1|\ldots,X_j=x_j+1,\ldots)}{\mathbb{P}(Y=1|\ldots,X_j=x_j,\ldots)}$$

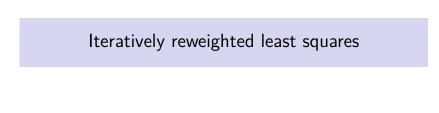
▶ Hypothetical example: in a lung cancer study, if X_j is an indicator of smoking or not, a β_j of 5 means for smoking vs. non-smoking, smokers are $e^5 \approx 150$ times more likely to develop lung cancer

▶ In flu example, the odds ratio for a 45 year old with health awareness 50 compared to a 35 year old with the same health awareness are $e^{-1.429284+3.647052} = 9.18$

```
## 1 2
## -3.647052 -1.429284
OR = exp(logodds[2])/exp(logodds[1]); OR
```

```
## 2
## 9.186801
```

▶ The estimated probabilities are below, yielding a ratio of $0.1932/0.0254 \approx 7.61$. Not too far from 9.18.



An algorithm to fit the model

- 1. Initialize $\hat{\pi}_i = \bar{Y}, 1 \leq i \leq n$
- 2. Define

$$Z_i = g(\widehat{\pi}_i) + g'(\widehat{\pi}_i)(Y_i - \widehat{\pi}_i),$$

where g is the logit function.

3. Fit weighted least squares model

$$Z_i \sim \sum_{j=1}^p \beta_j X_{ij}, \qquad w_i = \widehat{\pi}_i (1 - \widehat{\pi}_i)$$

- 4. Set $\widehat{\pi}_i = \operatorname{logit}^{-1} \left(\widehat{\beta}_0 + \sum_{j=1}^p \widehat{\beta}_j X_{ij} \right)$.
- 5. Repeat steps 2-4 until convergence.

Newton-Raphson

➤ The Newton-Raphson updates for logistic regression are (minimizing Deviance)

$$\hat{\beta} \mapsto \hat{\beta} - \nabla^2 DEV(\hat{\beta})^{-1} \nabla DEV(\hat{\beta})$$

- ► These turn out to be the same as the updates above (as in the Iteratively reweighted least squares).
- ▶ In earlier statistical software one might only have access to a weighted least squares estimator.

Inference

- One thing the IRLS procedure hints at is what the approximate limiting distribution is.
 - The IRLS procedure suggests using approximation $\widehat{\beta} \approx N(\beta, (X^T W X)^{-1})$
 - ▶ This allows us to construct Cls, test linear hypotheses, etc.
 - ▶ Intervals formed this way are called *Wald intervals*.

Covariance

➤ The estimated covariance vcov(flu.glm) uses the weights computed from the fitted model.

```
pi.hat = fitted(flu.glm)
W.hat = pi.hat * (1 - pi.hat)
X = model.matrix(flu.glm)
C = solve(t(X) %*% (W.hat * X))
c(SE, sqrt(C['Age', 'Age']))
```

```
## [1] 0.07435712 0.07435807
```

Confidence intervals in R

- ► The intervals above are slightly different from what R will give you if you ask it for confidence intervals.
- R uses so-called profile intervals.
- For large samples the two methods should agree quite closely.

Confidence intervals in R

```
CI = confint(flu.glm)
CI
                     2.5 % 97.5 %
##
## (Intercept) -38.0402235 -11.6669218
## Age
         0.1004533 0.4046856
## Health.Aware 0.1026984 0.3595480
# profile intervals are not symmetric around the estimate.
mean(CI[2,])
## [1] 0.2525694
# we computed center of the interval as follows
data.frame(L, center, U)
##
                center
```

Age 0.0760395 0.2217768 0.3675141

Testing in logistic regression

What about comparing full and reduced model?

- ▶ For a model \mathcal{M} , $DEV(\mathcal{M})$ replaces $SSE(\mathcal{M})$.
- ▶ In least squares regression (with σ^2 known), we use

$$\frac{1}{\sigma^2} \left(SSE(\mathcal{M}_R) - SSE(\mathcal{M}_F) \right) \stackrel{H_0:\mathcal{M}_R}{\sim} \chi^2_{df_R - df_F}$$

- ► This is closely related to F with large df_F : approximately $F_{df_R-df_F,df_R} \cdot (df_R-df_F)$.
- ▶ For logistic regression this difference in *SSE* is replaced with

$$DEV(\mathcal{M}_R) - DEV(\mathcal{M}_F) \overset{n \to \infty, H_0: \mathcal{M}_R}{\sim} \chi^2_{df_R - df_F}$$

Resulting tests do not agree numerically with those coming from IRLS (Wald tests). Both are often used.

```
anova(glm(Shot ~ 1,
         data=flu.table,
         family=binomial()),
     flu.glm)
## Analysis of Deviance Table
##
## Model 1: Shot ~ 1
## Model 2: Shot ~ Age + Health.Aware
##
    Resid. Df Resid. Dev Df Deviance
## 1
         49 68.029
                             35.613
          47
                  32.416
## 2
```

```
## Analysis of Deviance Table
##
## Model 1: Shot ~ Health.Aware
## Model 2: Shot ~ Age + Health.Aware
## Resid. Df Resid. Dev Df Deviance
## 1 48 49.279
## 2 47 32.416 1 16.863
```

We should compare this difference in deviance with a χ_1^2 random variable.

```
# testing ~1 vs ~1 + Health.Aware + Age
1 - pchisq(35.61, 2)

## [1] 1.850916e-08

# testing ~ 1 + Health.Aware vs ~1 + Health.Aware + Age
1 - pchisq(16.863, 1)
```

```
## [1] 4.017719e-05
```

Let's compare this with the Wald test:

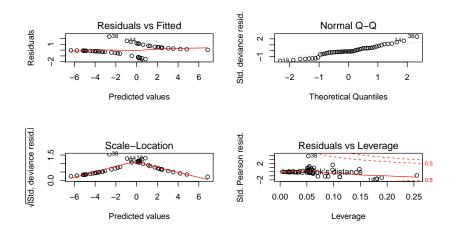
summary(flu.glm)

```
Call:
glm(formula = Shot ~ Age + Health.Aware, family = binomial(),
   data = flu.table)
Deviance Residuals:
             10 Median
-1.5522 -0.2962 -0.1124 0.4208 2.3244
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -21.58458
                        6.41824 -3.363 0.000771 ***
              0.22178
                        0.07436 2.983 0.002858 **
Health.Aware 0.20351
                         0.06273 3.244 0.001178 **
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: 32,416 on 47 degrees of freedom
ΔTC · 38 416
Number of Fisher Scoring iterations: 6
```

Diagnostics

- Similar to least square regression, only residuals used are usually deviance residuals $r_i = \text{sign}(Y_i \widehat{\pi}_i) \sqrt{DEV(\widehat{\pi}_i|Y_i)}$.
- ▶ These agree with usual residual for least square regression.

Diagnostics



Diagnostics

influence.measures(flu.glm)

	dfb.1	dfb.Age	dfb.Hl.A	dffit	cov.r	cook.d	hat	inf
	<dbl></dbl>	<dbi></dbi>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<fctr></fctr>
1	-0.017208450	0.015425632	0.015642750	-0.017627295	1.0826918	3.659998e-05	0.016044175	
2	-0.102896560	0.095601518	0.104158961	0.134913568	1.1016580	2.242955e-03	0.052309317	
3	-0.015043331	0.012796775	0.014423117	-0.015557954	1.0812268	2.849979e-05	0.014540618	
4	-0.058889061	0.024180020	0.119204481	0.287549399	1.0400288	1.178645e-02	0.058501495	
5	-0.103487667	0.038531289	0.171669954	0.234752910	1.1440718	6.941304e-03	0.097887286	
6	-0.130919008	0.118975462	0.110976921	-0.152033795	1.1089962	2.859279e-03	0.060396517	
7	-0.066733843	0.066912148	0.060032141	0.077608468	1.1041718	7.216821e-04	0.042487429	
8	-0.043827442	0.043992127	0.034380158	-0.047042275	1.1010477	2.622724e-04	0.035080574	
9	-0.018883246	0.018809963	0.015150022	-0.019796169	1.0854748	4.617103e-05	0.018665882	
10	-0.112977727	0.096952606	0.132645407	0.208414096	1.0760659	5.683995e-03	0.055255614	
11	-0.009577574	0.095836356	-0.043048893	0.364897254	1.0037014	2.083004e-02	0.063175325	
12	0.020211669	-0.133730542	0.058121041	-0.435658880	0.9792425	3.195699e-02	0.070590655	
13	0.192769578	-0.507763090	0.117899074	-0.937781945	1.0402263	1.632619e-01	0.189724920	*
14	0.372025379	-0.472612878	-0.145485378	0.688135732	0.9022852	1.019381e-01	0.098269672	
15	-0.038715894	0.035962655	0.033505165	-0.040345463	1.0954845	1.927046e-04	0.029695080	
16	-0.057483528	0.064804695	0.037346215	-0.068923294	1.1213473	5.647229e-04	0.053933004	
17	-0.046411886	0.139137544	-0.108584803	-0.479730861	0.9930315	3.855770e-02	0.084036358	
18	-0.029026018	0.024985096	0.030041389	0.032568615	1.0900109	1.253857e-04	0.024164623	
19	0.111761811	0.199472599	-0.490738781	-1.006689601	0.9788611	2.098408e-01	0.180843476	*
20	-0.063892521	0.051985794	0.062463199	-0.069722982	1.1049785	5.804322e-04	0.041691779	
21	-0.148883584	0.116208572	0.142755961	-0.193270807	1.0962350	4.759595e-03	0.061993468	
22	-0.046450729	0.036647120	0.052203167	0.056584320	1.1005070	3.808388e-04	0.036145888	
23	-0.058937986	0.036950964	0.069332741	-0.075873231	1.1164261	6.867114e-04	0.051205093	
24	-0.046667990	0.040386222	0.043379257	-0.049176718	1.0983427	2.870168e-04	0.033293002	
25	0.181347490	-0.108435013	-0.178659012	0.430487951	0.9213015	3.496902e-02	0.054530052	
26	-0.009162371	0.007591158	0.009034704	-0.009529635	1.0767247	1.068087e-05	0.009944897	

1-26 of 50 rows



Model selection

- ➤ As the model is a likelihood based model, each fitted model has an AIC.
- ► Stepwise selection can be used easily

Model selection

```
step(flu.glm, scope=list(upper= ~.^2),
    direction='both')
```

```
Start: AIC=38.42
Shot ~ Age + Health.Aware
                  Df Deviance AIC
+ Age: Health, Aware 1 24, 283 32, 283
<none>
                     32,416, 38,416
                1 49.279 53.279
- Health.Aware 1 56.078 60.078
Step: AIC=32.28
Shot ~ Age + Health.Aware + Age:Health.Aware
                  Of Deviance ATC
                       24 283 32 283
<none>
- Age: Health. Aware 1 32.416 38.416
Call: glm(formula = Shot ~ Age + Health.Aware + Age:Health.Aware, family = binomial(),
    data = flu.table)
Coefficients:
    (Intercept)
                                      Health.Aware
       26. 75944
                        -0.88151
                                          -0.82239
Age: Health. Aware
        0.02365
Degrees of Freedom: 49 Total (i.e. Null); 46 Residual
Null Deviance:
                   68 03
Residual Deviance: 24.28
                         AIC: 32.28
```



LASSO

Instead of just minimizing deviance, we can also look at penalized versions

$$\mathsf{minimize}_{\beta} \frac{1}{2n} DEV(\beta) + \lambda \|\beta\|_{1}$$

Flu shot example

```
library(glmnet)
X = model.matrix(flu.glm)[,-1]
Y = as.numeric(flu.table$Shot)
G = glmnet(X, Y, family="binomial")
plot(G)
         0
   0.20
Coefficients
   0.00
        0.0
                                  0.2
                                              0.3
                                                           0.4
```

L1 Norm

Spam data set

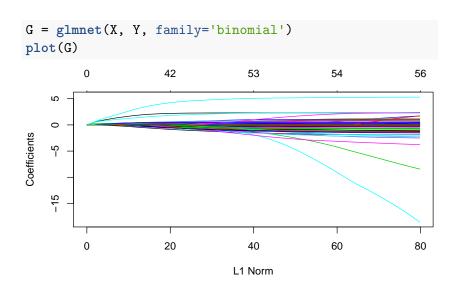
- ▶ A data frame with 4601 observations on the 57 numeric predictor variables and a response spam is factor variable with 2 levels email, spam.
- ▶ More information of the data is here.

```
library(ElemStatLearn)
data(spam)
dim(spam)

## [1] 4601 58

X = model.matrix(spam ~ ., data=spam)[,-1]
Y = as.numeric(spam$spam == 'spam')
```

Spam data set



Spam data set

```
CV = cv.glmnet(X, Y, family='binomial')
plot(CV)
                 57 54 53 54 53 52 50 42 36 27 26 17 8 4
Binomial Deviance
    1.0
    0.8
    9.0
    4.0
         -10
                                    Log(\lambda)
c(CV$lambda.min, CV$lambda.1se)
```

[1] 0.0003349517 0.0025934091

Extracting coefficients from glmnet

```
beta.hat = coef(G, s=CV$lambda.1se)
beta.hat
## 58 x 1 sparse Matrix of class "dgCMatrix"
##
## (Intercept) -1.5752618121
              -0.1716645042
## A.1
## A.2
               -0.0871840559
## A.3
               0.1318482487
## A.4
                0.0936079556
## A.5
               0.5081162007
## A.6
                0.5482723371
## A.7
                2.2785920925
## A.8
                0.5519184177
## A.9
                0.5002890226
## A.10
                0.0829896113
## A.11
## A.12
               -0.1157514617
```



Probit model

Probit regression model:

$$\Phi^{-1}(E(Y|X)) = \sum_{i=1}^{p} \beta_i X_i$$

where Φ is CDF of N(0,1), i.e. $\Phi(t) = pnorm(t)$, $\Phi^{-1}(q) = qnorm(q)$.

Regression function

$$\begin{split} E(Y|X) &= E(Y|X_1, \dots, X_p) \\ &= P(Y = 1|X_1, \dots, X_p) \\ &= \operatorname{pnorm}\left(\sum_{i=1}^p \beta_i X_i\right) \end{split}$$

- ▶ In logit, probit and cloglog $Var(Y_i) = \pi_i(1 \pi_i)$ but the model for the mean is different.
- Coefficients no longer have an odds ratio interpretation.

Probit model

```
Call:
alm(formula = Shot ~ Age + Health.Aware, family = binomial(link = "probit"),
   data = flu.table)
Deviance Residuals:
   Min
             10 Median
                                      Max
-1.5471 -0.2883 -0.0648 0.4060 2.2955
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -12.35039 3.22797 -3.826 0.000130 ***
         0.12786 0.03887 3.289 0.001005 **
Age
Health.Aware 0.11642 0.03237 3.596 0.000323 ***
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: 32.076 on 47 degrees of freedom
ATC: 38.076
Number of Fisher Scoring iterations: 7
```

Generalized linear models

Given a dataset $(Y_i, X_{i1}, \dots, X_{ip}), 1 \le i \le n$ we consider a model for the distribution of $Y | X_1, \dots, X_p$.

- ▶ If $\eta_i = g(E(Y_i|X_i)) = g(\mu_i) = \sum_{j=1}^{p} \beta_j X_{ij}$ then g is called the *link* function for the model.
- ▶ If $Var(Y_i) = \phi \cdot V(\mathbb{E}(Y_i)) = \phi \cdot V(\mu_i)$ for $\phi > 0$ and some function V, then V is the called *variance* function for the model.
- ► Canonical reference Generalized linear models.

Binary regression as GLM

- ▶ For a logistic model, $g(\mu) = \text{logit}(\mu)$, $V(\mu) = \mu(1 \mu)$.
- For a probit model, $g(\mu) = \Phi^{-1}(\mu)$, $V(\mu) = \mu(1 \mu)$.
- For a cloglog model, $g(\mu) = -\log(-\log(\mu)), \qquad V(\mu) = \mu(1-\mu).$
- ▶ All of these have dispersion $\phi = 1$.

Reference

- ► CH Chapter 12.
- ► Lecture notes of Jonathan Taylor .