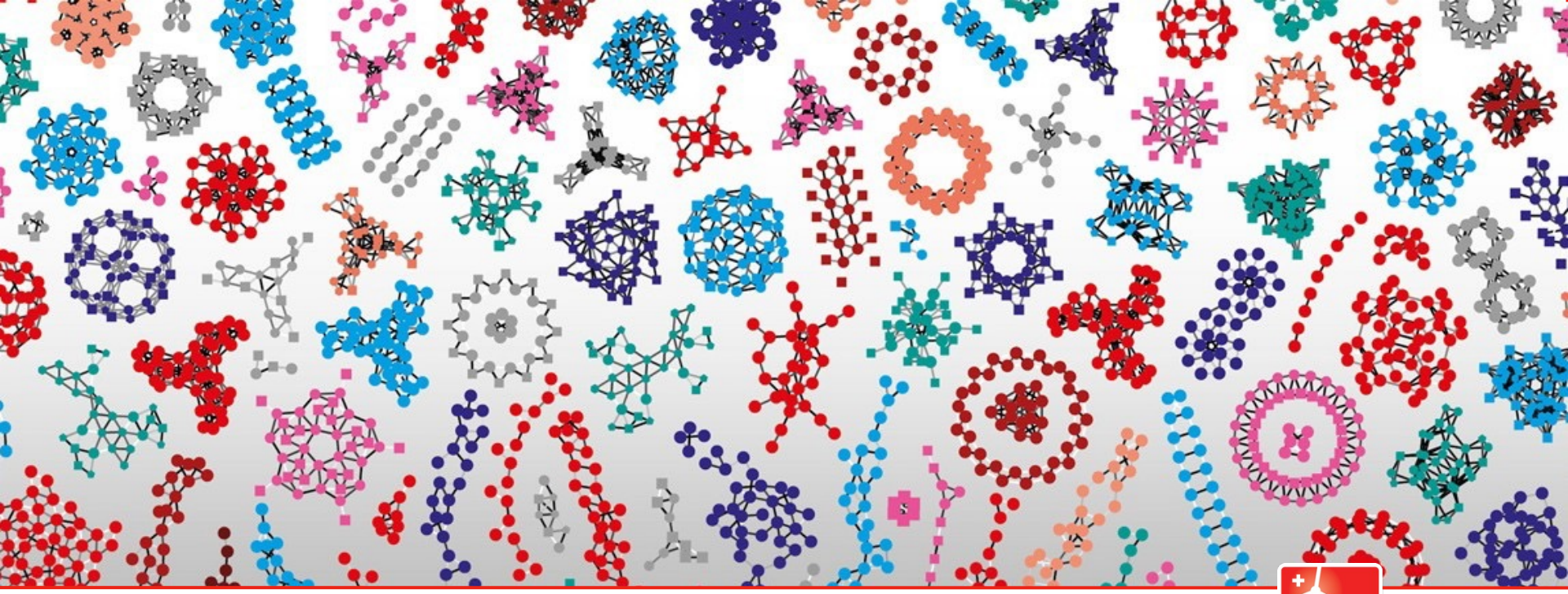


# Logistic Regression and GLM

*Adv.stat course Sept 2023*

*Rachel Marcone (Jeitziner) and Mauro Delorenzi*

*Slides credit also to Linda Dib, Frédéric Schütz, Isabelle Dupanloup, …*

# Statistical Models

Are used for explanation and prediction

*Statistical models predicts the mean Y for any combination of predictors.*

General form: g(Y) = f(X) (+ Error)

with a stochastic process (⇔ errors)

Y: dependent variable (response variable, observed outcome)

X: independent/ explanatory variable(s) (grouping variable, predictor)

# Types of response and predictors variables

- binary (2 groups)

(e.g. yes/no, passed/failed, male/female, ill/healthy, responder/NR, ...)

- categorical (k groups)

(e.g. phenotype, genotype, degree of physical activity, ...)

- continuous (i.e. pot. infinite number of groups)

(e.g. weight, blood pressure, gene expression value, ...)

- Censored data (e.g. survival data for patients, living beings, technical devices, ...)

# Types of variables

Response variable's type determines the suitable regression method(s) :

| | |
|---|---|
| continuous response | -> Linear regression |
| **binary response** | **-> Logistic regression** |
| count response | -> Poisson regression |

# Logistic regression

# What is Logistic Regression?

Form of regression that allows the prediction of discrete variables
by a mix of continuous and discrete predictors.

Discrete ~ continuous / discrete

Example: Responder status ~ dosis

# Binary Logistic Regression Model

*Y* = Binary response, ex. Responder status (1 / 0)
*X* = Quantitative predictor, ex. Dose, genotype for gene G, …

$\pi$ = Proportion / **Probability** of »event 1» at any X

Given $\pi$ we assume that a (always identical) stochastic process "determines" the event(s) observed outcome.

For a group with the same configurations of X, the same $\pi$:
there is a **binomial** distribution B(n,p) of »event 1»
n = number of observations at this X,
p = prob. of event 1 and

# Proportion of "success"

*In linear regression the model predicts the mean Y for any combination of prediction (the E [Y | X] ) resp. E [P(Y=1) | X] ) .*
*What's the mean of a 0/1 indicator variable?*
*The **Proportion** of "cases 1" among n observations.*

$$\pi = \bar{y} = \frac{\sum y_i}{n}$$

*Goal of logistic regression: Predict the **"true" probability** of success, π, at any value of the predictor(s).*

*Modeling overview revised*

**X** → E(Y) the expected value of Y → individual values $Y_i$

**stochastic error**
**(lm: normal; log: binomial)**

**now a prob. [0,1]**

**Deterministic function**
**( lm: Linear / affine function or polynomial etc. , linear in parameters**

**glm a new approach, linear in parameters, but with a transformation linking it to the E(Y) )**

# Relation probability – odds

$$\boldsymbol{odds} = \frac{\pi}{1-\pi} \Leftrightarrow \pi = \frac{odds}{1+odds}$$

π in [0 , 1] , odds in ( 0, + ∞),

π = 0.5 odds = 1

π = 0.9 odds = 9

π = 0.1 odds = 1/9 = 0.111

not symmetric

# Logistic curve

Probability of success

Logit is the **logarithm of the odds (log=ln=$\log_e$)**

$$\log\left(\frac{\pi}{1-\pi}\right)$$

Probability of failure

$\pi$ = 0.50 ⇔ logit = 0

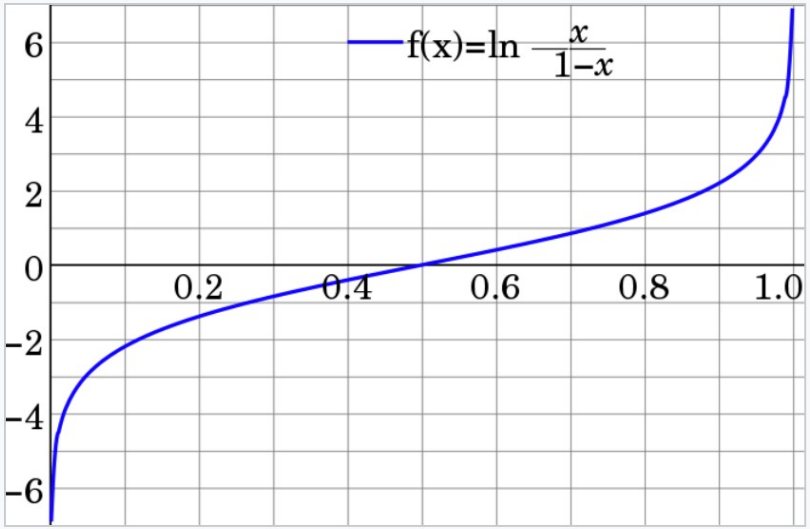
$\pi$ = 0.70 ⇔ logit = 0.84

$\pi$ = 0.30 ⇔ logit = -0.84

$\pi$ -> 1 ⇔ logit -> inf

$\pi$ -> 0 ⇔ logit -> - inf

Symmetric, range (-inf, +inf)




Plot of logit(*p*) in the domain of 0 to 1, where the base of logarithm is *e*.

https://en.wikipedia.org/wiki/Logit

# Binary Logistic Regression Model

$$\log\left(\frac{\pi}{1-\pi}\right) = \beta_0 + \beta_1 X$$

The predictors acts at the level of the log odds

**X** → logit → E(Y) → individual values $Y_i$

**prob. [0,1]**

**Deterministic function,**
**Linear in the parameters describing the effects of the expl. Vars.**

The logit is called a **link function**, links the level of the observed events (**response level**) to the level at which the predictors effects are acting (**link level**)

# GLM LOGISTIC

Predictors X => E( logit($\pi$) | X) => observations $Y_i$

=> The assumed model of effects

$\Rightarrow$ ex. Logit is linear in ß's

=> The assumed underlying stochastic process (generating the data)

=> ex. Binomial distribution

# Binary Logistic Regression Model

$$\boldsymbol{odds} = \frac{\pi}{1-\pi} \Leftrightarrow \pi = \frac{odds}{1+odds} = \frac{1}{1+1/odds}$$

**Logit form**

$$\log\left(\frac{\pi}{1-\pi}\right) = \beta_0 + \beta_1 X$$

**Link - Level**

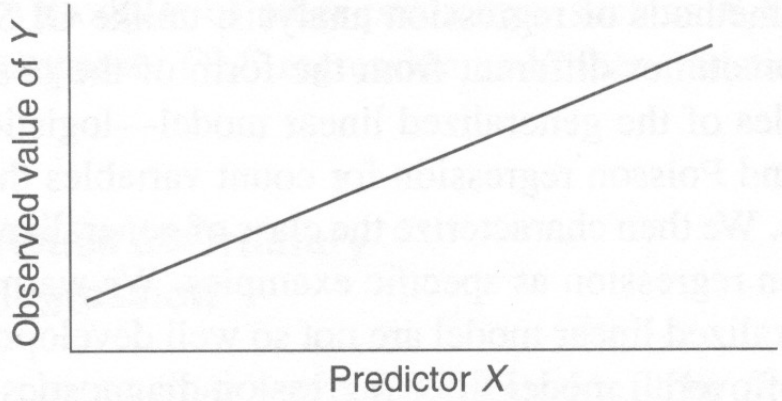
**Probability form**

$$\pi = \frac{e^{\beta_0+\beta_1 X}}{1+e^{\beta_0+\beta_1 X}} = \frac{1}{1+e^{-(\beta_0+\beta_1 X)}}$$

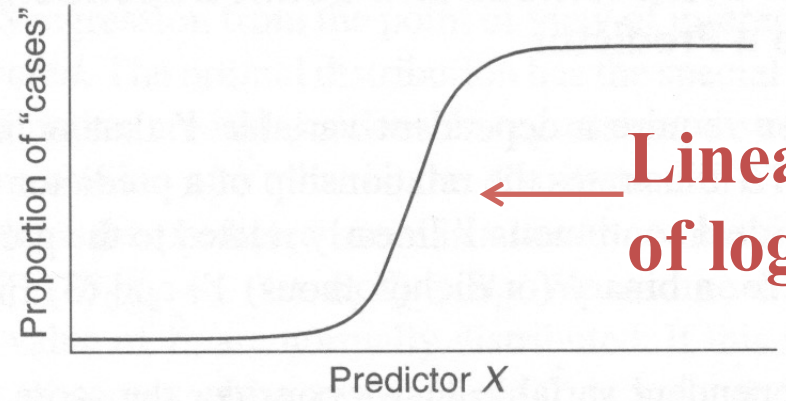
**Response - Level**

# The logistic function

(A) For a continuous outcome variable $Y$, the numerical value of $Y$ at each value of $X$.




(B) For a binary outcome variable, the proportion of individuals who are "cases" (exhibit a particular outcome property) at each value of $X$.




Change in probability is not constant (linear) with constant changes in X

**Linear part of logistic fit**

$$\pi = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$

Odds for X: $$odds = e^{\beta_0+\beta_1 X}$$

Odds for X+1: $$odds = e^{\beta_0+\beta_1 (X+1)}$$

Odds ratio (odds for X+1 / odds for X):

$$\frac{e^{\beta_0+\beta_1 (X+1)}}{e^{\beta_0+\beta_1 X}} = e^{\beta_0+\beta_1 (X+1)-(\beta_0+\beta_1 X)} = e^{\beta_1}$$

We increase $X_1$ by one unit **(+1**, **additive**)
The log odds is increased by **ß$_1$** (additive)

The odds is increased by a factor exp(**ß$_1$**) (**multiplicative**)

The probaility is increased by ? (**question!** )

# Assumptions

$$\log\left(\frac{\pi}{1-\pi}\right) = \beta_0 + \beta_1 X$$

**The logistic model assumes a linear relationship between the *predictors* and the *log(odds).***

$$odds = \frac{\pi}{1-\pi} = e^{\beta_0 + \beta_1 X}$$

# Logistic regression

## is a special case of a

# Generalized Linear Model

# GLM

Ordinary Least Squares regression provides linear models of continuous variables. However, much data of interest to statisticians and researchers are not continuous and so other methods must be used to create useful predictive models.

# GLM LOGISTIC

Predictors X => E( logit($\pi$) | X) => observations $Y_i$

=> The assumed model of effects

$\Rightarrow$ ex. Logit is linear in ß's

=> The assumed underlying stochastic process (generating the data)

=> ex. Binomial distribution

# GLM Poisson

Predictors X => E( link(Y) | X) => observations $Y_i$

=> **The assumed model of effects**

**Log ($\lambda_i$) linear in ß's**

$\Rightarrow$ **stochastic process**

Data $Y_i$ ~ Poisson distribution

Poi (mean $\lambda$ =E[Y])

Stdev = sqrt ($\lambda$)

The dispersion is the one expected for a »pure random sampling» that is without any factor of variability increasing the dispersion.

Stddev = sqrt(mean)

ML-estimation, deviance, LRT,
Wald test on coefficients etc:
Like Logistic Regression

# Poisson regression

- Basic standard model used for Count data
- Distribution: Poisson, (Restriction: mean = variance : E(Y)=V(Y)=λ)

- Default Link Function: log link:

$$\ln(\lambda) = \beta_0 + \beta_1 X_1 + \ldots + \beta_k X_k$$

$$\Rightarrow \lambda(X_1, \ldots, X_k) = e^{\beta_0 + \beta_1 X_1 + \ldots + \beta_k X_k}$$

Tests are conducted as in Logistic regression

# Poisson regression - assumptions

- Poisson at the Response Level : the response variable is a count per unit of time or space, described by a Poisson distribution.
- Linearity at Link Level : the log of the mean rate, log(λ), is be a linear function of the predictor x.
- Independence: the observations are independent of one another.
- Mean=Variance: the mean of a Poisson random variable is equal to its variance.

# Generalized Linear Models

Generalized linear models are fit using the **glm( )** function. The form of the **glm** function is

**glm(***formula*, **family=***familytype*(**link=***linkfunction*), **data=)**

| Family | Default Link Function |
|---|---|
| binomial | (link = "logit") |
| gaussian | (link = "identity") |
| Gamma | (link = "inverse") |
| inverse.gaussian | (link = "1/mu^2") |
| poisson | (link = "log") |
| quasi | (link = "identity", variance = "constant") |
| quasibinomial | (link = "logit") |
| quasipoisson | (link = "log") |

# How to find the »best fit«

Standard method: **maximum likelihood estimation MLE**
Probability of observations
(Likelihood of the model given the data) = maximum

The **MLE** is the preferred method for statisticians in many situations. It has a series of good properties (best method given some criteria).

The t-test for example is the maximum likelihood-based test to compare the mean of two normal distributions.

The MLE estimate for lm models leads to the same solution like the least squares (under given assumptions).

# How to find the »best fit«

Solution:
Generally there is no closed solution (formula) for the parameters in function of the data

The point estimates are determined by a multi-step iterative algorithms

# GLM diagnostic 1: Hat and Cook

- **Detection of influential observations and poor fitting**

1) **Hat values $h_i$** In analogy to LM there is a definition of a hat matrix for logistic regression fits and large diagonal values suggest a potential high influence (**leverage**) of a point on the obtained fit. Limit ~ 2p / n or 3p / n.

2) **Cook's distance $Cd_i$** is a measure of a change in estimated coefficients when the observation i is ignored. Large values (> ~ 4/n) suggest a large influence, pointing to observations one might want to "investigate".

3) (The square of the) individual **deviance residuals** or **studentized residuals** can also indicate single observation points with potential high influence or outlying character.

Plots: influencePlot (model);
residualPlot(model2, type = "response")
residualPlot(model2, type = "pearson")
residualPlot(model2, type = "deviance")

# GLM diagnostic 2: analysis of residuals

- Deviance residuals vs fitted values
- **Missing patterns**: **Deviance residuals vs each of the available covariates**
- **Dispersion check: Quantile Residuals**

Many more checking procedures are known, but **interpretation** and recommended actions rarely straightforward

# GLM diagnostic 3: analysis of residuals

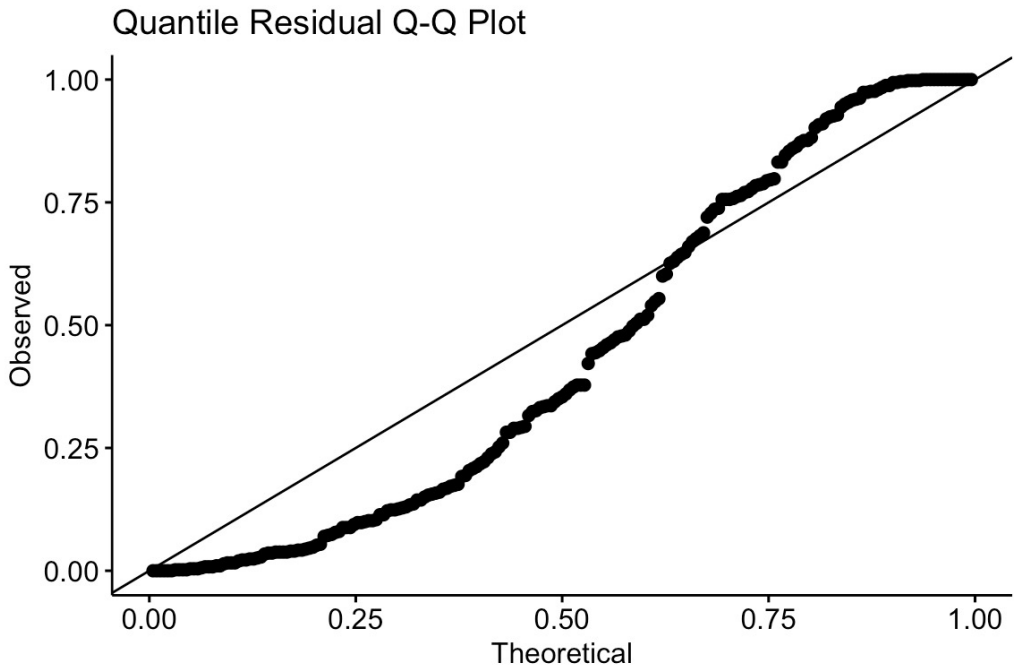
**Quantile Residuals $QR_i$**

Example: (Poisson GLM QRs)

Several excessively extreme (larger and smaller than expected) QRs in this checking

suggests overdispersion of data

might suggest the use of a **quasi-Poisson** or a **Negativ Binomial** approach instead of the Poisson, as these have higher variances



# GLM diagnostic 4: analysis of residuals

**Quantile Residuals $QR_i$**

One can generate faked simulated data from the fitted model, like distribution of predicted new values and compare to the observed values (for each data point, each $\mathbf{x}_i$).
The nb of fakes < obs, $y_i$ is called quantile residual $\mathbf{Qr}_i$ .

If the data are distributed as specified by the model these follow a uniform U[0,1] distribution.

A Q-Q plot of calculated vs. expected quantile residuals can detect significant departures and suggest modifications to the model.

# GLM diagnostic 5: analysis of residuals

"**Raw Residuals" $RR_i$ = $Y_i$ - fitted E [Y | X)** , where $Y_i$ = 0 or 1

**Pearson Residuals $PR_i$** :
are adjusted for expected variance (given X) and are expected to follow approximately a normal distribution at each $X_i$ (under assumptions).
Can reveal potential outliers.
Large residuals (in absolute value) are "somewhat strange" compared to their "neighbour points", but not necessarily to be considered outliers (in general some large residuals have to be expected).

A (linear) trend in a plot of **$PR_i$** against covariates might identify predictors **that have been** omitted in the model but should maybe be included.
Trend: add a loess to the graph

A curved trend might indicate that adding a higher order term of the covariate could be useful (ex. $x^2$).

# GLM diagnostic 6: autocorrelation

A quick test if there is any obvious evidence of **non-independence** of the observations**:**

Check for «autocorrelation», function  acf()

# Challenge 1

Using the babies dataset

- Fit a logistic regression to find parameters explaining the probability of prematurity ?
- What is the effect of birth weight on the probability of prematurity ?
- What about parity ?

# Solution

```
> model2 <- glm(prem ~ bwt, family=binomial)
> summary(model2)

Call:
glm(formula = prem ~ bwt, family = binomial)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.2879  -0.3985  -0.2784  -0.1810   3.0710

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  5.017338   0.717952   6.988 2.78e-12 ***
bwt         -0.067061   0.006808  -9.851  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 664.66  on 1173  degrees of freedom
Residual deviance: 545.31  on 1172  degrees of freedom
AIC: 549.31

Number of Fisher Scoring iterations: 6
```

# How to test »significance» and determine CI ?

Given standard errors SE of ß :

test-statistics = estimate / SE = z

approx. Normal (under the null hypothesis)

called a **Wald-test**

CI width = approx. 1.96 * SE

CI symmetric for ß and the log odds scale

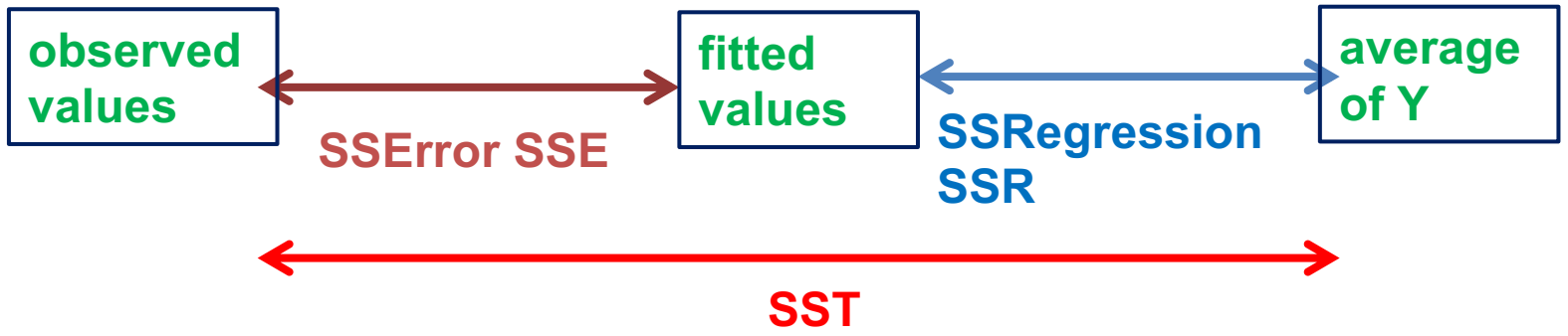
$\Rightarrow$ not symmetric for the multiplicative effect exp(ß) on the odds scale

$\Rightarrow$ not symmetric for the effect on the probability $\pi$

$$SST = SSR + SSE$$

*Total sum of squares = regression SS + residual SS*

**HEURISTIC REPRESENTATION**




$$R^2 = SSR / SST = 1 - (SSE / SST)$$

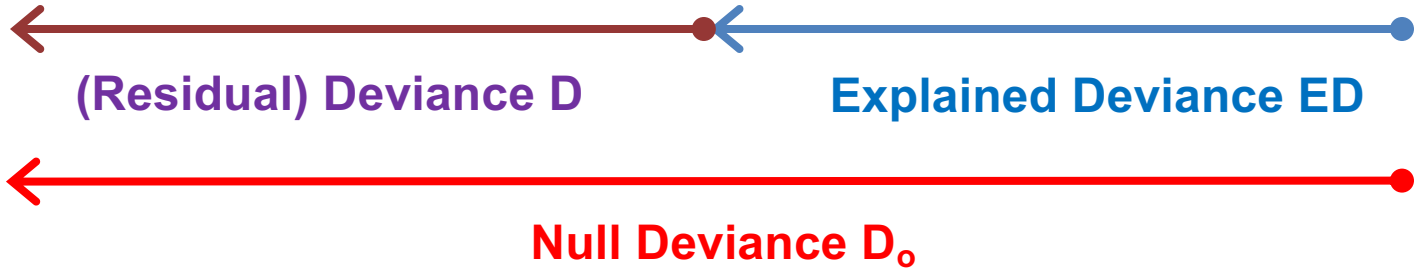
# MLE likelihood and deviance

**Highest (log) likelihood possible, predictors best adapted to each Yi**

*Deviance : difference in 2* Log Lik*

**(log) likelihood if data from a fixed distribution with no individual observation-predictors**

| **observed values, Saturated model** | **fitted , current proposed, Model** | **"Null model" , only 1 parameter** |
|---|---|---|




$$D_o = ED + D; \quad ED = D_o - D$$

$$R^2 \Rightarrow ED / D_o = (D_o - D) / D_o) = 1 - (D / D_o) = \text{called a pseudo-}R^2$$

Notes: log Lik ≤ 0 ; good Log Lik is close to 0;
Deviance > 0 : a measure of "lack of fitting",
good is small positive close to 0
Parameter Optimization: Maximal (Log) Likelihood ~ Minimal Deviance

# Deviance

- **Null deviance**: how well (or bad) the response variable is predicted by a model that includes only the intercept (overall mean, logistic: binomial with fixed p) compared to the best possible model

- **Residual deviance**: how much deviance is missing compared to the best model after including the proposed set of independent variables (residual lack of fit)

# Solution

```
> model2 <- glm(prem ~ bwt, family=binomial)
> summary(model2)

Call:
glm(formula = prem ~ bwt, family = binomial)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.2879  -0.3985  -0.2784  -0.1810   3.0710

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  5.017338   0.717952   6.988 2.78e-12 ***
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Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 664.66  on 1173  degrees of freedom
Residual deviance: 545.31  on 1172  degrees of freedom
AIC: 549.31

Number of Fisher Scoring iterations: 6
```

# Multiple Logistic Regression

Extension to more than one predictor variable (either numeric or dummy variables).

With *k* predictors, the model is written:

$$\pi = \frac{e^{\beta_0 + \beta_1 x_1 + .. + \beta_k x_k}}{1 + e^{\beta_0 + \beta_1 x_1 + .. + \beta_k x_k}}$$

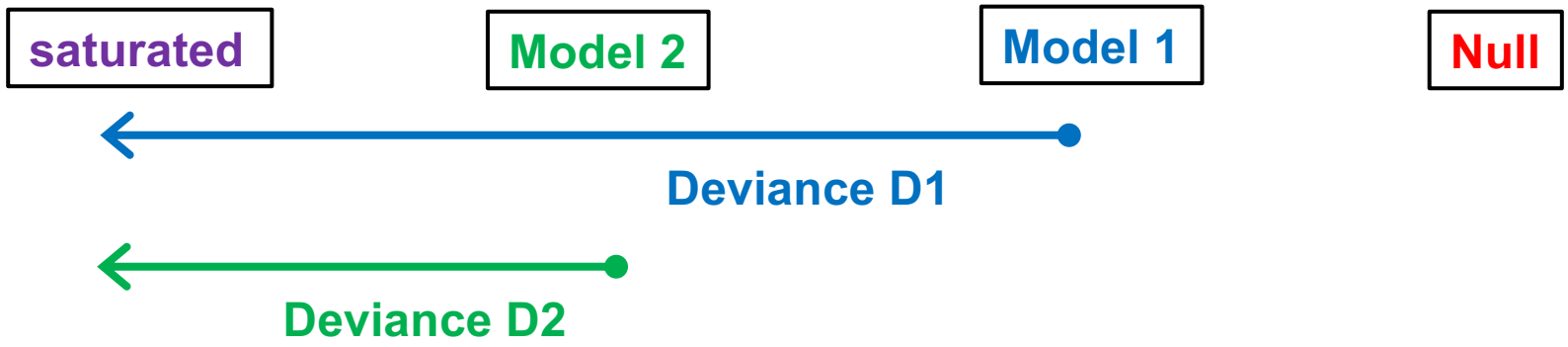
Adjusted Odds ratio for raising $x_i$ by 1 unit, holding all other predictors constant:

$$OR_i = e^{\beta_i}$$

# Solution

```
> model4 <- glm(prem ~ bwt*smoke+parity, family=binomial)
> summary(model4)

Call:
glm(formula = prem ~ bwt * smoke + parity, family = binomial)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.4798  -0.3998  -0.2784  -0.1682   2.9571

Coefficients:
                  Estimate Std. Error z value Pr(>|z|)
(Intercept)       4.839354   0.978834   4.944 7.65e-07 ***
bwt              -0.062082   0.008741  -7.103 1.22e-12 ***
smokesmoker       2.247047   1.609071   1.396   0.1626
paritynot first -0.470085   0.283836  -1.656   0.0977 .
bwt:smokesmoker -0.028043   0.015781  -1.777   0.0756 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 664.66  on 1173  degrees of freedom
Residual deviance: 532.93  on 1169  degrees of freedom
AIC: 542.93

Number of Fisher Scoring iterations: 6
```

# model comparison tests




**Likelihood Ratio Test LRT**

**Nested** models
- the smaller model 1 is a special case of the larger model 2;
- larger model 2 has all predictors of model 1 and some additional predictors

Comparison of **nested** models:
- we can test if the improvement of model 2 over model 1 is statistically significant with a **likelihood ratio test (LRT) = deviance test = Wilks test**

# model comparison tests

**Likelihood Ratio Test LRT**

Test statistic = 2 x Log Lik Ratio = **Deviance D1 - Deviance D2**

~ **chi2 distribution** with degrees of freedom = df for smaller model (higher df) - df for larger model

Example R code :

```
anova (model1, model2, test = "Chisq")
```

The same function encodes the analogous model comparison test for LM models
Example for the class data :

```
anova(model.0, model.3)
Model 1: Height ~ Age
Model 2: Height ~ Age + Weight
  Res.Df    RSS  Df  Sum of Sq      F    Pr(>F)
1     17 1042.71
2     16  524.94   1     517.77 15.781 0.0011 **
```

# Model quality indices

## R squared

Analogous of $R^2$ in LM

$R^2 = ED / D_o = (D_o - D) / D_o) = 1 - (D / D_o)$

**called a pseudo- $R^2$**

Many different R-Squared and adjusted R-Squared have been proposed for GLM
Some are fairly widely used but generally model selection is best done with LRT

## Akaike Information Criterion (AIC)

- allows to assess the quality of a model through comparison of related models
- based on the Deviance, but penalizes for the number of parameters (like adjusted R-squared, it's intent is to correct for irrelevant predictors)

# Solution

```
> model4 <- glm(prem ~ bwt*smoke+parity, family=binomial)
> summary(model4)

Call:
glm(formula = prem ~ bwt * smoke + parity, family = binomial)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
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paritynot first -0.470085   0.283836  -1.656   0.0977 .
bwt:smokesmoker -0.028043   0.015781  -1.777   0.0756 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 664.66  on 1173  degrees of freedom
Residual deviance: 532.93  on 1169  degrees of freedom
AIC: 542.93

Number of Fisher Scoring iterations: 6
```

# Model selection

**Nested Models: LRT !!!!**

Otherwise: complicated
¿ Nothing simple works reliably ?

**Multiple data methods** (separate datasets learning-testing, **cross-validation**, bootstraps)

Some methods incorporate cross-validation for optimization:
(ex. **penalized regression,** f.ex. package glmnet)

(See statistical learning / machine learning literature)

# Other Questions 1

Does another **link function** give a better fit ?
(example: binomial family regression: logit or complementary log-log which can better fit cases asymmetric about 0.5 , …)

For the Binomial Model

- There is the Probit link function, but very close to the Logit

- There is an asymmetric link function:
Complementary Log-Log transformation (cloglog)
$\log \{-\log [1- \pi(x) ] \}$ linear in X , $= X\beta$
$\pi(x) = 1 – \exp (- \exp (X\beta) )$
Results are frequently close to the Logit results

# Other Questions 2

Is the model appropriate ?

Does another model type («**family»)** give a better fit ?
(example: binomial vs. Poisson vs. Quasi Poisson)