

MASM22/FMSN30: Linear and Logistic Regression, 7.5 hp

FMSN40: ... with Data Gathering, 9 hp

Lecture 7, spring 2024

Logistic regression:
probabilities, odds and odds ratios
Maximum-likelihood estimates, Wald test

Mathematical Statistics / Centre for Mathematical Sciences
Lund University

22/4-24

Introduction

Why?

Binomial

Odds

Logistic regression model

Model

OR

Oslo

Maximum likelihood

log-likelihood

only intercept

full model

Newton-Raphson

Properties

Estimates

Distributions

Wald

Example

Probabilities

Introduction to Logistic regression

- ▶ In this part of the course we consider a *nonlinear model* (nonlinear in the β -parameters).
- ▶ However, it will be a monotonous transformation of a linear relationship making it a **Generalized Linear Model** (GLM)
- ▶ This time our response variable Y will be a **discrete, binary variable** (success/failure, yes/no, etc).
- ▶ The nature of the response will make the Bernoulli (a special case of the Binomial) distribution a natural choice.
- ▶ The resulting regression model is called **logistic regression**, because we will use a logistic transformation.
- ▶ Our expected response will be the probability of success.

Why is this relevant?

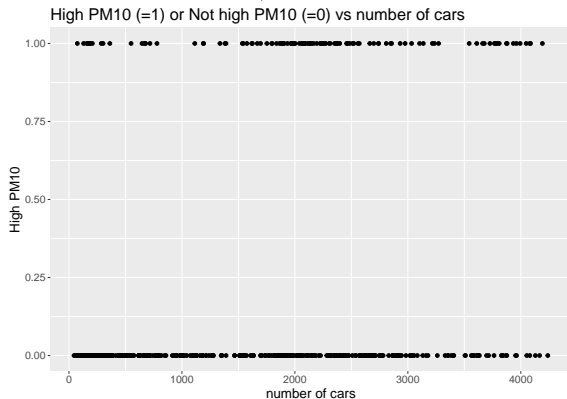
Examples:

- ▶ political election: response is win/lose. What factors (covariates) affect the probability to win? (e.g. money spent on campaign; age of the candidate etc.)
- ▶ result of some medical test (positive/negative): estimate the probability to have a “positive” result, depending on several physiological covariates.
- ▶ crash test dummies. Probability of “survival” of a dummy, depending on several test conditions.
- ▶ ...

We consider logistic regression with binary response. But extension to **multicategory** (or polytomous) response are possible, assuming a multinomial distributed response, see Lecture 11.

Example: particles in Oslo

A random subsample of 500 observations from the Norwegian Public Roads Administration measuring whether the concentration of atmospheric particles with a diameter between 2.5 and 10 μm , PM_{10} , exceeds the limit 50 $\mu\text{g}/\text{m}^3$.



Model???

Binomial distribution (a reminder)

Let Y be the number of successes in n independent trials, each with the same probability of success, p . Then $Y \sim \text{Bin}(n, p)$ with

$$\Pr(Y = k) = \binom{n}{k} p^k (1 - p)^{n-k}, \quad k = 0, 1, \dots, n$$

$$E(Y) = np, \quad V(Y) = np(1 - p).$$

For the estimate $\hat{p} = Y/n$ we have

$$\hat{p} \approx N\left(p, \frac{p(1-p)}{n}\right) \quad I_p \approx \left(\hat{p} \pm \lambda_{\alpha/2} \sqrt{\frac{\hat{p}(1-\hat{p})}{n}}\right)$$

when n is large enough, typically when $np(1-p) > 10$.

Warning: If n is too small the interval can go outside $[0, 1]$.

We will have $n = 1$. Not even close to “large enough”.

Before (linear regression)

Y_i was a continuous variable with

$$Y_i = \mathbf{x}_i\boldsymbol{\beta} + \epsilon_i \text{ where } \epsilon_i \sim N(0, \sigma^2) \Leftrightarrow Y_i \sim N(\mu_i, \sigma^2)$$
$$E(Y_i) = \mu_i = \mathbf{x}_i\boldsymbol{\beta} = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}$$

Now (logistic regression)

Y_i is discrete with two possible outcomes: success (1) or failure (0) with probabilities $Pr(Y_i = 1) = p_i$ and $Pr(Y_i = 0) = 1 - p_i$

$$Y_i \sim \text{Bin}(1, p_i) \text{ with } Pr(Y_i = k) = p_i^k (1 - p_i)^{1-k}, k = 0, 1$$
$$E(Y_i) = \mu_i = p_i = \text{some function of } \mathbf{x}_i$$
$$V(Y_i) = p_i(1 - p_i) \text{ also depends on } \mathbf{x}_i$$

Choosing $\mu_i = p_i = \mathbf{x}_i\boldsymbol{\beta}$ is *not* good since we need $0 \leq p_i \leq 1$.

Odds: number of successes for each failure

The odds of “success” is defined as

$$\text{odds} = \frac{Pr(\text{success})}{Pr(\text{failure})} = \frac{p}{1-p} \quad \Leftrightarrow p = \frac{\text{odds}}{1 + \text{odds}}$$

$$\text{log-odds} = \ln \text{odds} = \ln \frac{p}{1-p} = \text{logit}(p)$$

$$\text{odds}_{\text{failure}} = \frac{1}{\text{odds}_{\text{success}}} \quad \ln \text{odds}_{\text{failure}} = -\ln \text{odds}_{\text{success}}$$

	min	middle	max	
p	0	1/2	1	
odds	0	1	∞	
$\ln \text{odds}$	$-\infty$	0	∞	no bounds!

Introduction

Why?

Binomial

Odds

Logistic regression model

Model

OR

Oslo

Maximum likelihood

log-likelihood

only intercept

full model

Newton-Raphson

Properties

Estimates

Distributions

Wald

Example

Probabilities

Logistic regression model

We assume that

$$Y_i = \text{"success"} (= 1) \text{ or "failure"} (= 0)$$

$$Pr(Y_i = 1) = 1 - Pr(Y_i = 0) = p_i$$

$$Y_i \sim \text{Bin}(1, p_i), \quad i = 1, \dots, n, \text{ and pairwise independent}$$

$$\text{logodds}_i = \ln \frac{p_i}{1 - p_i} = \beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip} = \mathbf{x}_i \boldsymbol{\beta}.$$

$$\text{This gives } p_i = \frac{e^{\mathbf{x}_i \boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i \boldsymbol{\beta}}} \text{ as a non-linear function of } \boldsymbol{\beta}.$$

Parameter interpretation

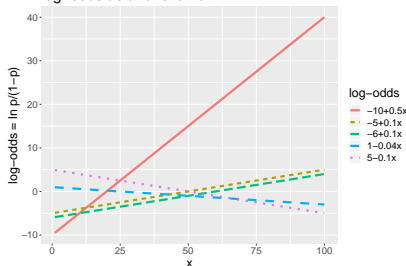
$$\beta_0 = \text{log-odds and } e^{\beta_0} = \text{odds when all } x_{ij} \text{ are 0,}$$

$$\beta_j = \text{additive change in log-odds and...}$$

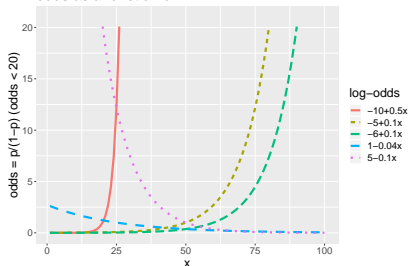
$$e^{\beta_j} = \text{relative change in odds when } x_{ij} \text{ is increased by 1, } j = 1, \dots, p$$

= odds ratio (OR)

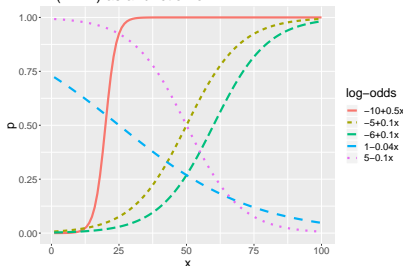
log-odds as a function of x



odds as a function of x



Pr(Y = 1) as a function of x



$$Y_i \sim \text{Bin}(1, p_i)$$

The log-odds is linear:

$$\ln \text{odds}_i = \beta_0 + \beta_1 x_i$$

The odds is exponential:

$$\text{odds}_i = e^{\beta_0 + \beta_1 x_i} = e^{\beta_0} \cdot (e^{\beta_1})^{x_i}$$

The probability is S-shaped:

$$p_i = \frac{e^{\beta_0 + \beta_1 x_i}}{1 + e^{\beta_0 + \beta_1 x_i}}$$

Interpretation of e^{β_1} : odds ratio

- What happens to the odds when we increase x by 1?

$$\text{odds ratio} = \text{OR} = \frac{e^{\beta_0 + \beta_1(x+1)}}{e^{\beta_0 + \beta_1 x}} = e^{\beta_1}$$

If $\beta_1 = 0.04$ then $e^{\beta_1} = 1.04$ and the odds increases by 4 %.

If $\beta_1 = -0.04$ then $e^{\beta_1} = 0.96$ and the odds decreases by 4 %.

- What happens to the odds when we increase x by 10?

$$\text{OR} = \frac{e^{\beta_0 + \beta_1(x+10)}}{e^{\beta_0 + \beta_1 x}} = e^{10\beta_1} = (e^{\beta_1})^{10}$$

If $\beta_1 = 0.04$ then $(e^{\beta_1})^{10} = 1.04^{10} = 1.49$ and the odds increases by 49 %.

If $\beta_1 = -0.04$ then $(e^{\beta_1})^{10} = 0.96^{10} = 0.67$ and the odds decreases by 33 %.

Size of the change

Marginal change = derivative ($\mathbf{x}\beta = \beta_0 + \beta_1 x$):

$$\frac{d \log \text{odds}}{dx} = \frac{d}{dx} \mathbf{x}\beta = \beta_1 \quad \text{constant,}$$

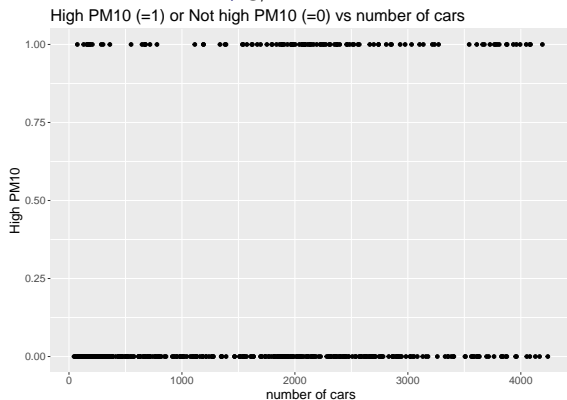
$$\frac{d \text{odds}}{dx} = \frac{d}{dx} e^{\mathbf{x}\beta} = \beta_1 e^{\mathbf{x}\beta} = \beta_1 \cdot \text{odds} \quad \text{prop. to the odds,}$$

$$\begin{aligned} \frac{dp}{dx} &= \frac{d}{dx} \frac{e^{\mathbf{x}\beta}}{1 + e^{\mathbf{x}\beta}} = \\ &= \beta_1 \cdot \frac{e^{\mathbf{x}\beta}}{1 + e^{\mathbf{x}\beta}} \left(1 - \frac{e^{\mathbf{x}\beta}}{1 + e^{\mathbf{x}\beta}}\right) = \\ &= \beta_1 \cdot p(1 - p) \quad \text{prop. to } V(Y|x) \end{aligned}$$

The size of the change in p is largest around $p = 0.5$ and gets smaller as $p \rightarrow 0$ or $\rightarrow 1$.

Example: particles in Oslo

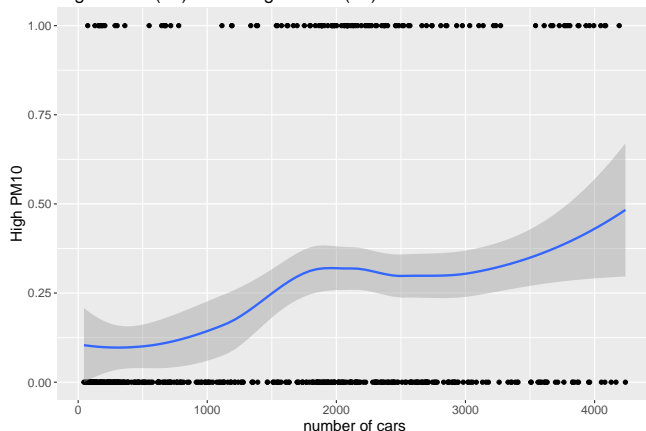
A random subsample of 500 observations from the Norwegian Public Roads Administration measuring whether the concentration of atmospheric particles with a diameter between 2.5 and 10 μm , PM_{10} , exceeds the limit 50 $\mu\text{g}/\text{m}^3$.



Does the data follow an S-shape? Well. . .

We can get a rough estimate of the shape using a moving average which calculates the average Y -value in an interval moving along the x -axis.

High PM10 (=1) or Not high PM10 (=0) vs number of cars



Sort of S-shaped. Obviously $\beta_1 > 0$. More cars give larger probability of exceeding the concentration limit.

Introduction

Why?

Binomial

Odds

Logistic regression model

Model

OR

Oslo

Maximum likelihood

log-likelihood

only intercept

full model

Newton-Raphson

Properties

Estimates

Distributions

Wald

Example

Probabilities

How should we estimate β

Least squares estimates?

- ▶ Minimize $Q(\beta) = \sum_{i=1}^n (\ln \frac{Y_i}{1-Y_i} - \mathbf{x}_i\beta)^2$?

No, $\ln \frac{Y_i}{1-Y_i} = \ln 0 = -\infty$ or $\ln \infty = \infty$. Useless!

- ▶ Minimize $Q(\beta) = \sum_{i=1}^n (Y_i - p_i)^2 = \sum_{i=1}^n (Y_i - \frac{e^{\mathbf{x}_i\beta}}{1+e^{\mathbf{x}_i\beta}})^2$?

No, since $V(Y_i) = p_i(1 - p_i)$ is not constant. We would need to do a weighted least squares but the weights $1/V(Y_i)$ are unknown.

- ▶ Minimize $Q(\beta) = \sum_{i=1}^n \frac{(Y_i - p_i)^2}{p_i(1-p_i)} = \sum_{i=1}^n \frac{(Y_i - \frac{e^{\mathbf{x}_i\beta}}{1+e^{\mathbf{x}_i\beta}})^2}{\frac{e^{\mathbf{x}_i\beta}}{1+e^{\mathbf{x}_i\beta}}(1 - \frac{e^{\mathbf{x}_i\beta}}{1+e^{\mathbf{x}_i\beta}})}$

using iteratively re-weighted least squares?

No, it can be done but it is a very inefficient method with a slow convergence rate.

Totally different method? Yes!

Maximum likelihood-method

Since we know what type of distribution our data come from, $Y_i \in \text{Bin}(1, p_i)$, we can find the β -values that maximize the probability of getting exactly the observation values that we got. That means that we should maximize the likelihood function

$$\begin{aligned} L(\beta; \mathbf{Y}) &= Pr(Y_1 = y_1, \dots, Y_n = y_n) = \prod_{i=1}^n Pr(Y_i = y_i) \\ &= \prod_{i=1}^n p_i^{Y_i} (1 - p_i)^{1-Y_i} = \prod_{i=1}^n \left(\frac{e^{\mathbf{x}_i \beta}}{1 + e^{\mathbf{x}_i \beta}} \right)^{Y_i} \left(1 - \frac{e^{\mathbf{x}_i \beta}}{1 + e^{\mathbf{x}_i \beta}} \right)^{1-Y_i} \\ &= \prod_{i=1}^n \left(\frac{e^{\mathbf{x}_i \beta}}{1 + e^{\mathbf{x}_i \beta}} \right)^{Y_i} \left(\frac{1}{1 + e^{\mathbf{x}_i \beta}} \right)^{1-Y_i} = \prod_{i=1}^n \frac{e^{\mathbf{x}_i \beta Y_i}}{1 + e^{\mathbf{x}_i \beta}} \end{aligned}$$

It is easier to maximize the log-likelihood function instead:

$$\ln L(\beta; \mathbf{Y}) = \sum_{i=1}^n \left(\mathbf{x}_i \beta Y_i - \ln(1 + e^{\mathbf{x}_i \beta}) \right)$$

ML-estimate for the Null model, $\ln \frac{p_i}{1-p_i} = \beta_0$

For the simplest model, having only an intercept, we have

$$p_i = \frac{e^{\beta_0}}{1 + e^{\beta_0}}$$

and the ML-estimate can easily be derived as

$$\begin{aligned}\ln L(\beta_0) &= \sum_{i=1}^n \left(\beta_0 Y_i - \ln(1 + e^{\beta_0}) \right) = \beta_0 \sum_{i=1}^n Y_i - n \ln(1 + e^{\beta_0}) \\ \frac{d \ln L(\beta_0)}{d \beta_0} &= \sum_{i=1}^n Y_i - \frac{n e^{\beta_0}}{1 + e^{\beta_0}} = 0 \Rightarrow \\ \hat{\beta}_0 &= \ln \frac{\bar{Y}}{1 - \bar{Y}} \Rightarrow \hat{p}_i = \bar{Y} = \frac{\text{number of successes}}{\text{number of observations}}\end{aligned}$$

ML-estimate for the full model: $\ln \frac{p_i}{1-p_i} = \mathbf{x}_i \boldsymbol{\beta}$

Find the $\boldsymbol{\beta}$ that maximizes the log-likelihood. This means setting all the partial derivatives equal to 0. First, rewrite using matrices as much as possible:

$$\begin{aligned} \ln L(\boldsymbol{\beta}) &= \sum_{i=1}^n \left(\mathbf{x}_i \boldsymbol{\beta} Y_i - \ln(1 + e^{\mathbf{x}_i \boldsymbol{\beta}}) \right) = \\ &= (\mathbf{X} \boldsymbol{\beta})^T \mathbf{Y} - \sum_{i=1}^n \ln(1 + e^{\mathbf{x}_i \boldsymbol{\beta}}) \\ &= \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{Y} - \sum_{i=1}^n \ln(1 + e^{\mathbf{x}_i \boldsymbol{\beta}}) \end{aligned}$$

Then use $\frac{\partial \boldsymbol{\beta}^T \mathbf{A}}{\partial \boldsymbol{\beta}} = \mathbf{A}$, $\frac{\partial \mathbf{A} \boldsymbol{\beta}}{\partial \boldsymbol{\beta}} = \mathbf{A}^T$, $\frac{d \ln x}{dx} = \frac{1}{x}$, $\frac{de^x}{dx} = e^x$ and

$$\frac{df(g(h(x)))}{dx} = f'(g(h(x))) \cdot g'(h(x)) \cdot h'(x).$$

The partial derivatives then become

$$\frac{\partial \ln L(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = \mathbf{X}^T \mathbf{Y} - \sum_{i=1}^n \mathbf{x}_i^T \cdot \underbrace{\frac{e^{\mathbf{x}_i \boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i \boldsymbol{\beta}}}}_{p_i} = \mathbf{X}^T \mathbf{Y} - \mathbf{X}^T \mathbf{p} = \mathbf{0}$$

where \mathbf{p} is a $n \times 1$ vector with elements p_i , $i = 1, \dots, n$.

The solution should satisfy the “Normal equations”

$$\mathbf{X}^T \mathbf{p} = \mathbf{X}^T \mathbf{Y}$$

These are nonlinear in $\boldsymbol{\beta}$ and there is no closed form solution. We need an iterative method, e.g. Newton-Raphson algorithm. (Not in this course.)

(*) Estimates via Newton-Raphson (a.k.a. Fisher-scoring)

- ▶ Start from an arbitrary guess $\hat{\beta}^{(0)}$, then iterate until $\|\hat{\beta}^{(k+1)} - \hat{\beta}^{(k)}\|$ is small enough.
- ▶ A generic iteration k of Newton-Raphson/Fisher-scoring is:
$$\hat{\beta}^{(k+1)} = \hat{\beta}^{(k)} + (\mathbf{X}^T \mathbf{W}^{(k)} \mathbf{X})^{-1} \mathbf{X}^T (\mathbf{Y} - \hat{\mathbf{p}}^{(k)}), \quad k = 0, 1, \dots$$
- ▶ Here $\hat{\mathbf{p}}^{(k)}$ is estimated using the current $\hat{\beta}^{(k)}$
- ▶ $\mathbf{W}^{(k)}$ is a diagonal matrix with elements $(w_{11}^{(k)}, \dots, w_{nn}^{(k)})$ where $w_{ii}^{(k)} = \hat{p}_i^{(k)}(1 - \hat{p}_i^{(k)})$.
- ▶ At convergence (k large) we write $\mathbf{W}^{(k)} \equiv \mathbf{W}$ and $\hat{\mathbf{p}}^{(k)} \equiv \hat{\mathbf{p}}$.

Introduction

Why?

Binomial

Odds

Logistic regression model

Model

OR

Oslo

Maximum likelihood

log-likelihood

only intercept

full model

Newton-Raphson

Properties

Estimates

Distributions

Wald

Example

Probabilities

ML-estimates of β

At convergence the ML-estimates of β become

$$\hat{\beta} = (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} \mathbf{Z}$$

where $\mathbf{W} = \hat{\text{Var}}(\mathbf{Y})$ is a diagonal matrix with elements

$$w_{ii} = \hat{p}_i(1 - \hat{p}_i), \quad i = 1, \dots, n,$$

\mathbf{Z} is a column vector with elements

$$Z_i = \mathbf{x}_i \hat{\beta} + \frac{Y_i - \hat{p}_i}{\hat{p}_i(1 - \hat{p}_i)}, \quad i = 1, \dots, n$$

and

$$\hat{p}_i = \frac{e^{\mathbf{x}_i \hat{\beta}}}{1 + e^{\mathbf{x}_i \hat{\beta}}}, \quad i = 1, \dots, n.$$

Asymptotics from likelihood estimation

For all maximum likelihood estimates, $\hat{\boldsymbol{\theta}}$, we have

$$\sqrt{n}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) \rightarrow N(\mathbf{0}, \mathbf{I}_{\text{Fish}}^{-1}) \quad (n \rightarrow \infty)$$

where \mathbf{I}_{Fish} is the Fisher information matrix (see any reference in inference theory and some numerical analysis).

In this case, it means that

$$\hat{\boldsymbol{\beta}} \sim N_{p+1}(\boldsymbol{\beta}, (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1}) \quad (n \rightarrow \infty)$$

$$\mathbf{x}_0 \hat{\boldsymbol{\beta}} \sim N(\mathbf{x}_0 \boldsymbol{\beta}, \mathbf{x}_0 (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{x}_0^T) \quad (n \rightarrow \infty)$$

Motivates the Wald test and confidence interval for β_j and constructing intervals for p_0 based on the log odds $\mathbf{x}_0 \boldsymbol{\beta}$.

Warning: for small and medium n the normal approximation is not good. Confidence intervals for $\mathbf{x}_0 \boldsymbol{\beta}$ are usually OK. For $\boldsymbol{\beta}$, use likelihood based tests and intervals instead, see Lecture 8.

Wald test for β_j (when n is very large)

Does variable x_j have a significant effect on the probability of success, i.e., does it change the log-odds of success?

Wald test

We want to test $H_0: \beta_j = 0$ against $H_1: \beta_j \neq 0$. If H_0 is true then

$$Z = \frac{\hat{\beta}_j - 0}{d(\hat{\beta}_j)} \sim N(0, 1) \quad \text{if } n \text{ is large}$$

and we should reject H_0 at significance level α if

$$\frac{|\hat{\beta}_j - 0|}{d(\hat{\beta}_j)} > \lambda_{\alpha/2}$$

Using `summary(model)` gives Wald tests for the β -parameters.

Warning: For small and medium size data ($n \ll \infty$) you should use a likelihood ratio test instead, see Lecture 8.

Wald based confidence intervals for log odds (ratios)

If n is large, so that the normal approximation of $\hat{\beta}$ is good, we can construct confidence intervals for β_j in the usual way (define λ_α as the α -percentile from $N(0, 1)$):

$$I_{\ln \text{OR}_j} = I_{\beta_j} = (\hat{\beta}_j \pm \lambda_{\alpha/2} \cdot d(\hat{\beta}_j)).$$

Warning: For small and medium size data, use a profile likelihood based confidence interval instead, see Lecture 8. This is what `confint(model)` does if the MASS package is installed.

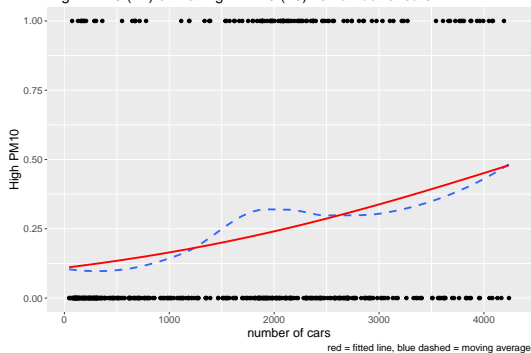
Confidence interval for odds and odds ratios

With $I_{\beta_j} = (c_1, c_2)$ we just exponentiate the bounds to get confidence intervals for the intercept odds, e^{β_0} , and the odds ratios, e^{β_j} , $j = 1, \dots, p$:

$$I_{\text{OR}_j} = I_{e^{\beta_j}} = e^{I_{\beta_j}} = (e^{c_1}, e^{c_2})$$

	param.	est.	s.e.	P-value (Wald)	95 % C.I. (profile)
Intercept	β_0	-2.10	0.22	< 0.001	(-2.55, -1.68)
cars/1000	β_1	0.48	0.10	< 0.001	(0.29, 0.67)
	param.	est.	95 % C.I.		
Intercept	e^{β_0}	$e^{-2.10} = 0.12$	$(e^{-2.55}, e^{-1.68}) = (0.08, 0.19)$		
cars/1000	e^{β_1}	$e^{0.48} = 1.61$	$(e^{0.29}, e^{0.67}) = (1.34, 1.95)$		

High PM10 (=1) or Not high PM10 (=0) vs number of cars



Interpretation:

OR = $e^{\hat{\beta}_1} = 1.61$.

The odds of having High PM₁₀ increases by 61 % when the number of cars increases by 1000.

Probability estimates

Since the log-odds is a linear function

$$\ln \frac{p_i}{1 - p_i} = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} = \mathbf{x}_i \boldsymbol{\beta}$$

the corresponding probability of success becomes

$$p_i = \frac{e^{\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}}}{1 + e^{\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}}} = \frac{e^{\mathbf{x}_i \boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i \boldsymbol{\beta}}}$$

which is a non-linear function of the $\boldsymbol{\beta}$ -parameters.

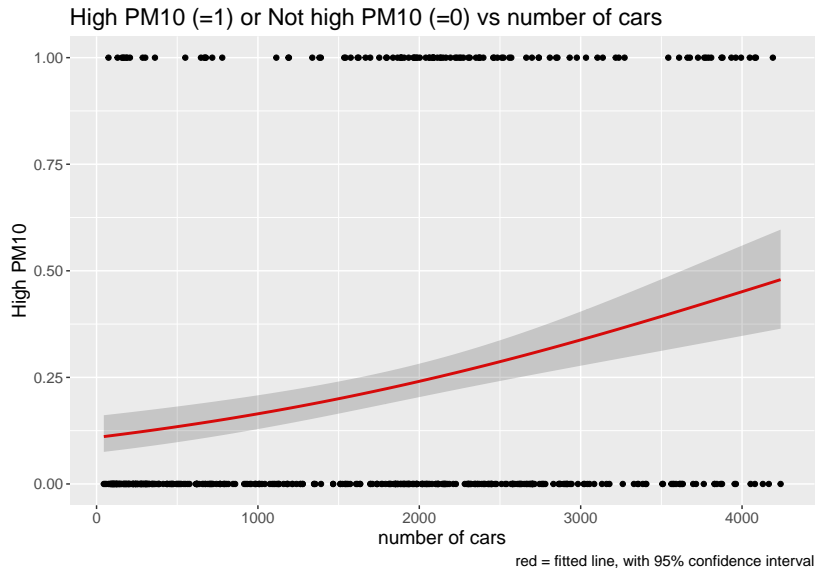
Since $\mathbf{x}_i \hat{\boldsymbol{\beta}}$ is a linear function of (dependent, approx.) normally distributed $\boldsymbol{\beta}$ -estimates we can construct confidence intervals for the log odds:

$$I_{\mathbf{x}_i \boldsymbol{\beta}} = (\mathbf{x}_i \hat{\boldsymbol{\beta}} \pm \lambda_{\alpha/2} \cdot d(\mathbf{x}_i \hat{\boldsymbol{\beta}}))$$

Since \hat{p}_i is a monotonous, increasing, function of $\mathbf{x}_i \hat{\boldsymbol{\beta}}$ we get

$$I_{p_i} = \frac{e^{I_{\mathbf{x}_i \boldsymbol{\beta}}}}{1 + e^{I_{\mathbf{x}_i \boldsymbol{\beta}}}}$$

which always lies in $[0, 1]!$



Prediction interval? The observations will always be either 0 or 1 so we will need other methods than intervals here, see Lecture 9.