A-B-C

Data Mining - CdL CLAMSES

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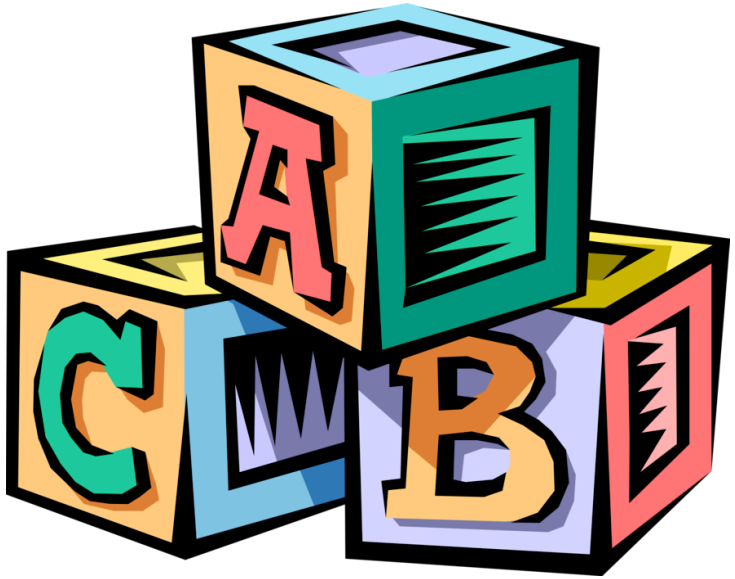


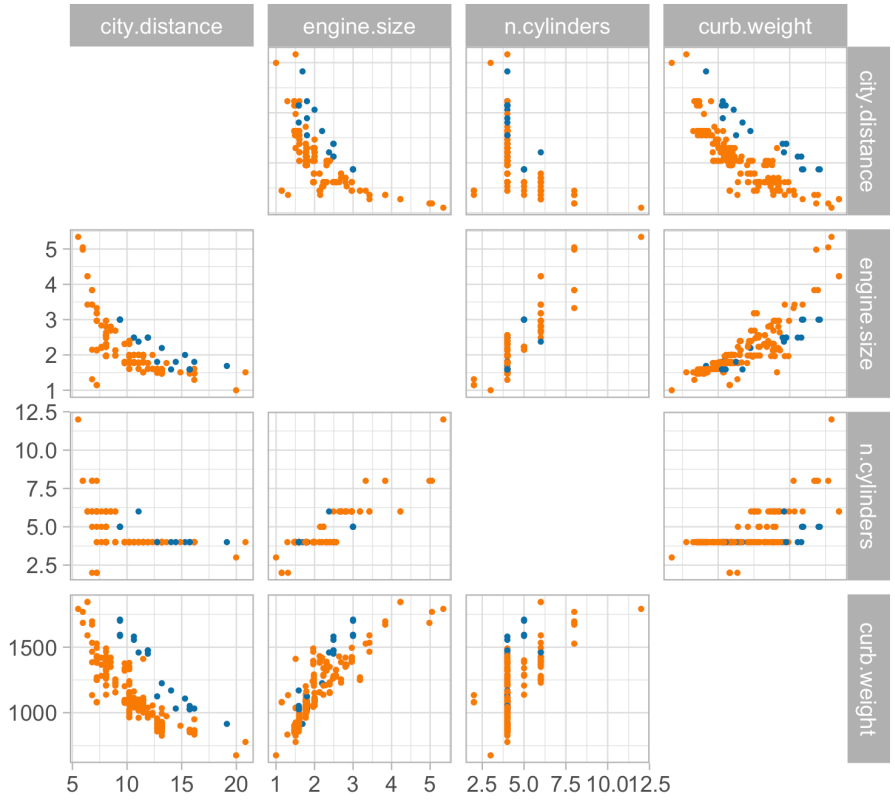
"Everything should be made as simple as possible, but not simpler"

Attributed to **Albert Einstein**

- This unit will cover the following **topics**:
  - Linear models and the modeling process
  - Cholesky factorization
  - Orthogonalization and QR decomposition
  - Iterative methods
  - Generalized linear models
- The **computational aspects** of linear models will be novel to most of you...
- ... but you should be already **very familiar** with linear models!

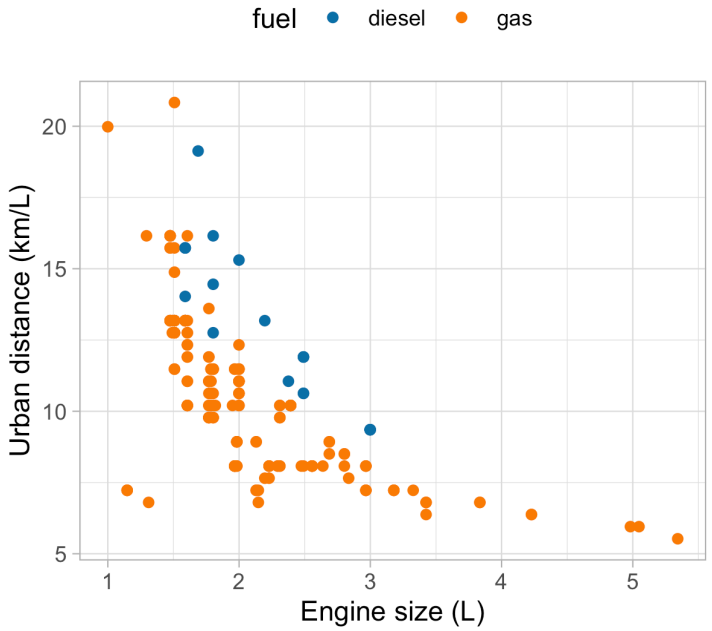
Old friends: linear models

Car data (diesel or gas)



- We consider data for $n = 203$ models of cars in circulation in 1985 in the USA.
- We want to **predict** the distance per unit of fuel as a function of the vehicle features.
- We consider the following **variables**:
  - The city distance per unit of fuel (km/L, `city.distance`)
  - The engine size (L, `engine.size`)
  - The number of cylinders (`n.cylinders`)
  - The curb weight (kg, `curb.weight`)
  - The fuel type (gasoline or diesel, `fuel`).

Linear regression



- Let us consider the variables `city.distance` (y), `engine.size` (x) and `fuel` (z).
- A **simple linear regression**

$$Y_i = \beta_1 + \beta_2 x_i + \epsilon_i, \qquad i = 1, \dots, n,$$

  could be easily fit by least squares...
- ... but the plot suggests that the relationship between `city.distance` and `engine.size` is **not** well approximated by a **linear** function.
- ... and also that `fuel` has a non-negligible effect on the response.

Regression models

- A **general** and **more flexible formulation** for modeling the relationship between a vector of **fixed covariates** $\boldsymbol{x}_i = (x_{i1}, \ldots, x_{ip})^T \in \mathbb{R}^p$ and a random variable $Y_i \in \mathbb{R}$ is

$$Y_i = f(\boldsymbol{x}_i; \beta) + \epsilon_i, \qquad i = 1, \ldots, n,$$

  where the "errors" ϵ_i are iid random variables, having zero mean and variance σ^2.

- To estimate the unknown parameters β, a possibility is to rely on the **least squares criterion**: we seek the **minimum** of the objective function

$$D(\beta) = \sum_{i=1}^{n} \{y_i - f(\boldsymbol{x}_i; \beta)\}^2,$$

  using n pairs of covariates $\boldsymbol{x}_i = (x_{i1}, \ldots, x_{ip})^T$ and the observed realizations y_i of the random variables Y_i, for $i = 1, \ldots, n$. The **optimal value** is denoted by $\hat{\beta}$.

- The **predicted values** are $\hat{y}_i = \mathbb{E}(Y_i) = f(\boldsymbol{x}_i; \hat{\beta})$, for $i = 1, \ldots, n$.

Linear models

- Let us consider again the variables `city.distance` (y), `engine.size` (x) and `fuel` (z).
- Which function $f(x, z; \beta)$ should we choose?
- A first attempt is to consider a **polynomial term** combined with a **dummy variable**

$$f(x, z; \beta) = \beta_1 + \beta_2 x + \beta_3 x^2 + \beta_4 x^3 + \beta_5 I(z = \texttt{gas}),$$

which is a special instance of **linear model**.

Definition (Linear model)

In a **linear model** the response variable Y_i is related to the covariates through the function

$$\mathbb{E}(Y_i) = f(\boldsymbol{x}_i; \beta) = \beta_1 x_{i1} + \cdots + \beta_p x_{ip} = \boldsymbol{x}_i^T \beta,$$

where $\boldsymbol{x}_i = (x_{i1}, \ldots, x_{ip})^T$ is a vector of **covariates** and $\beta = (\beta_1, \ldots, \beta_p)^T$ is the corresponding vector of **coefficients**.

Matrix notation

- The **response random variables** are collected in the random vector $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^T$, whose **observed realization** is $\boldsymbol{y} = (y_1, \ldots, y_n)^T$.
- The **design matrix** is a $n \times p$ matrix, comprising the covariate's values, defined by

$$\boldsymbol{X} = \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix}.$$

- The jth variable (column) is denoted with $\tilde{\boldsymbol{x}}_j$, whereas the ith observation (row) is $\boldsymbol{x}_i$:

$$\boldsymbol{X} = (\tilde{\boldsymbol{x}}_1, \ldots, \tilde{\boldsymbol{x}}_p) = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)^T.$$

- Then, a **linear model** can be written using the **compact notation**:

$$\boldsymbol{Y} = \boldsymbol{X}\beta + \boldsymbol{\epsilon},$$

where $\boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_n)^T$ is a vector of iid error terms with zero mean and variance σ^2.

Linear regression: estimation I

- The optimal set of coefficients $\hat{\beta}$ is the minimizer of the **least squared criterion**

$$D(\beta) = (\boldsymbol{y} - \boldsymbol{X}\beta)^T(\boldsymbol{y} - \boldsymbol{X}\beta) = ||\boldsymbol{y} - \boldsymbol{X}\beta||^2,$$

  also known as **residual sum of squares (RSS)**, where

$$||\boldsymbol{y}|| = \sqrt{y_1^2 + \cdots + y_n^2},$$

  denotes the **Euclidean norm**.

Least square estimate (OLS)

If the design matrix has **full rank**, that is, if $\mathrm{rk}(\boldsymbol{X}^T\boldsymbol{X}) = p$, then the **least square estimate** has an explicit solution:

$$\hat{\beta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}.$$

Linear regression: estimation II

- In matrix notation, the predicted values can be obtained as

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\hat{\beta} = \boldsymbol{H}\boldsymbol{y}, \qquad \boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T.$$

- $\boldsymbol{H}$ is a $n \times n$ **projection matrix** matrix sometimes called **hat matrix**.
- It can be shown that $\mathrm{tr}(\boldsymbol{H}) = \mathrm{rk}(\boldsymbol{H}) = p$. Moreover, it holds $\boldsymbol{H} = \boldsymbol{H}^T$ and $\boldsymbol{H}^2 = \boldsymbol{H}$.
- The quantity $D(\hat{\beta})$ is the so-called residual **deviance**, which is equal to

$$D(\hat{\beta}) = ||\boldsymbol{y} - \hat{\boldsymbol{y}}||^2 = \boldsymbol{y}^T(I_n - \boldsymbol{H})\boldsymbol{y}.$$

- Moreover, a typical estimate for the **residual variance** σ^2 is obtained as follows:

$$s^2 = \frac{D(\hat{\beta})}{n-p} = \frac{1}{n-p}\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T\hat{\beta})^2.$$

Linear regression: inference

- Let us additionally assume that the errors follow a Gaussian distribution: $\epsilon_i \overset{\text{iid}}{\sim} N(0, \sigma^2)$.
- This implies that the **distribution** of the **estimator** $\hat{\beta}$ is

$$\hat{\beta} \sim N_p(\beta, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}).$$

- Hence, the estimator $\hat{\beta}$ is **unbiased** and its **variance** can be estimated by

$$\widehat{\text{var}}(\hat{\beta}) = \boldsymbol{s}^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}.$$

- The **standard errors** of the components of $\hat{\beta}$ correspond to the square root of the diagonal of the above covariance matrix.
- Confidence interval and Wald's tests can be obtained through classical inferential theory.
- Ok, we are ready to get back to the original problem...

Car data, a first model

- Our first attempt for predicting `city.distance` (y) via `engine.size` (x) and `fuel` (z) is:

$$f(x, z; \beta) = \beta_1 + \beta_2 x + \beta_3 x^2 + \beta_4 x^3 + \beta_5 I(z = \mathbf{gas}).$$

- Indeed, by looking at the plot of the data, it is plausible that we need a **polynomial** of degree 3 or 4
- It is also clear from the plot that `fuel` is a relevant variable. Categorical variables are **encoded** using **indicator variables**.

- To evaluate the goodness of fit, we can calculate the **coefficient of determination**:

$$R^2 = 1 - \frac{(\text{“Residual deviance”})}{(\text{“Total deviance”})} = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}.$$

A first model: estimated coefficients

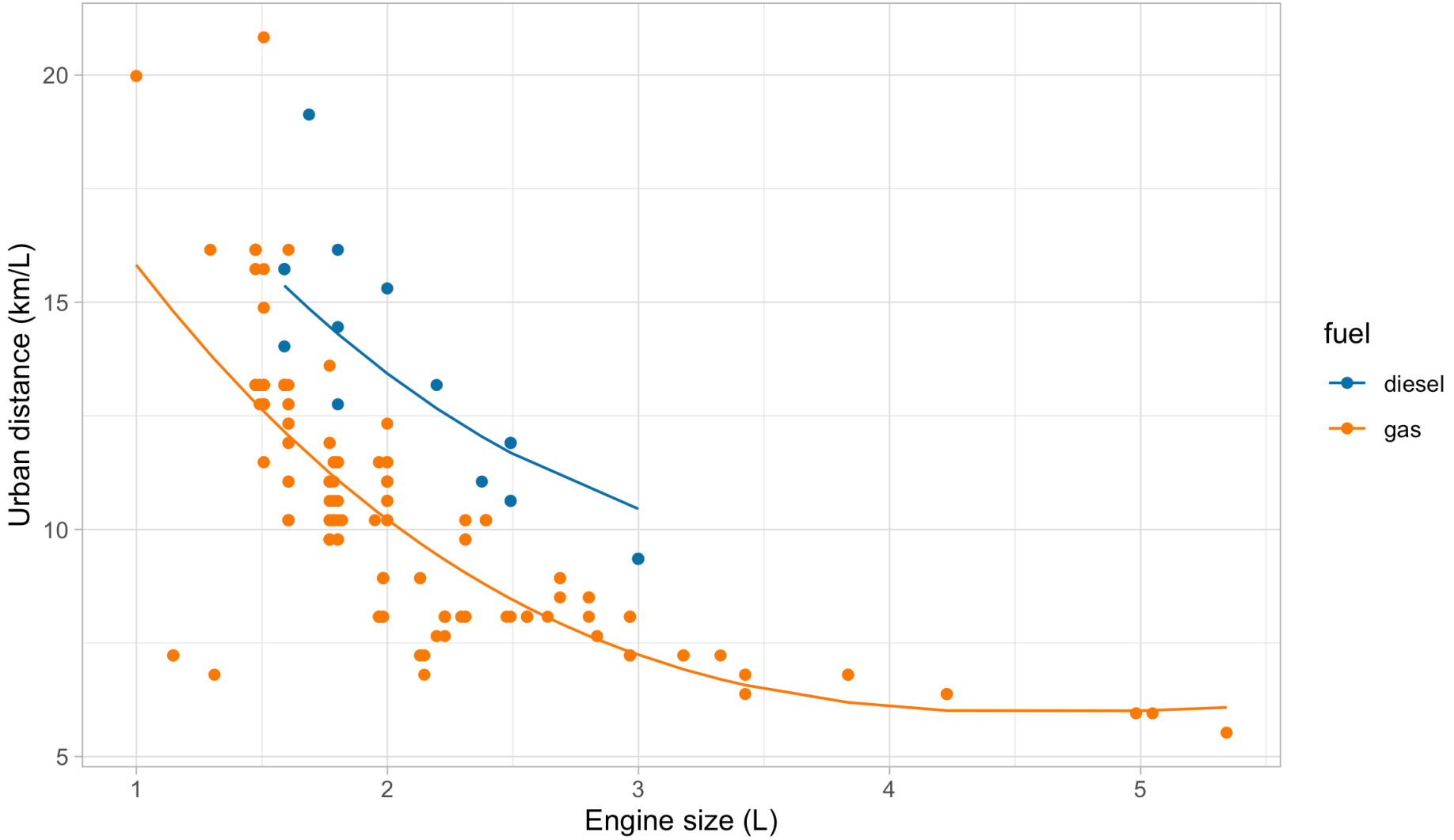
- We obtain the following **summary** for the regression coefficients $\hat{\beta}$.

term	estimate	std.error	statistic	p.value
(Intercept)	28.045	3.076	9.119	0.000
engine.size	-10.980	3.531	-3.109	0.002
engine.size^2	2.098	1.271	1.651	0.100
engine.size^3	-0.131	0.139	-0.939	0.349
fuel_gas	-3.214	0.427	-7.523	0.000

- Moreover, the coefficient R^2 and the residual standard deviation s are:

r.squared	sigma	deviance
0.5973454	1.790362	634.6687

A first model: fitted values



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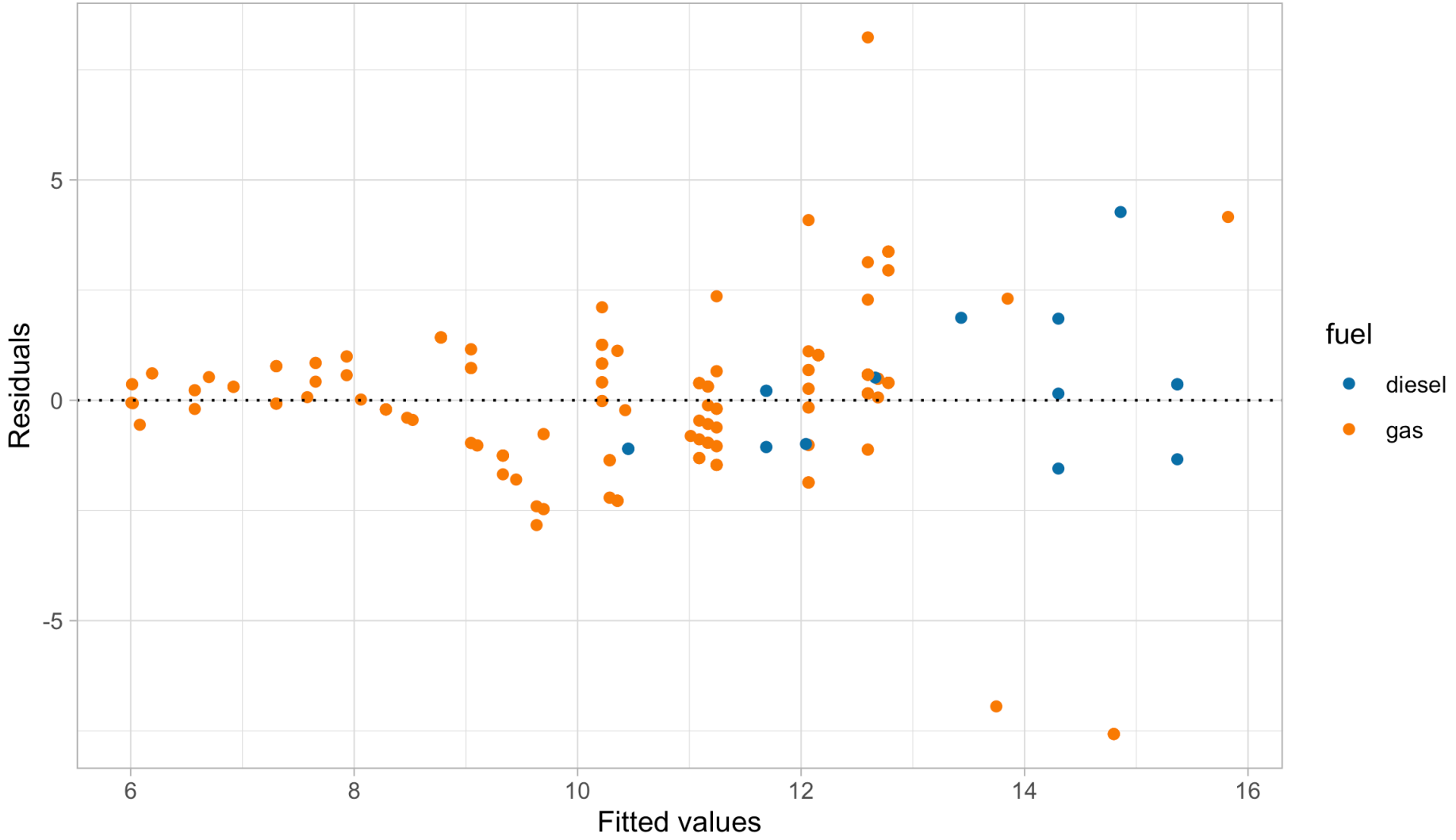
A first model: graphical diagnostics



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Comments and criticisms

- Is this a good model?
- The overall fit **seems satisfactory** at first glance, especially if we aim at predicting the urban distance of cars when average engine size (i.e., between $1.5L$ and $3L$).
- However, the plot of the **residuals** $r_i = y_i - \hat{y}_i$ suggests that the homoscedasticity assumption, i.e. $\mathrm{var}(\epsilon_i) = \sigma^2$, might be violated.
- Also, this model is unsuitable for **extrapolation**. Indeed:
  - It has no grounding in physics or engineering, leading to difficulties when interpreting the trend and to paradoxical situations.
  - For example, the curve of the set of gasoline cars shows a local minimum around $4.6L$ and then rises again!
- It is plausible that we can find a better one, so what's next?

Linear models and non-linear patterns

- A significant advantage of linear models is that they can describe non-linear relationships via **variable transformations** such as polynomials, logarithms, etc.

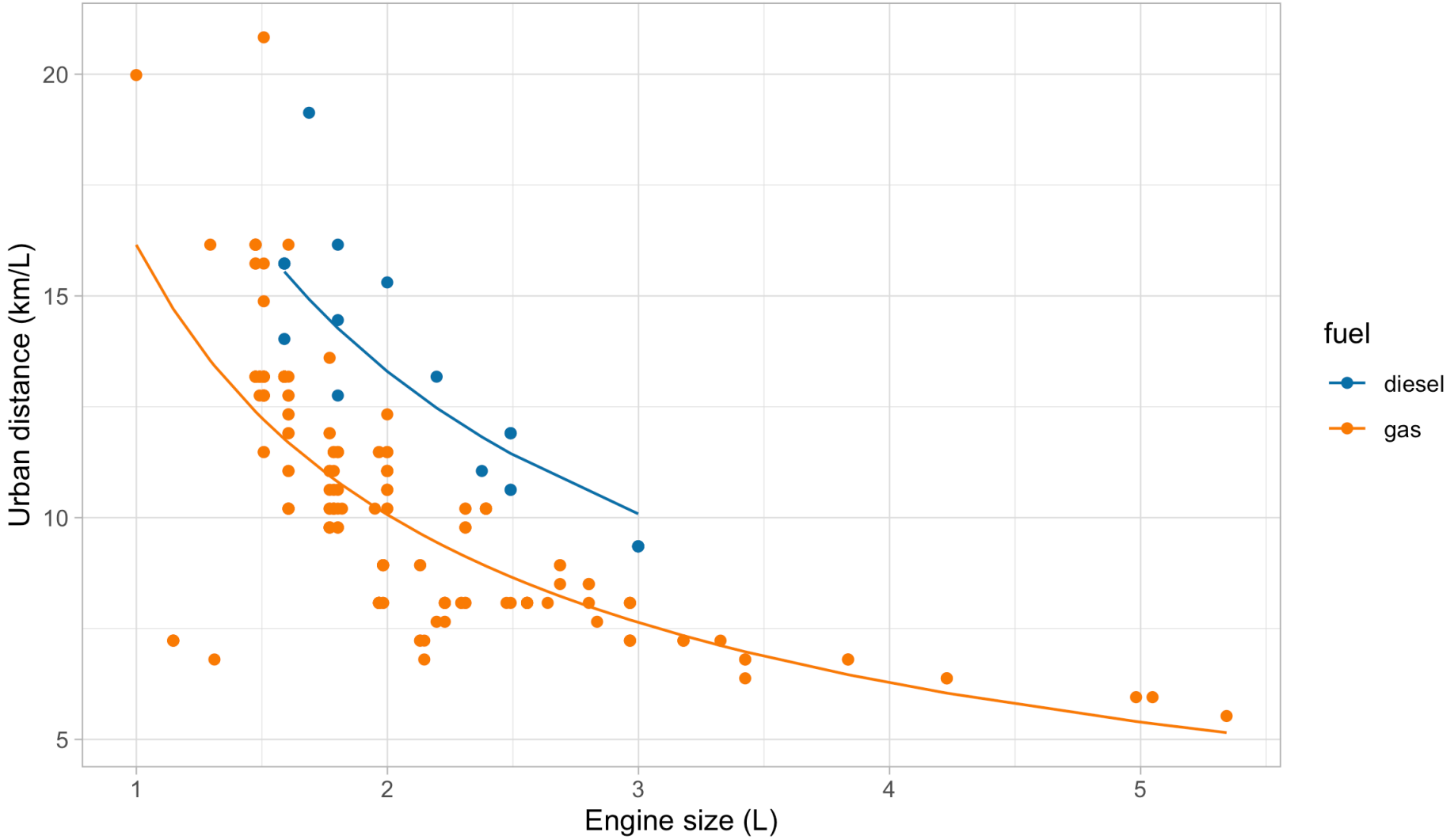
- This gives the statistician a lot of modeling flexibility. For instance, we could let:

$$\log Y_i = \beta_1 + \beta_2 \log x_i + \beta_3 I(z_i = \textbf{gas}) + \epsilon_i, \qquad i = 1, \ldots, n.$$

- This specification is **linear in the parameters**, it fixes the domain issues, and it imposes a monotone relationship between engine size and consumption.

term	estimate	std.error	statistic	p.value
(Intercept)	3.060	0.047	64.865	0
log(engine.size)	-0.682	0.040	-17.129	0
fuel_gas	-0.278	0.038	-7.344	0

Second model: fitted values



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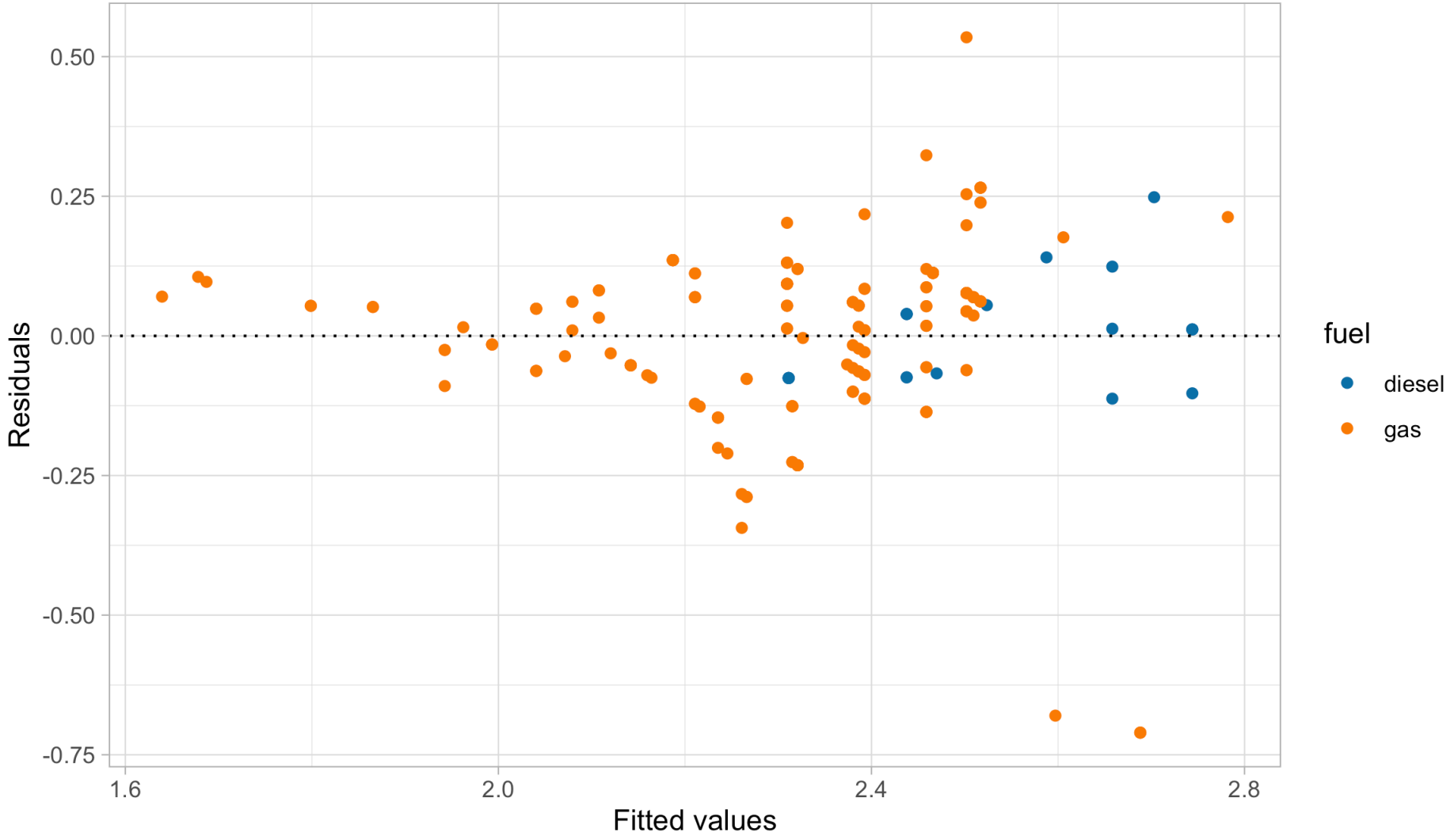
Second model: graphical diagnostics



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Comments and criticisms

- The **goodness of fit** indices are the following:

r.squared.original	r.squared	sigma	deviance
0.5847555	0.6196093	0.1600278	5.121777

- Do not mix **apple** and **oranges**! Compare R^2s only if they refer to the same scale!

- This second model is **more parsimonious**, and yet it reaches satisfactory predictive performance.
- It is also more coherent with the nature of the data: the predictions cannot be negative, and the relationship between engine size and the consumption is monotone.
- Yet, there is still some heteroscedasticity in the residuals — is this is due to a missing covariate that has not been included in the model?

A third model: additional variables

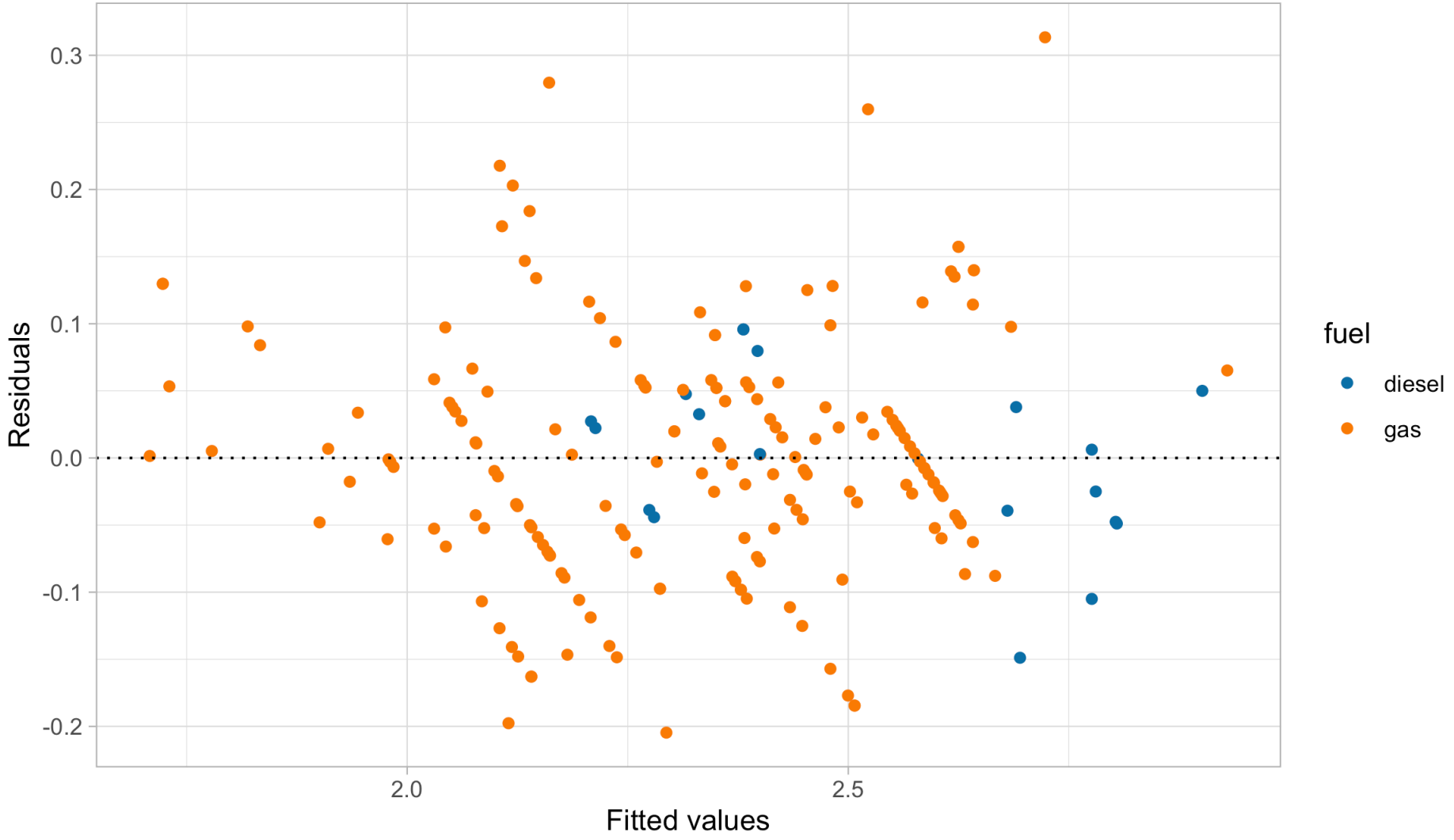
- Let us consider **two additional variables**: `curb.weight` (w) and `n.cylinders` (v).
- A richer model, therefore, could be:

$$\log Y_i = \beta_1 + \beta_2 \log x_i + \beta_3 \log w_i + \beta_4 I(z_i = \texttt{gas}) + \beta_5 I(v_i = 2) + \epsilon_i,$$

for $i = 1, \ldots, n$. The estimates are:

term	estimate	std.error	statistic	p.value
(Intercept)	9.423	0.482	19.549	0.000
log(engine.size)	-0.180	0.051	-3.504	0.001
log(curb.weight)	-0.943	0.072	-13.066	0.000
fuel_gas	-0.353	0.022	-15.934	0.000
cylinders2_TRUE	-0.481	0.052	-9.301	0.000

A third model: graphical diagnostics



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Comments and criticisms

- The goodness of fit greatly **improved**:

r.squared.original	r.squared	sigma	deviance
0.869048	0.8819199	0.0896089	1.589891

- In this third model, we handled the **outliers** appearing in the residual plots, which it turns out are identified by the group of cars having 2 cylinders.
- The diagnostic plots are also very much improved, although still not perfect.
- The estimates are coherent with our expectations, based on common knowledge. Have a look at the textbook (A&S) for a detailed explanation of β_4!
- The car dataset is available from the textbook (A&S) website:
  - Dataset http://azzalini.stat.unipd.it/Book-DM/auto.dat
  - Variable description http://azzalini.stat.unipd.it/Book-DM/auto.names

A tour inside old-fashioned statistics

- The first part of the unit is a tour in the "old style" data modeling, the kind of culture that Leo Breiman so **heavily criticized** in his 2001 *Statistical Science* paper.
- However, this dataset was sufficiently small, meaning it could be "manually" analyzed and modeled. We gained much **understanding** by doing so.
- Hence, these old tools should not be considered useless or irrelevant.
- The second half of the unit will have an entirely different flavor, though.
- Given the vast amount of data we now have, it makes sense to focus on **computations** for fitting linear models.
- As we will see, the mathematical simplicity of linear models leads to extremely **fast computations**, an important advantage in the era of big data.

Normal equations

How to obtain the least squares estimate?

- In B.Sc. courses, it is often suggested that the least square estimate should be computed using the formula

$$\hat{\beta} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y},$$

  that is, using the R code `solve(t(X) %*% X) %*% t(X) %*% y`.

- This approach works reasonably well in many **simple cases**.

- Unfortunately, in more challenging scenarios, e.g., when we have a lot of data (large n) and correlated variables, the above code is
  - **computationally inefficient**
  - **numerically inaccurate**
- The main computational bottleneck is the calculation of the inverse of $\boldsymbol{X}^T \boldsymbol{X}$, which is very costly and often numerically unstable, especially when the predictors are almost collinear.

The normal equations

- The least square estimate is the solution of the system of equations (**normal equations**):

$$\boldsymbol{X}^T\boldsymbol{X}\beta = \boldsymbol{X}^T\boldsymbol{y}.$$

- This system could be solved using `solve(crossprod(X), crossprod(X, y))`.
- This avoids the explicit computation of $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$ and it is preferable compared to the "direct solution." However, it does not exploit the properties of the matrix $\boldsymbol{X}^T\boldsymbol{X}$.
- Recall (from your favorite linear algebra textbook) that a **symmetric** matrix $\boldsymbol{A} \in \mathbb{R}^{p\times p}$ is **positive definite** if and only if one of the following properties is satisfied
  - The quadratic form $\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} > 0$ for all $\boldsymbol{x} \in \mathbb{R}^p$ such that $\boldsymbol{x} \neq 0$.
  - The eigenvalues $\lambda_1, \ldots, \lambda_p$ of $\boldsymbol{A}$ are all strictly positive.
- We now describe a strategy to compute $\hat{\beta}$ that exploits the fact that $\boldsymbol{X}^T\boldsymbol{X}$ is **positive definite**, resulting in more **efficient computations**.

Cholesky factorization

Proposition A.1

Suppose $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ with $n \geq p$ has full rank, that is $\mathrm{rk}(\boldsymbol{X}) = p$. Then, the matrix

$$\boldsymbol{X}^T \boldsymbol{X}$$

is **symmetric** and **positive definite**.

Theorem (Cholesky factorization)

Let $\boldsymbol{A} \in \mathbb{R}^{p \times p}$ be a symmetric and positive definite matrix. Then, there exists a unique **upper triangular** $p \times p$ matrix $\boldsymbol{R}$ with positive entries such that

$$\boldsymbol{A} = \boldsymbol{R}^T \boldsymbol{R}.$$

Cholesky factorization and least squares

- The Cholesky factorization is incredibly helpful for computing least squares. Indeed:
- Let $\boldsymbol{R}^T\boldsymbol{R}$ be the Cholesky factorization of the matrix $\boldsymbol{X}^T\boldsymbol{X}$. Then, the **normal equations** can be written as

$$\boldsymbol{R}^T\boldsymbol{R}\beta = \boldsymbol{X}^T\boldsymbol{y}.$$

This system can now solved in **two steps**:

- **Step 1 (Forwardsolve)**. Solve with respect to $\boldsymbol{z}$ the system of equations

$$\boldsymbol{R}^T\boldsymbol{z} = \boldsymbol{X}^T\boldsymbol{y}.$$

- **Step 2 (Backsolve)**. Given $\boldsymbol{z}$, now solve with respect to β the system of equations

$$\boldsymbol{R}\beta = \boldsymbol{z}.$$

- Why is this procedure computationally more efficient than the naïve solution?

Forward and backward substitutions

- The key observation is that the solution of **triangular systems** is computationally **straightforward**.
- As an example, consider the following 3×3 lower triangular system:

$$\begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}.$$

- The solution for x_1, x_2, x_3 can be found sequentially:

$$x_1 = \frac{b_1}{l_{11}}, \qquad x_2 = \frac{b_2 - l_{21}x_1}{l_{22}}, \qquad x_3 = \frac{b_3 - l_{31}x_1 - l_{32}x_2}{l_{33}}.$$

- Finding the **inverse** $\boldsymbol{R}^{-1}$ is simple, again because $\boldsymbol{R}$ is upper triangular. Also, note that

$$(\boldsymbol{X}^T\boldsymbol{X})^{-1} = (\boldsymbol{R}^T\boldsymbol{R})^{-1} = \boldsymbol{R}^{-1}(\boldsymbol{R}^{-1})^T.$$

Computational complexity

- The solution via Cholesky factorization is a **fast direct approach** for finding $\hat{\beta}$.
- The expensive steps are:
  - The formation of the matrix $\boldsymbol{X}^T\boldsymbol{X}$ requires $\sim np^2$ elementary operations
  - The Cholesky factorization of $\boldsymbol{X}^T\boldsymbol{X}$ requires $\sim p^3/3$ elementary operations.
- This gives an overall computational complexity of order

$$\sim np^2 + p^3/3,$$

  which corrects the typographical error of the A&S textbook.
- This means, unfortunately, that in **high-dimensional** settings (large p) computations become **very costly**, since the complexity is cubic in p.

Error propagation in normal equations

- The normal equations method is typically **quicker** than other algorithms, as it removes the dependency on n, but it is in general numerically more **unstable**.
- Consider, for example, the following matrix:

$$\boldsymbol{X} = \begin{bmatrix} 1 & 1 \\ \epsilon & 0 \\ 0 & \epsilon \end{bmatrix},$$

for a small value $\epsilon > 0$. Then, we obtain that

$$\boldsymbol{X}^T \boldsymbol{X} = \begin{bmatrix} 1+\epsilon^2 & 1 \\ 1 & 1+\epsilon^2 \end{bmatrix}.$$

- The numerical computation of ϵ^2 in $\boldsymbol{X}^T \boldsymbol{X}$ requires a higher precision compared to ϵ, leading to numerical instabilities and/or a **loss in accuracy**.

Condition numbers and normal equations

- Suppose $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ with $n \geq p$ has full rank and singular values $d_1 \geq d_2 \geq \cdots \geq d_p$. Then its **condition number** is

$$\kappa(\boldsymbol{X}) = ||\boldsymbol{X}|| \cdot ||\boldsymbol{X}^+|| = \frac{d_1}{d_p},$$

  where $\boldsymbol{X}^+$ is the Moore-Penrose pseudo-inverse. Note that $\kappa(\boldsymbol{X}) \geq 1$.

- If $\kappa(\boldsymbol{X})$ is small, the matrix $\boldsymbol{X}$ is **well conditioned**. Otherwise, we say it is **ill conditioned**.
- The condition number determines how accurately we can solve linear systems.
- An important fact is:

$$\kappa(\boldsymbol{X}^T\boldsymbol{X}) = \kappa(\boldsymbol{X})^2,$$

  implying that there is an evident loss of numerical accuracy when using normal equations.

The QR decomposition

Orthogonal predictors

- Another approach for computing least squares is based on the notion of orthogonality.
- If the **predictors** were mutually **orthogonal**, the problem would be much simpler.
- In other words, consider a linear model of the form

$$\boldsymbol{Y} = \boldsymbol{Z}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where $\boldsymbol{Z} = (\tilde{\boldsymbol{z}}_1, \ldots, \tilde{\boldsymbol{z}}_p)$. **Orthogonality** means that $\boldsymbol{Z}^T\boldsymbol{Z} = \text{diag}(\tilde{\boldsymbol{z}}_1^T\tilde{\boldsymbol{z}}_1, \ldots, \tilde{\boldsymbol{z}}_p^T\tilde{\boldsymbol{z}}_p)$.

Proposition A.2. OLS with orthogonal predictors

The least square estimate $\hat{\boldsymbol{\beta}} = (\hat{\beta}_1, \ldots, \hat{\beta}_p)^T$ with orthogonal predictors is

$$\hat{\beta}_j = \frac{\tilde{\boldsymbol{z}}_j^T\boldsymbol{y}}{\tilde{\boldsymbol{z}}_j^T\tilde{\boldsymbol{z}}_j}, \qquad j = 1, \ldots, p.$$

Regression by successive orthogonalization

- Clearly, the predictors in $\boldsymbol{X}$ are generally not orthogonal. Hence, we want to find a suitable transformation $\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{\Gamma}^{-1}$ that **orthogonalizes** the **predictors**.
- Suppose, for example, that $p = 2$. We set **first orthogonal predictor** $\tilde{\boldsymbol{z}}_1 = \tilde{\boldsymbol{x}}_1$.
- We then consider the following **univariate** regression problem

$$\tilde{\boldsymbol{x}}_2 = \gamma \tilde{\boldsymbol{z}}_1 + \boldsymbol{\epsilon}, \qquad \text{which leads} \qquad \hat{\gamma} = \frac{\tilde{\boldsymbol{z}}_1^T \tilde{\boldsymbol{x}}_2}{\tilde{\boldsymbol{z}}_1^T \tilde{\boldsymbol{z}}_1}.$$

- The **second orthogonal predictor** is obtained as the **residual term**:

$$\tilde{\boldsymbol{z}}_2 = \tilde{\boldsymbol{x}}_2 - \hat{\gamma} \tilde{\boldsymbol{z}}_1.$$

- The geometry of linear models guarantees that $\tilde{\boldsymbol{z}}_1^T \tilde{\boldsymbol{z}}_2 = 0$.

Gram-Schmidt algorithm

- Let us now consider the **general case**, valid for any value of p.
- **Initialization**. Set $\tilde{\boldsymbol{z}}_1 = \tilde{\boldsymbol{x}}_1$.
- **For** $j = 2, \ldots, p$. Consider the regression problem with $j-1$ orthogonal predictors

$$\tilde{\boldsymbol{x}}_j = \sum_{k=1}^{j-1} \gamma_{kj} \tilde{\boldsymbol{z}}_k + \boldsymbol{\epsilon}_j, \quad \text{which leads} \quad \hat{\gamma}_{kj} = \frac{\tilde{\boldsymbol{z}}_k^T \tilde{\boldsymbol{x}}_j}{\tilde{\boldsymbol{z}}_k^T \tilde{\boldsymbol{z}}_k}, \quad k = 1, \ldots, j-1,$$

  Then, compute the new vector $\boldsymbol{z}_j$ as the **residual** term

$$\tilde{\boldsymbol{z}}_j = \tilde{\boldsymbol{x}}_j - \sum_{k=1}^{j-1} \hat{\gamma}_{kj} \tilde{\boldsymbol{z}}_k$$

- The geometry of linear models guarantees **orthogonality**, that is $\tilde{\boldsymbol{z}}_j^T \tilde{\boldsymbol{z}}_{j'} = 0$ for any $j \neq j'$.

The QR decomposition I

- By construction, the Gram-Schmidt algorithm produces the following decomposition

$$\boldsymbol{X} = \boldsymbol{Z}\boldsymbol{\Gamma}, \qquad \boldsymbol{\Gamma} = \begin{bmatrix} 1 & \hat{\gamma}_{12} & \hat{\gamma}_{13} & \cdots & \hat{\gamma}_{1p} \\ 0 & 1 & \hat{\gamma}_{23} & \cdots & \hat{\gamma}_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}, \qquad \boldsymbol{Z} = (\tilde{\boldsymbol{z}}_1, \ldots, \tilde{\boldsymbol{z}}_p).$$

- The $p \times p$ matrix $\boldsymbol{\Gamma}$ is **upper triangular**, whereas the columns of the $n \times p$ matrix $\boldsymbol{Z}$ are **mutually orthogonal**, due to the properties of the residuals of a linear model.
- It is often convenient to **standardize** the columns of $\boldsymbol{Z}$, dividing them by their norm $||\tilde{\boldsymbol{z}}_j||$. Let $\boldsymbol{D} = \text{diag}(||\tilde{\boldsymbol{z}}_1||, \ldots, ||\tilde{\boldsymbol{z}}_p||)$, then in matrix notation:

$$\boldsymbol{X} = \boldsymbol{Z}\boldsymbol{\Gamma} = \boldsymbol{Z}\boldsymbol{D}^{-1}\boldsymbol{D}\boldsymbol{\Gamma} = \boldsymbol{Q}\boldsymbol{R}, \quad \text{with} \quad \boldsymbol{Q} = \boldsymbol{Z}\boldsymbol{D}^{-1} \quad \text{and} \quad \boldsymbol{R} = \boldsymbol{D}\boldsymbol{\Gamma}.$$

- **Remark**. Note that $\boldsymbol{Q}^T\boldsymbol{Q} = I_p$, i.e. the columns of $\boldsymbol{Q}$ are **orthonormal**.

The QR decomposition II

Theorem (QR factorization)

Suppose $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ with $n \geq p$ has full rank, that is $\mathrm{rk}(\boldsymbol{X}) = p$. Then, there exists a factorization of the form

$$\boldsymbol{X} = \boldsymbol{Q}\boldsymbol{R},$$

where $\boldsymbol{Q} \in \mathbb{R}^{n \times p}$ has **orthonormal columns** and $\boldsymbol{R} \in \mathbb{R}^{p \times p}$ is an **upper triangular** matrix.

Corollary (QR factorization)

The QR decomposition is **unique** up to **sign flips** of the columns of $\boldsymbol{Q}$ and the rows of $\boldsymbol{R}$. Moreover, if $\boldsymbol{R}$ has positive diagonal entries, as the one obtained using Gram-Schmidt, then it coincides with the **Cholesky factor** of $\boldsymbol{X}^T\boldsymbol{X}$.

The QR decomposition and least squares

- The QR decomposition greatly facilitates computations for linear models. Indeed:

$$\begin{aligned}\hat{\beta} &= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} = [(\boldsymbol{Q}\boldsymbol{R})^T\boldsymbol{Q}\boldsymbol{R}]^{-1}(\boldsymbol{Q}\boldsymbol{R})^T\boldsymbol{y} \\ &= (\boldsymbol{R}^T\boldsymbol{Q}^T\boldsymbol{Q}\boldsymbol{R})^{-1}\boldsymbol{R}^T\boldsymbol{Q}^T\boldsymbol{y} \\ &= \boldsymbol{R}^{-1}(\boldsymbol{R}^T)^{-1}\boldsymbol{R}^T\boldsymbol{Q}^T\boldsymbol{y} \\ &= \boldsymbol{R}^{-1}\boldsymbol{Q}^T\boldsymbol{y}.\end{aligned}$$

- Hence, the least square estimate is obtained as the solution of the **triangular system**

$$\boldsymbol{R}\beta = \boldsymbol{Q}^T\boldsymbol{y},$$

  which can be easily solved via **backward substitution**.

- As a particular case of the above equation, one gets $\hat{\beta}_p = (\tilde{\boldsymbol{z}}_p^T\boldsymbol{y})/(\tilde{\boldsymbol{z}}_p^T\tilde{\boldsymbol{z}}_p)$.

The QR decomposition and linear models

- An important advantage of the QR factorization is that many other useful quantities can be readily computed. For example, the **covariance matrix** is obtained as:

$$s^2(\boldsymbol{X}^T\boldsymbol{X})^{-1} = s^2\boldsymbol{R}^{-1}(\boldsymbol{R}^{-1})^T.$$

- The **predicted values** and the **projection matrix** are also easily obtained as

$$\hat{\boldsymbol{y}} = \boldsymbol{H}\boldsymbol{y} = \boldsymbol{Q}\boldsymbol{Q}^T\boldsymbol{y}.$$

- The diagonal elements $h_i = [\boldsymbol{H}]_{ii}$ of the hat matrix $\boldsymbol{H}$ are called **leverages** and one may want to compute them without evaluating the full $n \times n$ matrix, using

$$h_i = \sum_{j=1}^{p} q_{ij}^2, \qquad i = 1, \ldots, n,$$

where q_{ij} are the entries of $\boldsymbol{Q}$.

Computational complexity

- The solution via QR factorization is **numerically reliable** and it facilitates the computation of other quantities of interest.
- In practice, the QR is computed via a **modified Gram-Schmidt**, that fixes the instabilities of the naïve Gram-Schmidt algorithm, or via **Householder reflections**.
- The expensive step is the QR factorization. The overall computational complexity is

$$\sim 2np^2,$$

  which is about twice that of the Cholesky, when n is much larger than p, and about the same when $p \approx n$.
- Depending on the context and assuming we only care about $\hat{\beta}$, we may prefer the Cholesky (**fast** but **imprecise**) or the QR (**slower** but more **reliable**).
- The default approach in R, i.e., the one implemented in the `lm` function is the QR factorization because one typically also needs to compute $\boldsymbol{H}$, or the leverages.

☠️ - Pivoting and rank deficiencies

- If $\text{rk}(\boldsymbol{X}) = k < p$ (**rank deficiency**) then it is still possible to obtain a "QR" factorization of the form

$$\boldsymbol{X}\boldsymbol{P} = \boldsymbol{Q}\begin{bmatrix} \boldsymbol{R}_{11} & \boldsymbol{R}_{12} \\ 0 & 0 \end{bmatrix},$$

  where $\boldsymbol{P}$ is a $p \times p$ permutation matrix and $\boldsymbol{R}_{11}$ is an $k \times k$ upper triangular and non-singular matrix.

- This operation is sometimes called **pivoting**, and it is particularly important even when $\text{rk}(\boldsymbol{X}) = p$ to prevent numerical issues when the condition number $\kappa(\boldsymbol{X})$ is high.
- In the presence of perfect collinearity, the implementation of the QR decomposition in R (`qr`) relies on pivoting. This is why the `lm` function can automatically "omit" a predictor.

Iterative methods

When n is very large...

- When the **sample size** n is **extremely large**, as it is common in data mining problems, then the QR factorization cannot be computed.
- Indeed, even **loading** $\boldsymbol{X}$ into **memory** could be problematic.
- In the normal equations approach, we only need to compute the **sufficient statistics**:

$$\boldsymbol{W} = \boldsymbol{X}^T\boldsymbol{X}, \qquad \boldsymbol{u} = \boldsymbol{X}^T\boldsymbol{y},$$

  which are of dimension $p \times p$ and $p \times 1$, respectively.
- If we knew $\boldsymbol{W}$ and $\boldsymbol{u}$, then we could obtain the least square estimate $\hat{\beta}$ using the Cholesky factorization.
- However, when n is extremely large, the difficult part is indeed computing $\boldsymbol{W}$ and $\boldsymbol{u}$!

Recursive data import

- Using matrix notation, we express $\boldsymbol{W} = \boldsymbol{W}_{(n)}$ and $\boldsymbol{u} = \boldsymbol{u}_{(n)}$ as follows

$$\boldsymbol{W}_{(n)} = \sum_{i=1}^{n} \boldsymbol{x}_i \boldsymbol{x}_i^T, \qquad \boldsymbol{u}_{(n)} = \sum_{i=1}^{n} \boldsymbol{x}_i y_i.$$

- Let us define the **initial conditions** $\boldsymbol{W}_{(1)} = \boldsymbol{x}_1 \boldsymbol{x}_1^T$ and $\boldsymbol{u}_{(1)} = \boldsymbol{x}_1 y_1$.
- Then, the following **recursive relationship** holds:

$$\boldsymbol{W}_{(i)} = \boldsymbol{W}_{(i-1)} + \boldsymbol{x}_i \boldsymbol{x}_i^T, \qquad \boldsymbol{u}_{(i)} = \boldsymbol{u}_{(i-1)} + \boldsymbol{x}_i y_i, \qquad i = 2, \ldots, n,$$

  where $\boldsymbol{W}_{(i)}$ is the matrix formed by the first i summands of $\boldsymbol{W}_{(n)}$ and analogously $\boldsymbol{u}_{(i)}$.
- Hence $\boldsymbol{W}_{(n)}$ and $\boldsymbol{u}_{(n)}$ can be calculated by **importing a single record** at a time, which does not create memory issues.

Recursive estimates

- In many occasions, the data flows continuously, meaning that we get a new pair of observations $(\boldsymbol{x}_{n+1}, y_{n+1})$ every minute, or even every second.
- In these cases, we would like to **update** the current least square estimate $\hat{\beta}_{(n)}$ with the new information $(\boldsymbol{x}_{n+1}, y_{n+1})$, but ideally without re-doing all the calculations.
- The **recursive data import** of the previous slide is partially unsatisfactory, because one would need to invert (or factorize) a $p \times p$ matrix every time, which could be costly.
- Let us define some useful quantity:

$$\boldsymbol{V}_{(n)} = \boldsymbol{W}_{(n)}^{-1} = (\boldsymbol{X}_{(n)}^T \boldsymbol{X}_{(n)})^{-1},$$

where $\boldsymbol{X}_{(n)}$ denotes the design matrix with n observations and analogously $\boldsymbol{y}_{(n)}$.

Sherman-Morrison formula

- When the new data points arrive, we can write the updated quantities

$$\boldsymbol{X}_{(n+1)} = (\boldsymbol{X}_{(n)}, \boldsymbol{x}_{n+1})^T, \quad \boldsymbol{W}_{(n+1)} = (\boldsymbol{X}_{(n+1)}^T \boldsymbol{X}_{(n+1)}) = (\boldsymbol{X}_{(n)}^T \boldsymbol{X}_{(n)} + \boldsymbol{x}_{n+1}\boldsymbol{x}_{n+1}^T).$$

- The difficult part is to **efficiently** compute $\boldsymbol{V}_{(n+1)} = \boldsymbol{W}_{(n+1)}^{-1}$. The following result of linear algebra is of incredible help in this regard.

Sherman-Morrison formula

Let $\boldsymbol{A} \in \mathbb{R}^{p \times p}$ be an invertible matrix and let $\boldsymbol{b}, \boldsymbol{d}$ be p-dimensional vectors. Then

$$(\boldsymbol{A} + \boldsymbol{b}\boldsymbol{d}^T)^{-1} = \boldsymbol{A}^{-1} - \frac{1}{1 + \boldsymbol{d}^T \boldsymbol{A}^{-1} \boldsymbol{b}} \boldsymbol{A}^{-1} \boldsymbol{b}\boldsymbol{d}^T \boldsymbol{A}^{-1}.$$

The recursive least squares algorithm I

- Using the Sherman-Morrison formula, then we can express the new matrix $\boldsymbol{V}_{(n+1)}$ as a function of previously computed quantities:

$$\boldsymbol{V}_{(n+1)} = \boldsymbol{V}_{(n)} - v_n \boldsymbol{V}_{(n)} \boldsymbol{x}_{n+1} \boldsymbol{x}_{n+1}^T \boldsymbol{V}_{(n)}, \quad v_n = \frac{1}{(1 + \boldsymbol{x}_{n+1}^T \boldsymbol{V}_{(n)} \boldsymbol{x}_{n+1})}.$$

- The **updated least square estimate** therefore becomes

$$\begin{aligned}
\hat{\beta}_{(n+1)} &= \boldsymbol{V}_{(n+1)} (\boldsymbol{X}_{(n)}^T \boldsymbol{y}_{(n)} + \boldsymbol{x}_{n+1} y_{n+1}) \\
&= \hat{\beta}_{(n)} + \underbrace{v_n \boldsymbol{V}_{(n)} \boldsymbol{x}_{n+1}}_{\boldsymbol{k}_n} \underbrace{(y_{n+1} - \boldsymbol{x}_{n+1}^T \hat{\beta}_{(n)})}_{e_{n+1}} \\
&= \hat{\beta}_{(n)} + \boldsymbol{k}_n e_{n+1}.
\end{aligned}$$

- The quantity e_{n+1} is the **prediction error** of y_{n+1} based on the previous estimate $\hat{\beta}_{(n)}$.

The recursive least squares algorithm II

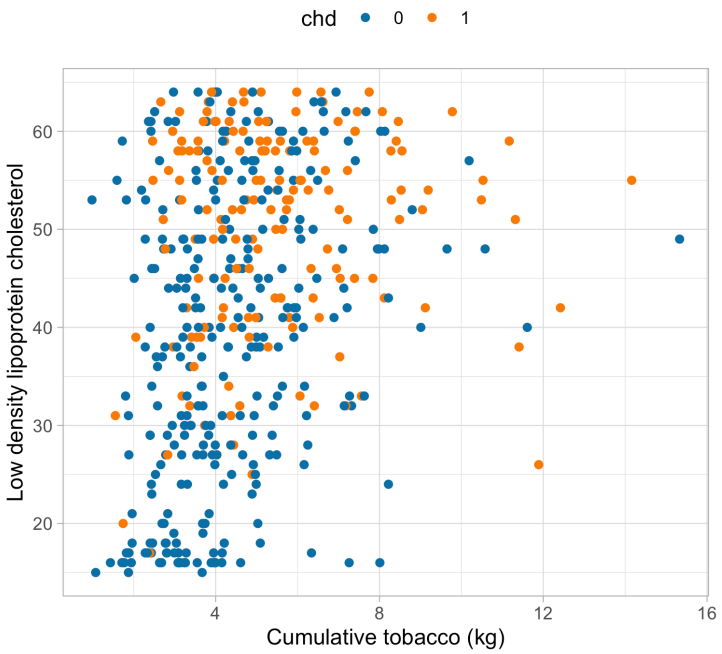
- The recursive estimation $\hat{\beta}_{(n+1)} = \hat{\beta}_{(n)} + \boldsymbol{k}_n e_{n+1}$ takes the form of a **linear filter**, in which the new estimate $\hat{\beta}_{(n+1)}$ is obtained by modifying the old one $\hat{\beta}_{(n+1)}$.
- This is performed according to the **prediction error** ϵ_{n+1} and the **gain** k_n of the filter.
- Using a terminology typical of the machine learning field, we say that the estimator "learns from its errors."
- If n is sufficiently high, it is also possible to get an **approximate** solution by initializing the algorithm by setting $\boldsymbol{V}_{(0)} = I_p$, to avoid any matrix inversion / factorization.
- With further algebraic steps, we also obtain a **recursive formula** for the **deviance**

$$||\boldsymbol{y}_{(n+1)} - \boldsymbol{X}_{(n+1)}\hat{\beta}_{(n+1)}||^2 = ||\boldsymbol{y}_{(n)} - \boldsymbol{X}_{(n)}\hat{\beta}_{(n)}||^2 + v_n e_{n+1}^2.$$

- The complete algorithm is provided in A&S, Algorithm 2.2.

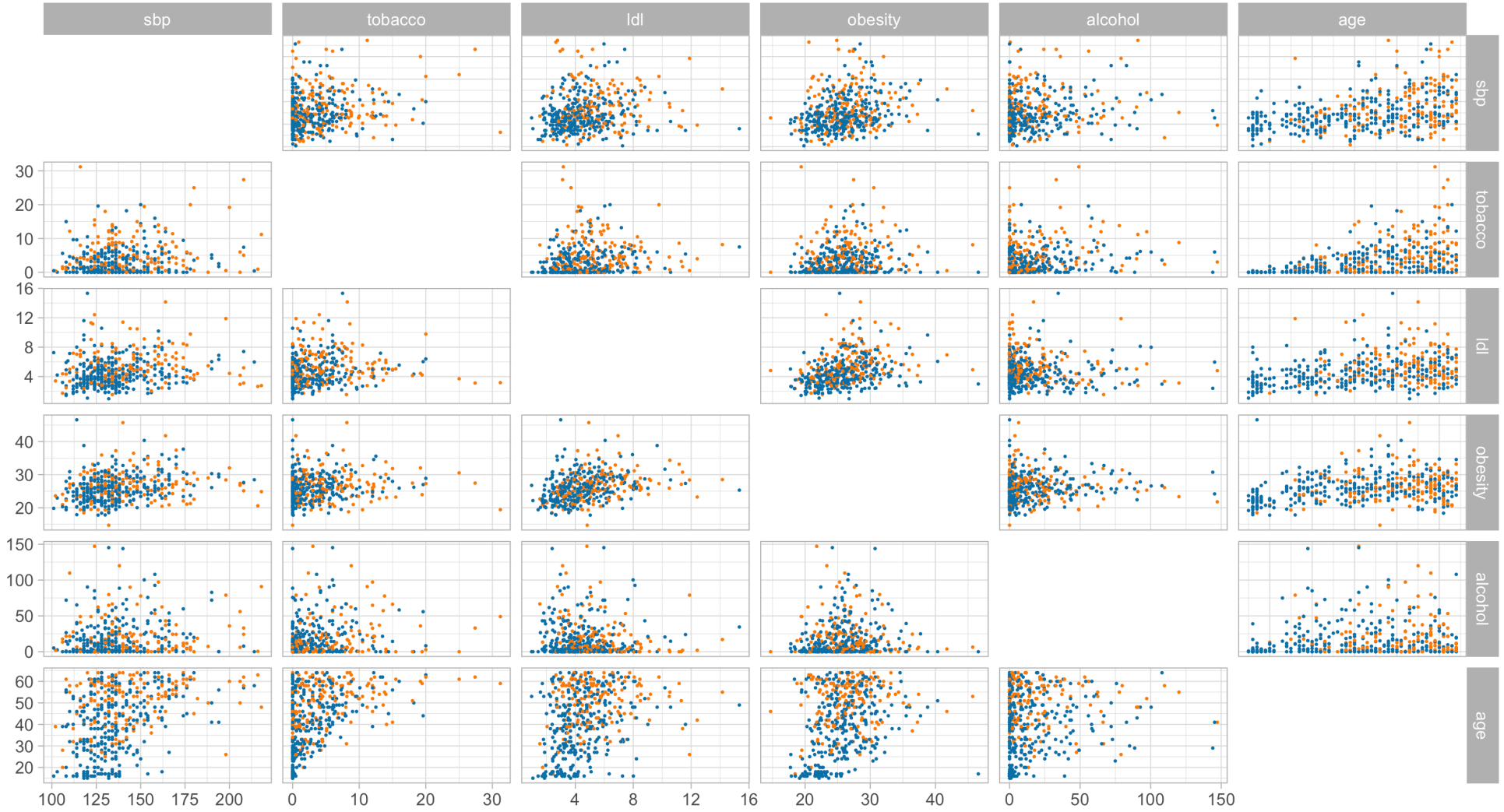
Generalized linear models

The `heart` dataset



- Let us consider the South African `heart` dataset, described is **Section 4.4.2** of HTF (2009).
- We want to **predict** the insurgence of **coronary heart disease** (`chd`) as a function of known risk factors:
  - Cholesterol level (`ldl`) and obesity (`obesity`)
  - Consumption of tobacco (`tobacco`) and alcohol (`alcool`)
  - Systolic blood pressure (`sbp`)
  - Age (`age`) and family history (`famhist`)
- The response variable is **binary**: we cannot rely on linear regression models.

The heart dataset



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Generalized linear models

- If the outcome is binary, a count, or if the errors are heteroscedastic, then the Gaussian linear regression model might be inappropriate.
- We let Y_i be iid draws from an **exponentialy dispersion family**, which includes the Binomial, the Poisson, and the Gaussian distribution as special cases.
- The canonical statistical solution are **generalized linear models**, which are usually taught in undergraduate courses (e.g. Statistica III). This is just a **short recap**.

Generalized linear model (GLMs)

In a **generalized linear model**, the response variable is related to the covariates through:

$$\mathbb{E}(Y_i) = g^{-1}\{f(\boldsymbol{x}_i; \beta)\} = g^{-1}(\beta_1 x_{i1} + \cdots + \beta_p x_{ip}) = g^{-1}(\boldsymbol{x}_i^T \beta),$$

where $g(\cdot)$ is the so-called **link function**, which is known and invertible.

Likelihood-based inference

- Let $\pi(y; \boldsymbol{x}, \theta)$ be the **density** associated to each Y_i. Here θ is a vector of parameters.
- The **log-likelihood** of a GLM is

$$\ell(\theta) = \ell(\theta; \boldsymbol{y}) = \sum_{i=1}^{n} \log \pi(y_i; \boldsymbol{x}_i, \theta) + c,$$

  where c is an additive constant not depending on β.
- The **maximum likelihood estimate** for the regression coefficients β is

$$\hat{\theta} = \arg\max_{\theta} \ell(\theta).$$

- Standard errors, tests, and confidence intervals can be easily obtained from (derivatives of) the log-likelihood, as you have seen in undergraduate courses (e.g., Statistica II and III).
- The aforementioned inferential results are often grounded on **asymptotic theory** and **quadratic approximations** of the log-likelihood.

Linear models with Gaussian errors

- When Y_i are Gaussian random variables, then the log-likelihood is

$$\ell(\beta, \sigma^2) = -\frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} D(\beta),$$

  where $D(\beta)$ is the same quantity we have defined before.

- Hence, the **ordinary least squares** estimate $\hat{\beta}$ is also the **maximum likelihood** estimate. Indeed, the maximizer of the log-likelihood with respect to β is also the minimizer of $D(\beta)$.
- Instead, the maximum likelihood estimate for the variance is $\hat{\sigma}^2 = D(\hat{\beta})/n$.
- Note in addition that the log-likelihood, evaluated at its maximum, is

$$-2\ell(\hat{\beta}, \hat{\sigma}^2) = n \log\{D(\hat{\beta})/n\} + n,$$

  a quantity that will turn useful in Unit B.

Binary classification via logistic regression

- The `heart` dataset presents a **classification** problem, in which we assume that

$$Y_i \overset{\text{ind}}{\sim} \text{Bern}\{p(\boldsymbol{x}_i; \beta)\}, \qquad i = 1, \dots, n.$$

- The **canonical link** function $g^{-1}(x) = e^x/(1+e^x)$ leads to the GLM

$$\mathbb{P}(Y_i = 1) = p(\boldsymbol{x}_i; \beta) = \frac{\exp\{f(\boldsymbol{x}_i; \beta)\}}{1 + \exp\{f(\boldsymbol{x}_i; \beta)\}} = \frac{\exp(\beta_1 x_{i1} + \cdots + \beta_p x_{ip})}{1 + \exp(\beta_1 x_{i1} + \cdots + \beta_p x_{ip})},$$

  known as **logistic regression**. Note that in this model $\mathbb{E}(Y_i) = \mathbb{P}(Y_i = 1)$.

- After some algebra, it can be shown that the log-likelihood is

$$\ell(\beta) = \sum_{i=1}^{n} y_i(\boldsymbol{x}_i^T \beta) - \log\{1 + \exp(\boldsymbol{x}_i^T \beta)\}.$$

- Moreover, the **predicted values** $p(\boldsymbol{x}_i; \hat{\beta})$ are **probabilities** and they belong to $(0, 1)$.

Iteratively re-weighted least squares I

- Let us define the so-called **score function**:

$$\ell'(\beta) = \frac{\partial}{\partial \beta}\ell(\beta) = \sum_{i=1}^{n} \boldsymbol{x}_i\{y_i - p(\boldsymbol{x}_i;\beta)\},$$

- Moreover, the so-called **observed information matrix** is

$$j(\beta) = -\frac{\partial^2}{\partial\beta\partial\beta^T}\ell(\beta) = -\sum_{i=1}^{n} \boldsymbol{x}_i\boldsymbol{x}_i^T w_i(\beta), \quad w_i(\beta) = p(\boldsymbol{x}_i;\beta)\{1 - p(\boldsymbol{x}_i;\beta)\}.$$

- In **matrix notation**, we will write

$$\ell'(\beta) = \boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{p}), \qquad j(\beta) = \boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X},$$

  where $\boldsymbol{p} = (p(\boldsymbol{x}_1;\beta), \ldots, p(\boldsymbol{x}_n;\beta))$ and $\boldsymbol{W} = \text{diag}(w_1(\beta), \ldots, w_n(\beta))$.

- Unfortunately, a closed-form expression for $\hat{\beta}$, solving the **likelihood equations** $\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{p}) = 0$, is not available. We need to use **iterative algorithms**.

Iteratively re-weighted least squares II

- As you may remember, in the Newton-Raphson **iterative method** we consider a **quadratic approximation** of the log-likelihood on β_0, so that:

$$\ell(\beta) \approx \ell(\beta_0) + \ell'(\beta_0)^T(\beta - \beta_0) - \frac{1}{2}(\beta - \beta_0)^T j(\beta)(\beta - \beta_0).$$

- By maximizing the quadratic approximation, in logistic regression we get the update

$$\begin{aligned}\beta^{(\text{new})} &= \beta^{(\text{old})} + j(\beta^{\text{old}})^{-1}\ell'(\beta^{\text{old}}) = \beta^{(\text{old})} + (\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{p}) \\ &= (\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{z},\end{aligned}$$

  where $\boldsymbol{z} = \boldsymbol{X}\beta^{(\text{old})} + \boldsymbol{W}^{-1}(\boldsymbol{y} - \boldsymbol{p})$, which we **cycle repeatedly** until **convergence**.

- This algorithm is sometimes called **iteratively re-weighted least squares** (IRLS), because **each step** can be seen as the solution of the weighted least squares problem

$$\beta^{(\text{new})} = \arg\min_{\beta}(\boldsymbol{z} - \boldsymbol{X}\beta)^T\boldsymbol{W}(\boldsymbol{z} - \boldsymbol{X}\beta).$$

Computational considerations

- Each **step** of the IRLS algorithm finds the solution of the likelihood equations

$$(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X})\beta = \boldsymbol{X}^T\boldsymbol{W}\boldsymbol{z}.$$

- Once again, the Cholesky and the QR decomposition can be exploited to speed up computations. See Section 5.4 of Arnold et al. (2019) for further details.
- It can be shown that $\beta = (0, \ldots, 0)^T$ is a good starting point for the initialization.
- Unfortunately, the IRLS is **not** guaranteed to **converge** nor to increase the log-likelihood at every step, but there are easy fixes.
- See this tutorial for an example of the **failure** of IRLS.
- These considerations and the IRLS algorithm can be easily generalized to all GLMs.

The estimated model

term	estimate	std.error	statistic	p.value
(Intercept)	-4.130	0.964	-4.283	0.000
sbp	0.006	0.006	1.023	0.306
tobacco	0.080	0.026	3.034	0.002
ldl	0.185	0.057	3.219	0.001
famhist_Present	0.939	0.225	4.177	0.000
obesity	-0.035	0.029	-1.187	0.235
alcohol	0.001	0.004	0.136	0.892
age	0.043	0.010	4.181	0.000

- Results of the IRLS algorithm applied to the logistic regression model using `heart` data.
- The coefficient of the variable `obesity` is **negative**. Why do you think this is the case?

Prediction and model assessment I

- The **predicted probabilities** $p(\boldsymbol{x}_i; \hat{\beta})$ are often **thresholded**, to obtain 0-1 predicted values, mostly useful for interpretative reasons

$$\hat{y}_i = \mathbb{I}(p(\boldsymbol{x}_i; \hat{\beta}) > c), \qquad i = 1, \ldots, n$$

  for some threshold c, which is **usually** set equal to $1/2$.

- We can then compare the responses with the predicted values using the **confusion matrix**:

	Actual response		
Prediction	**0**	**1**	**Total**
0	n_{00}	n_{01}	$n_{0.}$
1	n_{10}	n_{11}	$n_{1.}$
Total	$n_{.0}$	$n_{.1}$	n

Prediction and model assessment II

- In the `heart` dataset, using $c = 0.5$, we get the following **confusion matrix**:

	Actual 0	Actual 1	Actual total
Predicted 0	255	78	333
Predicted 1	47	82	129
Predicted total	302	160	462

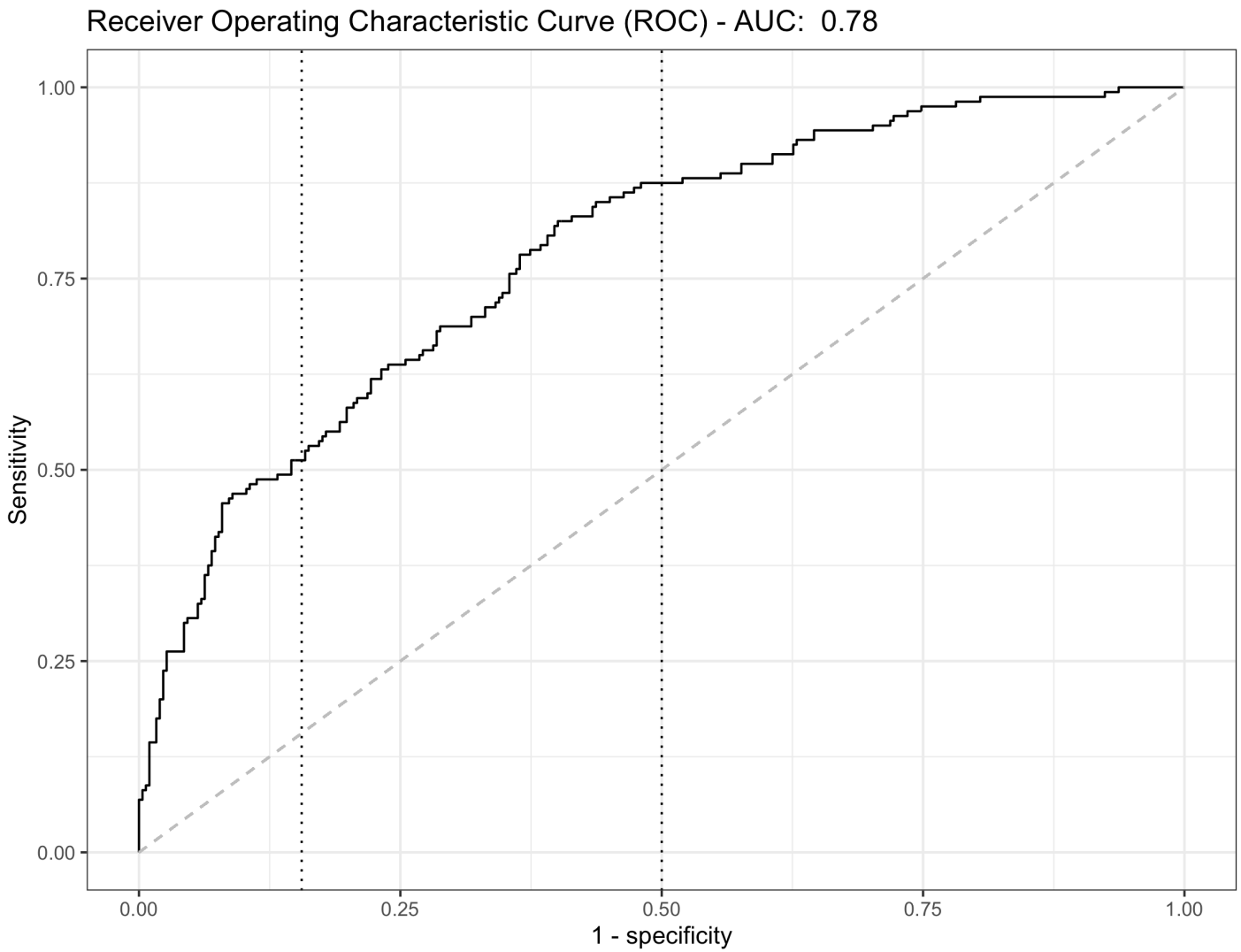
- Hence, the **overall accuracy** is $(255 + 82)/462 \approx 0.72$.
- The **true positive rate** (**specificity**) is defined as

$$\text{specificity} = 1 - \mathbb{P}(\text{“false positive”}) \approx \frac{n_{00}}{n_{00} + n_{10}} = \frac{255}{255 + 47} = 0.844.$$

- On the other hand, the **true negative rate** (**sensitivity**) is defined as

$$\text{sensitivity} = 1 - \mathbb{P}(\text{“false negative”}) \approx \frac{n_{11}}{n_{01} + n_{11}} = \frac{82}{72 + 82} = 0.532.$$

The ROC curve



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Other topics

- When the number of responses labels $K > 2$, we cannot use any more logistic regression.
- The natural extension is called **multinomial regression**, in which we model the probabilities

$$\mathbb{P}(Y_i = k) = p_k(\boldsymbol{x}_i, \beta), \qquad k = 1, \dots, K,$$

  for example, using **multinomial logit**. The ideas of GLMs can be easily borrowed.
- An alternative and straightforward approach is **linear discriminant analysis**, which is based on Bayes theorem.
- You can find these topics in the textbook A&S (2011), although you have likely seen these models in the previous courses.

References

- **Main references (M.Sc. level)**
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  - **Chapters 3 and 4** of Hastie, T., Tibshirani, R. and Friedman, J. (2009), *The Elements of Statistical Learning*, Second Edition, Springer.
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  - **Chapters 5 and 6** of Azzalini, A. (2000), *Inferenza Statistica. Una presentazione basata sul concetto di verosimiglianza*, Springer.
- **Specialized references**
  - **Chapters 1–3** of Quarteroni, A., Sacco, R., and Saleri F. (2007). *Numerical mathematics*. Second Edition, Springer.
  - **Chapters 1–5** of Golub, G.H., and Van Loan, C.F. (1983). *Matrix computations*. Hopkins University Press.