Linear models and misspecification

Statistics III - CdL SSE

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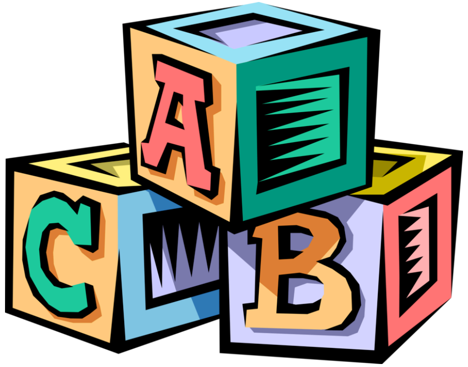
Home page

Homepage



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

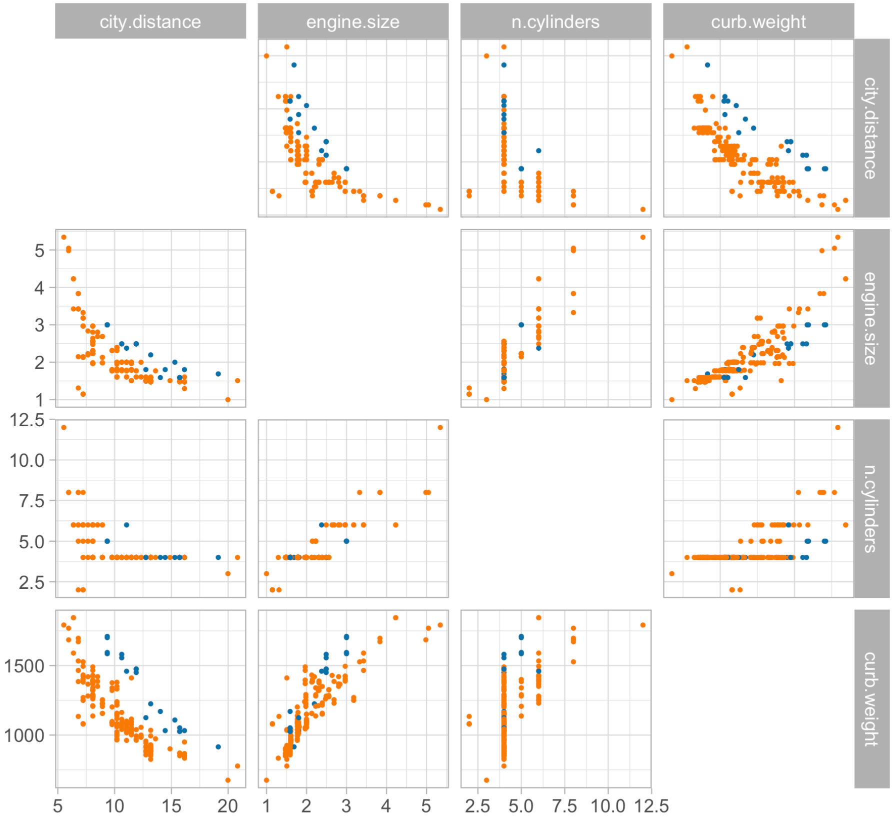
Attributed to **Albert Einstein**

- This unit will cover the following **topics**:
    - **Recap**: linear models and the modeling process
    - Robustness of OLS estimates, sandwich estimators
    - Weighted least squares
    - Box-Cox transform, variance stabilizing transformations
- The main theme is: what should we do when the **assumptions** of linear models are **violated**?
- We will push the linear model to its limit, using it even when is not supposed to work.
- The symbol 📖 means that a few extra steps are discussed in the **handwritten notes**.

The content of this Unit is covered in **Chapter 1** of Salvan et al. (2020). Alternatively, see **Chapter 2** of Agresti (2015) or **Chapter 5** of Azzalini (2008).

The modeling process

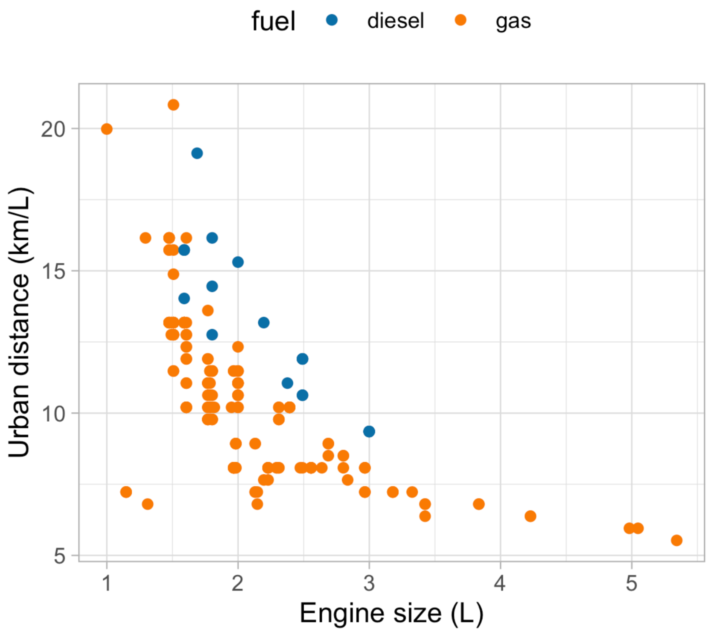
Car data (diesel or gas)



- 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`).

> We assume you are already familiar with linear models. The following is a brief recap rather than a full discussion.

Linear regression



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

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

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** $\boldsymbol{x}_i = (x_{i1}, \dots, x_{ip})^T \in \mathbb{R}^p$ and a random variable $Y_i \in \mathbb{R}$ is

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

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

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

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**

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

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

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 $\boldsymbol{Y} = (Y_1, \dots, Y_n)^T$, whose **observed realization** is $\boldsymbol{y} = (y_1, \dots, y_n)^T$.
- 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 $\boldsymbol{x}_i$:

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

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

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

where $\boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_n)^T$ 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

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

  where $\boldsymbol{H}$ is a $n \times n$ **projection matrix** matrix sometimes called **hat matrix**. The matrix is idempotent, meaning that $\boldsymbol{H} = \boldsymbol{H}^T$ and $\boldsymbol{H}^2 = \boldsymbol{H}$.

- The quantity $D(\hat{\beta})$ is the so-called **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:

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

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

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

Linear regression: inference

- Recall that the errors $\boldsymbol{\epsilon}$ have zero mean $\mathbb{E}(\boldsymbol{\epsilon}) = 0$ and are **uncorrelated** $\mathrm{var}(\boldsymbol{\epsilon}) = \sigma^2 I_n$.
- Then, the estimator $\hat{\beta}$ is **unbiased** $\mathbb{E}(\hat{\beta}) = \beta$ and its **variance** is $\mathrm{var}(\hat{\beta}) = \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}$. Since σ^2 is also unknown, we can estimate the variances of $\hat{\beta}$ as follows:

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

- The **standard errors** of the components of $\hat{\beta}$ correspond to the square root of the diagonal of the above covariance matrix.

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

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

- Confidence interval and Wald's tests can be obtained through classical inferential theory.

Linear regression: diagnostic

- The diagonal elements $h_i \in [0,1]$ of the matrix $\boldsymbol{H}$ are called **leverages** and it holds

$$\operatorname{var}(\hat{Y}_i) = \sigma^2 h_i, \qquad \operatorname{var}(Y_i - \hat{Y}_i) = \sigma^2(1-h_i), \qquad \operatorname{cor}(Y_i, \hat{Y}_i) = \sqrt{h_i}.$$

  The leverage h_i determines the **precision** with which $\hat{Y}_i$ predicts Y_i. For large h_i close to 1, $\operatorname{cor}(Y_i, \hat{Y}_i) \approx 1$, therefore changes of a single point Y_i leads to significant changes in $\hat{Y}_i$.

- Leverages also appear in the definition of **standardized residuals**:

$$\tilde{r}_i = \frac{r_i}{\sqrt{s^2(1-h_i)}} = \frac{y_i - \boldsymbol{x}_i^T\hat{\beta}}{\sqrt{s^2(1-h_i)}},$$

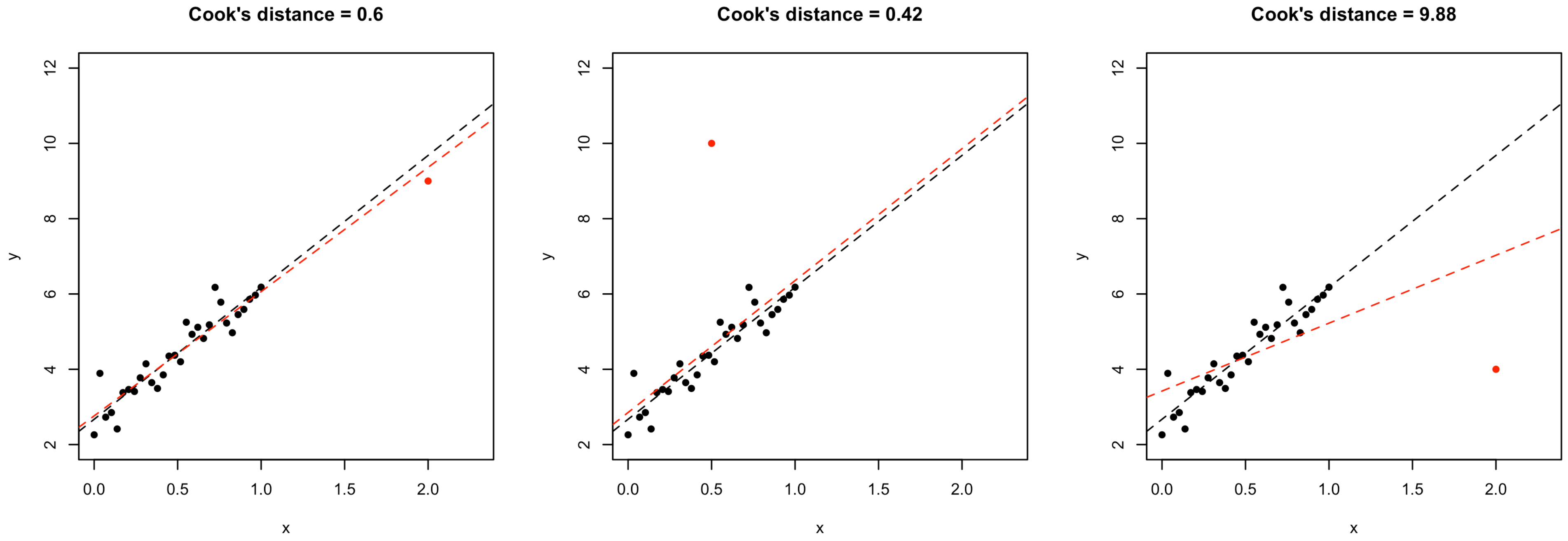
  where $r_i = y_i - \boldsymbol{x}_i^T\hat{\beta}$ are the (raw) **residuals**.

- An observation is **influent** if it has high leverage and high squared residual. **Cook's distance** c_i is based on the change in $\hat{\beta}$ when the observation is removed:

$$p \cdot c_i = (\hat{\beta} - \hat{\beta}_{-i})^T \widehat{\operatorname{var}}(\hat{\beta})^{-1}(\hat{\beta} - \hat{\beta}_{-i}) = \tilde{r}_i^2 \frac{h_i}{p(1-h_i)}.$$

  Cook's distance is considered relatively large when $c_i \geq 1$.

Leverages, outliers and influence points



- **Left plot**: leverage, not outlier. **Central plot**: outlier, not leverage. **Right plot**: influence point = leverage + outlier.

A first model: estimated coefficients

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

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

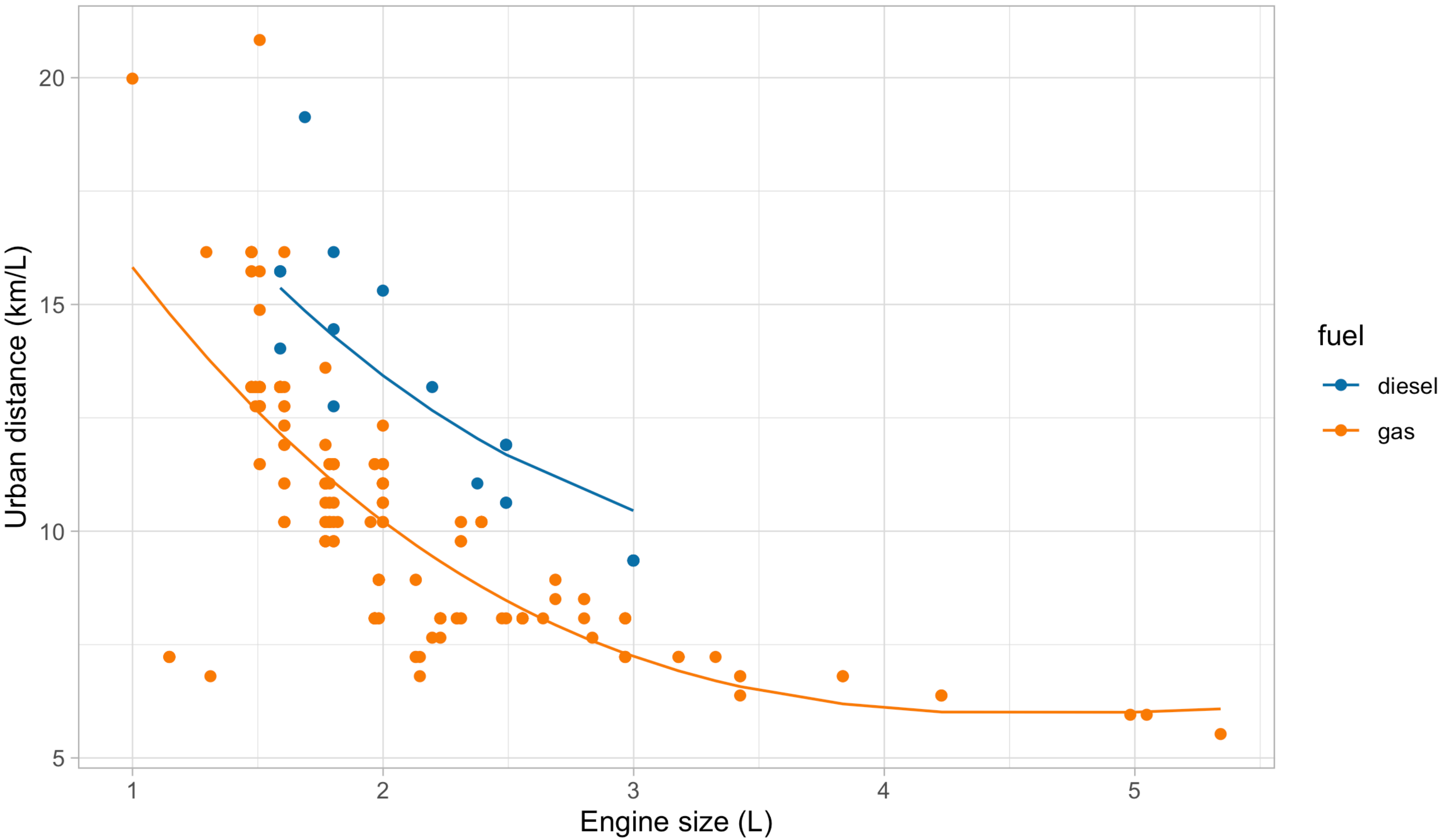
- We obtain the following **summary** for the regression coefficients $\hat{\beta}$.

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

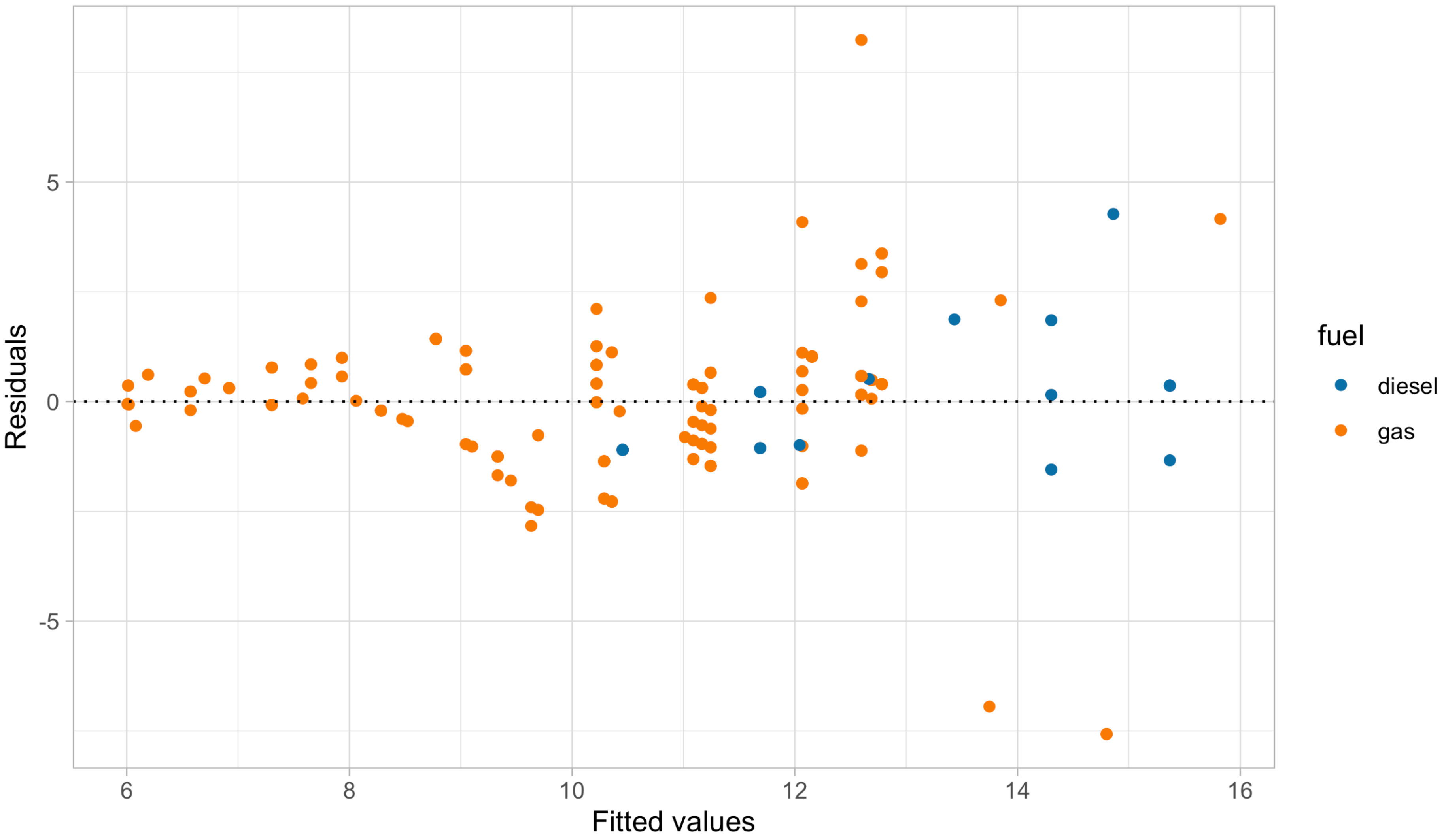
- Moreover, the coefficient R^2 and the residual standard deviation s are:

r.squared	sigma	deviance
0.5973454	1.790362	634.6687

A first model: fitted values



A first model: graphical diagnostics



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 homoschedasticity assumption, i.e. $\text{var}(\epsilon_i) = \sigma^2$, 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.

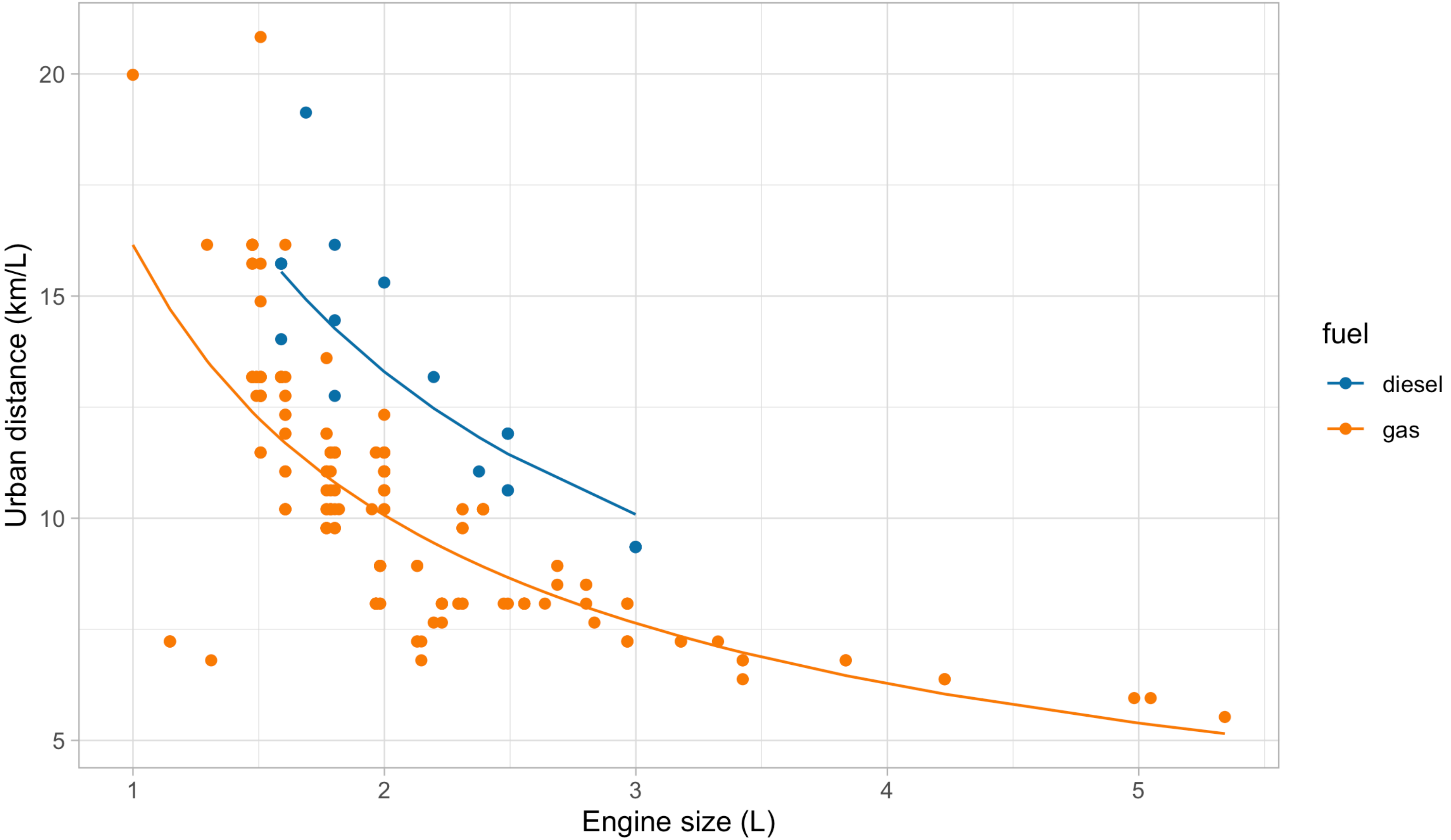
- This gives the statistician a lot of modeling flexibility. For instance, we could let:

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

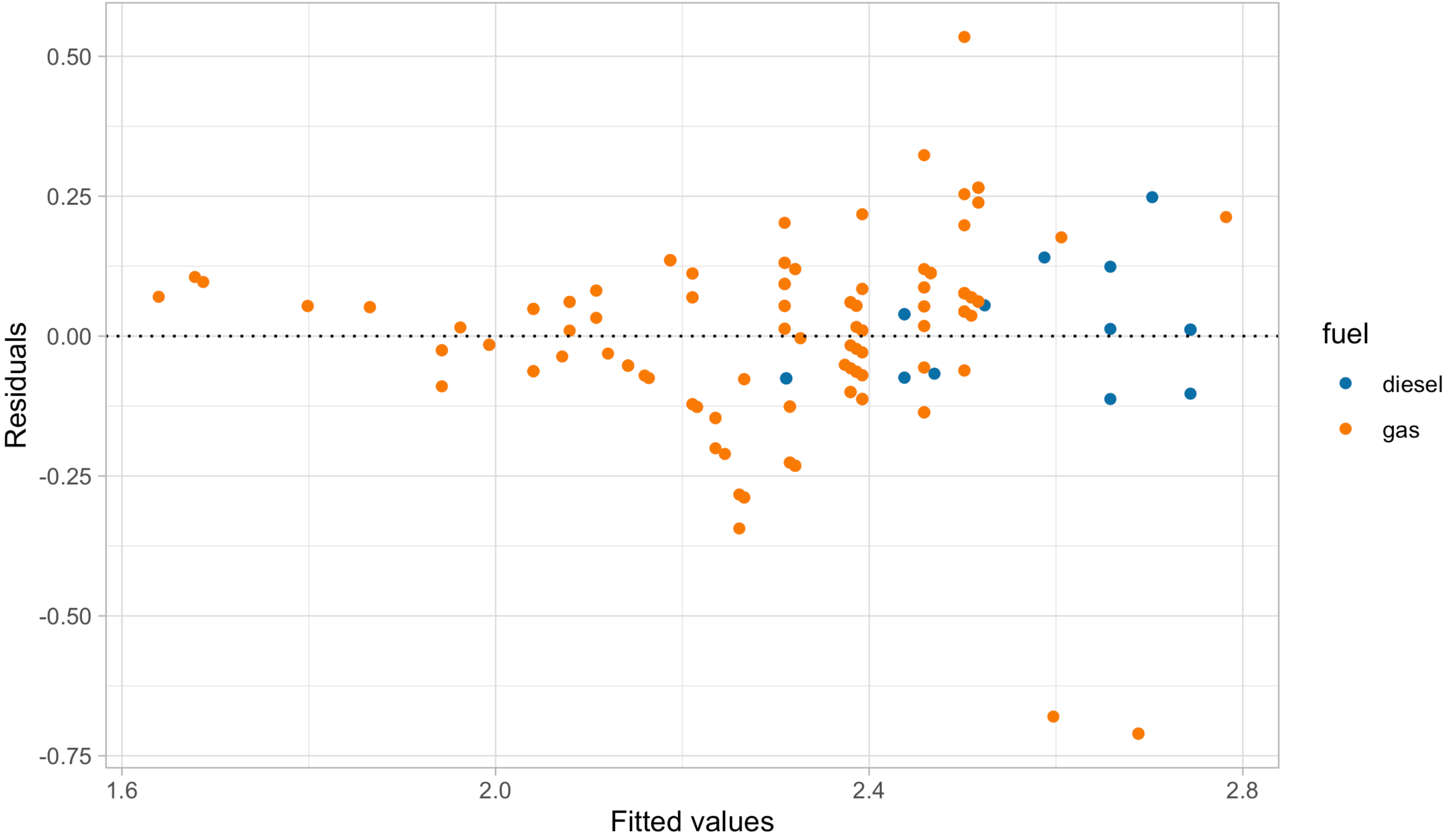
- This specification is **linear in the parameters**, it fixes the domain issues, and it imposes a monotone relationship between engine size and consumption.

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



Second model: graphical diagnostics



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

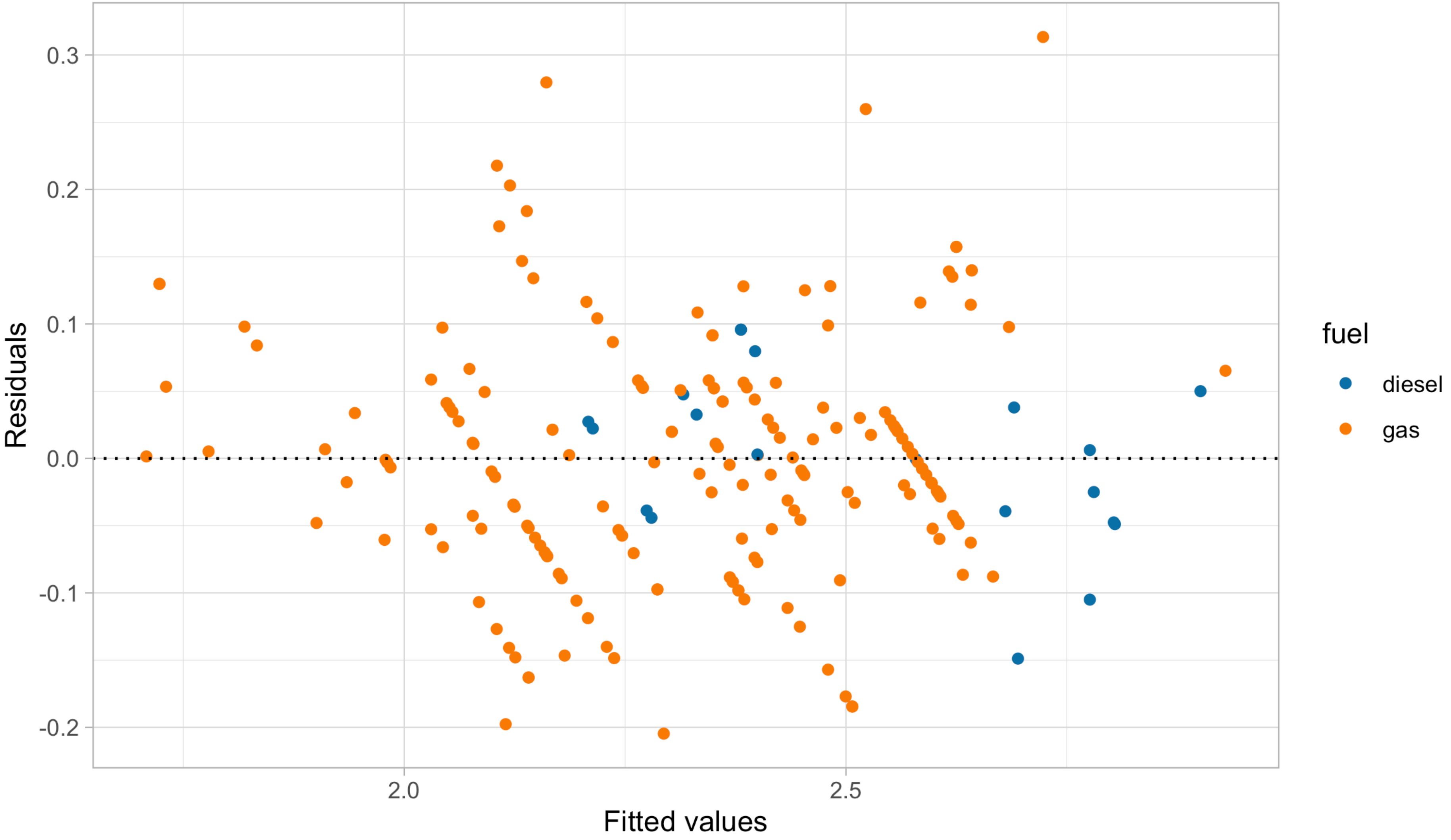
- Let us consider **two additional variables**: `curb.weight` (w) and `n.cylinders` (v).
- A richer model, therefore, could be:

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

for $i = 1, \dots, n$. 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



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 book (Azzalini and Scarpa (2012)) 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

Misspecification and remedies

Assumptions and misspecification

Classical assumptions of linear models

- **(A.1)** **Linear structure**, namely $\boldsymbol{Y} = \boldsymbol{X}\beta + \boldsymbol{\epsilon}$ with $\mathbb{E}(\boldsymbol{\epsilon}) = 0$, implying $\mathbb{E}(\boldsymbol{Y}) = \boldsymbol{X}\beta$. [1]
- **(A.2)** **Homoschedasticity** and **uncorrelation** of the errors, namely $\mathrm{var}(\boldsymbol{\epsilon}) = \sigma^2 I_n$.
- **(A.3)** **Gaussianity**, namely $\boldsymbol{\epsilon} \sim \mathrm{N}_n(0, \sigma^2 I_n)$. In other words, the errors $\epsilon_i \overset{\text{iid}}{\sim} N(0, \sigma^2)$ are iid Gaussian random variables with zero mean and variance σ^2.

It is also commonly asked that $\mathrm{rk}(\boldsymbol{X}) = p$, otherwise the model is not identifiable.

- If one of the above assumptions is violated, it is not necessarily a huge problem, because
  - the OLS estimator $\hat{\beta}$ is fairly **robust** to misspecification;
  - simple **fixes** (variable transformations, standard error corrections) are available.

[1] If the intercept is included in $\boldsymbol{X}$, the errors automatically satisfy the property $\mathbb{E}(\boldsymbol{\epsilon}) = 0$.

Robust estimation and assumptions

- A plane can still fly with one of its **engines on fire**, but this is hardly an appealing situation.
- Similarly, robust estimators may work under **model misspecification**, but this does not mean we should neglect **checking** whether the original **assumptions** hold.

Non-normality of the errors I 📖

- Let us consider the case in which assumptions **(A.1)-(A.2)** are **valid** but **(A.3)** **is not**, that is $\mathbb{E}(\boldsymbol{\epsilon}) = 0$ and $\text{var}(\boldsymbol{\epsilon}) = \sigma^2 I_n$, but ϵ does **not** follow **a Gaussian** distribution.
- For example, ϵ_i may follow a Laplace distribution, a skew-Normal, a logistic distribution, a Student's t distribution, etc.
- The OLS estimate $\hat{\beta}$ is **not** anymore the **maximum likelihood** estimator, but it **preserves** most of its **properties** and a **geometric interpretation**.

> Under **(A.1)-(A.2)**, even without requiring normality of the errors **(A.3)**, we obtain the usual formulas:
>
> $$\mathbb{E}(\hat{\beta}) = \beta, \qquad \text{var}(\hat{\beta}) = \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}.$$
>
> Moreover, because of **Gauss-Markov** theorem, the OLS estimator $\hat{\beta}$ is the most **efficient** within the class of linear and unbiased estimators (**BLUE**) for any distribution of the errors $\boldsymbol{\epsilon}$.

- In fact, note that the **proof** of the Gauss-Markov theorem requires **(A.1)-(A.2)** but **not** **(A.3)**.

Non-normality of the errors II

- When the errors are non Gaussian the **exact inferential results** are not valid. In particular $\hat{\beta}$ does not follow anymore a Gaussian distribution.
- However, a **central limit theorem** can be invoked under very mild conditions on the design matrix $\boldsymbol{X}$.
- Thus, when the sample size n is large enough, then the following **approximation** holds

$$\hat{\beta} \mathrel{\dot\sim} \mathrm{N}_p(\beta, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}),$$

  from which **confidence intervals** and **test statistics** can be obtained as usual. The approximation is **excellent** if the errors are **symmetric** around 0.

Non-normality of the errors is **not a major concern**: the OLS estimator preserves most of its properties, including approximate normality for sufficiently large n.

There is often an **over-emphasis** on testing whether the residuals are Gaussian. However, even if normality is rejected, the practical implications are minimal.

Heteroschedasticity of the errors I 📖

- Suppose now that the linearity assumption **(A.1)** is valid but **homoschedasticity** of the errors **(A.2)** is **not**. Instead, we consider **heteroschedastic errors**:

$$\operatorname{var}(\boldsymbol{\epsilon}) = \boldsymbol{\Sigma}, \quad \text{or equivalenty} \quad \operatorname{var}(Y_i) = \sigma_i^2, \quad i = 1, \dots, n$$

  where $\boldsymbol{\Sigma} = \operatorname{diag}(\sigma_1^2, \dots, \sigma_n^2)$ is a diagonal matrix with positive entries.

- The OLS estimator is still **unbiased**, with a **modified covariance** structure[1]

$$\mathbb{E}(\hat{\beta}) = \beta, \qquad \operatorname{var}(\hat{\beta}) = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}.$$

  If in addition we assume Gaussianity of the errors, that is $\boldsymbol{\epsilon} \sim \mathrm{N}_n(0, \boldsymbol{\Sigma})$, then

$$\hat{\beta} \sim \mathrm{N}_p(\beta, (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}).$$

  Under suitable but mild conditions on $\boldsymbol{X}$ and $\boldsymbol{\Sigma}$, the estimator is also **consistent**.

[1] These results are valid even when the matrix $\boldsymbol{\Sigma}$ is non-diagonal. This is useful to model correlated responses.

Heteroschedasticity of the errors II

> The OLS estimator in presence of heteroschedasticity still gives a **good point estimate**. However, the OLS estimator is **not efficient** and the classical **standard errors** are **wrong**.

- A potential approach is to **accept the inefficiency** of the OLS estimator in this scenario and **correct** the standard errors.
- The elements of $\mathbf{\Sigma}$ are **unknown**, but we can estimate them from the data. Note that

$$\text{var}(r_i) = \text{var}(y_i - \boldsymbol{x}_i^T\hat{\beta}) = \sigma_i^2(1 - h_i),$$

  suggesting the **estimate** $\hat{\sigma}_i^2 = r_i^2/(1 - h_i)$.
- This leads to the so-called **sandwich estimator** of the covariance matrix:

$$\widehat{\text{var}}(\hat{\beta}) = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\hat{\mathbf{\Sigma}}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1},$$

  where $\hat{\mathbf{\Sigma}} = \text{diag}(\hat{w}_1, \dots, \hat{w}_n)$ and $\hat{w}_i = r_i^2/(1 - h_i)$.
- These are known as **White's** heteroscedasticity-consistent **standard errors**. [1]

[1] White originally proposed the simpler version $\hat{\sigma}_i^2 = r_i^2$. Another variant is $\hat{\sigma}_i^2 = r_i^2/(1 - h_i)^2$.

Weighted least squares I 📖

- Let us consider again the case of **heteroschedastic errors**:

$$\text{var}(\boldsymbol{\epsilon}) = \sigma^2\boldsymbol{\Omega}^{-1}, \quad \text{or equivalenty} \quad \text{var}(Y_i) = \sigma_i^2 = \frac{\sigma^2}{\omega_i}, \quad i = 1, \dots, n$$

  where $\boldsymbol{\Omega} = \text{diag}(\omega_1, \dots, \omega_n)$ are positive **weights**. However, here we assume that the weights $\omega_1, \dots, \omega_n$ are **known**, a common situation in survey design.

- Let us define the **standardized** quantities:

$$\boldsymbol{Y}^* = \boldsymbol{\Omega}^{1/2}\boldsymbol{Y}, \qquad \boldsymbol{X}^* = \boldsymbol{\Omega}^{1/2}\boldsymbol{X}.$$

  This is equivalent to say that $Y_i^* = \sqrt{\omega_i}Y_i$ and $x_{ij}^* = \sqrt{\omega_i}x_{ij}$. Then, it is easy to show that

$$\mathbb{E}(\boldsymbol{Y}^*) = \boldsymbol{X}^*\beta, \qquad \text{var}(\boldsymbol{Y}^*) = \sigma^2\boldsymbol{\Omega}^{1/2}\boldsymbol{\Omega}^{-1}\boldsymbol{\Omega}^{1/2} = \sigma^2 I_n,$$

  namely the **assumptions** **(A.1)** and **(A.2)** are valid in the **transformed scale**.

- In other words, **after** a suitable **transformation**, we reconducted the problem to a **standard linear model**.

Weighted least squares II 📖

- Thus an estimator for β, based on the transformed data, is obtained minimizing the deviance

$$\begin{aligned} D_{\text{wls}}(\beta) &= (\boldsymbol{y}^* - \boldsymbol{X}^*\beta)^T(\boldsymbol{y}^* - \boldsymbol{X}^*\beta) = (\boldsymbol{y} - \boldsymbol{X}\beta)^T\boldsymbol{\Omega}(\boldsymbol{y} - \boldsymbol{X}\beta) \\ &= \sum_{i=1}^{n}\omega_i(y_i - \boldsymbol{x}_i^T\beta)^2. \end{aligned}$$

  which is a **weighted** version of the original **quadratic loss**, with **high weight = low variance**.

- The resulting OLS estimate minimizing $D_{\text{wls}}(\beta)$ in the transformed and original scales is

$$\hat{\beta}_{\text{wls}} = [(\boldsymbol{X}^*)^T\boldsymbol{X}^*]^{-1}(\boldsymbol{X}^*)^T\boldsymbol{y}^* = (\boldsymbol{X}^T\boldsymbol{\Omega}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Omega}\boldsymbol{y}$$

  and it is referred to as **weighted least squares** estimator of β.

- Such an estimator is **unbiased** and **efficient** (**BLUE**), with

$$\mathbb{E}(\hat{\beta}_{\text{wls}}) = \beta, \qquad \text{var}(\hat{\beta}_{\text{wls}}) = \sigma^2(\boldsymbol{X}^T\boldsymbol{\Omega}\boldsymbol{X})^{-1}.$$

  Moreover, if $\boldsymbol{\epsilon} \sim \text{N}_n(0, \sigma^2\boldsymbol{\Omega}^{-1})$ it also coincides with the **maximum likelihood** estimator.

Variable transformations

- Another remedy for **misspecification** was already applied in the analysis of the car dataset, namely through **variable transformation**.

> While the model may have been incorrectly specified for the original data, it could become **appropriate** once the **transformations** are considered, namely
>
> $$g(Y_i) = h_1(\boldsymbol{x}_i)\beta_1 + \cdots + h_p(\boldsymbol{x}_i)\beta_p + \epsilon_i, \qquad i = 1, \dots, n,$$
>
> where $g(\cdot)$ and $h_j(\cdot)$ for $j = 1, \dots, p$ are **non-linear** and **known** functions.

- This idea is conceptually **simple** and **powerful**. It also shows that linear models are capable of capturing non-linear relationships, as long as they remain **linear in the parameters**.
- However, choosing $g(\cdot)$ and $h_j(\cdot)$ in practice is **not simple**. In our case study, we proceeded by trial and error and used **contextual information** to guide our final choice.
- Regarding the functions $h_j(\cdot)$, **polynomial** terms are a simple and common option. More advanced approaches based on **splines** will be discussed in Data Mining.

Box-Cox transform

Box-Cox transform

If the data are y_i are **positive**, we may consider a **parametric class** of transformations:

$$g_\lambda(y) = \frac{y^\lambda - 1}{\lambda}, \qquad \lambda \neq 0.$$

and $g_\lambda(y) = \log y$ when $\lambda = 0$. This is the celebrated **Box-Cox transform**.

The case $\lambda = 1$ corresponds to no transformation, $\lambda = 1/2$ to the square root, $\lambda = 0$ to the logarithm, and $\lambda = -1$ to the reciprocal.

- We estimate λ from the data using **maximum likelihood**, so that the data themselves can inform us about the best transformation. We assume

$$g_\lambda(Y_i) = \boldsymbol{x}_i^T \beta + \epsilon_i, \qquad \epsilon_i \sim \mathrm{N}(0, \sigma^2), \qquad i = 1, \dots, n.$$

- The aim of the transformation is to produce a response for which the **variance** of ϵ_i is **constant** with an **approximately normal** distribution.

Box-Cox transform: derivation I 📖

- By assumption, the distribution of the **transformed data** $\boldsymbol{Z}_\lambda = (g_\lambda(Y_1), \dots, g_\lambda(Y_n))^T$ is Gaussian, therefore their joint density is

$$f_Z(\boldsymbol{z}_\lambda) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left\{-\frac{1}{2\sigma^2}(\boldsymbol{z}_\lambda - \boldsymbol{X}\beta)^T(\boldsymbol{z}_\lambda - \boldsymbol{X}\beta)\right\}.$$

- Using standard tools of probability theory, we can obtain the density of the **original data**:

$$f_Y(\boldsymbol{y}) = f_Z(g_\lambda(y_1), \dots, g_\lambda(y_n)) \prod_{i=1}^n \left|\frac{\partial g_\lambda(y_i)}{\partial y_i}\right|, \quad \text{where} \quad \left|\frac{\partial g_\lambda(y_i)}{\partial y_i}\right| = y_i^{\lambda-1}.$$

  The additional term is the determinant of the **Jacobian** of the transformation.

- The **log-likelihood** therefore is

$$\ell(\beta, \sigma^2, \lambda) = -\frac{n}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(\boldsymbol{z}_\lambda - \boldsymbol{X}\beta)^T(\boldsymbol{z}_\lambda - \boldsymbol{X}\beta) + (\lambda - 1)\sum_{i=1}^n \log y_i.$$

Box-Cox transform: derivation II 📖

- Note that, for any given value of λ, the maximum likelihood estimates are

$$\hat{\beta}_\lambda = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{z}_\lambda, \qquad \hat{\sigma}^2_\lambda = \frac{1}{n}(\boldsymbol{z}_\lambda - \boldsymbol{X}\hat{\beta}_\lambda)^T(\boldsymbol{z}_\lambda - \boldsymbol{X}\hat{\beta}_\lambda),$$

- We can **plug-in** the above estimates into the log-likelihood. This gives the **profile log-likelihood** for λ, which admits a very simple expression:

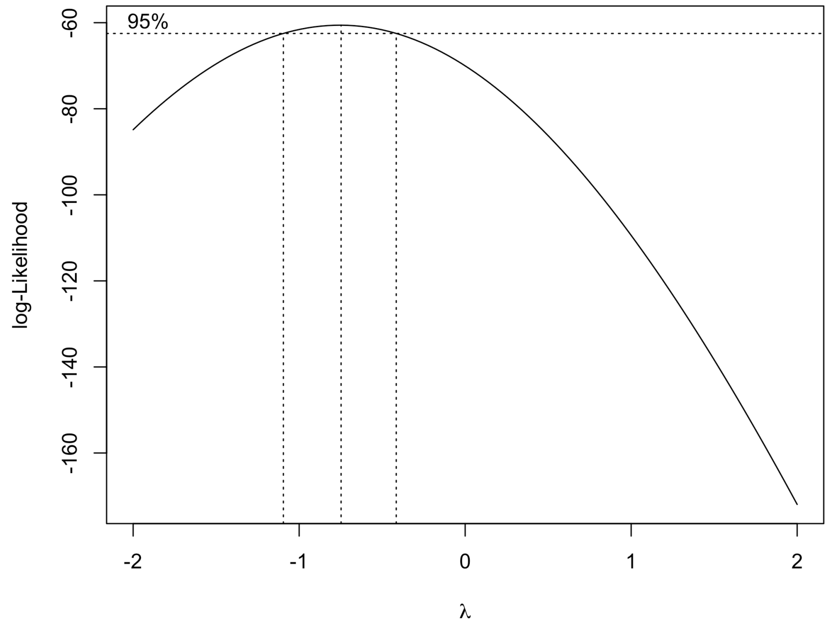
$$\ell_P(\lambda) = \ell(\hat{\beta}_\lambda, \hat{\sigma}^2_\lambda, \lambda) = -\frac{n}{2}\log\hat{\sigma}^2_\lambda + (\lambda - 1)\sum_{i=1}^n \log y_i,$$

  which must be **numerically maximized** over λ, e.g. using `optim`.

- The optimal value $\hat{\lambda} = \arg\max \ell_P(\lambda)$, as well as a confidence interval for it, may offer guidance in choosing the right transformation.

> Box and Cox suggested using this approach as an **exploratory tool**. For instance, an optimal value $\hat{\lambda} = 0.4210283$ is **hard to interpret** but it could suggest a square root transformation.

Box-Cox transform for the auto dataset

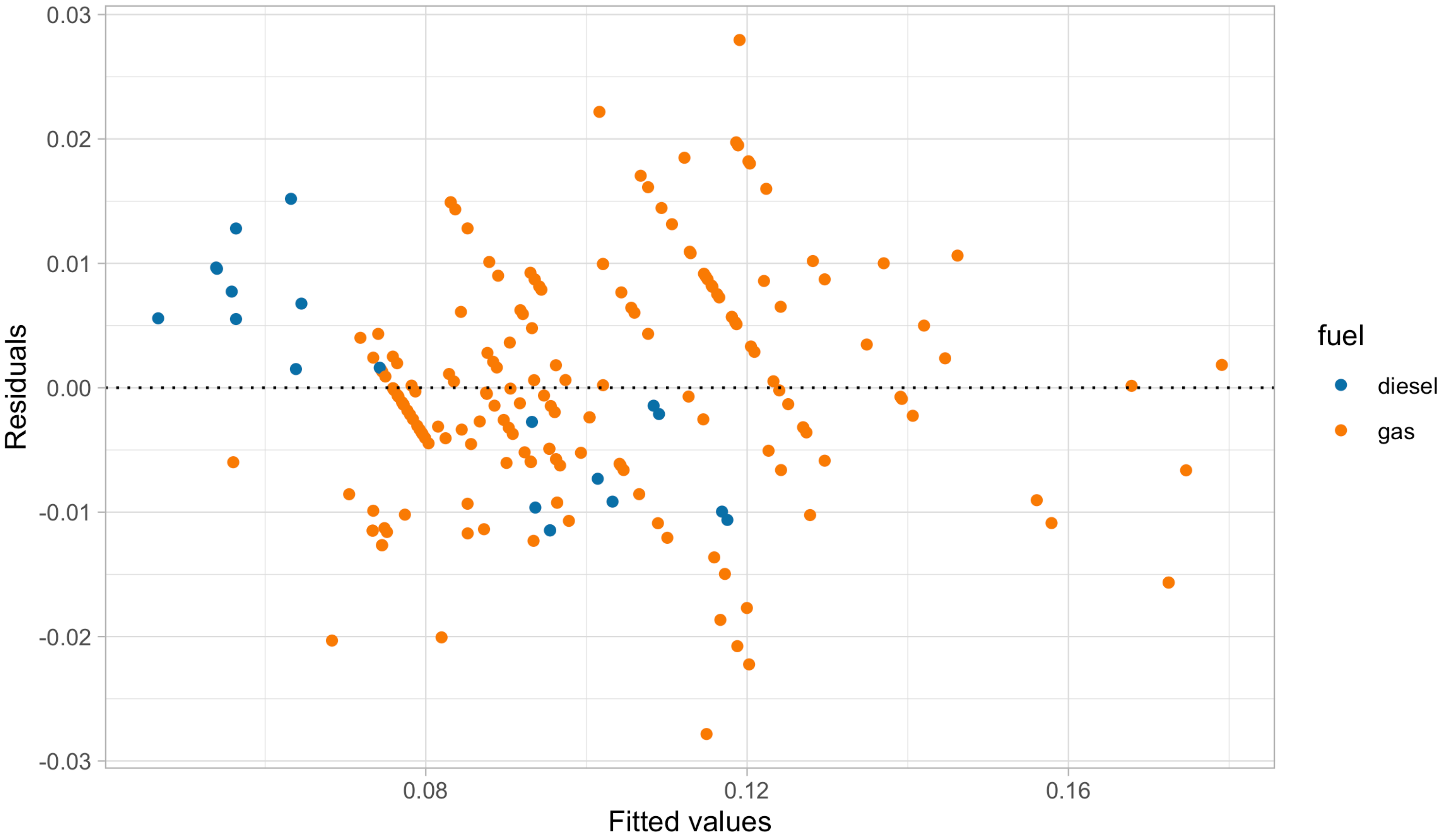


- The **Box-Cox transform** in the auto dataset suggests a **reciprocal** transformation:

$$\frac{1}{Y_i} = \beta_1 + \beta_2 x_i + \beta_3 w_i + \beta_4 I(z_i = \texttt{gas}) + \beta_5 I(v_i = 2) + \epsilon_i,$$

which is a good alternative to our model based on logarithms of y_i, x_i, and w_i (**but**...).

A fourth model: graphical diagnostics



Variance stabilizing transformations I 📖

- Let $Y_i \sim \text{Poisson}(\mu_i)$ with mean $\mathbb{E}(Y_i) = \mu_i = f(\boldsymbol{x}_i; \beta) = \text{var}(Y_i)$. Note that
$$Y_i \,\dot{\sim}\, \text{N}(\mu_i, \mu_i),$$
is **asymptotically Gaussian** for large values of μ_i. However, data are **heteroschedastic**.
- In modeling count data, we could transform the counts so that, at least **approximately**, the **variance** of $g(Y_i)$ is **constant** and ordinary least squares methods can be used.
- As an application of the **delta method**, the following linearization holds
$$g(Y_i) - g(\mu_i) \approx (Y_i - \mu_i)g'(\mu_i), \quad \text{which implies} \quad \text{var}\{g(Y_i)\} \approx g'(\mu_i)^2 \text{var}(Y_i).$$
In the Poisson case $\text{var}\{g(Y_i)\} \approx \mu_i \, g'(\mu_i)^2$ and we would like this to be **constant**.
- The choice $g(y) = \sqrt{y}$, called **variance stabilizing** transformation, gives
$$\text{var}(\sqrt{Y_i}) \approx \left(\frac{1}{2\sqrt{\mu_i}}\right)^2 \mu_i = \frac{1}{4}.$$

Variance stabilizing transformations II 📖

- Let $Y_i \sim \text{Binomial}(\pi_i, m_i)$, with **success probability** $\pi_i = f(\boldsymbol{x}_i; \beta)$ and **trials** m_i. For large values of m_i, the **Gaussian approximation** holds
$$Y_i \,\dot\sim\, \text{N}(m_i\pi_i, m_i\pi_i(1-\pi_i)).$$
However, the data are **heteroschedastic**, because $\text{var}(Y_i) = m_i\pi_i(1-\pi_i)$.
- Thus, a **variance stabilizing** transformation in this case is
$$g_{m_i}(y) = \sqrt{m_i}\arcsin\left(\frac{2y}{m_i} - 1\right),$$
because in fact we have that
$$\text{var}(g_{m_i}(Y_i)) \approx \left(\frac{\sqrt{m_i}}{\sqrt{1-(2\pi_i-1)^2}}\frac{2}{m_i}\right)^2 m_i\pi_i(1-\pi_i) = 1.$$
- If the data are **gamma distributed**, the **variance stabilizing** transform is $g(y) = \log y$.

Limitations of variable transformations I

- Variable transformations are appealing for their simplicity and have a long history in statistics. However, they also have some **drawbacks**.

- In the case of transformations applied only to the **explanatory variables**, the model is

$$Y_i = h_1(\boldsymbol{x}_i)\beta_1 + \cdots + h_p(\boldsymbol{x}_i)\beta_p + \epsilon_i, \qquad i = 1, \dots, n,$$

  Thus, the coefficient β_j can **no longer** be **interpreted** as the change in the mean of Y_i corresponding to a **one-unit increase** $x_{ij} \to x_{ij} + 1$ of the jth covariate.

- In the case of transformations of the **response** variable we let $\mathbb{E}(g(Y_i)) = \boldsymbol{x}_i^T\beta$. However:

$$g(\mathbb{E}(Y_i)) \neq E(g(Y_i)) \quad \implies \quad \mathbb{E}(Y_i) \neq g^{-1}(\boldsymbol{x}_i^T\beta).$$

  Thus $\hat{y}_i = g^{-1}(\boldsymbol{x}_i^T\hat{\beta})$ is a **reasonable prediction** for Y_i and **not an estimate** for its **mean**.

- When $g(y) = \log y$ this distinction can be made explicit, because we have

$$g^{-1}(\mathbb{E}\{g(Y_i)\}) = g^{-1}(\boldsymbol{x}_i^T\beta) = \exp(\boldsymbol{x}_i^T\beta), \qquad \mathbb{E}(Y_i) = \exp(\boldsymbol{x}_i^T\beta + \sigma^2/2),$$

  the former being the **geometric mean** of Y_i, whereas the latter is the usual **mean**.

Limitations of variable transformations II

Suppose $Y_i \sim \text{Binomial}(\pi, m_i)$. The variance stabilizing transformation is not fully satisfactory:

- It **complicates** the **interpretation**, because it models $\mathbb{E}\{g(Y_i)\}$ instead of $\mathbb{E}(Y_i)$;
- It is an **asymptotic approximation**, and is only valid for $m_i \to \infty$.
- The transform depends on m_i, therefore we cannot make predictions for a generic covariate value $\boldsymbol{x}_i$ without knowing the associated m_i.

Besides, this transform is clearly not applicable when $m_i = 1$ and $Y_i \in \{0, 1\}$, a very common problem called **binary regression**.

- If we know that Y_i follows, say, a Bernoulli or a Gamma distribution, then we should use the **appropriate likelihood** rather than a **Gaussian approximation**.
- **Generalized Linear Models** provide a **much more elegant solution** to the above problem.

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