



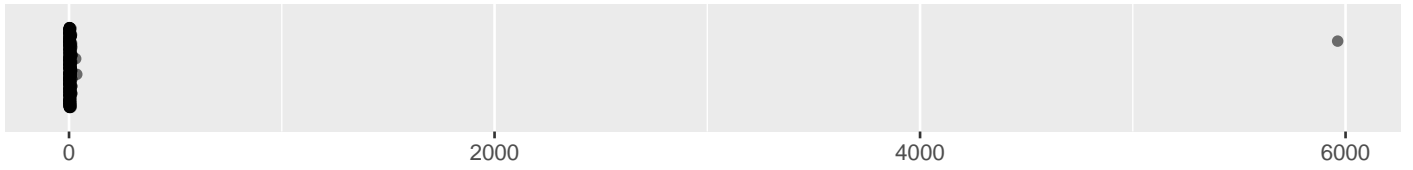
Katholieke
Universiteit
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Statistische Modellen & Data-analyse
Practicum 2

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Robust distance



(zoomed in)

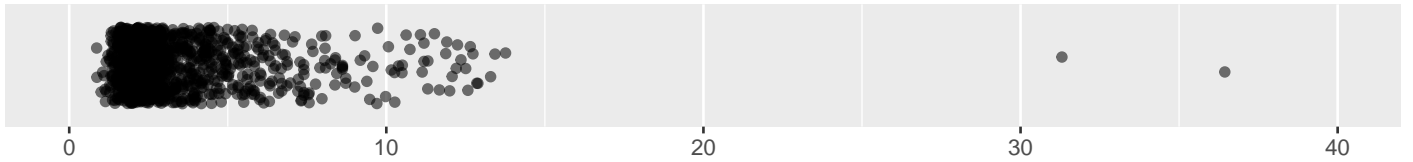


Figure 1: Robust distance-to-center of each car in the training set.

1 Linear regression

The complete dataset of 1500 cars was split into a 1000-car training set and a 500-car test set. We continue this analysis with the training set.

Exploratory analysis & outlier removal

We search for outliers by calculating, for each data point, its statistical distance to the multivariate distribution – using robust estimates for the center and the covariance matrix. Specifically, the Minimum Covariance Determinant estimator [1] was used, approximated by the **Fast** MCD algorithm [2]. Figure 1 shows the resulting robust distances.

Three strong outliers are found:

- the “Volkswagen *Jetta (from NOV 06 Wk 45 >) 1.4 TSI (170 PS) Sport*” with an abnormal `noise_level` of 0.3;
- the “Vauxhall *Signum MY2008 3.0CDTi V6 24v with 16/17/18" wheel*” with an abnormal `nox_emissions` value of 237000;
- the “MG Rover Group *Streetwise 1.8*” without any individually abnormal variables.

Note that this third outlier would not have been found had we only looked at univariate (or even bivariate) distributions of the data.

The found strong outliers are removed from the training set.

Figure 2 shows the uni- and bivariate distributions in the data set. Note the very strong correlations between `urban_metric`, `extra_urban_metric`, `combined_metric`, and `co2` – and to a lesser extend `engine_capacity`. This is in accordance with

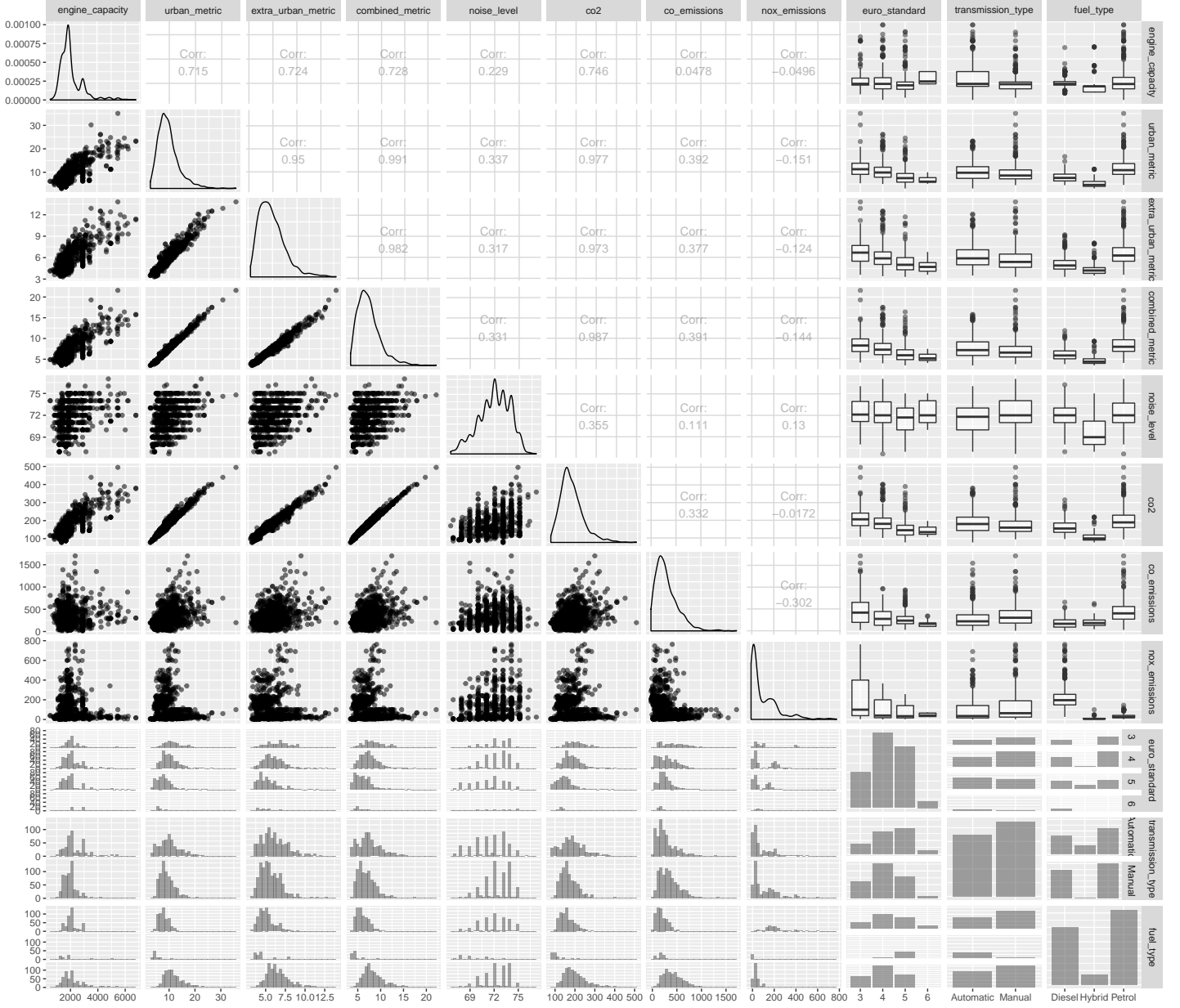


Figure 2: Uni- and bivariate sample distributions (after the strongest robust distance-outliers have been removed).

their meanings: cars with larger engine volumes consume more liters of fuel (all three `_metrics` measure fuel consumption), and every liter of fuel corresponds to a fixed amount of CO₂. These strong pairwise correlations point to the problem of multicollinearity in the data set. We explore this more formally further on.

We also note that for the variable `noise_level`, a large subset of cars take on discrete values. (There are also cars with `noise_levels` in between). This discrete character would negatively impact a cluster analysis, as the clusters would tend to form around the discrete values; while other variables would have disproportionately less impact on the clustering. However, we decide this will probably not impact the subsequent regression and classification tasks too much, so we keep this variable, for now.

Additionally, we note that none of the continuous variables seem to be univariate normally distributed (further on we do numeric normality tests, and normal QQ plots have been checked). Rather, they are positively skewed, with heavy right tails.

Finally, note the multimodality of `engine_capacity` and `nox_emissions`, and the fact that `fuel_type` tends to split the other variables into groups – see e.g. Diesel versus Hybrid or Petrol for `nox_emissions`.

Model construction

We will construct a general linear model to predict the `co2` variable. The predictor variables to include in the model will be selected via bidirectional stepwise regression. The Akaike Information Criterion (AIC) is used to compare models. The least squares estimator will always be used to estimate the coefficients β for a candidate model. The categorical variables `euro_standard`, `transmission_type`, and `fuel_type` are expanded into indicator variables (e.g. `fuel_type_Petrol`, taking on either a 0 or a 1).

Predictor variable transformations

The AIC assumes the residuals to be normally distributed. As they are an affine transformation of the predictor variables, the predictor variables need to be normally distributed as well. Thus, before starting the stepwise variable selection procedure, we find a Box-Cox power transformation [3] for all continuous predictor variables that maximises their normality in the maximum likelihood sense. The thusly found exponents λ are listed in table 1, along with the p -values for the Shapiro-Wilk test of normality before and after the transformation. Note that, except for `noise_level`, the normality of each variable greatly increases after the transformation. This was confirmed using normal QQ plots of the variables. We apply the maximum likelihood transformation to all continuous predictor variables, except for `noise_level` (as its maximum likelihood exponent falls outside the usual range, and its normality does not significantly improve after transforma-

Variable	λ_{ML}	p_{before}	p_{after}
engine_capacity	-0.65	4E-33	2E-12
urban_metric	-0.06	2E-23	0.164
extra_urban_metric	-0.64	3E-22	0.002
combined_metric	-0.37	3E-23	0.011
noise_level	7.11	2E-14	3E-12
co_emissions	0.29	7E-26	0.093
nox_emissions	0.04	1E-35	1E-12

Table 1: Maximum likelihood transformation exponents λ , and p -values for the Shapiro-Wilk test of normality before and after transformation, for each possible continuous predictor variable.

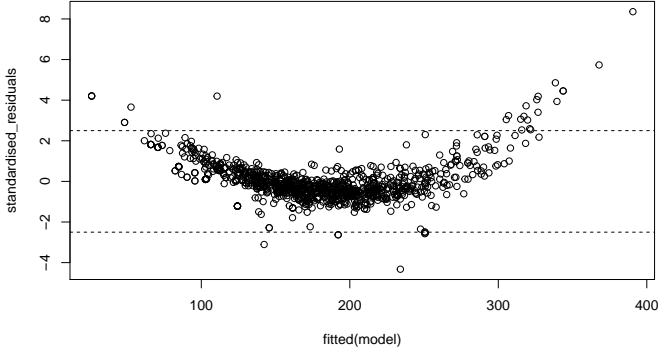


Figure 3: Standardised residuals of the linear model versus fitted values, before the response variable has been transformed.

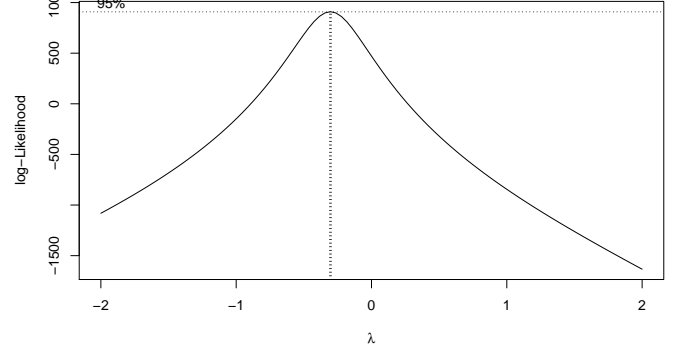


Figure 4: Log-likelihood of λ for the Box-Cox transformation of the response variable.

tion).

Response variable transformation

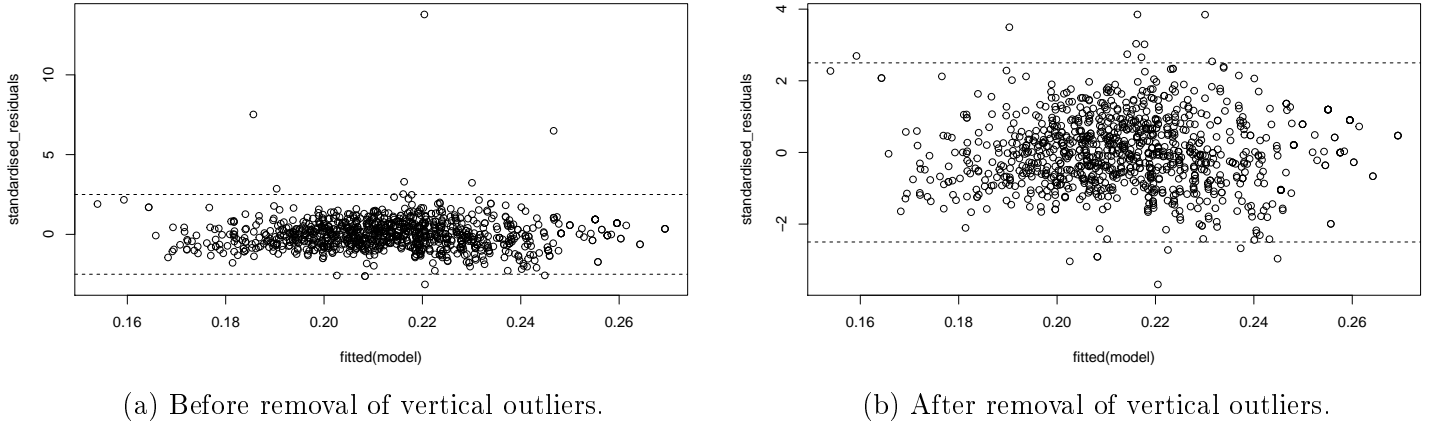
We now create a first linear model (via stepwise AIC regression starting from a model containing all predictor variables). Figure 3 shows the residuals of the resulting model. The strong (nonlinear) correlation between the predicted `co2` values and the residuals prompts us to transform the response variable. The optimal Box-Cox power transformation of the response variable [3] is found for $\lambda = -0.3$ (see fig. 4). We create a new linear model with the transformed response variable.

Removal of residual outliers

The residuals of the model with transformed response variable are shown in fig. 5a. We find three strong vertical outliers. They are:

- the “Volkswagen *LT 35 Kombi MWB - LWB* 2.8 (158 PS) TDI Axle Ratio 3.727”;
- the “Honda *Insight, Model Year 2012* 1.3 IMA HS, HS-T, HX”;

Figure 5: Standardised residuals of the linear model versus fitted values, after the response variable has been transformed.



- and the “Renault *New Mégane Hatchback* 2.0 dCi 160 FAP”.

(These cars do not have higher robust distances than other cars (as in fig. 1); they can however be spotted as outliers when the Mahalanobis distance is considered). These three additional outliers are removed from the training set. We note that removing these outliers has no effect on the maximum-likelihood λ of the Box-Cox transformation of the response variable.

Variable selection & final model

With optimal input and output transformations and the strongest outliers removed, we can now construct our final model, by selecting an appropriate subset of predictor variables. As already mentioned, bidirectional stepwise AIC regression is used. The procedure is started both from a model containing all predictor variables, and from an empty model containing only a constant term. Both procedures converge to the same model. The included variables, along with estimates for their coefficient and an analysis of variance (ANOVA), are shown in table 2. The variables that are not included, are `noise_level` and `transmission_type_Manual`. We find a final R^2 value of 0.9987, an adjusted R^2 value of 0.9987, and a mean squared error $\hat{\sigma}^2$ of 4.750×10^{-7} . The standardised residuals are shown in fig. 5b.

Discussion

Performance on the test set

As we have a proper test set at our disposal, we can check whether our model generalises well. It does. The mean absolute relative error (defined as $\frac{1}{n-p} \sum_{i=1}^n \left| \frac{\hat{y}_i - y_i}{y_i} \right|$) on the test set is 2.9×10^{-3} , demonstrating excellent predictive power – the CO₂ emissions of a car can be predicted with an error of on average only 0.3%. The

Predictor variable j	λ_j	$\hat{\beta}_j$	$s(\hat{\beta}_j)$	t	p	SS	F	$Pr(> F)$
<i>Intercept</i>	–	5.3E–1	2.8E–2	18.9	3E–68	45.6	95 972 309	< 2E–16
engine_capacity	–0.65	–9.3E–2	1.8E–2	–5.1	5E–7	0.1663	350 125	< 2E–16
urban_metric	–0.06	–2.2E–2	1.2E–3	–18.4	3E–65	0.1771	372 852	< 2E–16
extra_urban_metric	–0.64	–5.5E–2	3.7E–3	–14.7	2E–44	0.0032	6710	< 2E–16
combined_metric	–0.37	–5.4E–2	4.5E–3	–12.0	7E–31	0.0001	229	< 2E–16
co_emissions	0.29	–2.6E–5	7.6E–6	–3.5	6E–4	0.0010	2149	< 2E–16
nox_emissions	0.04	7.2E–5	3.7E–5	2.0	5E–2	0.0058	12 130	< 2E–16
euro_standard_4	–	3.7E–4	7.0E–5	5.2	2E–7	0.0002	506	< 2E–16
euro_standard_5	–	1.4E–3	7.9E–5	18.0	5E–63	0.0002	391	< 2E–16
euro_standard_6	–	1.0E–3	1.6E–4	6.0	2E–9	0.0002	388	< 2E–16
fuel_type_Hybrid	–	7.5E–3	1.7E–4	44.0	2E–234	0.0002	390	< 2E–16
fuel_type_Petrol	–	7.5E–3	1.4E–4	54.7	2E–300	0.0014	2993	< 2E–16
<i>Residuals</i>	–	–	–	–	–	0.0005	–	–

Table 2: Coefficients and ANOVA of the final general linear model. λ_j ’s taken from table 1. Note that both the predictor variables and the response variable are transformed non-linearly. That is why some coefficients may seem counterintuitive at first – e.g. a negative slope for `engine_capacity` with respect to `co2`.

mean squared error on the test set is 8.00×10^{-7} , indicating that our previous estimate $\hat{\sigma}^2 = 4.75 \times 10^{-7}$ was a decent one.

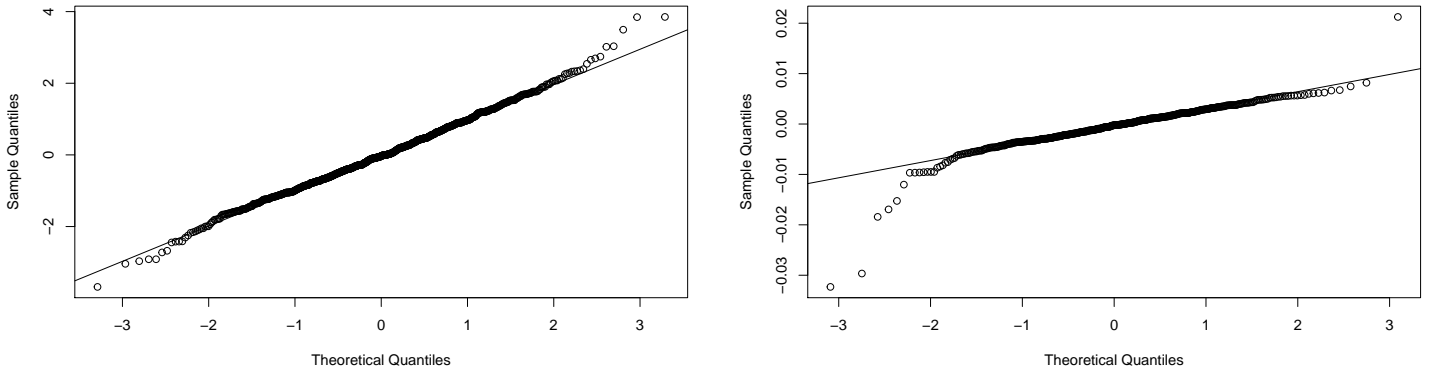
Gauss-Markov conditions

We check whether our final model satisfies the Gauss-Markov conditions. The first condition, that the errors have expectation zero, is satisfied by construction. The other two conditions – that the errors have equal variance and are uncorrelated – cannot be proven to be satisfied, but we can check whether some necessary conditions seem to be satisfied. All residual plots – residuals versus their index, residuals versus the fitted values, and residuals versus each of the independent variables – need to be free of correlation. No curvature, funnel or trend should be visible. All named residual plots have been checked – both for the training set as well as for the test set. (One such plot can be seen in fig. 5b). No visible correlations were found, supporting the hypothesis that the Gauss-Markov conditions are reasonably well satisfied.

Normality

Most steps in the construction and analysis of our model assume the errors to be normally distributed (e.g. the Box-Cox transformation of the response variable, the AIC, and the statistics for the coefficients and the ANOVA in table 2). Based on the normal QQ plots of fig. 6, we pose that the errors are roughly normally distributed, but with tails that are too heavy. (The p values for the Shapiro-Wilk test of normality are 0.01 and < 2E–16 for the training and test set, respectively). This less-than-ideal normality does not seem to be a problem during model construction. It does have the result however that the statistics and p -values in table 2

Figure 6: Normal QQ plots of linear model residuals



(a) Training set standardised residuals

(b) Test set residuals

need to be taken with a grain of salt.

Multicollinearity

In the exploratory analysis, we noted the strong pairwise correlations between `urban_metric`, `extra_urban_metric`, `combined_metric`, and `co2`. This points to the problem of multicollinearity. Indeed, when we perform more formal tests, strong evidence is found for multicollinearity in the data: the variance inflation factors (VIF) of the mentioned variables are all larger than 100, and the mean VIF is 456, significantly larger than 1. The condition number $\sqrt{\lambda_{\max}/\lambda_{\min}} = 129$ is greater than 30 (where λ are the eigenvalues of the correlation matrix of the data). In the preceding linear regression, we have ignored this multicollinearity. In the following exercise however, we will use a biased regression method with smaller variance as a remedy.

2 Classification

blablie

References

- [1] Rousseeuw, P. J. and Leroy, A. M. *Robust Regression and Outlier Detection*. Wiley, 1987.
- [2] Rousseeuw, P. J. and van Driessen, K. *A fast algorithm for the minimum covariance determinant estimator*. Technometrics 41, 212–223, 1999.
- [3] Box, G. E. P. and Cox, D. R. *An analysis of transformations (with discussion)*. Journal of the Royal Statistical Society B, 26, 211–252, 1964.

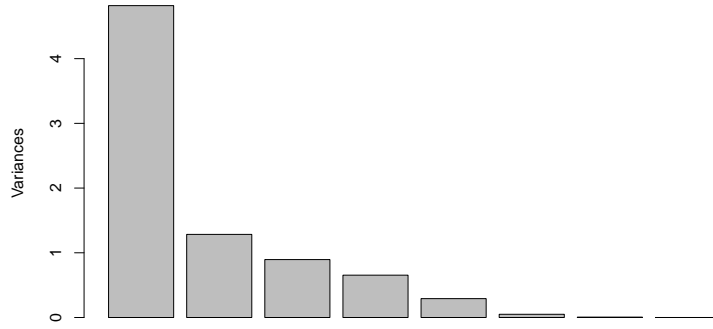


Figure 7

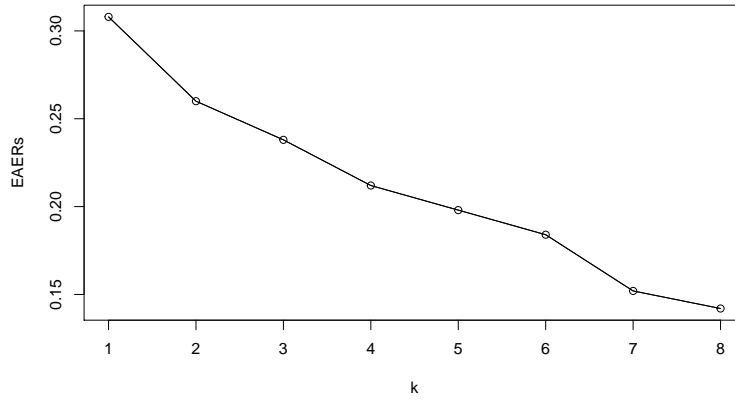


Figure 8

Predictor variable j	$\hat{\beta}^+$	PC1	PC2	PC3	PC4	PC5
engine_capacity	0.89	0.355	0.192	-0.371	-0.220	0.806
urban_metric	-0.26	0.447	-0.021	-0.040	0.042	-0.222
extra_urban_metric	-0.39	0.444	-0.003	-0.065	0.073	-0.201
combined_metric	-0.31	0.451	-0.016	-0.052	0.054	-0.214
noise_level	0.01	0.182	0.337	0.757	-0.527	0.044
co2	-0.84	0.447	0.092	-0.052	0.112	-0.184
co_emissions	-0.15	0.190	-0.557	0.508	0.474	0.412
nox_emissions	-4.73	0.065	0.728	0.140	0.653	0.094
transmission_type_Manual	-0.59					
fuel_type_Hybrid	-4.99					
fuel_type_Petrol	-4.44					
Intercept	1.70					

Table 3

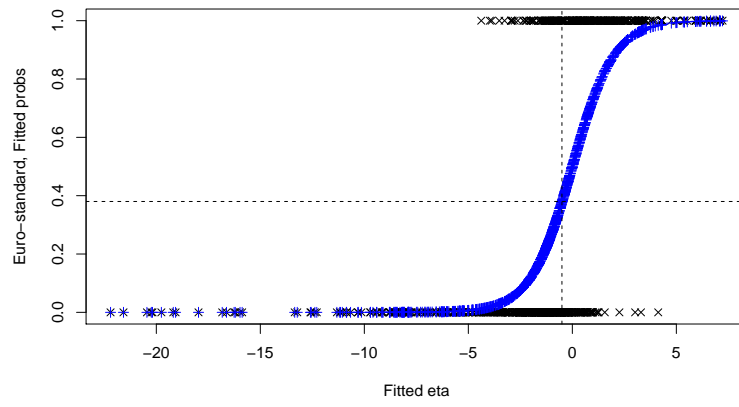


Figure 9

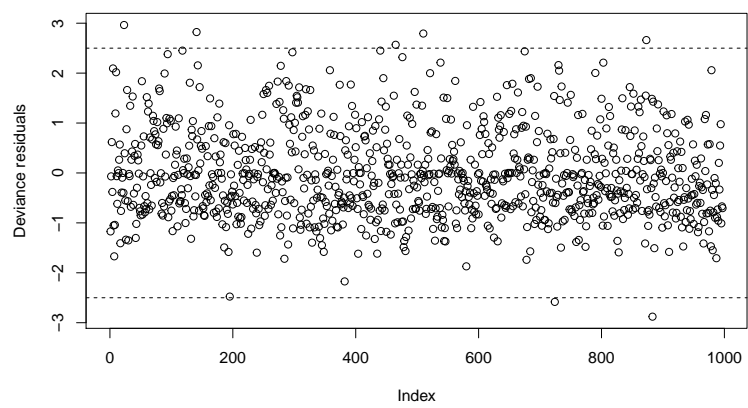


Figure 10

A Code

src/init.R

```
rm(list = ls()) # Clear environment
options(digits = 4) # Set output display precision
cat("\014") # Clear console
# Hit Ctrl+Shift+L to clear plots

X = read.table('data.txt', header=TRUE)
X$euro_standard = factor(X$euro_standard)

set.seed(0380267)
selVec <- c(sample(1:dim(X)[1], 1000))
XTrain <- X[selVec,]
XTest <- X[-selVec,]

# These identifying variables will not be included in any models
id_col_names = c('manufacturer',
                  'model',
                  'description')
id_cols = which(names(X) %in% id_col_names)

factor_col_names = c('euro_standard',
                     'transmission_type',
                     'fuel_type')
factor_cols = which(names(X) %in% factor_col_names)

continuous_cols = which(!(names(X) %in% id_col_names)
                        & !(names(X) %in% factor_col_names))

# Plotting init
library(ggplot2)
univariate_plot_theme = theme(axis.title.y=element_blank(),
                              axis.title.x=element_blank(),
                              axis.text.y=element_blank(),
                              axis.ticks.y=element_blank(),
                              panel.grid.major.y=element_blank(),
                              panel.grid.minor.y=element_blank(),
                              legend.position='none')

plot_stdres_bounds = function() {
  abline(-2.5, 0, lty=2)
  abline(+2.5, 0, lty=2)
}
```

src/remove_RD_outliers.R

```
# Find, save, and remove all outliers

library(robustbase)

data = XTrain[, continuous_cols]
mcd = covMcd(data)
d = sqrt(mahalanobis(data, mcd$center, mcd$cov))
outlier_indexes = which(d > 20)

outliers = XTrain[outlier_indexes,]
XTrain = XTrain[-outlier_indexes,]
```

src/outliers_plot.R

```
source('init.R')
source('remove_RD_outliers.R')

save = function(affix) {
  filename = paste('../multivar_outlier_', affix, '.pdf', sep='')
  ggsave(filename, width=8, height=1.25)
}

df = data.frame(robust_distance=d)

p = ggplot(df, aes(x=seq_along(robust_distance), y=robust_distance, alpha=0.2)) +
  scale_x_continuous(expand=c(0.3,0.3)) +
  geom_point() +
  coord_flip() +
  ggtitle('Robust_distance') +
  univariate_plot_theme
print(p)
save('all')

p +
  coord_flip(ylim=c(0,40)) +
  ggtitle('(zoomed_in)')
save('zoom')
```

src/pairs.R

```
source('init.R')
source('remove_RD_outliers.R')

library(GGally)

# Pairwise plots
ggpairs(XT, columns=c(continuous_cols, factor_cols),
  aes(alpha=0.01),
  labeller='label_parsed')
ggsave('../pairs.pdf', width=15, height=13)
```

src/transformer.R

```
# ML power transform of continuous variables

transform = function(XX, ignored_col='co2', verbose=FALSE, XSource=NULL) {
  # The maximum likelihood transforms are calculated using XSource (default: XX)
  if (is.null(XSource)) {
    XSource = XX
  }
  for (col in continuous_cols) {
    name = names(XX)[col]
    pt = powerTransform(XSource[,col])
    pt$lambda = pt$lambda
    transf_coldata = bcPower(XX[,col], pt$lambda)
    if ((abs(pt$lambda) < 3) && (name != ignored_col)) {
      XX[,col] = transf_coldata
    }
    if (verbose) {
      qqnorm(XX[,col], main=name)
      qqline(XX[,col])
      p_before = shapiro.test(XX[,col])$p
      #
    }
  }
}
```

```

    qqnorm(transf_coldata, main=name)
    qqline(transf_coldata)
    p_after = shapiro.test(transf_coldata)$p
    #
    print(name)
    print(as.numeric(pt$lambda), digits=3)
    print(p_before, digits=3)
    print(p_after, digits=3)
  }
}
return(XX)
}

```

src/lm.R

```

# Model selection by bidirectional stepwise regression using AIC.

source('init.R')
source('remove_RD_outliers.R')
source('transformer.R')

library(MASS)
library(car)

transform_predictors = TRUE
remove_stdres_outliers = TRUE
transform_response = TRUE

# Copy training set
XT = XTrain

# (Extra plot: MD-RD)
cont_cols = XT[,continuous_cols]
mcd = covMcd(cont_cols)
rd = sqrt(mahalanobis(cont_cols, mcd$center, mcd$cov))
md = sqrt(mahalanobis(cont_cols, colMeans(cont_cols), cov(cont_cols)))

# Remember: data got shuffled in init.R.
# First/top number is original row;
# Second/bottom number is current row / indexing number.

# ML power transform of continuous variables
if (transform_predictors) {
  XT = transform(XT, verbose=TRUE)
}

# Define, save and remove lm outliers
# (These were found with 'which(abs(stdres(lm1)) > 5))')
if (remove_stdres_outliers) {
  lm_outliers_idx = c(176, 317, 635)
  lm_outliers = XT[lm_outliers_idx,]
  XT = XT[-lm_outliers_idx,]
}

expand_factors = function(full_X) {
  data = full_X[,c(continuous_cols, factor_cols)]
  # Expand factor columns into a set of 'one hot' columns
  # eg: fuel_type -> (fuel_typeHybrid, fuel_typePetrol)
  # (fuel_type=Diesel is then encoded as (0,0))
  design_matrix = model.matrix(lm(co2~., data))
  X_encoded = cbind(design_matrix[, -1], data[, 'co2', drop=FALSE])
}

```

```

    return(X_encoded)
}

XT_encoded = expand_factors(XT)

vars = colnames(XT_encoded)
vars = vars[-length(vars)] # Remove 'co2'
full_formula = as.formula(paste("~", paste(vars, collapse="+")))

if (transform_response) {
  # The power is determined by running:
  # b = boxcox(model_without_transformed_responses)
  # lambda = b$x[which.max(b$y)]
  response = 'co2^-0.3'
} else {
  response = 'co2'
}

# Start with a full linear model
full_lm = lm(as.formula(paste(response, '~.')), XT_encoded)
lm1 = stepAIC(full_lm, list(lower=~1, upper=full_formula), direction='both')

# Start with an empty model
empty_model = lm(as.formula(paste(response, '~1')), XT_encoded)
lm2 = stepAIC(empty_model, list(lower=~1, upper=full_formula), direction='both')

# (Extra: model with interaction terms)
# full2_lm = lm(as.formula(paste(response, '~.^2')), XT_encoded)
# lm1 = stepAIC(full2_lm, list(lower=~1, upper=~.^2), direction='both')

# Check whether the two seeds converged to the same model
same_vars = setequal(names(lm1$coefficients), names(lm2$coefficients))
diff = lm1$coefficients[names(XT_encoded)] - lm2$coefficients[names(XT_encoded)]
same_coeffs = all((diff < 1e-12) | (is.na(diff)))
stepAIC_convergence = same_vars & same_coeffs

```

src/evaluate_lm.R

```

# Evaluate the found linear model

source('lm.R')

model = lm1

print(summary(model))
print(model$anova)

standardised_residuals = stdres(model)

for (col in c(factor_cols, continuous_cols)) {
  plot(XT[[col]], standardised_residuals, xlab=names(X)[col])
  plot_stdres_bounds()
}

plot(standardised_residuals)
plot_stdres_bounds()

plot(fitted(model), standardised_residuals)
plot_stdres_bounds()

b = boxcox(model)

```

```

lambda = b$x[which.max(b$y)]

qqnorm(standardised_residuals)
qqline(standardised_residuals)
shapiro.test(standardised_residuals)

# Compare with robust linear model
# lmrob = ltsreg(log(co2)^., data)
# ltsPlot(lmrob, which=c('rfit'))

# Diagnostic plot
if (!remove_stdres_outliers) {
  plot(rd, stdres(lm1))
  plot_stdres_bounds()
}

# Find strong stdres outliers
which(abs(stdres(lm1)) > 5)

print(sum(model$residuals^2))
print(lambda, digits=5)
print(stepAIC_convergence)

# Test the model on the test set
# Important: needs to use same transform for unbiased predictions.
XTT = expand_factors(transform(XTest, XSource=XTrain))
y = XTT$co2^-0.3
yhat = predict(lm1, XTT)

plot(y, yhat)
abline(0, 1)

e = (y - yhat)
e_rel = e/y
qqnorm(e_rel)
qqline(e_rel)
plot(e_rel)
plot(yhat, e_rel)

n = 500
p = 11
sigma = sum(e^2)/(n-p)
print(sigma)

msre = sum(e_rel^2)/(n-p)
print(msre, digits=5)

mare = sum(abs(e_rel))/(n-p)
print(mare, digits=5)

# Manual prediction
# x = c(1, as.numeric(XTT[1, -c(5, 11, 14)]))
# w = as.numeric(summary(lm1)$coeff[, 1])
# y[1]
# yhat[1]
# w %*% x
#
# plot(XT_encoded$combined_metric, XT_encoded$co2^-0.3)
# points(XTT$combined_metric, XTT$co2^-0.3, col='blue')

```

src/multicol.R

```
source('init.R')
source('remove_RD_outliers.R')

c = cor(XTrain[continuous_cols])
I = diag(nrow=dim(c)[1])
ridge = 0
diag(solve(c+ridge*I))
ev = eigen(c)$values
sqrt(max(ev)/ev)
```