Topic 11 – Multiple Linear Regression

ENVX1002 Introduction to Statistical Methods

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Module overview

- **Week 9. Describing relationships**
  - Correlation → calculation, interpretation, things to watch out for
  - Regression → Why do we care? model structure, model fitting
- **Week 10. Linear functions**
  - Is the model worth fitting? → Assumptions, hypothesis testing
  - How good is the model? → Measures of model fit
- **Week 11. Linear functions - multiple predictors**
  - Parsimonious models
  - Introduction to Multiple Linear Regression (MLR) modelling
  - Assumptions and interpretation
- **Week 12. Nonlinear functions**
  - Common nonlinear functions
  - Transformations
  - Performing nonlinear regression

Module overview

- **Week 11. Linear functions - multiple predictors**
    - ➟ Parsimonious models
    - ➟ Introduction to Multiple Linear Regression (MLR) modelling
    - ➟ Assumptions and interpretation

Recap

Simple linear regression

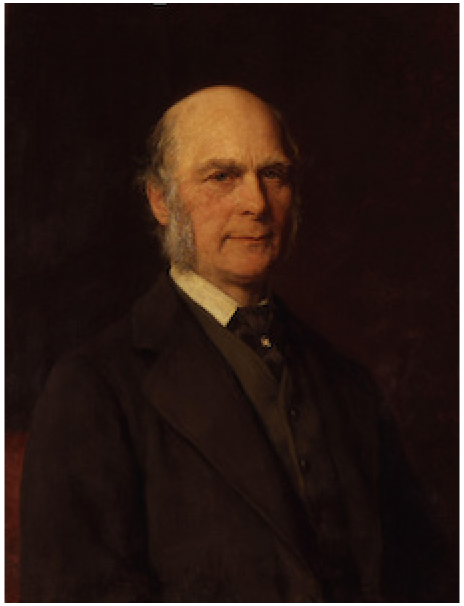
$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

Ideal for predicting a continuous response variable from a single predictor variable: *"How does $\boldsymbol{y}$ change as $\boldsymbol{x}$ changes?"*

What if we have more than one predictor?

What is the model and how do we interpret the results?

Multiple linear regression

Francis Galton and Karl Pearson

History

- First raised by **Francis Galton** in 1886, after studying genetic variations in sweet peas over several generations.
- **Karl Pearson** developed the mathematical formalism for the multiple linear regression model in the early 1900s.

> *"The somewhat complicated mathematics of multiple correlation, with its repeated appeals to the geometrical notions of hyperspace, remained a closed chamber to him."*

– Pearson (1930), on Galton's work with MLR

Air Quality in New York (1973)

Air quality

```
Rows: 153
Columns: 6
$ Ozone   <int> 41, 36, 12, 18, NA, 28, 23, 19, 8, NA, 7, 16, 11, 14, 18, 14, …
$ Solar.R <int> 190, 118, 149, 313, NA, NA, 299, 99, 19, 194, NA, 256, 290, 27…
$ Wind    <dbl> 7.4, 8.0, 12.6, 11.5, 14.3, 14.9, 8.6, 13.8, 20.1, 8.6, 6.9, 9…
$ Temp    <int> 67, 72, 74, 62, 56, 66, 65, 59, 61, 69, 74, 69, 66, 68, 58, 64…
$ Month   <int> 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5,…
$ Day     <int> 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18,…
```

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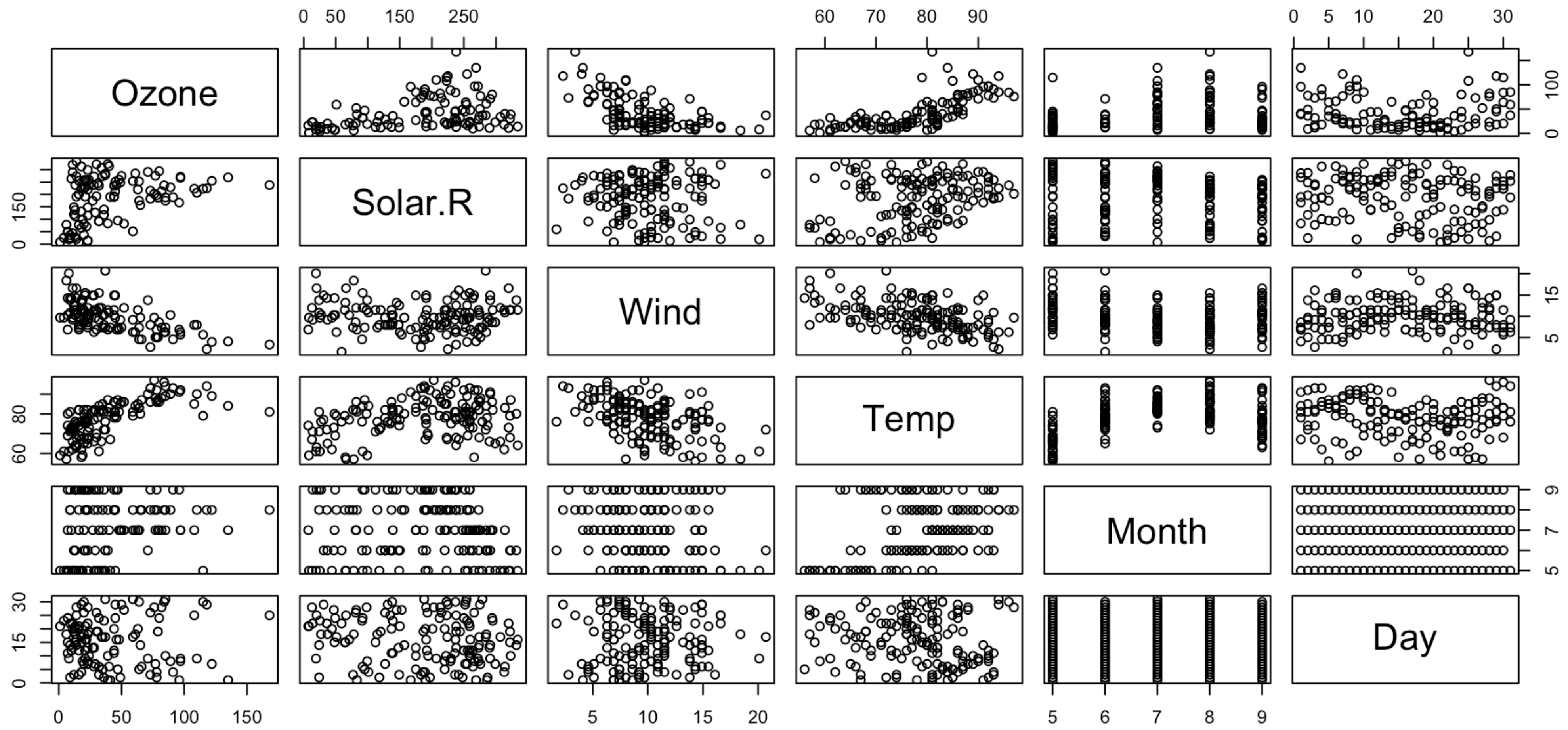
$ Month   <int> 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5,…
$ Day     <int> 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18,…
```

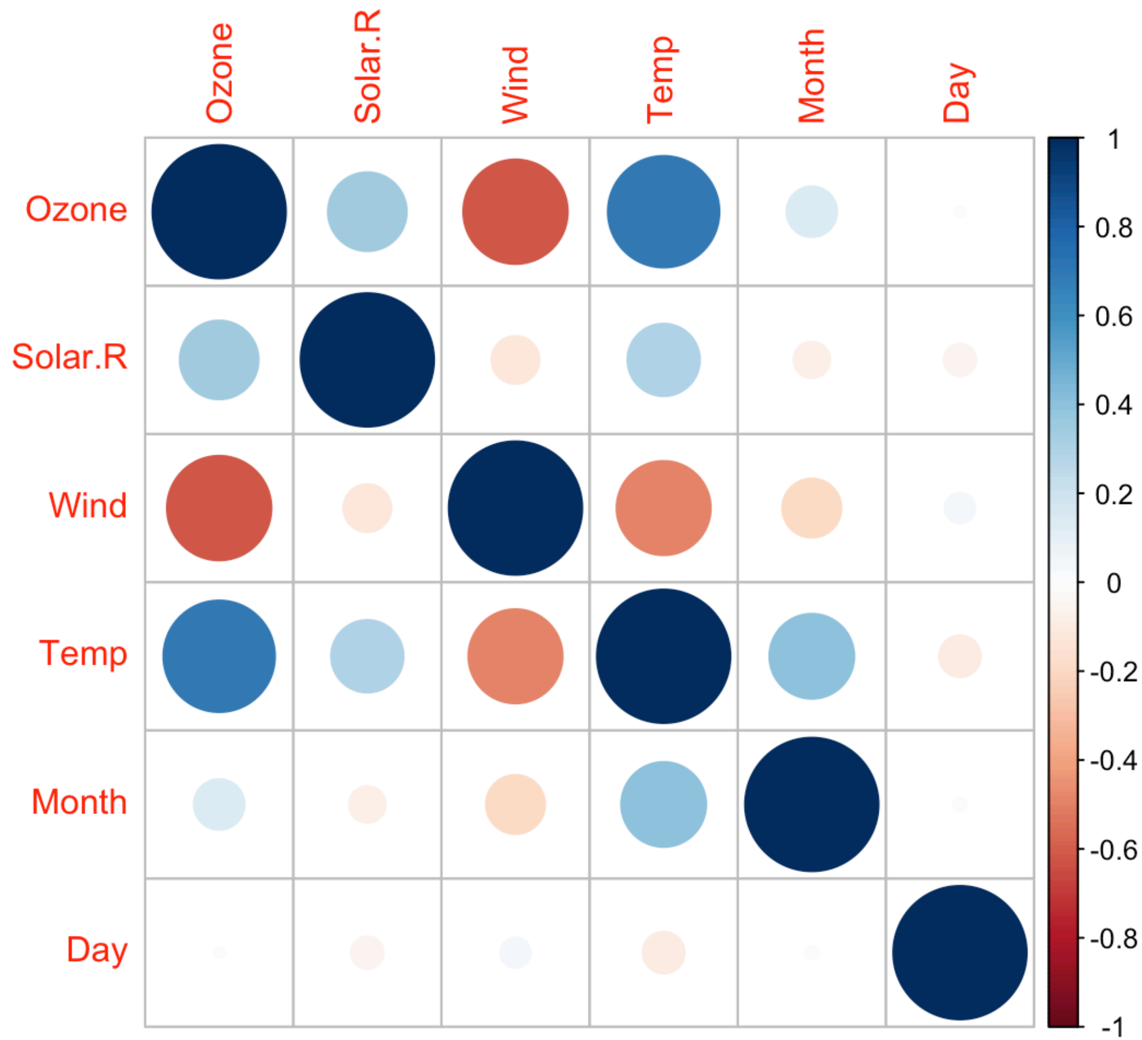
Ozone: harmful air pollutant when present at ground level; main component of smog:

- `Ozone`: ozone concentration (ppb)
- `Solar.R`: solar radiation (lang)
- `Wind`: wind speed (mph)
- `Temp`: ambient temperature (degrees F)
- `Month`: month (1-12)
- `Day`: day of the month (1-31)

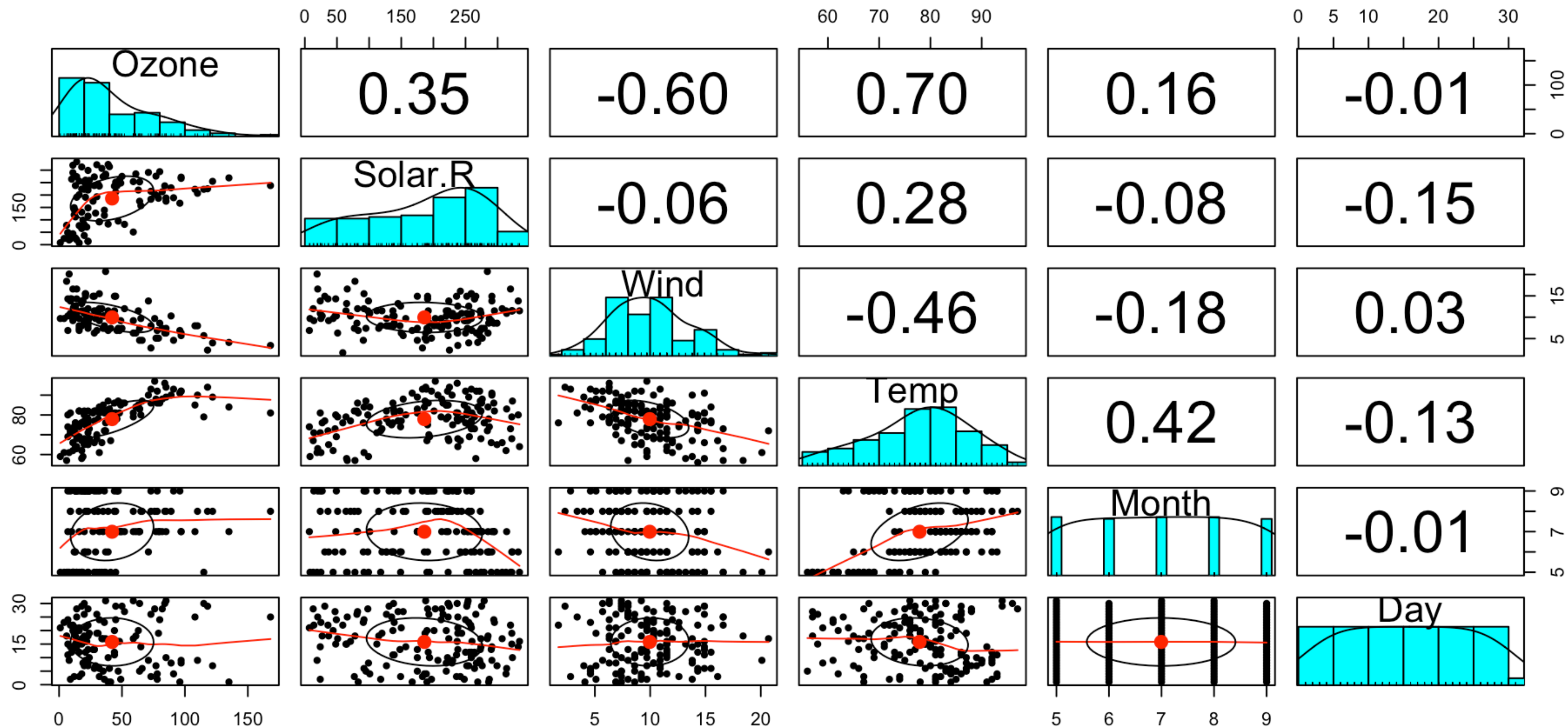
Correlations



`corrplot`



psych


Ozone
Solar.R
Wind
Temp
Month
Day
0.35
-0.60
0.70
0.16
-0.01
-0.06
0.28
-0.08
-0.15
-0.46
-0.18
0.03
0.42
-0.13
-0.01

The simplest model

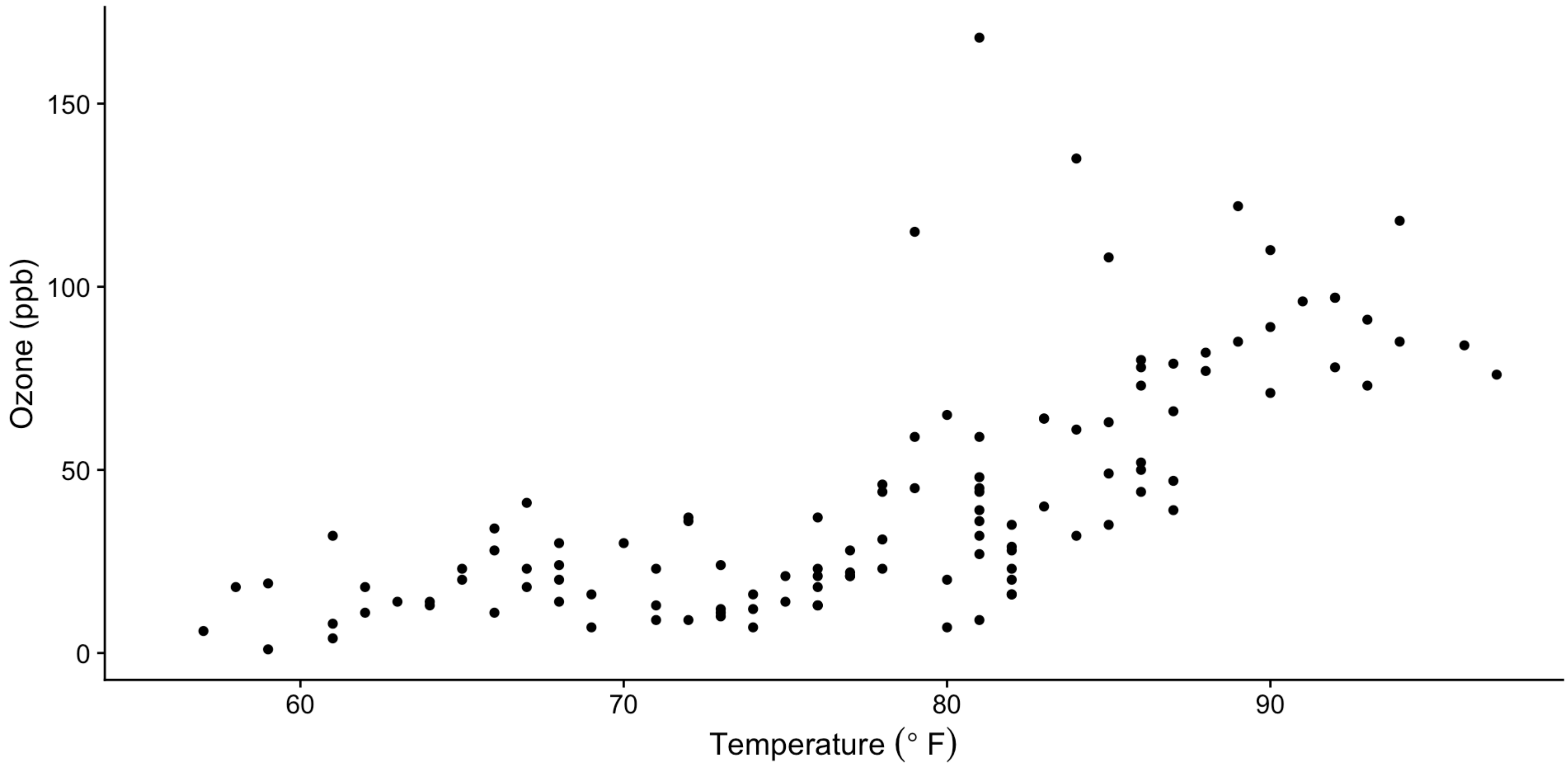
Pick the predictor that has the highest correlation coefficient with the response variable.

```
                Ozone     Solar.R        Wind       Temp        Month
Ozone     1.000000000  0.34834169 -0.61249658  0.6985414  0.142885168
Solar.R   0.348341693  1.00000000 -0.12718345  0.2940876 -0.074066683
Wind     -0.612496576 -0.12718345  1.00000000 -0.4971897 -0.194495804
Temp      0.698541410  0.29408764 -0.49718972  1.0000000  0.403971709
Month     0.142885168 -0.07406668 -0.19449580  0.4039717  1.000000000
Day      -0.005189769 -0.05775380  0.04987102 -0.0965458 -0.009001079
                  Day
Ozone    -0.005189769
Solar.R  -0.057753801
Wind      0.049871017
Temp     -0.096545800
Month    -0.009001079
Day       1.000000000
```

What can we understand about the relationship between `Ozone` and `Temp` (r = 0.7)?

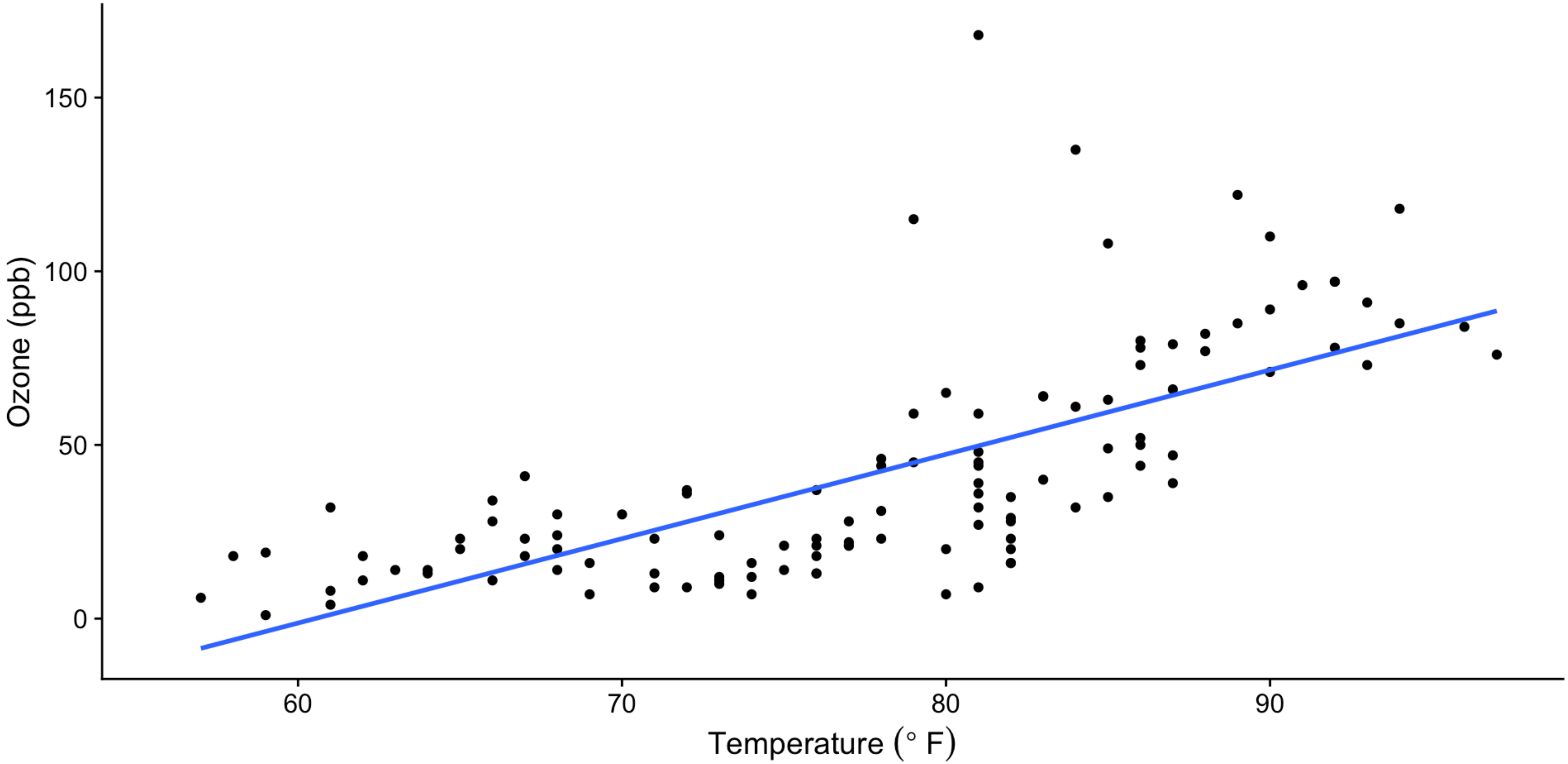
Relationship

What can we understand about the relationship between `Ozone` and `Temp` (r = 0.7)?



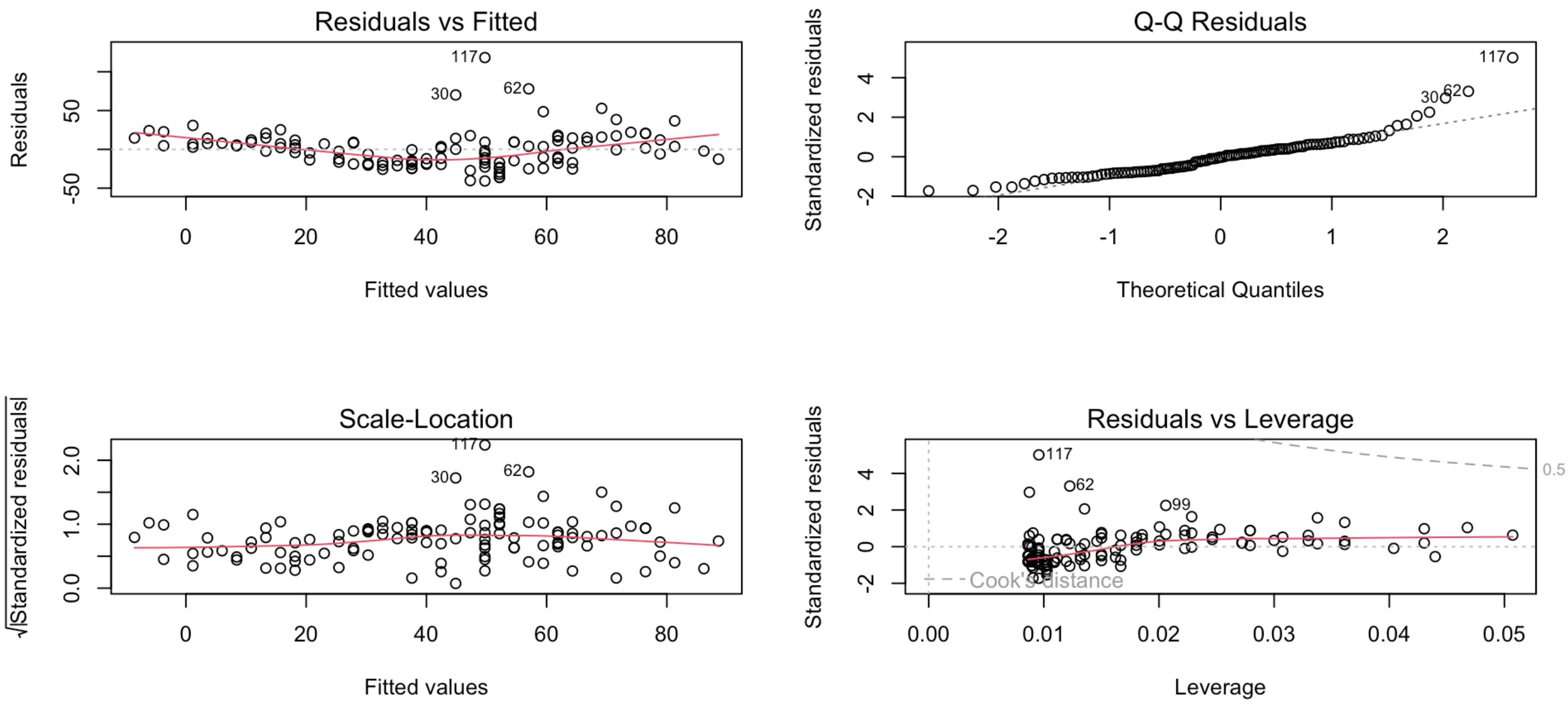
Relationship

What can we understand about the relationship between `Ozone` and `Temp` (r = 0.7)?

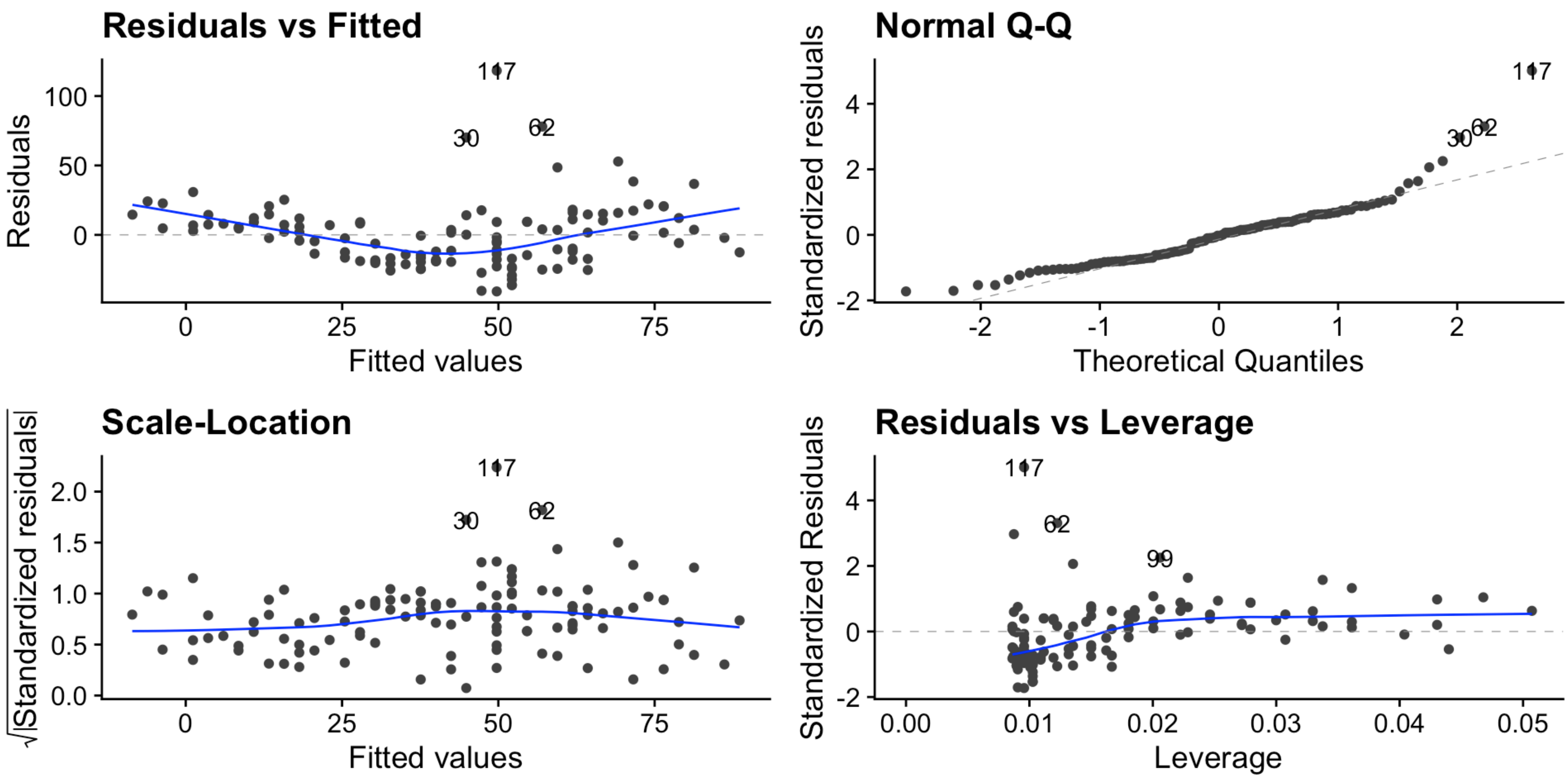


Fitting the model

Assumptions



`ggfortify`


Residuals vs Fitted
Residuals
Fitted values
117
30
62
100
50
0
0
25
50
75
Normal Q-Q
Standardized residuals
Theoretical Quantiles
117
30
62
4
2
0
-2
-2
-1
0
1
2
Scale-Location
√|Standardized residuals|
Fitted values
117
30
62
2.0
1.5
1.0
0.5
0.0
0
25
50
75
Residuals vs Leverage
Standardized Residuals
Leverage
117
62
99
4
2
0
-2
0.00
0.01
0.02
0.03
0.04
0.05

Interpretation

```
Call:
lm(formula = Ozone ~ Temp, data = airquality)

Residuals:
    Min      1Q  Median      3Q     Max 
-40.729 -17.409  -0.587  11.306 118.271 

Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept) -146.9955    18.2872  -8.038 9.37e-13 ***
Temp           2.4287     0.2331  10.418  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 23.71 on 114 degrees of freedom
  (37 observations deleted due to missingness)
Multiple R-squared:  0.4877,	Adjusted R-squared:  0.4832 
F-statistic: 108.5 on 1 and 114 DF,  p-value: < 2.2e-16
```

- `Temp` is a statistically significant predictor of `Ozone` ($p < .001$).
- The (simple linear) model explains 49% of variance ($r^2 = 0.49$).

Can we improve the model in other ways?

Multiple linear regression

Important concepts

- The “best” model is the one that best describes the relationship between the response and the predictors.
    - ➟ **NOT** the model that includes all possible predictors (data dredging).

Principle of parsimony

A good model:

- Has only *useful* predictors.
- Has no *redundant* predictors (principle of orthogonality).
- Is *interpretable* (principle of transparency) or *predicts well* (principle of accuracy).

The MLR model

An extension of simple linear regression to include **more than one** predictor variable: *"How does y change as x_1, x_2, ..., x_k change?"*

$$Y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_k x_k + \epsilon_i$$

Therefore, estimating the model involves *estimating the values of* β_0, β_1, β_2, ..., β_k.

- β_0 is the intercept
- β_1 to β_k are the partial regression coefficients
- ϵ is the error term

Explore

```
Rows: 153
Columns: 6
$ Ozone   <int> 41, 36, 12, 18, NA, 28, 23, 19, 8, NA, 7, 16, 11, 14, 18, 14, …
$ Solar.R <int> 190, 118, 149, 313, NA, NA, 299, 99, 19, 194, NA, 256, 290, 27…
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$ Month   <int> 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5,…
$ Day     <int> 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18,…
```

The "best" model

The variables `Month` and `Day` are not useful predictors, so we will exclude them from the model.

Visualisation: not easy

Are the plots useful?

3D plot

WebGL is not supported by your browser - visit https://get.webgl.org for more info

Visualisation: not easy

Are the plots useful?

4D plot

WebGL is not supported by your browser - visit https://get.webgl.org for more info

Partial regression coefficients

Given the multiple linear model:

$$Y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_k x_k + \epsilon_i$$

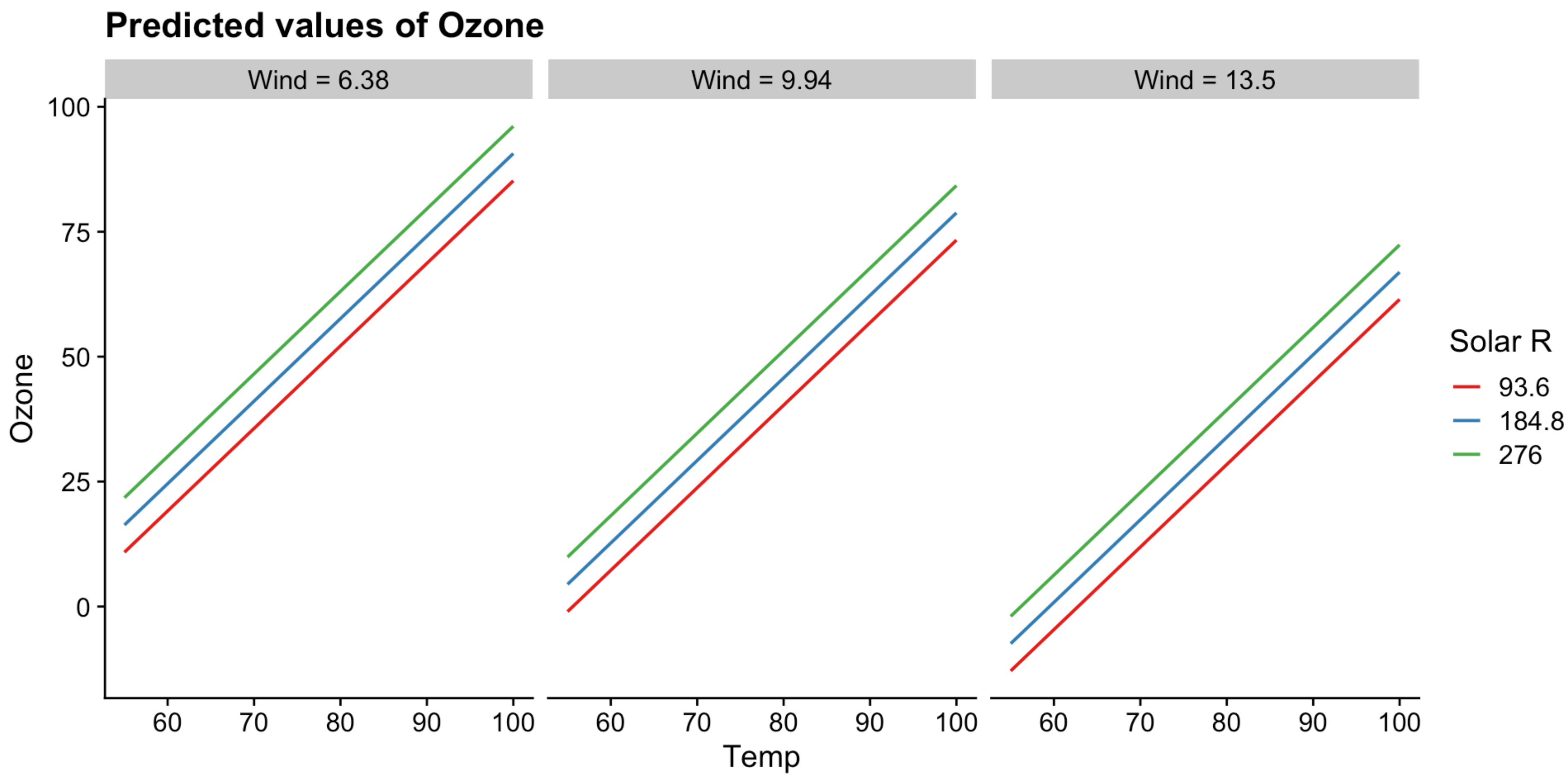
The partial regression coefficient for a predictor x_i is the amount by which the response variable Y changes when x_k is increased by one unit, **while all other predictors are held constant**.

$$\beta_k = \frac{\Delta Y}{\Delta x_k}$$

$$\text{Ozone} = \alpha + \beta_1(\text{Solar.R}) + \beta_2(\text{Wind}) + \beta_3(\text{Temp}) + \epsilon$$

> *With `Wind` and `Solar.R` held constant, how does `Temp` affect `Ozone`?*

Partial regression coefficients: visualisation



> *With `Wind` and `Solar.R` held constant, how does `Temp` affect `Ozone`?*

Interpreting the partial regression coefficients

```
Call:
lm(formula = Ozone ~ Solar.R + Wind + Temp, data = airquality)

Coefficients:
(Intercept)      Solar.R         Wind         Temp  
  -64.34208      0.05982     -3.33359      1.65209  
```

Holding **all** other variables constant:

- For every 1 unit increase in `Solar.R`, `Ozone` increases by a mean value of 0.06 ppb.
- For every 1 degree increase in `Temp`, `Ozone` increases by a mean value of 1.65 ppb.
- For every 1 unit increase in `Wind`, `Ozone` decreases by a mean value of 3.33 ppb.

Caution

If the model is not "valid", then the partial regression coefficients are not meaningful.

Assumptions

LINE

As with Simple Linear Regression, we need to check the assumptions of the model (LINE):

- **L**inearity: the relationships between the response and the predictors are all linear.
- **I**ndependence: the observations are independent of each other.
- **N**ormality: the residuals are normally distributed.
- **E**qual variance: the variance of the residuals is constant.

Recall

In SLR, the model is made up of the **deterministic** component (the line) and the ***random*** component (the error term).

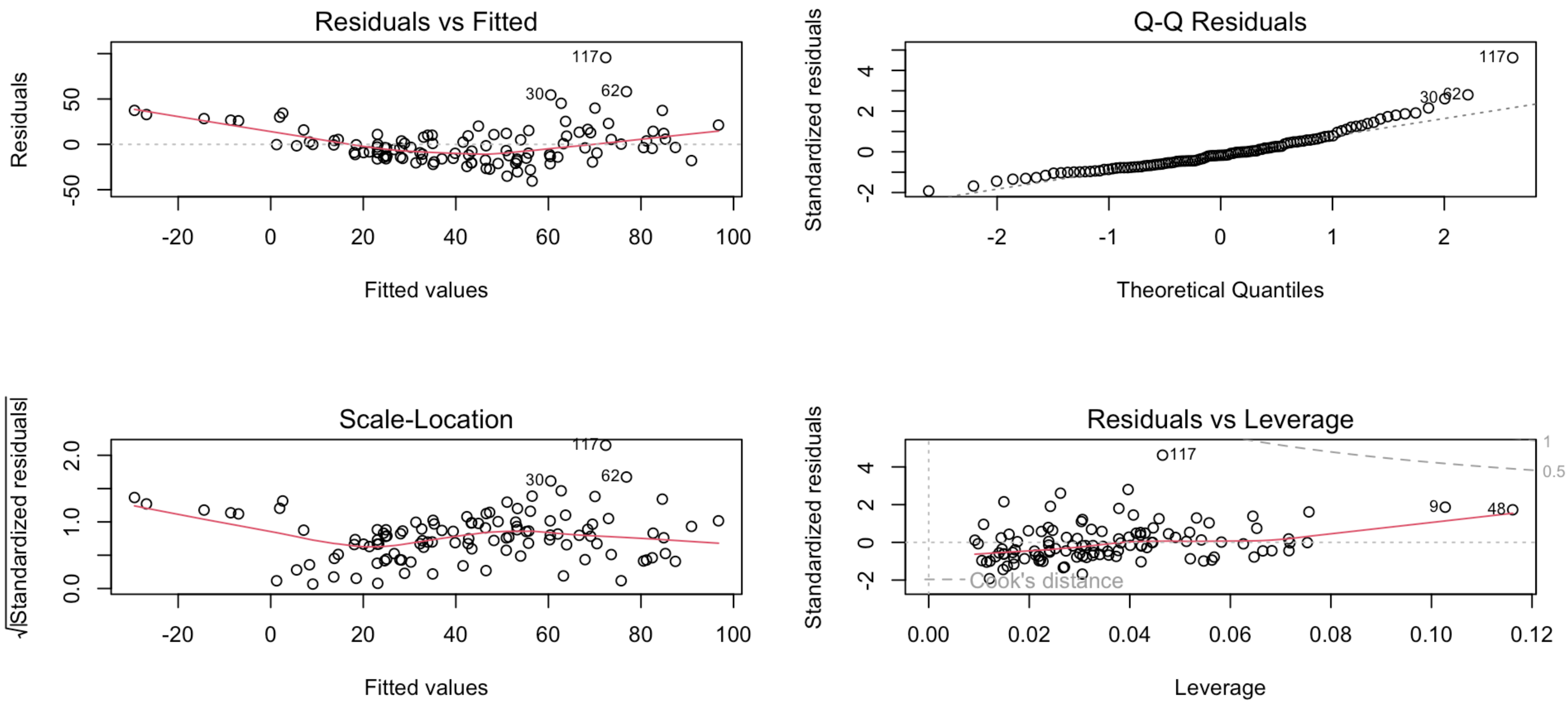
$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

This is the same for MLR:

$$Y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_k x_k + \epsilon_i$$

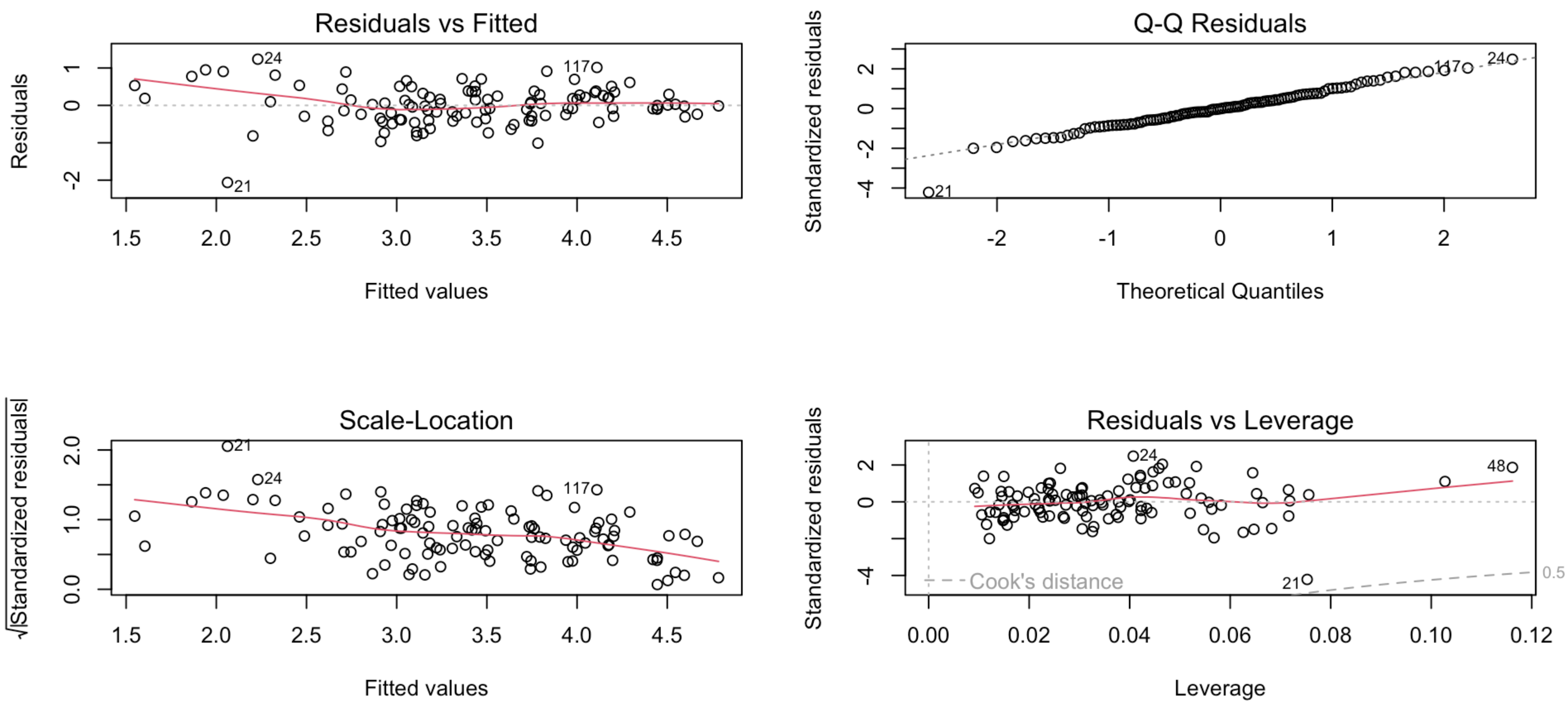
Since *only* the error term is random, the assumptions are *still* about the error term, $\hat{\epsilon}$, which is simple to assess!

Assumptions of MLR



Transformation using `log()`

Some evidence of nonlinearity in the diagnostic plots. Transform and re-check assumptions.



Results

```
Call:
lm(formula = log(Ozone) ~ Solar.R + Wind + Temp, data
= airquality)

Residuals:
     Min       1Q   Median       3Q      Max
-2.06193 -0.29970 -0.00231  0.30756  1.23578

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.2621323  0.5535669  -0.474 0.636798
Solar.R      0.0025152  0.0005567   4.518 1.62e-05 ***
Wind        -0.0615625  0.0157130  -3.918 0.000158 ***
Temp         0.0491711  0.0060875   8.077 1.07e-12 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.'
0.1 ' ' 1

Residual standard error: 0.5086 on 107 degrees of
freedom
  (42 observations deleted due to missingness)
```

- All three predictors are statistically significant ($p < .001$).
- The model explains 66% of variance ($r^2 = 0.66$).

Results compared to SLR

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0.4832
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```

- All three predictors are statistically significant ($p < .001$).
- The model explains 66% of variance ($r^2 = 0.66$ vs. 0.48 in SLR).

Interpretation

Coefficients

All three predictors are statistically significant ($p < .001$).

- For every 1 unit increase in `Solar.R`, `log(Ozone)` increases by a mean value of 0.0025 ppb, holding all other variables constant.
- For every 1 unit increase in `Wind`, `log(Ozone)` decreases by a mean value of 0.062 ppb, holding all other variables constant.
- For every 1 degree increase in `Temp`, `log(Ozone)` increases by a mean value of 0.049 ppb, holding all other variables constant.

Residual standard error

On average, the model predicts `log(Ozone)` within 0.51 ppb of the true value. *Not bad?*

```
[1] 1.665291
```

- On average, the model predicts `Ozone` within 1.6652912 ppb of the true value.
- Number of observations = degrees of freedom (107) + number of parameters in the model (4) = 111.

R-squared

If there are >1 predictors, use the **Adjusted R-Squared** as it penalises the model for having more predictors that are not useful.

F-stat

- The F-statistic tests the null hypothesis that all the regression coefficients are equal to zero, i.e. $H_0 : \beta_1 = \beta_2 = ... = \beta_k = 0$.
- As a ratio, it tells us how much better the model is than the null model (i.e. a model with no predictors).
- If the p-value is less than our specified critical value (e.g. 0.05), we reject the null hypothesis and conclude that the current model is better than the null model.

Reporting

Solar radiation, wind speed and temperature are **significant predictors** of Ozone concentration (**$p < 0.001$**) with the model accounting for **66% of the variation** in weight.

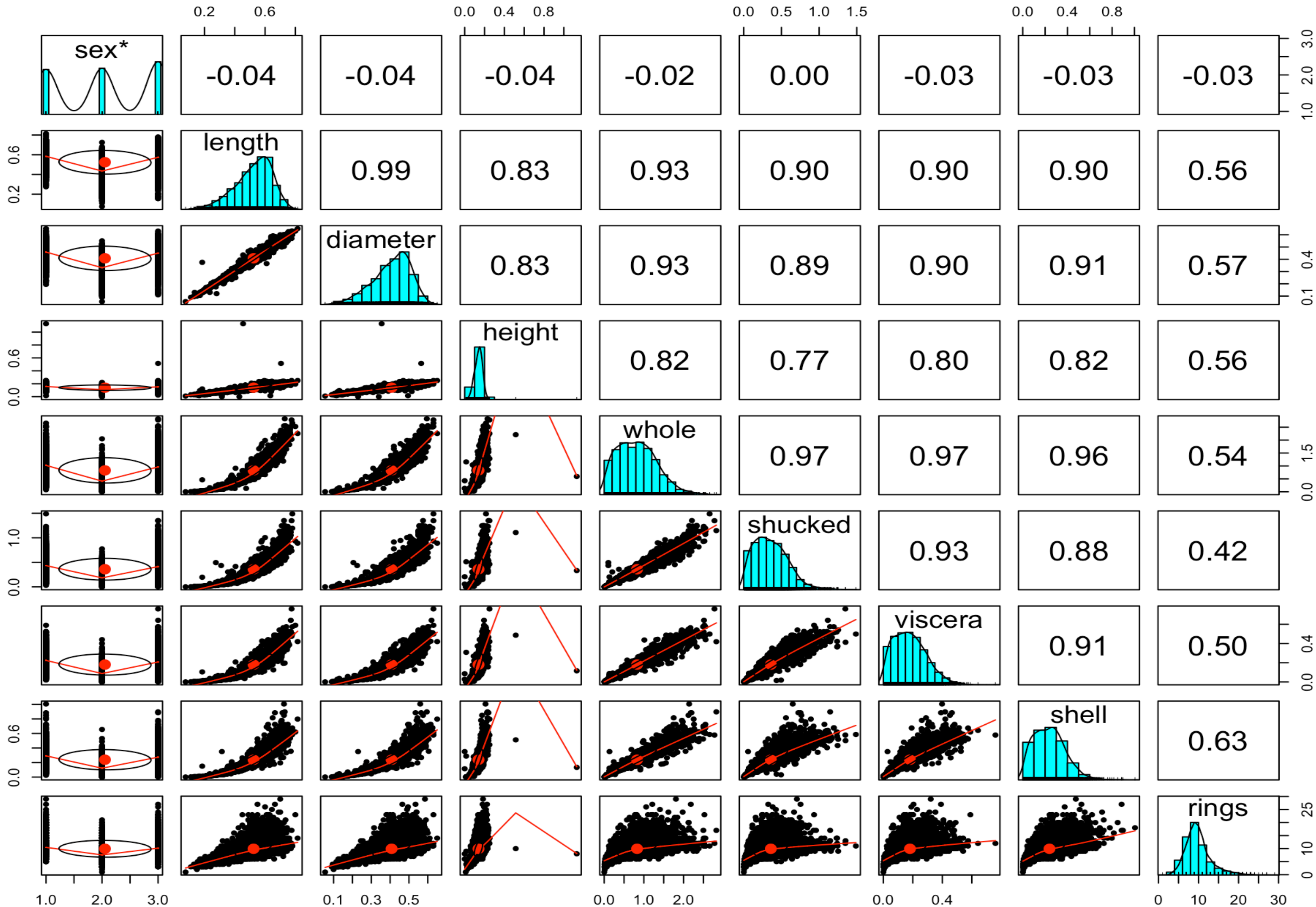
Abalone: full example

Data

Data from the UCI Machine Learning Repository.

```
Rows: 4,177
Columns: 9
$ sex      <chr> "M", "M", "F", "M", "I", "I", "F", "F", "M", "F", "F", "M", "…
$ length   <dbl> 0.455, 0.350, 0.530, 0.440, 0.330, 0.425, 0.530, 0.545, 0.475…
$ diameter <dbl> 0.365, 0.265, 0.420, 0.365, 0.255, 0.300, 0.415, 0.425, 0.370…
$ height   <dbl> 0.095, 0.090, 0.135, 0.125, 0.080, 0.095, 0.150, 0.125, 0.125…
$ whole    <dbl> 0.5140, 0.2255, 0.6770, 0.5160, 0.2050, 0.3515, 0.7775, 0.768…
$ shucked  <dbl> 0.2245, 0.0995, 0.2565, 0.2155, 0.0895, 0.1410, 0.2370, 0.294…
$ viscera  <dbl> 0.1010, 0.0485, 0.1415, 0.1140, 0.0395, 0.0775, 0.1415, 0.149…
$ shell    <dbl> 0.150, 0.070, 0.210, 0.155, 0.055, 0.120, 0.330, 0.260, 0.165…
$ rings    <dbl> 15, 7, 9, 10, 7, 8, 20, 16, 9, 19, 14, 10, 11, 10, 10, 12, 7,…
```

Preview


sex*
length
diameter
height
whole
shucked
viscera
shell
rings
-0.04
-0.04
-0.04
-0.02
0.00
-0.03
-0.03
-0.03
0.99
0.83
0.93
0.90
0.90
0.90
0.56
0.83
0.93
0.89
0.90
0.91
0.57
0.82
0.77
0.80
0.82
0.56
0.97
0.97
0.96
0.54
0.93
0.88
0.42
0.91
0.50
0.63

Live coding session

Data import → EDA → Model fitting → Diagnostics → Transform/Select → Interpret

Let's fit a model to predict the whole weight of abalone from other measured variables – I will now switch to RStudio.

And we're back!

A quick recap on sub-sampling the dataset:

What we did

- Fitted a model to predict the whole weight of abalone from other measured variables.
- Performed a transformation of the response variable to improve model fit.
- Checked the assumptions of the model.
- Interpreted the model coefficients.
- Interpreted the model fit.

Model complexity: overfitting

> Why can’t we just use ALL the predictors?

The problem with using too many predictors

- The more predictors you add, the better the model fits the data.
- However, the model may not be able to **generalise** to new data: **overfitting**.

Model	r.squared	adj.r.squared
sqrt(whole) ~ shucked	0.892	0.891
sqrt(whole) ~ shucked + shell	0.952	0.951
sqrt(whole) ~ height + shucked + shell	0.963	0.962
sqrt(whole) ~ length + height + shucked + shell	0.982	0.981
sqrt(whole) ~ length + height + shucked + shell + rings	0.982	0.981
sqrt(whole) ~ length + height + shucked + viscera + shell + rings	0.982	0.981
sqrt(whole) ~ .	0.982	0.981

The r^2 value

The R-squared value is the proportion of variance explained by the model.

$$r^2 = \frac{SS_{reg}}{SS_{tot}} = 1 - \frac{SS_{res}}{SS_{tot}}$$

The adjusted R-squared value is the proportion of variance explained by the model, adjusted for the number of predictors.

$$r^2_{adj} = 1 - \frac{SS_{res}}{SS_{tot}} \frac{n-1}{n-p-1}$$

where n is the number of observations and p is the number of predictors.

Full model vs reduced model

```
Call:
lm(formula = sqrt(whole) ~ ., data = abalone)

Residuals:
      Min        1Q    Median        3Q       Max
-0.218383 -0.016249  0.000771  0.020543  0.105263

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.027849   0.036151  -0.770 0.443065
length       0.959033   0.296239   3.237 0.001678 **
diameter    -0.024686   0.377611  -0.065 0.948019
height       0.969022   0.265067   3.656 0.000427 ***
shucked      0.317776   0.055354   5.741 1.20e-07 ***
viscera      0.107616   0.104461   1.030 0.305614
shell        0.433048   0.095434   4.538 1.72e-05 ***
rings        0.001984   0.001800   1.103 0.273097
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.'
0.1 ' ' 1
```

```
Call:
lm(formula = sqrt(whole) ~ shell + height + diameter,
data = abalone)

Residuals:
      Min        1Q    Median        3Q       Max
-0.149252 -0.030922 -0.004514  0.023821  0.160182

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.13051    0.03854  -3.386 0.001028 **
shell        0.56407    0.09945   5.672 1.49e-07 ***
height       1.33325    0.34613   3.852 0.000212 ***
diameter     1.62282    0.14862  10.919  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.'
0.1 ' ' 1

Residual standard error: 0.05209 on 96 degrees of
freedom
Multiple R-squared:  0.9674,    Adjusted R-squared:
```

- Is the 0.015 improvement in the adjusted R-squared – *an extra 1.5% of the variance explained* – worth the extra predictors?
- Recall: **principle of parsimony** - the simplest model that explains the data is the best.
- But how do we know which predictors to keep?

Model selection

- Covered in **second year (ENVX2001)**.
- Using techniques of **stepwise regression**, we can select the best model from a set of “candidate” models.
- If we have non-significant predictors, we can consider the effect of removing them from the model (**partial F-test**).
- Aim is to achieve the best balance between **model fit** and **model complexity**.

Summary

- MLR is an extension of SLR to include more than one predictor.
    - ➟ Instead of a line, we are fitting a “hyperplane” i.e. multiple dimensions.
    - ➟ However, the principles are the same: we are still trying to minimise the sum of squared residuals.
    - ➟ Assumptions of MLR are the same as SLR.
    - ➟ Instead of the multiple R-squared value, we use the adjusted R-squared value to assess model fit.
- Follow the rules of parsimony: the simplest model that explains the data is the best, given similar model fit.
    - ➟ Consider the effect of removing non-significant predictors from the model.

Thanks!