Experimental Design and Data Analysis, Lecture 7

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Lecture overview

1. contingency tables
   1. chisquare test
   2. Fisher test
2. simple linear regression
3. multiple linear regression

contingency tables

Setting

An experiment with:

- a count of individuals or units in different categories of two factors.

Interest is in a possible dependence of the two factors.

EXAMPLE Study possible dependency between blood group and disease by counting the number of patients having a certain blood group (A, B or O) and a certain disease (stomach cancer, kidney cancer, no disease).

EXAMPLE Study possible dependency between web layout and size of a company by counting the number of companies of a certain size (small, moderate, large) using a certain web design (relative, fixed, elastic, liquid) .

EXAMPLE Consider the following (fictive) counts amongst 60 VU-students:

	exact	arts	total
men	23	17	40
women	7	13	20
total	30	30	60

Question: `study` and `gender` independent?

Design

Design A:

- Take a random sample of experimental units from the relevant population.
- Count for each cross-category the number of units falling into that cross-category.

Design B:

- Take for each category of the first (row) factor a random sample of experimental units.
- Count for each category of the second factor the number of units falling into that cross-category.

Design C:

- Take for each category of the second (column) factor a random sample of experimental units.
- Count for each category of the first factor the number of units falling into that cross-category.

Analysis (1)

The general form of a contingency table is

n_{11}	n_{12}	$\cdots$	n_{1J}	$n_{1\cdot}$
n_{21}	n_{22}	$\cdots$	n_{2J}	$n_{2\cdot}$
$\vdots$		$\ddots$	$\vdots$	$\vdots$
n_{I1}	n_{I2}	$\cdots$	n_{IJ}	$n_{I\cdot}$
$n_{\cdot 1}$	$n_{\cdot 2}$	$\cdots$	$n_{\cdot J}$	$n_{\cdot\cdot}$

We want to test whether the two factors are independent (under design A):

$$H_0 : \textit{row variable and column variable are independent}.$$

Or, we want to test whether the distributions are homogeneous over rows (design B) or columns (design C):

$$H_0 : \textit{the distributions over row (column) factors are equal}.$$

Analysis (2)

Let $n = n_{\cdot\cdot}$ be the total number of observations. Under the null hypothesis of no dependence (or homogeneity), the counts are expected to be in proportion:

$$E_{ij} = np_{ij} = np_{i\cdot}p_{\cdot j} = n\frac{n_{i\cdot}}{n}\frac{n_{\cdot j}}{n} = \frac{n_{i\cdot}n_{\cdot j}}{n}.$$

Expected counts in the example data set:

	exact	arts	total
men	?	?	40
women	?	?	20
total	30	30	60

$\Longrightarrow$

	exact	arts	total
men	$60 \cdot \frac{40}{60} \cdot \frac{30}{60}$	$60 \cdot \frac{40}{60} \cdot \frac{30}{60}$	40
women	$60 \cdot \frac{20}{60} \cdot \frac{30}{60}$	$60 \cdot \frac{20}{60} \cdot \frac{30}{60}$	20
total	30	30	60

The test statistic is based on the (appropriately normalized) differences between the expected counts E_{ij} under H_0 and the observed counts n_{ij}:

$$T = \sum_{i=1}^{I}\sum_{j=1}^{J}\frac{(n_{ij} - E_{ij})^2}{E_{ij}} \sim \chi^2_{(I-1)(J-1)}, \quad \text{(approx. a chisquare distribution).}$$

The p-value is always right-sided: $p_{right} = P(T > t)$. Why?
Condition: For the test to be reliable, at least 80% of the E_{ij}'s should be at least 5.

In R: `chisq.test(data)`

Analysis in R: data input

First, we need to create a table of the counts in the form of a matrix.

The following data consists of grade counts in an elementary statistics class, classified by the students' majors.

```
> grades=matrix(c(8,15,13,14,19,15,15,4,7,3,1,4),byrow=TRUE,ncol=3,nrow=4,
+ dimnames=list(c("A","B","C","D-F"),c("Psychology","Biology","Other")))
> grades
    Psychology Biology Other
A            8      15    13
B           14      19    15
C           15       4     7
D-F          3       1     4
```

For the calculations on the next slide, *R* needs the data in a `matrix` object, rather than in a `dataframe` format.

Analysis in R: testing (1)

```
> rowsums=apply(grades,1,sum); colsums=apply(grades,2,sum)
> total=sum(grades); expected=(rowsums%*%t(colsums))/total
> round(expected,0)
     Psychology Biology Other
[1,]         12      12    12
[2,]         16      16    16
[3,]          9       9     9
[4,]          3       3     3
> sum((grades-expected)^2/expected) # realization of statistics T
[1] 12.18346
> 1-pchisq(12.18346,6)   # p-value for the observed T=12.18346
[1] 0.05799897
```

Less than 80% of the expected counts are above 5. Hence, the approximation by a chi-square test is not reliable.

Analysis in R: testing (2)

Of course, no need to perform all these computations, just use build-in R command: `chisq.test`, which executes the χ^2-test.

```
> z=chisq.test(grades); z
                      Pearson's Chi-squared test
data:  grades
X-squared = 12.1835, df = 6, p-value = 0.058

Warning message:
In chisq.test(grades) : Chi-squared approximation may be incorrect
```

R gives a warning because the chi-squared approximation in this case is not reliable. In such a case one can use the setting `simulate.p.value=TRUE`, which computes a *p*-value in a bootstrap fashion. This may yield a very different *p*-value.

```
> chisq.test(grades,simulate.p.value=TRUE)
Pearson's Chi-squared test with simulated p-value (based on 2000 replicates)

data:  grades
X-squared = 12.1835, df = NA, p-value = 0.05647
```

Analysis in R: testing (3)

You can extract information from `z=chisq.test(grades)`: `z$expected` gives the table of expected values, `z$observed` recovers the observed values.
We can look at the (square root) contributions of each cell to the chi-squared statistics, by using `residuals(z)` (or `z$residuals`), to determine which observed values deviate most from the expected under H_0.

```
> residuals(z)  # = (z$observed-z$expected)/sqrt(z$expected)
    Psychology    Biology      Other
A   -1.2032599  0.8992005  0.3193881
B   -0.5630451  0.7872412 -0.2170232
C    2.0838439 -1.5668929 -0.5434979
D-F  0.1749697 -1.0110751  0.8338764
```

- From this table we see that psychology students have relatively more C's,
- biology students have relatively less C's,
- psychology students have relatively less A's,

than expected under H_0 (the differences are not significant though ($p \approx 0.06$)).

Alternatively, we can look at the standardized residuals using the command `z$stdres` (=(z\$observed-z\$expected)/sqrt(V), where V is the residual cell variance, see Agresti, 2007, section 2.4.5) and compare this to $z_{\alpha/2}$=`qnorm(0.975)`≈1.96.

Fisher's exact test for 2x2-tables

For 2x2-tables it is possible to compute an exact *p*-value, that does not use approximation or simulation. This is called Fisher's exact test.
Data on right- and left-handed people, classified according to gender.

```
> handed=matrix(c(2780,3281,311,300),nrow=2,ncol=2,byrow=TRUE,
+ dimnames=list(c("right-handed","other"),c("men","women")))
> handed
             men  women
right-handed 2780  3281
left-handed   311   300
```

We can compare this to picking without replacement 3091 balls from a vase which contains 6672 balls, 6061 white and 611 red. The number of white balls amongst the picked 3091 balls is $n_{11} = 2780$.

n_{11}	...	6061
...	...	611
3091	3581	6672

$\Longrightarrow$

n_{11}	$6061 - n_{11}$
$3091 - n_{11}$	$3581 - (6061 - n_{11})$

The number n_{11} determines all other numbers. Fisher's exact test is based on this number. Under the null hypothesis of no dependence between the two factors it has a hypergeometric distribution.

Analysis in R: testing

```
> fisher.test(handed)
        Fisher's Exact Test for Count Data

data:  handed
p-value = 0.01918
alternative hypothesis: true odds ratio is not equal to 1
95 percent confidence interval:
 0.6894895 0.9688105
sample estimates:
odds ratio
 0.8173619
> chisq.test(handed)
        Pearson's Chi-squared test with Yates' continuity correction

data:  handed
X-squared = 5.4542, df = 1, p-value = 0.01952
```

The chisquare approximation is also fine for these data. The odds ratio is computed as $\frac{2780/311}{3281/300} = 0.8173619$ and can be interpreted as “for one right-handed women there is ≈ 0.82 right-handed men", there are relatively more left handed men than women.

Recap: simple linear regression

Setting, design and data

An experiment with a numerical outcome Y (dependent variable) and a numerical explanatory variable X (independent variable). The purpose is to explain Y by a numerical function of X.

> EXAMPLE Chemical production process with outcome total yield and explanatory variable temperature.

Design

- Fix a set of values X of the explanatory variable.
- Perform the corresponding experiments and measure the outcome Y.

It is natural to let the explanatory variable X vary over a grid of values.

Data: $(X_1, Y_1), \dots, (X_n, Y_n)$. The simple linear regression model assumes that

$$Y_i = \beta_0 + \beta_1 X_i + e_i, \quad i = 1, \dots, n, \quad e_1, \dots, e_n \sim N(0, \sigma^2).$$

We test the null hypothesis $H_0 : \beta_1 = 0$ that the explanatory variable does *not* influence the outcome. We also want to estimate the parameters β_0, β_1.

The function $x \mapsto \beta_0 + \beta_1 x$ is a line with intercept (value at $x = 0$) β_0 and slope (change per unit) β_1. This is a simple function and may give a bad fit!

Analysis in R: data input, graphics, estimation and testing

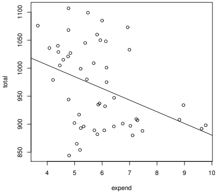
The column `total` of the dataset `sat.txt` is the average score on the *scolastic aptitude test* of pupils in US states in 1994/95; the column `expend` is the amount of dollars spent per pupil in the state.

```
> sat=read.table("sat.txt",header=TRUE); sat1=sat[,c(1,7)]; sat1[1:2,]
          expend total
Alabama    4.405  1029
Alaska     8.963   934
```

```
> sat1lm=lm(total~expend,data=sat1); summary(sat1lm)
[ some output deleted ]
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 1089.294     44.390  24.539  < 2e-16 ***
expend       -20.892      7.328  -2.851  0.00641 **
```

The parameters β_0 and β_1 are estimated to be 1089.294 and -20.892. The p-value for testing $H_0 : \beta_1 = 0$ is 0.00641. The slope is significantly negative!

```
> plot(total~expend,data=sat1)
> abline(sat1lm)
```



Compare to Pearson's correlation test

Compare simple linear regression to Pearson's correlation test (treated earlier) which tests whether the response and explanatory variable (in our case columns `total` and `expand`) are uncorreleted.

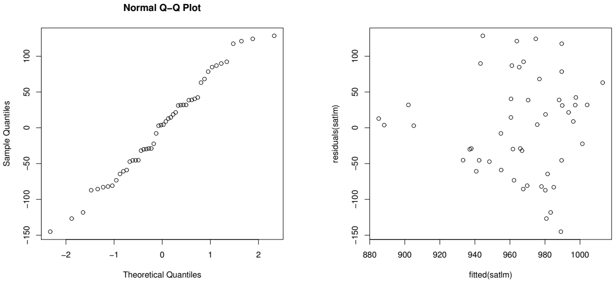
```
> cor.test(sat1$total,sat1$expend)

Pearson's product-moment correlation

data:  sat1$total and sat1$expend
t = -2.8509, df = 48, p-value = 0.006408
```

Notice that the *p*-value of the correlation test between response and covariate is equal to the *p*-value for testing the zero slope in simple linear regression. In fact, this is the same test: testing $H_0 : \rho = 0$ is the same as testing $H_0 : \beta_1 = 0$.

Analysis in R: diagnostics

We can use the data to check whether the assumptions on the errors $e_i = Y_i - \beta_0 - \beta_1 X_i$ are not totally untrue.
The residuals are $\hat{e}_i = Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i$; the fitted values $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$.
The residuals should look normal, and their spread should not vary with the fitted values.

```
> qqnorm(residuals(sat1lm))
> plot(fitted(sat1lm),residuals(sat1lm))
```



The two plots look ok.

multiple linear regression

Setting and design

Setting: an experiment with

- a numerical outcome Y (“dependent variable”);
- p numerical explanatory variables $X_1, \dots, X_p$ (“independent variables", "predictors").

The purpose is to explain Y by a numerical function of $X_1, \dots, X_p$.

EXAMPLE Chemical production process with outcome total yield and explanatory variables temperature and pressure.

EXAMPLE Educational study with outcome score on final exam and explanatory variables teacher salaries and number of pupils per teacher.

Design:

- Fix a set of combinations $(X_1, \dots, X_p)$ of explanatory variables.
- Perform the corresponding experiments and measure the outcome Y.

It is natural to let each explanatory variable vary over a grid and use all their possible combinations, but this may necessitate many experiments. (Regression analysis is also often used in non-experimental situations, with the explanatory variables not under control.)

Analysis

Data $Y_i, X_{i1}, X_{i2}, \dots, X_{ip}$, $i = 1, \dots, n$. The linear regression model:

$$Y_i = \beta_0 + \beta_1 X_{i1} + \ldots + \beta_p X_{ip} + e_i, \quad i = 1, \dots, n, \quad (\text{matrix notation } Y = X\beta + e)$$

where errors $e_1, e_2, \dots, e_n$ are viewed as a random sample from $N(0, \sigma^2)$, $\beta_0, \dots, \beta_p$ are unknown population parameters.

We test the null hypotheses $H_0 : \beta_j = 0$ that the jth explanatory variable does *not* influence the outcome for $j = 1, \dots, p$.
We also want to estimate the parameters β_j's.

Possible explanatory variables (prediction variables):

- all x_j different $Y = \beta_0 + \beta_1 x_1 + \ldots + \beta_7 x_7 + e$,
- powers of x_j's $y = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \beta_3 x_1^3 + e$,
- interactions between x_j's $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + e$.

Essential: all models are linear in β_j's, but not necessarily in x_j's.
All ANOVA models can also be written in the matrix notation $Y = X\beta + e$, for some design matrix X (composed of "dummy variables"), where β is the vector of all the ANOVA coefficients involved. Thus the rest of this part also relates to all ANOVA models.

Estimating parameters, SSE

To find the best parameters we minimize the sum of squared errors:

$$\min_{\beta_0,\ldots\beta_p} \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_{i1} - \ldots - \beta_p X_{ip})^2 = \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_{i1} - \ldots - \hat{\beta}_p X_{ip})^2 = RSS,$$

$\hat{\beta}_0, \ldots, \hat{\beta}_p$ are the least squares estimates, RSS is the Residual Sum of Squares.

Notation: $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \ldots + \hat{\beta}_p x_{ik}$ is called prediction/predicted response.

The Residual Sum of Squares RSS (also called Sum of Squared Errors, SSE) and the estimated variance of the errors e_n:

$$RSS = SSE = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n} \hat{e}_i^2, \qquad \hat{\sigma}^2 = s^2 = \frac{RSS}{n-p-1} = \frac{SSE}{n-p-1}.$$

$\hat{\sigma}^2$ is the estimated variance of the e_i's, $\hat{e}_i = Y_i - \hat{Y}_i$ is the i-th residual (the estimated error e_i of the i-th observation).

In R: `model=lm(y∼x1+...+xp,data=...)`

Coefficient of determination R^2

- The coefficient of determination (also called the proportion of explained variance) R^2 compares the fits for the models

$$\omega: \ Y = \beta_0 + e \qquad \text{and} \qquad \Omega: \ Y = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p + e.$$

- For model ω, $\hat{\beta}_0 = \bar{Y}$, the fit is $SS_y = \sum_{i=1}^n (Y_i - \bar{Y})^2$, called total SS.
- For model Ω, the fit is $SSE = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$, the residual SS.
- explained variation$=\overset{\textit{total variation}}{\sum_{i=1}^n (Y_i - \bar{Y})^2} - \overset{\textit{unexplained variation}}{\sum_{i=1}^n (Y_i - \hat{Y}_i)^2}$.
- The coefficient of determination R^2 is defined as

$$R^2 = \frac{SS_y - RSS}{SS_y} = \frac{\sum_{i=1}^n (Y_i - \bar{Y})^2 - \sum_{i=1}^n (Y_i - \hat{Y}_i)^2}{\sum_{i=1}^n (Y_i - \bar{Y})^2} = \frac{\text{explained variation}}{\text{total variation}}.$$

  $0 \leq R^2 \leq 1$ because always $SS_y \geq SSE \geq 0$.
- R^2 yields a global check on the multiple linear regression model. The higher R^2, the more variation the model explains.
- If $p = 1$, then $R^2 = r^2$ (the squared correlation between X_1 and Y).

$R^2 \approx 1$ means that the linear regression model can explain the measured response values Y very well using a linear function of the explanatory variables $(X_1, \ldots, X_p)$. $R^2 \approx 0$ means that the linear model does not explain much.

Global model fit

- Data: $X_{i1}, X_{i2}, \ldots, X_{ip}, Y_i,, \ i = 1, \ldots, n.$
- Assumption: the ind. errors follow a $N(0, \sigma^2)$-distribution.
- When is the linear regression model adequate as a whole? In linear regression we compare the models

$$\omega : Y = \beta_0 + e \qquad \text{and} \qquad \Omega : Y = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p + e.$$

- Test if $X_1, \ldots, X_p$ together have significant explanatory power in the model: $H_0 : \beta_1 = \ldots = \beta_p = 0$ versus H_1 : at least one $\beta_i \neq 0$.
- The test statistic: $T = \frac{R^2/p}{(1-R^2)/(n-(p+1))} = \frac{(SS_y - RSS)/p}{RSS/(n-(p+1))} \sim F_{p,n-(p+1)}$ under H_0. Notice that the case $p = 1$ corresponds to Pearson's correlation test.
- The larger R^2 (hence T is large), the more evidence against H_0, hence we reject H_0 if T is large.
- The right-sided test: for $T \sim F_{p,n-(p+1)}$, reject H_0 if $p = P(T > t) < \alpha$.
- In R: this p-value is in the last line of `summary(model)`.

Relevance of individual coefficients

- Not all available explanatory variables may have explanatory power.
- From all explanatory variables, we need to find relevant ones by testing for individual coefficients.
- Test $H_0 : \beta_i = 0$ vs. $H_1 : \beta_i \neq 0$ for individual β_i's (usually two-sided).
- The setting and assumptions are the same as before.
- Test statistic: under H_0,

$$T_i = \frac{\hat{\beta}_i}{s_{\hat{\beta}_i}} \sim t_{n-(p+1)}, \quad \text{where } s^2_{\hat{\beta}_i} = \hat{\sigma}^2 \nu_{ii}, \, [\nu_{ij}] = (X^T X)^{-1}, \, Y = X\beta + e.$$

- In R: the estimates $\hat{\beta}_i$, standard errors $s_{\hat{\beta}_i}$, the statistics values T_i and the p-values are (in the column `Pr(>|t|)`) all given in the output of `summary(model)`.
- In case $p = 1$, testing for $\beta_1 = 0$ is the same as Pearson's correlation test. Thus, if $p = 1$, Pearson's correlation test = Global model fit test = test for $H_0 : \beta_1 = 0$ vs. $H_1 : \beta_i \neq 0$.

Example: bodyfat data

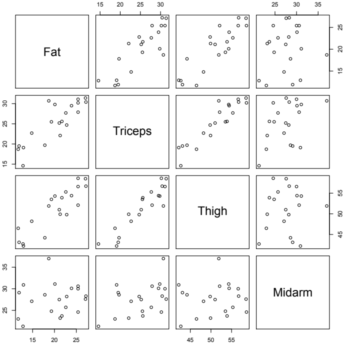
Data of 20 individuals between 25 and 30 years old on amount of body fat, triceps skinfold thickness, thigh circumference and midarm circumference. Body fat is hard to measure, while the other 3 variables are easy to measure.

Question: can we predict `Fat` from the other 3 variables?

```
> bodyfat=read.table("bodyfat.txt",header=T)
> bodyfat
    Fat  Triceps Thigh Midarm
1  11.9    19.5  43.1   29.1
2  22.8    24.7  49.8   28.2
3  18.7    30.7  51.9   37.0
...
19 14.8    22.7  48.2   27.1
20 21.1    25.2  51.0   27.5
```

Scatter plots of all pairs:

```
> pairs(bodyfat)
```



Example: bodyfat data

```
> bodyfatlm=lm(Fat~Triceps+Thigh+Midarm,data=bodyfat); summary(bodyfatlm)
 [some output is deleted]
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  117.085     99.782   1.173    0.258
Triceps        4.334      3.016   1.437    0.170
Thigh         -2.857      2.582  -1.106    0.285
Midarm        -2.186      1.595  -1.370    0.190

Residual standard error: 2.48 on 16 degrees of freedom
Multiple R-squared: 0.8014, Adjusted R-squared: 0.7641
F-statistic: 21.52 on 3 and 16 DF,  p-value: 7.343e-06
```

Many things can be read from this output. The estimates $\hat{\beta}_i$ are in the column `Estimate`, $\hat{\sigma} = 2.48$ (so $\hat{\sigma}^2 = 6.15$), $s^2_{\hat{\beta}_i}$'s are in the column `Std. Error`, T_i's in the column `t value`, the p-values for individual tests $\beta_i = 0$ are in column `Pr(>|t|)`. The CI's for the β_i's are $\hat{\beta}_i \pm t_{\alpha/2,n-(p+1)} s_{\hat{\beta}_i}$, obtained in R by `confint(bodyfatlm)`. Next, $R^2 = 0.8014$, $R^2_{adj} = 0.7641$. For testing the global model fit, statistics $T = 21.52$, the `p-value=7.343e-06`. From this output: none of the β_i's is individually significant, but all together they are significant and explain 80%!

Adjusted R^2

- We want a good fit (high R^2) and a small number of explan. variables.
- Since more explanatory variables always explain more, R^2 always increases with more variables. R^2 can be found in the output of `summary(model)`.
- For p of explanatory variables in the model, R^2 adjusted is

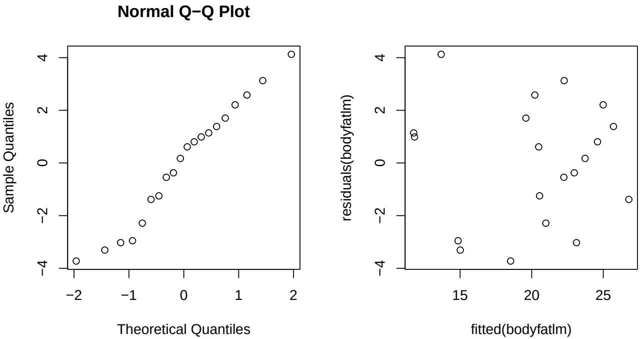
  $$R^2_{adj} = 1 - \frac{n-1}{n-(p+1)}(1 - R^2).$$

  The more variables, the more conservative R^2_{adj} becomes (as compared to R^2), it can be used to choose between models with different amounts of variables. R^2_{adj} can also be found in the output of `summary(model)`.
- The interpretation of R^2_{adj} is not fraction of explained variance anymore.

Analysis in R: diagnostics

The residuals $\hat{e}_i = Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_{i1} - \cdots - \hat{\beta}_p X_{ip}$ (in R: `residuals(model)`); the fitted values $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_{i1} + \cdots + \hat{\beta}_p X_{ip}$ (in R: `fitted(model)`).

```
> qqnorm(residuals(bodyfatlm))
> plot(fitted(bodyfatlm),residuals(bodyfatlm))
```



Both plots look ok.

If the assumptions fail?

One can consider:

- transforming the outcomes (e.g., use $\log Y$, Y^3).
- transforming the explanatory variables (e.g. use $\log X$, X^2).
- adding powers $X_i^2, X_i^3, \ldots$ of the regression variables.
- adding “interactions” like $X_i X_j$.
- performing nonparametric or additive regression.
- something else (there is no fix that always works).

To finish

Today we discussed:

- contingency tables
    - chi-square test
    - Fisher test
- simple linear regression
- multiple linear regression

Next time: more on linear regression.