Case Studies

"Data Analytics"

Topic

Summer Term 2013

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2.1.3 Pearson's chi-squared test

Pearson's chi-squared goodness of fit test is used to test whether data from a sample are distributed according to a given theoretical distribution. The main idea of this test is to divide the observations $X_1, \ldots, X_N$ into several pairwise disjoint classes $C_1, \ldots, C_K$ and compare the empirical frequencies within these classes to the theoretical frequencies, which are expected if the data complies to the hypothetical distribution. If the histograms of the sample data and the expected densities are plotted together (see figure 1), the area of density that is not overlapped by both histograms can be understood as a kind of indicator for the likelihood that the sample is drawn from a population which is distributed according to the hypothetical distribution: The more area is not overlapping, the less likely it is that the sample is drawn from a population with the assumed distribution. However, the test statistic of the chi-squared test is calculated differently, namely by the sum of the squared differences between observed frequencies O_k and expected frequencies E_k divided by the expected frequencies for each class k of the overall K classes. Thus, the test statistic is calculated by

$$\chi^2 = \sum_{k=1}^{K} \frac{(O_k - E_k)^2}{E_k}$$

Larger differences of observed and expected values indicate a lower compliance to the assumed distribution. However, the addends are not weighted (neither by the size of a class nor by the frequencies within a class nor by any other means). Therefore, the class bounds should be chosen equidistant or in such a way that the classes contain preferably the same number of observations or according to similar reasonable rationales. The test statistic is approximately χ^2-distributed with $K - 1$ degrees of freedom – the larger the sample size, the better the approximation. A sample size that is too small can be a reason for the approximation being insufficient. Moreover, for each parameter of the hypothetical distribution which is estimated from the data sample, one degree of freedom is lost; the number of estimated parameters is denoted by p. The test statistic is determined under the null hypothesis that the sample is distributed according to the assumed distribution and the chi-squared test is defined as

$$\delta(Y) = \begin{cases} 1 & \text{if } \chi^2 > F^{-1}(1-\alpha) \\ 0 & \text{otherwise} \end{cases} \qquad \text{with } F = \chi^2_{K-1-p}$$

for a given significance level α where Y is a multinomial distributed random variable denoting the counts of observations in each class with $Y_k = |\{i : X_i \in C_k\}|$.

As a common requirement for a sufficient approximation, the minimum number of observations in each class should not fall below five. Hence, marginal or even inner classes have to be unified in some cases in order to achieve a sufficient class size. The following R-function is used here for this purpose.

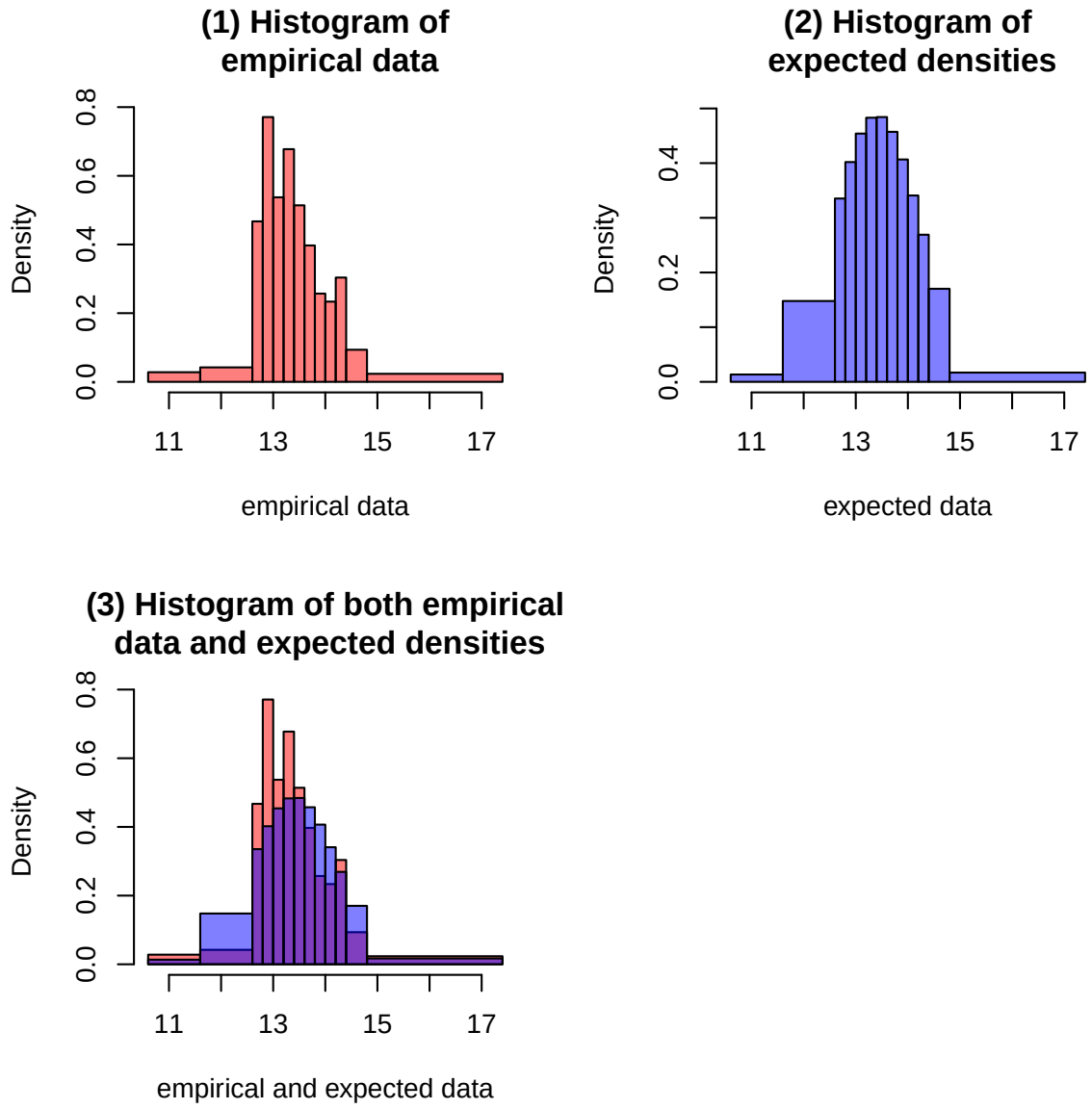


Figure 1: Exemplary histrograms of a data sample, expected densities for a normal distribution with parameters estimated from the sample and a combined histogram of these both histograms.

```
> # Calculates bounds of bins (classes) of a data sample.
> # The initial bounds are given by initial_breaks,
> # k denotes the minimum class size.
> makebins = function(data, initial_breaks, k) {
+   h = hist(data, breaks=initial_breaks, plot=FALSE)
+
+   br = h$breaks
+   changed = TRUE
+
+   while(changed) {
+     h = hist(data, breaks=br, plot=FALSE)
+     br = h$breaks
```

```
+     changed=FALSE
+
+     for(i in 1:length(h$counts)) {
+       if(h$counts[i] < k) {
+         if(i > 1 && i < length(h$counts)) {
+           if(h$counts[i-1] < h$counts[i+1]) {
+             br = br[-i]
+             changed = TRUE
+             break
+           }
+           else {
+             br = br[-(i+1)]
+             changed = TRUE
+             break
+           }
+         }
+         # index on first class
+         else if(i == 1) {
+           br = br[-2]
+           changed = TRUE
+           break
+         }
+         # index on last class
+         else {
+           br = br[-(length(h$counts))]
+           changed = TRUE
+           break
+         }
+       }
+     }
+   }
+   return(br)
+ }
```

Further functions are needed for calculating the expected frequencies, the test statistic and the result of the test (since the mean and the standard deviation are estimated from the sample, two degrees of freedom are additionally lost):

```
> # Calculates the expected probabilities of a normal distribution
> # with the given parameters mean and sd
> # for the given bin (class) bounds
> probabilities.exp = function(bins, mean, sd) {
+   result = rep(0, length(bins)-1)
+
+   result[1] = pnorm(q=bins[2], mean=mean, sd=sd)
+
+   for(i in 2:(length(bins)-1)) {
+     result[i] <- pnorm(q=bins[i+1], mean=mean, sd=sd)
```

```
+       - pnorm(q=bins[i], mean=mean, sd=sd)
+   }
+
+   result[length(bins)-1] = pnorm(q=bins[length(bins)-1],
+     mean=mean, sd=sd, lower.tail=FALSE)
+
+   return(result)
+ }
> # Returns the chi squared test statistics
> # for the given actual and expected values.
> teststat.chi = function(actual, expected) {
+   sum((actual - expected)^2 / expected)
+ }
> # Performs a chi squared goodness of fit test on the given data
> # for the assumption of a normal distribution.
> # Returns true if the null hypothesis (sample drawn from a
> # normal distributed population) is rejected, false otherwise.
> # The parameters are estimated from the sample.
> # The initial bounds for the classes are given by initial_breaks,
> # min denotes the minimum class size.
> # The significance level is determined by sig.
> chisq.test.norm = function(data, initial_breaks, min, sig) {
+   bins = makebins(data, initial_breaks, min)
+   hist = hist(data, breaks=bins, plot=FALSE)
+   expected_probabilities = probabilities.exp(bins, mean(data), sd(data))
+   expected_frequencies = expected_probabilities * length(data)
+   teststat = teststat.chi(hist$counts, expected_frequencies)
+
+   # length(bin) - 1 classes, 2 estimated parameters (mean, sd)
+   df=length(bins)-4
+   critical_value = ifelse(df < 1, NA, qchisq(p=1-sig, df=df))
+
+   print(teststat > critical_value)
+
+   return(list(hist = hist,
+               expected_probabilities = expected_probabilities,
+               expected_frequencies = expected_frequencies,
+               teststat = teststat,
+               critical_value = critical_value,
+               p_value =
+                 ifelse(df < 1, NA, 1 - pchisq(q=teststat, df=df)),
+               rejected = teststat > critical_value))
+ }
```

A drawback of Pearson's chi-squared test is its inconsistency caused by information reduction, i. e. information about the data sample is lost in the process of categorising the observations in classes. As a consequence, different class bounds can lead to different test

results. Furthermore, this test is rather suited for large sample sizes.

2.1.4 Kolmogorov-Smirnov test

The Kolmogorov-Smirnov (KS later on) test as all other tests is used for testing whether a given univariate sample $X_1, \dots X_2$ with unknown distribution $\mathbb{P}$ is distributed according to a completely determined distribution $\mathbb{P}_0$. It implies a decision making between the following two hypotheses:

$$\begin{aligned} H_0 &: \mathbb{P} = \mathbb{P}_0, \\ H_1 &: \mathbb{P} \neq \mathbb{P}_0. \end{aligned}$$

The decision is made according to the value of KS test statistics and a given significance level α.

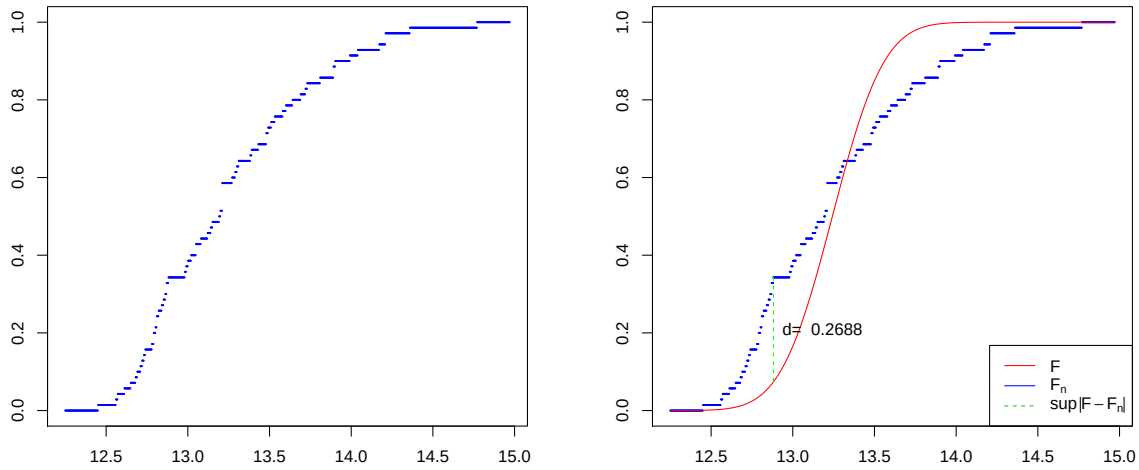
Definition 1 *For a given univariate sample $X_1, X_2, \dots, X_n$ the function*

$$F_n = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{X_i \leq x\}}$$

is called empirical cumulative distribution function (c. d. f.), where $\mathbb{1}_{\{X_i \leq x\}}$ is an indicator function defined as follows: $\mathbb{1}_{\{X_i \leq x\}}(x) = \begin{cases} 1 & \text{if } X_i \leq x \\ 0 & \text{otherwise.} \end{cases}$

The exemplary graph of such a function is depicted in the Figure 2a.

The main idea of the KS test is the analysis of the difference between the given cumulative distribution function (c. d. f.) F and the empirical c. d. f. F_n. Since both theoretical and empirical functions belong to normed space of bounded functions $\mathbb{B}(\mathbb{R})$ (all values are between 0 and 1), this difference can be measured as a distance $\|F_n - F\|_\infty = \sup_{x \in \mathbb{R}} |F_n(x) - F(x)|$. Figure 2b illustrates the calculated distance between the empirical c. d. f. and the theoretical normal c. d. f. with parameters of sample mean and sample variance.



(a) **(b)**

Figure 2: Empirical c. d. f. for Natrium vector (a) and theoretical normal c. d. f. with sample mean and sample variance (b)

The KS statistics is defined as follows:

$$D_n = \sqrt{n} \cdot \sup_{x \in \mathbb{R}} |F_n(x) - F(x)|.$$

If value D_i is considered for different $1 \leq i \leq n$, then the sample $\hat{D}_n = (D_1, \ldots, D_n)$ is obtained that also complies with some distribution $\mathbb{D}_n$. It can be shown that if hypothesis H_0 is true, then this distribution does not depend on the c. d. f. F and therefore can be tabulated. Moreover, Kolmogorov proved that if n is large enough then the distribution function of $\mathbb{D}_n$ can be approximated by Kolmogorov-Smirnov distribution function $H(t) = 1 - 2\sum_{i=1}^{\infty}(-1)^{i-1} \exp^{-2i^2t^2}$, i. e. for each positive value t the probability $P(D_n \leq t) \to H(t)$ when $n \to \infty$. More details can be found in the textbook [**?**].

The KS test uses the decision rule

$$\delta = \begin{cases} H_0 & : \quad D_n \leq c \\ H_1 & : \quad D_n > c \end{cases},$$

where the critical value c depends on the significance level α and can be calculated from the following equations:

$$\alpha = P(\delta \neq H_0 | H_0) = P(D_n > c | H_0) = 1 - P(D_n \leq c | H_0) \approx 1 - H(c).$$

As was mentioned above the last equality can be considered only when n is relatively high. Otherwise the table values for $\mathbb{D}_n$ distribution should be used. Hence, $c \approx H^{-1}(1 - \alpha)$.

Although the KS test is commonly used is has a huge drawback. Namely it considers only completely defined theoretical c. d. f. . In case of normality testing both parameters μ and σ have to be predefined. But usually they are a priori unknown when a sample is going to be tested. Of course it can be managed by assigning sample mean and sample variance as unknown parameters (and initial KS test suggests to do that) but they are not always the best choice. Further example of Natrium distribution illustrates this proposition.

For Natrium (Na) univariate sample of 70 observatons the sample mean $\bar{\mu}$ =13.2423 and the sample variance $\bar{\sigma} = 0.2493$ are calculated. For these values of theoretical c.d.f. is determined (Figure 2b). Then the value of KS statistics is calculated: $D_n = \sqrt{n} \cdot \sup_x |F_n(x) - F(x)|$ =2.2493. Critical value for the significance level $\alpha = 0.01$ is equal to $c = H^{-1}(1 - \alpha)$=1.6276. To calculate this value the following R functions are used:

```
> #Calculates KS distribution function
> H= function(t) {
+         i=1
+         sum=0
+         while(abs(f(t,i) - f(t,i+1))>0.000000000001) {
+                 sum=sum+f(t,i)
+                 i=i+1
+         }
+         1-2*sum
+ }
> #Summand of H function
> f=function(t,i) {
+         (-1)^(i-1)*exp(-2*i^2*t^2)
```

```
+ }
> #Returns value c such that H(c)=a
> Inverse = function(H,a) {
+         newFunction = function(t) {
+                 H(t)-a
+         }
+         #Returns the root of the equation H(x)-a=0
+         uniroot(newFunction,c(0.2,4),tol=0.001)$root
+ }
```

Since $D_n > c$ the null hypothesis is rejected by KS test. But that does not mean that the sample is not normal distributed. That means only that it is not normal distributed with sample mean and sample variance as parameters of that distribution.

In order to manage that issue KS test is improved by solving the following optimization problem

$$KS(\mu, \sigma) = \sup_{x \in \mathbb{R}} |F_n(x) - F(x, \mu, \sigma)| \to \min .$$

When the new values $\hat{\mu}$ and $\hat{\sigma}$ that minimize the value $KS(\mu, \sigma)$ are found the general KS test is performed with respect to these values of parameters. For solving this optimization problem the following R code is used:

```
> KS= function(param) {
+         #discretization of a line segment
+         seq = seq(from = min(dat)-0.2, to = max(dat)+0.2, length.out=1000)
+         #values of empirical c.d.f.
+         empdat = sapply(seq, function(x) {empiric(x,dat)})
+         #values of theoretical c.d.f.
+         theordat = pnorm(seq,param[1],abs(param[2]))
+         #difference between the values
+         diff=theordat-empdat
+         absdiff=abs(diff)
+         max(absdiff)
+ }
> #optim is a predifined R function in stats package
> #defalut method of optimization is Nelder and Mead (1965)
> KSoptim = optim(c(mean,Cov),KS)
> KSoptim$par

[1] 13.1769501  0.4682486

> KSoptim$value

[1] 0.07870673
```

These new parameters $\hat{\mu}$ =13.1770 and $\hat{\sigma}$ =0.4682 are taken as parameters of a new theoretical normal c. d. f. and a new distance is calculated (Figure 3).

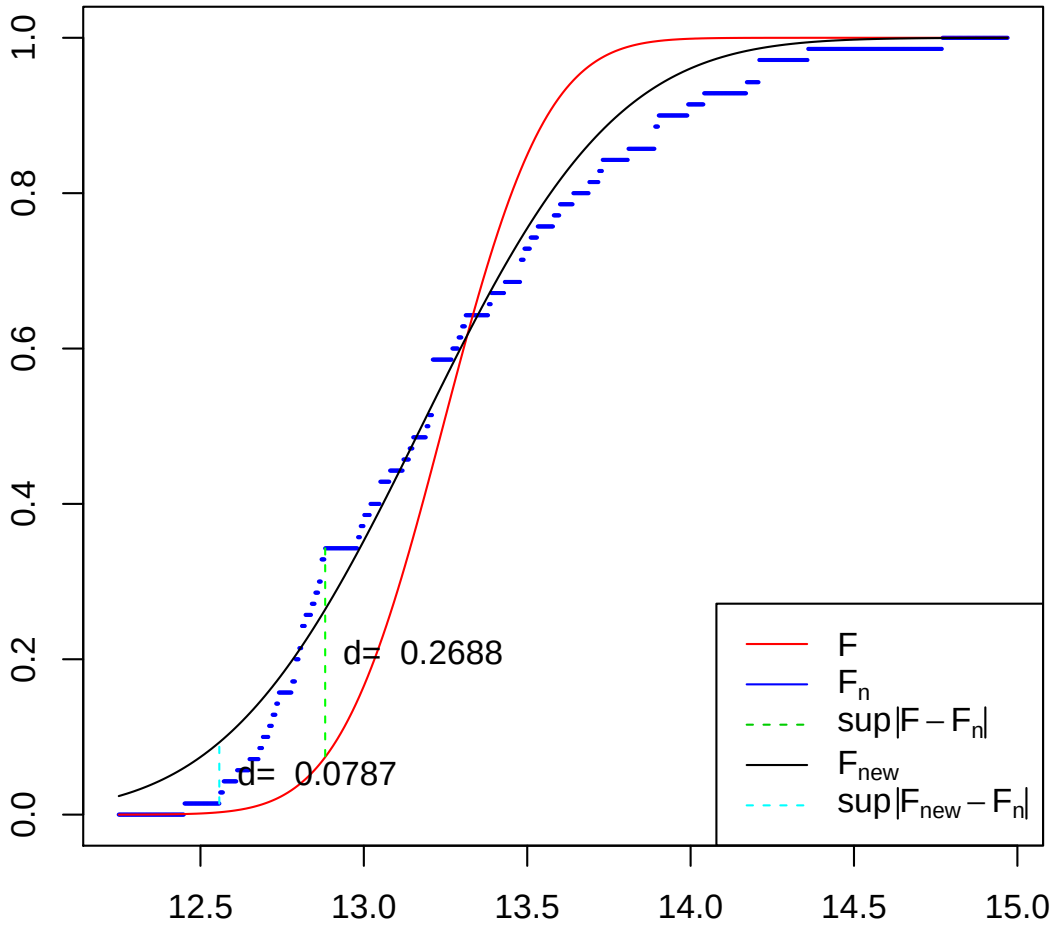


Figure 3: Normal c. d. f. with optimized parameters in comparison to the old c. d. f. with sample mean and sample variance.

The new value of KS statistics is $D_n = \sqrt{n}\sup_{x\in\mathbb{R}} |F_n(x) - F(x, \hat{\mu}, \hat{\sigma})|$ =0.6585 that is smaller than the critical value c =1.6276. Therefore the null hypothesis H_0 is accepted by KS-test. For all further samples the improved KS test is used. It was implemented in *R* and has the following code.

```
> # Performs a Kolmogorov-Smirnov goodness of fit test on the given data
> # for the assumption of a normal distribution.
> # Returns true if the null hypothesis (sample drawn from a
> # normal distributed population) is rejected, false otherwise.
> # The parameters are optimized.
> # The significance level is determined by sig.
> KSimpr.test.norm = function(data, sig) {
```

```
+         critical_value = Inverse(H,1-sig)
+         #Sample mean and sample variance calculation
+         mu = mean(data)
+         sigma = var(data)
+         #KS function that has to be minimized.
+         KS= function(param) {
+                 #discretization of a line segment
+                 seq = seq(from = min(data)-0.2,
+                                 to = max(data)+0.2, length.out=1000)
+                 #values of empirical c.d.f.
+                 empdat = sapply(seq, function(x) {empiric(x,data)})
+                 #values of theoretical c.d.f.
+                 theordat = pnorm(seq,param[1],abs(param[2]))
+                 #difference between the values
+                 diff=theordat-empdat
+                 absdiff=abs(diff)
+                 max(absdiff)
+                 }
+         #optim is a predifined R function in stats package
+         #defalut method of optimization is Nelder and Mead (1965)
+         KSoptim = optim(c(mu,sigma),KS)
+         teststat = sqrt(length(data))*KSoptim$value
+         p_value = 1-H(teststat)
+
+         print(teststat > critical_value)
+
+         return(list( mean = mu,
+                                 var = sigma,
+                                 mu_opt = KSoptim$par[1],
+                                 sigma_opt = KSoptim$par[2],
+                                 teststat = teststat,
+                                 critical_value = critical_value,
+                                 p_value = p_value,
+                                 rejected = teststat > critical_value))
+ }
> KSimpr.test.norm(dat,0.01)

[1] FALSE
$mean
[1] 13.24229

$var
[1] 0.2493019

$mu_opt
[1] 13.17695
```

```
$sigma_opt
[1] 0.4682486

$teststat
[1] 0.6585078

$critical_value
[1] 1.627616

$p_value
[1] 0.7787185

$rejected
[1] FALSE
```

The problem of approximation with H function remains in the improved KS test as well. Therefore this approximation is only applicable when the sample size is relatively high. Otherwise the tabular values for $\mathbb{D}_n$ distribution should be used.

2.2 Box-Cox-Transformation

3 Testing the data sample for normality

3.1 Testing original data

3.1.1 Q-Q-plot

3.1.2 Shapiro-Wilk test

3.1.3 Pearson's chi-squared test

As mentioned in section 2.1.3, Pearson's chi-squared test is not suited for rather small sample sizes because of the approximation via the chi-squared distribution. Concerning the given data, the samples of type 3 glass (17 observations), type 5 glass (13 observations) and type 6 glass (9 observations) are not large enough to ensure a viable test result. Hence, the data belonging to those types will not be considered for separate tests. However, it will remain in the overall data sample of all types. The minimum size of observations in each class is set to five and the number of initial classes (i. e. number of classes before unifying) will be ten. The first tests are conducted on the whole data set for each variable. The results are shown in table 1.

variable	test statistic	sig. level	critical value	p-value	rejected
RI	64.95	0.01	13.28	2.64011035255862e-13	yes
Na	36.99	0.01	13.28	1.80797974702607e-07	yes
Mg	158.3	0.01	11.34	$<$ 1.0e-15	yes
Al	27.2	0.01	9.21	1.24084046404516e-06	yes
Si	38.85	0.01	13.28	7.4876188027595e-08	yes
K	95.97	0.01	NA	NA	NA
Ca	131.13	0.01	13.28	$<$ 1.0e-15	yes
Ba	31.37	0.01	NA	NA	NA
Fe	70.96	0.01	13.28	1.4210854715202e-14	yes

Table 1: Test results of the chi-squared test on the whole data sample with ten initial classes

For two variables, it is not possible to determine a test result with the given parameters: The observations of the variables Potassium (K) and Barium (Ba) are divided only into three classes respectively after the unification of classes in order to fulfill the requirement of minimum class size. Since one degree of freedom is subtracted always and two degrees of freedom are subtracted for the estimation of the mean value and the standard deviation, zero degrees of freedom remain and so the critical value cannot be calculated. For each of the other variables, the hypothesis of normality is clearly rejected for the given significance level. The results for type 1 glass (table 2) are slightly different; in this case, the results can be determined for each variable (except for Barium (Ba), which has been dropped beforehand) and the hypothesis of normality is rejected for each variable but Natrium (Na). The p-value for Natrium is comparably high amounting to approximately 0.52. It is well recognisable that the observed class frequencies for Natrium fluctuate around the expected class frequencies under the hypothesis of a normal distribution with the according parameters (table 3). The good compliance of empirical and hypothetical data for this variable is illustrated in figure 4. In general, the p-values for this part of the sample are higher than those for the whole sample.

variable	test statistic	sig. level	critical value	p-value	rejected
RI	28.01	0.01	9.21	8.26265138420545e-07	yes
Na	3.25	0.01	13.28	0.51688441877949	no
Mg	18.81	0.01	6.63	1.44068580684165e-05	yes
Al	23.55	0.01	11.34	3.10284613768141e-05	yes
Si	23.68	0.01	13.28	9.26014020323773e-05	yes
K	114.86	0.01	11.34	< 1.0e-15	yes
Ca	22.58	0.01	15.09	0.000405198755082603	yes
Fe	18.65	0.01	9.21	8.91413549507503e-05	yes

Table 2: Test results of the chi-squared test on type 1 glass with ten initial classes

class	frequencies	
(interval)	observed	expected
]12.4, 12.8]	15	13.15
]12.8, 13]	12	8.81
]13, 13.2]	9	10.68
]13.2, 13.4]	11	11.04
]13.4, 13.6]	8	9.74
]13.6, 14]	9	12.06
]14, 14.8]	6	4.52

Table 3: Observed end expected frequencies of items in the classes for the variable Natrium of type 1 glass

variable	test statistic	sig. level	critical value	p-value	rejected
RI	27.92	0.05	9.21	8.6430973300633e-07	yes
Na	8.2	0.05	6.63	0.00418393039163056	yes
Mg	66.57	0.05	6.63	< 1.0e-15	yes
Al	9.41	0.05	11.34	0.024332262426528	no
Si	6.24	0.05	9.21	0.0441247638253744	no
K	41.06	0.05	6.63	1.47495904379014e-10	yes
Ca	71.68	0.05	9.21	< 1.0e-15	yes
Fe	16.75	0.05	11.34	0.00079487617843276 8	yes

Table 4: Test results of the chi-squared test on type 2 glass

variable	test statistic	sig. level	critical value	p-value	rejected
RI	19.93	0.01	NA	NA	NA
Na	1.4	0.01	NA	NA	NA
Al	3.42	0.01	6.63	0.0644860281274806	no
Si	4.84	0.01	NA	NA	NA
K	13.14	0.01	NA	NA	NA
Ca	11.93	0.01	NA	NA	NA
Ba	0.2	0.01	NA	NA	NA

Table 5: Test results of the chi-squared test on type 7 glass

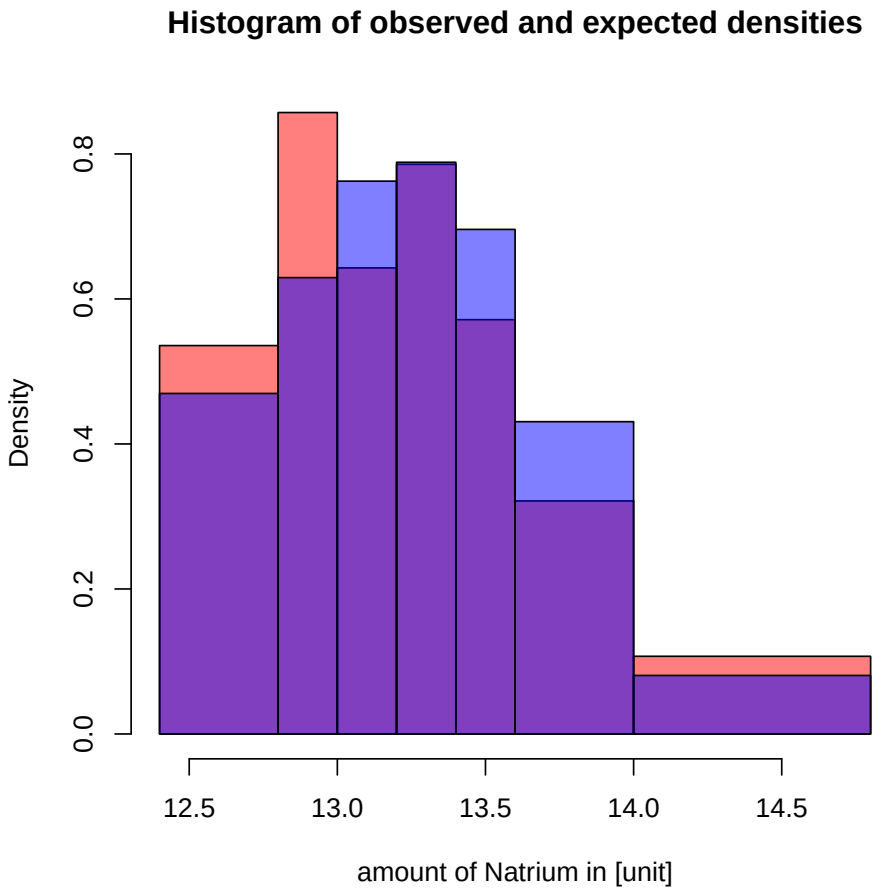


Figure 4: Histogram of observed densities (red) and expected densities (blue) within the classes for the variable Natrium of type 1 glass

3.1.4 Kolmogorov-Smirnov test

3.2 Testing transformed data

3.2.1 Q-Q-plot

3.2.2 Shapiro-Wilk test

3.2.3 Pearson's chi-squared test

3.2.4 Kolmogorov-Smirnov test

4 Conclusion

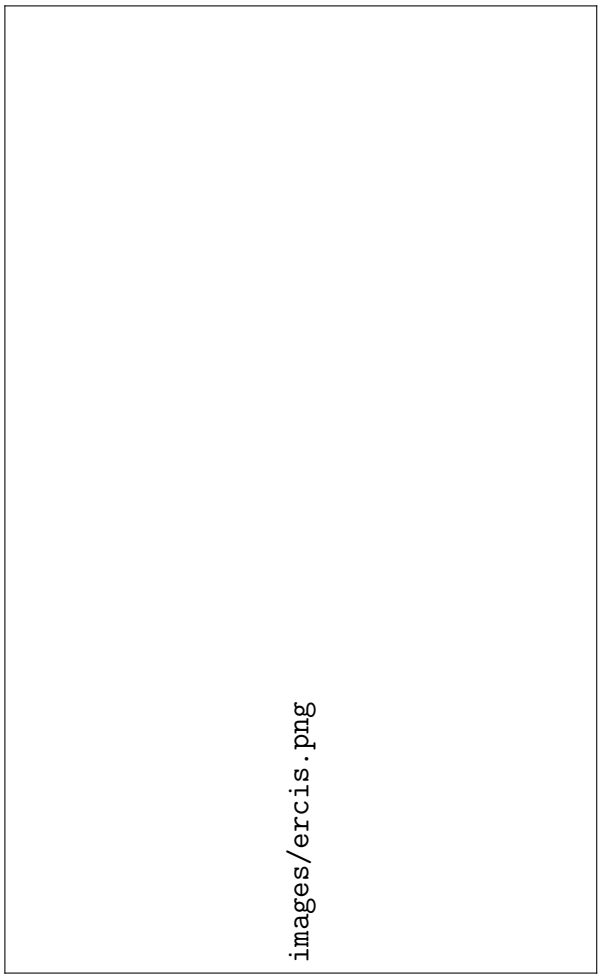


Figure 5: Logo of ERCIS as an example for figures

5 Section 1

Example for referring to a chapter: As written in section **??** ...

5.1 First Subsection

Example for a citation: [**?**],[**?**], [**?**]

5.2 Second Subsection

6 Section 2

Here could be a table, e.g. table 6 (which is on page 17):

Feature 1	Feature 2			
	case		studies	
	ca	te	go	ry
data	63,50%	9,56%	2,16%	1,17%
analytics	1,57%	0,41%	0,29%	0,41%

Table 6: This is the label of the table

If you want to relate to a figure or table from a different page, you could do it this way: Figure 5, see page 16, shows the ERCIS-Logo.

A Appendix

here starts the appendix

A.1 Slides

here could be some slides

List of Figures

List of Tables