Normal Distribution

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Case Studies
"Data Analytics"

Outline

Normality as a requirement for statistical methods

Data Set Overview

- `Glass` data set from package `mlbench`
- sample of 214 observations
- 7 types of glass (but only 6 present in this sample)
- Variables: refractive index (RI) and 8 elements (Na, Mg, Al, Si, K, Ca, Ba, Fe)

Box-Cox Transformation
Definition

Box-Cox Transformation

If data are not normally distributed, they can possibly be transformed by the parameterised power transformation

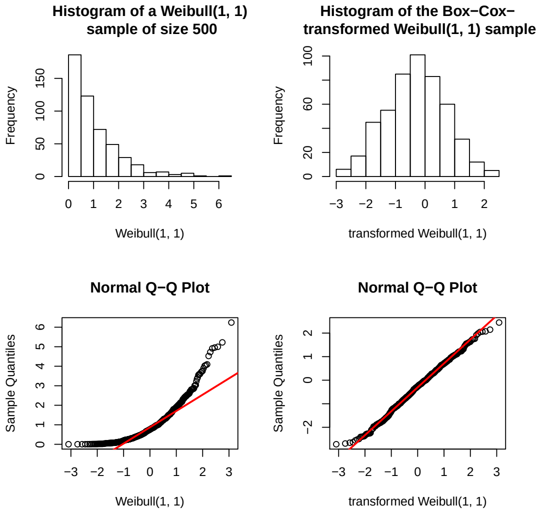
$$x^{(\lambda)} = \begin{cases} \frac{x^\lambda - 1}{\lambda} & \lambda \neq 0 \\ \ln(x) & \lambda = 0 \end{cases} \qquad \text{for } x > 0$$

The optimal parameter λ for specific observations $x_1, \ldots, x_n$ can be obtained by a maximum-likelihood estimation, maximising the log likelihood

$$l(\lambda) = -\frac{n}{2} \ln \left[\frac{1}{n} \sum_{j=1}^{n} (x_j^{(\lambda)} - \overline{x^{(\lambda)}})^2 \right] + (\lambda - 1) \sum_{j=1}^{n} \ln(x_j)$$

with $\overline{x^{(\lambda)}} = \frac{1}{n} \sum_{j=1}^{n} x_j^{(\lambda)}$

Box-Cox Transformation
Transformation issues



Box-Cox Transformation
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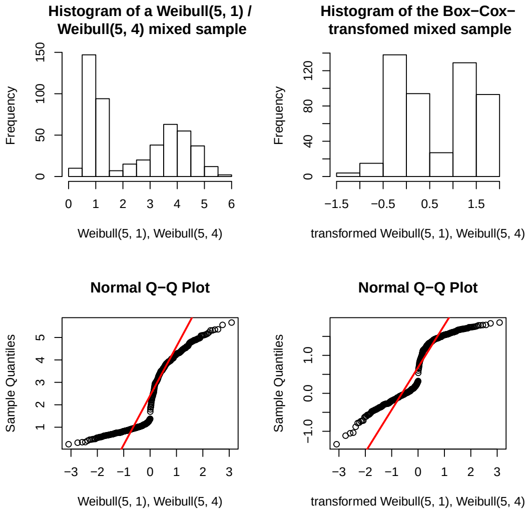


Q-Q-Plots

Sample:

$$x = (x_1, x_2, \dots, x_n)$$

Empirical quantiles:

$$x_{(1)} \le x_{(2)} \le \dots \le x_{(n)}$$

Theoretical quantiles:

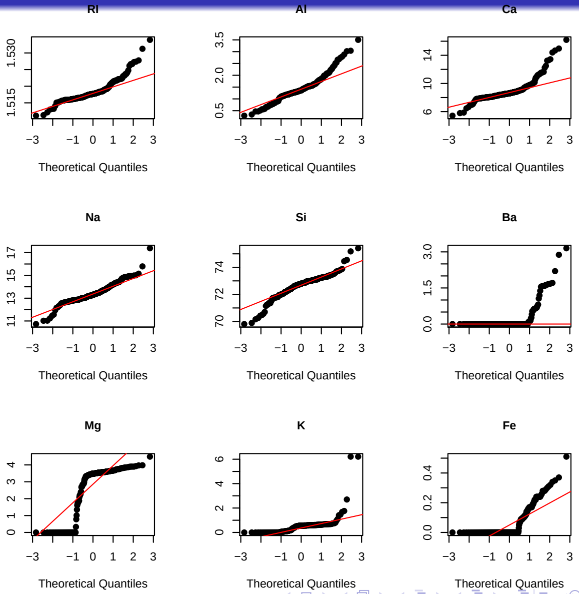
$$q_{(j)} = \Phi^{-1}(p_{(j)}),$$

where

$$p_{(j)} = \frac{j - \frac{1}{2}}{n},$$

Φ - $N(0,1)$ c. d. f. .

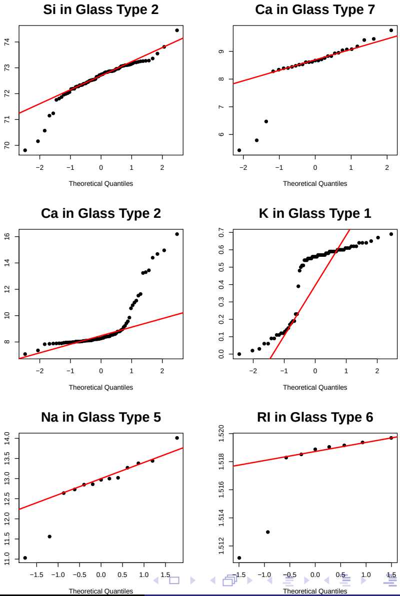
$\Longrightarrow$ Plot $x_{(i)}$ against $q_{(i)}$



Q-Q-Plots

QQ-Plots of the subdatasets:

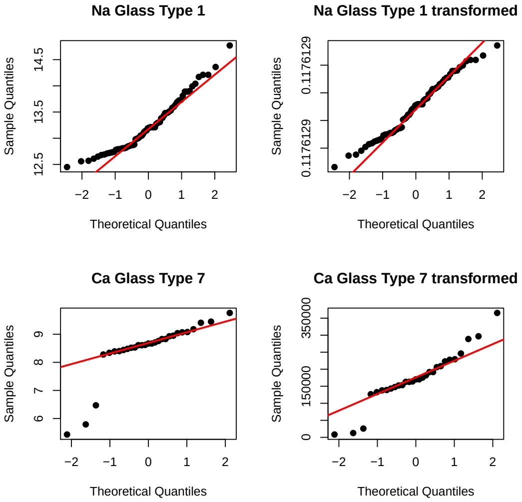
- Variables could be normally distributed within the subclasses
- For some cases there appear to be a linear relationships
- For other cases a linear relationship is questionable
- In some subdatasets a linear relationship seems plausible, however n is very small



Q-Q-Plots

Results of the Transformation of the Full Dataset :

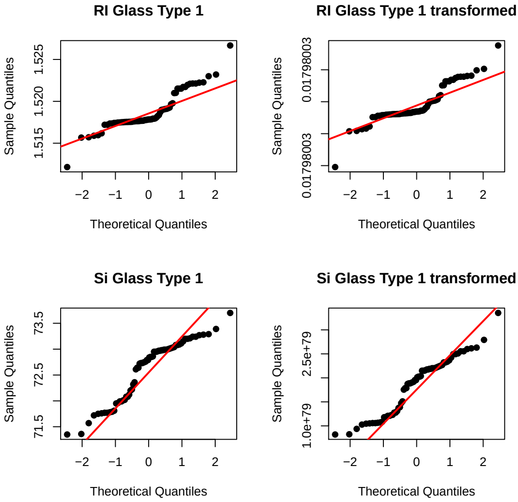
- For some of the cases there seems to be a slight improvement
- For non-unimodal cases the transformation does not show significant improvements towards normality



Q-Q-Plots

Results of the Transformation of the Subdatasets :

- For unimodal cases the transformation shapes the distribution closer to normality
- For non-unimodal cases the transformation does not show significant improvements towards normality



Shapiro-Wilk Test

The test statistic W indicates the deviation of the observed quantile values from the assumed cumulative distribution function quantiles

$$W = \frac{\sum_{i=1}^{n} (a_i y_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2},$$

where

- a_i denotes the normalised "best linear unbiased" coefficients,
- y_i denotes the observations.

The critical value for W is obtained by the Monte Carlo Method
$\Longrightarrow$ p-value is calculated

Important: If a variable contains only zeros the Shapiro-Wilk test is not applicable, since the term in the denominator sums up to zero.

Shapiro-Wilk Test

Testing the Full Dataset :

Null hypothesis is rejected for all variables at a 1 % significance level

After the Transformation :

The null hypothesis can be rejected for the four transformed variables

$\Longrightarrow$ Possible Explanation: Combination of different distributions in the different glass types

variable	test statistic	sig. level	critical value	p-value	rejected
RI	0.87	0.01	NA	1.0766713449726e-12	yes
Na	0.95	0.01	NA	3.4655430546966e-07	yes
Mg	0.7	0.01	NA	$<$ 1.0e-15	yes
Al	0.94	0.01	NA	2.08315629600399e-07	yes
Si	0.92	0.01	NA	2.17503176825416e-09	yes
K	0.44	0.01	NA	$<$ 1.0e-15	yes
Ca	0.79	0.01	NA	$<$ 1.0e-15	yes
Ba	0.41	0.01	NA	$<$ 1.0e-15	yes
Fe	0.65	0.01	NA	$<$ 1.0e-15	yes

Test results of the Shapiro-Wilk test on the whole data sample

variable	test statistic	sig. level	critical value	p-value	rejected
RI	NA	NA	NA	NA	NA
Na	0.95	0.01	NA	8.75605777309153e-07	yes
Mg	NA	NA	NA	NA	NA
Al	0.97	0.01	NA	0.000244326513056066	yes
Si	0.93	0.01	NA	1.58998125691823e-08	yes
K	NA	NA	NA	NA	NA
Ca	0.89	0.01	NA	1.13880689831982e-11	yes
Ba	NA	NA	NA	NA	NA
Fe	NA	NA	NA	NA	NA

Test results of the Shapiro-Wilk test on the whole transformed data sample

Shapiro-Wilk Test

Testing the Subdatasets Example – Glass Type 1 :

Null hypothesis is rejected for all variables at a 1 % significance level

variable	test statistic	sig. level	critical value	p-value	rejected
RI	0.88	0.01	NA	6.36192013015468e-06	yes
Na	0.95	0.01	NA	0.00459078607995831	yes
Mg	0.82	0.01	NA	8.02702432879544e-08	yes
Al	0.9	0.01	NA	5.42971629496434e-05	yes
Si	0.91	0.01	NA	0.000117060780025464	yes
K	0.77	0.01	NA	3.14049093233846e-09	yes
Ca	0.93	0.01	NA	0.00103561283726753	yes

Test results of the Shapiro-Wilk test on type 1 glass

After the Transformation :

The null hypothesis cannot be rejected for 3 of the transformed variables

$\Longrightarrow$ Appeerently the transformation was successful

variable	test statistic	sig. level	critical value	p-value	rejected
RI	0.89	0.01	NA	1.62433657125306e-05	yes
Na	0.98	0.01	NA	0.353792914291578	no
Mg	0.83	0.01	NA	1.40023833110547e-07	yes
Al	0.96	0.01	NA	0.0459207068393172	no
Si	0.94	0.01	NA	0.00269629206710463	yes
K	NA	NA	NA	NA	NA
Ca	0.97	0.01	NA	0.148237775100495	no

Test results of the Shapiro-Wilk test on the transformed type 1 glass

Pearson's Chi-Squared Test

Theoretical foundations

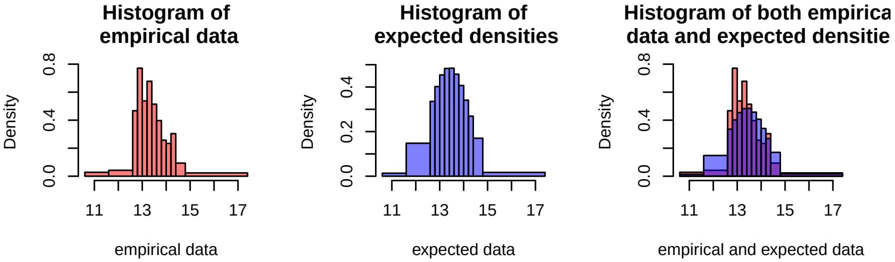
- Divide observations $X_1, \dots, X_N$ into pairwise disjoint classes $C_1, \dots, C_K$
- Common requirement: minimum class size of 5
- Compare observed class frequencies to expected theoretical class frequencies for a certain distribution

$$\text{test statistic:} \quad \chi^2 = \sum_{k=1}^{K} \frac{(O_k - E_k)^2}{E_k}$$

- The test statistic is approximately χ^2-distributed with $K - 1$ degrees of freedom (minus one degree of freedom per estimated parameter)

Pearson's Chi-Squared Test

Theoretical foundations



Pearson's Chi-Squared Test

Theoretical foundations

- Test under the null hypothesis that the sample is drawn from a population with unknown distribution $\mathbb{P}$ which is equal to the assumed distribution $\mathbb{P}_0$:

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

Decision rule

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

(significance level α, number of estimated parameters p)

Pearson's Chi-Squared Test

Test results for the whole sample

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

Pearson's Chi-Squared Test

Test results for type 1 glass

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

Pearson's Chi-Squared Test

Test results for type 1 glass

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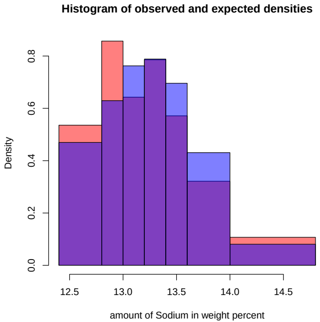
K	114.86	0.01	11.34	$<$ 1.0e-15	yes
Ca	22.58	0.01	15.09	0.000405198755082603	yes
Fe	18.65	0.01	9.21	8.91413549507503e-05	yes

Pearson's Chi-Squared Test

Test results for sodium of type 1 glass

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



Pearson's Chi-Squared Test

Test results for transformed type 1 glass

variable	test statistic	sig. level	critical value	p-value	rejected
RI	27.81	0.01	6.63	1.33864150764218e-07	yes
Na	1.59	0.01	13.28	0.810360513797024	no
Mg	17.87	0.01	NA	NA	NA
Al	6.41	0.01	11.34	0.093110657016404	no
Si	16.87	0.01	13.28	0.00205136639513992	yes
K	NA	0.01	NA	NA	NA
Ca	3.35	0.01	11.34	0.341234021909645	no
Fe	NA	0.01	NA	NA	NA

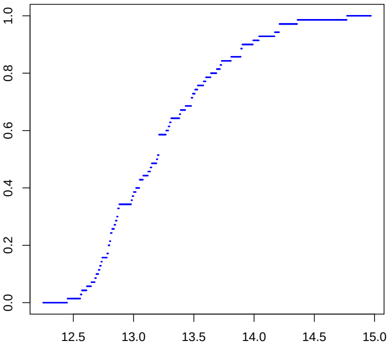
Kolmogorov-Smirnov Test
Preliminaries

Let $x = (x_1, x_2, \ldots, x_n)$ be a sample of unknown distribution $\mathbb{P}$.

Definition

$F_n(x) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{x_i \le x\}}(x)$
- empirical c. d. f. , where

$$\mathbb{1}_{\{x_i \le x\}}(x) = \begin{cases} 1 & \text{if } x_i \le x \\ 0 & \text{otherwise.} \end{cases}$$



Glass Type 1, Sodium (Na)

Kolmogorov-Smirnov Test

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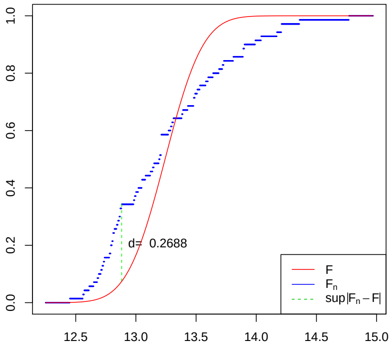
$$\mathbb{1}_{\{x_i \leq x\}}(x) = \begin{cases} 1 & \text{if } x_i \leq x \\ 0 & \text{otherwise.} \end{cases}$$

$F(x)$ - theoretical normal c. d. f. with

$$\bar{x} = \frac{1}{n} \sum_i x_i, \quad \sigma_x^2 = \frac{1}{n} (x_i - \bar{x})^2$$



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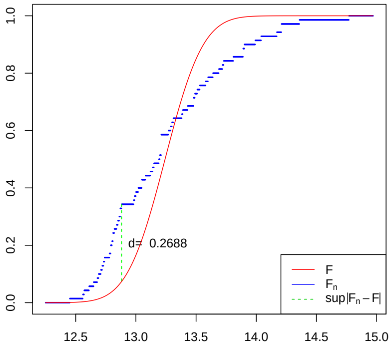
$$\bar{x} = \frac{1}{n} \sum_i x_i, \quad \sigma_x^2 = \frac{1}{n} (x_i - \bar{x})^2$$

$d = \sup_{x \in \mathbb{R}} |F_n(x) - F(x)|$
- distance between them.



Glass Type 1, Sodium (Na)

Kolmogorov-Smirnov Test

Let $x = (x_1, x_2, \ldots, x_n)$ be a sample of unknown distribution $\mathbb{P}$.
Theoretical c. d. f. F defines a distribution $\mathbb{P}_0$.

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

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KS test statistics:

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

Kolmogorov-Smirnov Test

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Properties of D_n in case H_0 is TRUE:

- Distribution of $\hat{D}_n := (D_1, D_2, \ldots, D_n)$ does not depend on F

Kolmogorov-Smirnov Test

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- Distribution of $\hat{D}_n := (D_1, D_2, \dots, D_n)$ does not depend on F $\implies$ tabulated

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

Properties of D_n in case H_0 is TRUE:

- Distribution of $\hat{D}_n := (D_1, D_2, \dots, D_n)$ does not depend on F $\Longrightarrow$ tabulated
- $\forall t > 0$:

$$P(D_n \leq t) \xrightarrow[n \to \infty]{} H(t) = 1 - 2 \sum_{i=1}^{\infty} (-1)^{i-1} \exp^{-2i^2 t^2}$$

Kolmogorov-Smirnov Test

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 c - critical value

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

where c - critical value that
depends on a significance level α:

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$\alpha = P(\delta \neq H_0 | H_0)$

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

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depends on a significance level α:

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

$$\Longrightarrow \; c \approx H_{1-\alpha}$$

Kolmogorov-Smirnov Test

The KS test uses the decision rule for a given significance level α

$$\delta = \begin{cases} H_0 & : \quad D_n \leq H_{1-\alpha} \\ H_1 & : \quad D_n > H_{1-\alpha} \end{cases} , \quad H(t) = 1 - 2\sum_{i=1}^{\infty}(-1)^{i-1}\exp^{-2i^2t^2}$$

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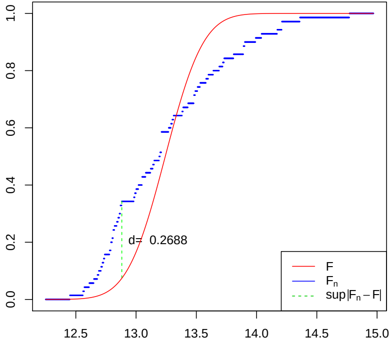
Example:



Glass Type 1, Sodium (Na)

Kolmogorov-Smirnov Test

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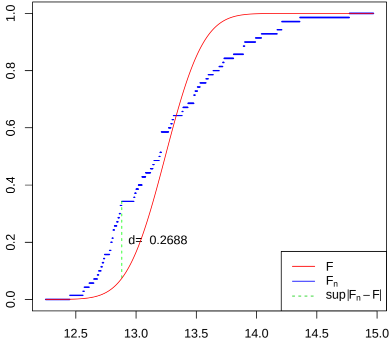
Example:

- $n = 70$



Glass Type 1, Sodium (Na)

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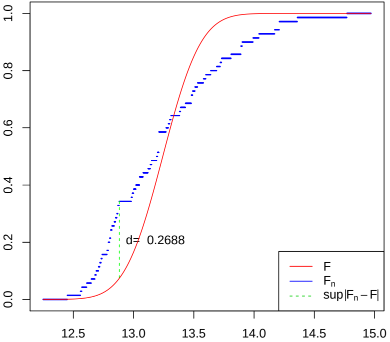
Example:

- $n = 70$
- $D_n = \sqrt{n}\sup|F_n - F| = 2.2493$



Glass Type 1, Sodium (Na)

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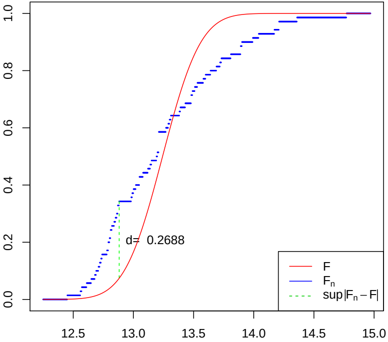
Example:

- $n = 70$
- $D_n = \sqrt{n}\sup|F_n - F| = 2.2493$
- $\alpha = 0.01$

$$\Longrightarrow \quad c = H_{1-\alpha} = 1.6276$$



Glass Type 1, Sodium (Na)

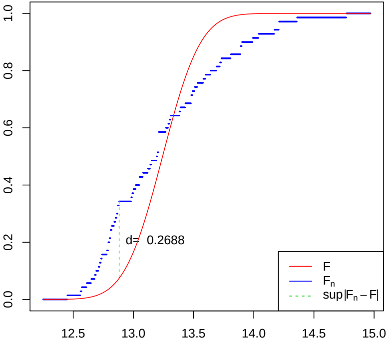
Kolmogorov-Smirnov Test

The KS test uses the decision rule for a given significance level α

$$\delta = \begin{cases} H_0 & : \quad D_n \leq H_{1-\alpha} \\ H_1 & : \quad D_n > H_{1-\alpha} \end{cases}, \quad H(t) = 1 - 2\sum_{i=1}^{\infty}(-1)^{i-1}\exp^{-2i^2t^2}$$

Example:

- $n = 70$
- $D_n = \sqrt{n}\sup|F_n - F| = 2.2493$
- $\alpha = 0.01$
  $\implies \quad c = H_{1-\alpha} = 1.6276$
- $D_n > c \implies H_0$ rejected



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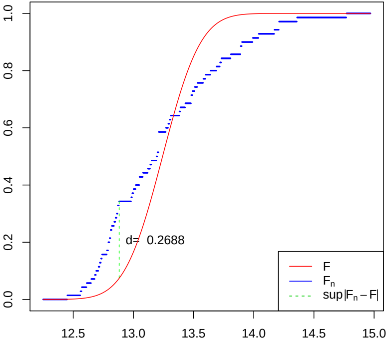

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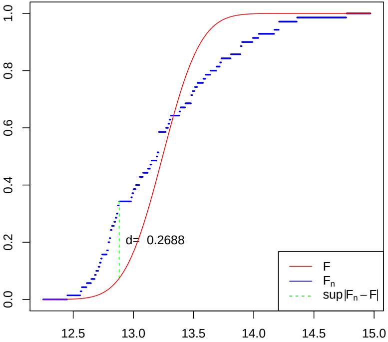
- $\implies \mathbb{P} \neq \mathbb{P}_0$
- $\not\Longrightarrow$ data not normally distributed!!!



Glass Type 1, Sodium (Na)

Kolmogorov-Smirnov Test

Improvement

KS test is improved by solving the following optimization problem

$$KS(\mu, \sigma^2) = \sup_{x \in \mathbb{R}} |F_n(x) - F(x, \mu, \sigma^2)| \to \min .$$

R code used:

Kolmogorov-Smirnov Test
Improvement

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R code used:

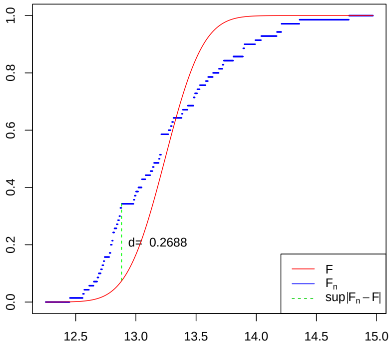
```
c(mean(dat),var(dat))
[1] 13.2422857  0.2493019
#optim is a predifined R function in stats package
#defalut method of optimization is Nelder and Mead
result = optim(c(mean(dat),var(dat)),KS)
result$par
[1] 13.1769501  0.4682486
result$value
[1] 0.07870673
```

Kolmogorov-Smirnov Test
Improvement

KS test is improved by solving the following optimization problem

$$KS(\mu, \sigma^2) = \sup_{x \in \mathbb{R}} |F_n(x) - F(x, \mu, \sigma^2)| \to \min .$$

- Initial vector of parameters
  $\mu = 13.2423, \quad \sigma^2 = 0.2493$
- Optimized vector of parameters
  $\hat{\mu} = 13.1770, \quad \hat{\sigma}^2 = 0.4682$



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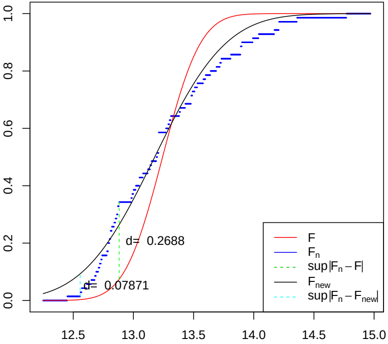

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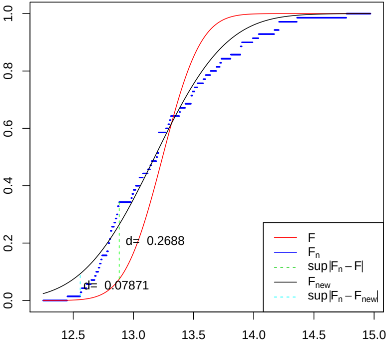
- $D_n = \sqrt{n} \sup |F_n - F_{new}| = 0.6585$



Glass Type 1, Sodium (Na)

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$$KS(\mu,\sigma^2) = \sup_{x\in\mathbb{R}} |F_n(x) - F(x,\mu,\sigma^2)| \to \min .$$

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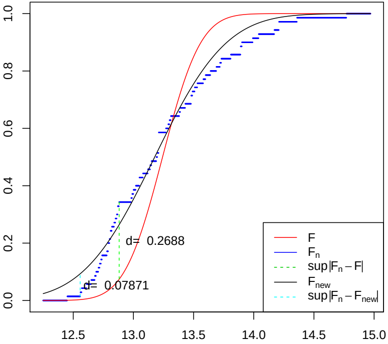

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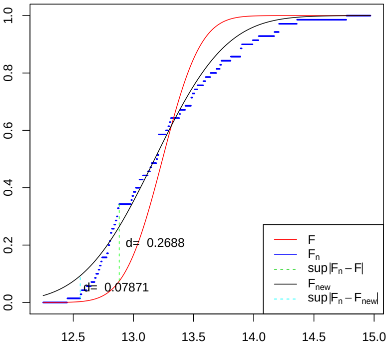
- $D_n < c \implies H_0$ not rejected



Glass Type 1, Sodium (Na)

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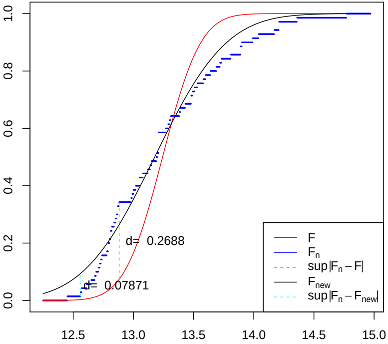

Glass Type 1, Sodium (Na)

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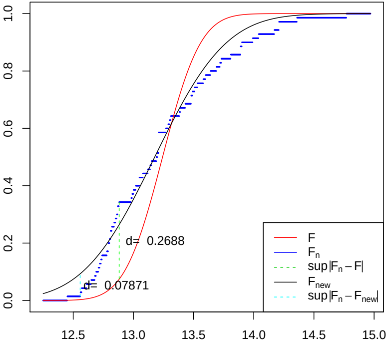
- $D_n < c \implies H_0$ not rejected
- $\implies \mathbb{P} = \mathbb{P}_0$
- $\implies$ data normally distributed!



Glass Type 1, Sodium (Na)

Kolmogorov-Smirnov Test

Results of the improved test on the whole data set

variable	test statistic	sig. level	critical value	p-value	rejected
RI	1.34	0.01	1.63	0.0561963016778131	no
Na	0.87	0.01	1.63	0.43825271603342	no
Mg	2.94	0.01	1.63	6.18457917100912e-08	yes
Al	0.84	0.01	1.63	0.474757887353829	no
Si	0.96	0.01	1.63	0.314710019077325	no
K	2.14	0.01	1.63	0.000212776619708754	yes
Ca	1.33	0.01	1.63	0.057710602872685	no
Ba	2.60	0.01	1.63	2.75476085742632e-06	yes
Fe	4.68	0.01	1.63	$<$ 1.0e-15	yes

Kolmogorov-Smirnov Test

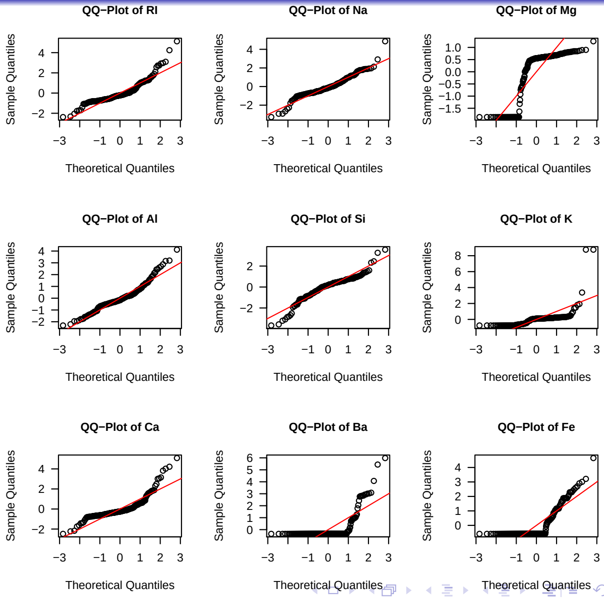
Test Results:

variable	rejected
RI	no
Na	no
Mg	yes
Al	no
Si	no
K	yes
Ca	no
Ba	yes
Fe	yes

Kolmogorov-Smirnov Test

Test Results:

variable	rejected
RI	no
Na	no
Mg	yes
Al	no
Si	no
K	yes
Ca	no
Ba	yes
Fe	yes



Kolmogorov-Smirnov Test

Results on the data subsets

variable	test statistic	sig. level	critical value	p-value	rejected
RI	1.31	0.01	1.63	0.0630043926883292	no
Na	0.66	0.01	1.63	0.77871853343362	no
Mg	0.49	0.01	1.63	0.967729719418776	no
Al	0.92	0.01	1.63	0.366854549713195	no
Si	1.06	0.01	1.63	0.208027646546284	no
K	1.73	0.01	1.63	0.00491847745617136	yes
Ca	0.84	0.01	1.63	0.48064266616439	no
Fe	2.65	0.01	1.63	1.63244296669252e-06	yes

Test results of the improved KS test on type 1 glass

variable	test statistic	sig. level	critical value	p-value	rejected
RI	0.67	0.01	1.63	0.767837508224946	no
Na	0.52	0.01	1.63	0.951658259816235	no
Al	0.49	0.01	1.63	0.968495966845634	no
Si	0.56	0.01	1.63	0.915628110530136	no
K	1.43	0.01	1.63	0.0340401962712393	no
Ca	0.56	0.01	1.63	0.91558957374917	no
Ba	0.76	0.01	1.63	0.61288183743927	no

Test results of the improved KS test on type 7 glass

Chi-Square Plot for Multivariate Normality

Sample mean and covariance matrix

Multivariate sample $X = (X_1, X_2, \dots, X_n)$ with p variables

$X = (X_1, X_2, \dots, X_n)$

$$\bar{X} = \frac{1}{n}\left(\sum_j X_j\right) \qquad S = \frac{1}{n-1}\left(\sum_j (X_j - \bar{X})(X_j - \bar{X})'\right)$$

Generalized squared distances

$$d_j^2 = (X_j - \bar{X})' S (X_j - \bar{X})', \quad j = 1, 2, \dots n$$

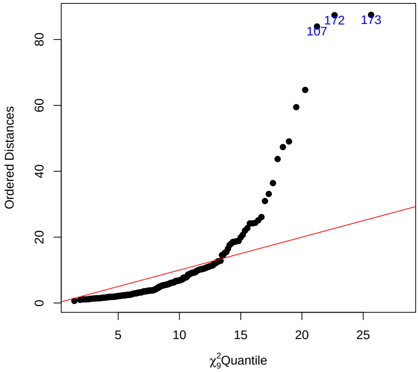
$$d_j^2 \approx \chi_p^2$$

$d_{(1)}^2 \leq d_{(2)}^2 \leq \cdots \leq d_{(n)}^2$ - empirical quantiles

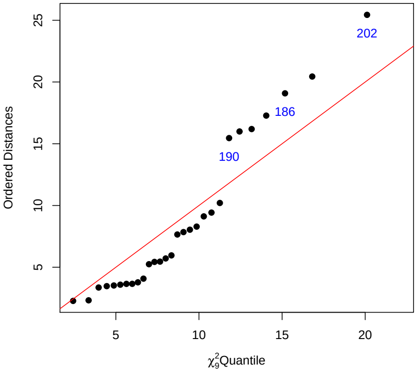
$q_{(j)} = (\chi_p^2)^{-1}\left(\frac{j - \frac{1}{2}}{n}\right)$ - theoretical quantiles

$\Longrightarrow$ Plot $d_{(i)}^2$ against $q_{(i)}$

Chi-Square Plot for Multivariate Normality



The whole data set



Type 7 Glass

Plot of multivariate normal distribution

Theoretical foundations

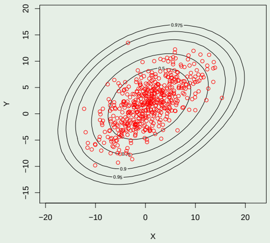
- Contour lines of the plot of a multivariate normal distribution are shaped elliptically
- Ellipsoids are centered at $\mu : \left\{x : (x-\mu)' \Sigma^{-1} (x-\mu) = c^2\right\}$ with some constant c.

Example

Multivariate normal distribution with sample size 500 and parameters

$$\mu = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

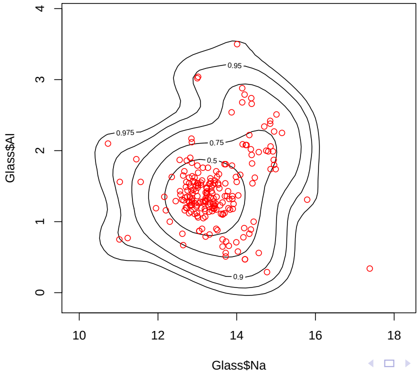
$$\Sigma = \begin{bmatrix} 27 & 15 \\ 15 & 18 \end{bmatrix}$$



Plot of multivariate normal distribution

Application

- Concerning the complete sample, the p-values for the variables Na and Al are highest among all used test methods.
- Plot data points and determine contour lines.



Plot of multivariate normal distribution

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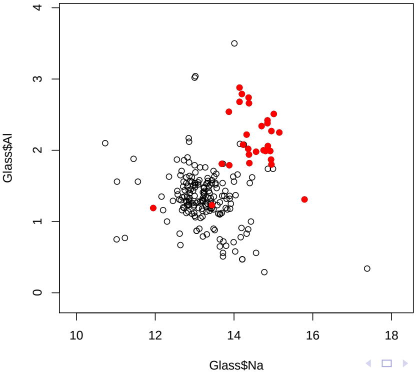

Plot of multivariate normal distribution
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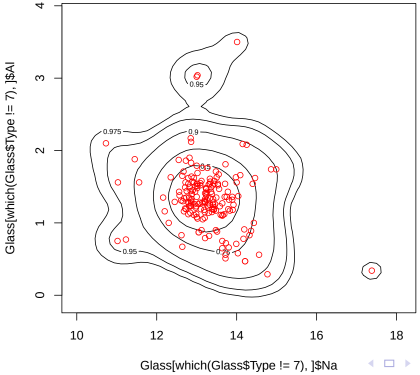

Summary

Pearson's Chi-Squared Test
Theoretical foundations