

Normal Distribution

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Case Studies
"Data Analytics"

Outline

① Introduction

- Normality as a requirement for statistical methods
- Data Set Overview

② Normality Testing

- Graphical Methods for Normality Testing
 - Q-Q-Plots
 - Chi-Square Plot
- Quantitative Methods for Normality Testing
 - Shapiro-Wilk Test
 - Pearson's Chi-Squared Test
 - Kolmogorov-Smirnov Test

③ Transformation to Normality

- Box-Cox Transformation
- Transformation Results Testing

④ Summary

Normality as a requirement for statistical methods

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Q-Q-Plots

Sample:

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

Empirical quantiles:

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

Theoretical quantiles:

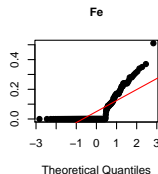
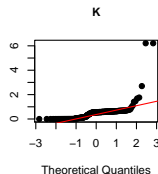
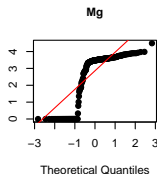
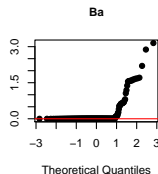
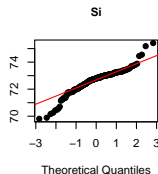
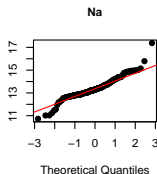
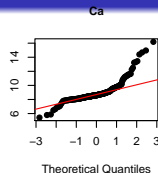
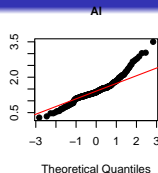
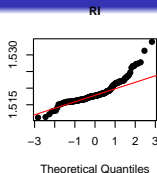
$$q_{(j)} = \Phi^{-1}(p_{(j)}),$$

where

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

$\Phi - N(0, 1)$ c. d. f. .

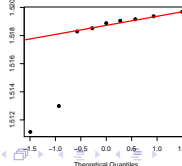
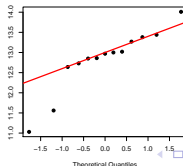
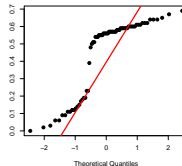
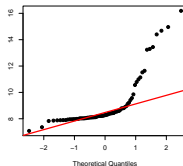
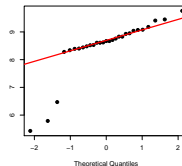
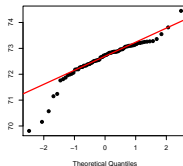
\Rightarrow Plot $x_{(i)}$ against $q_{(i)}$



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

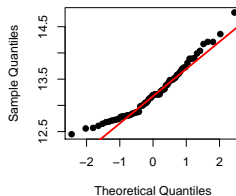


Q-Q-Plots

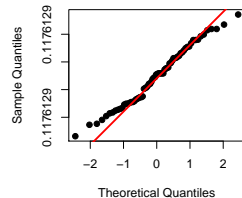
Results of the Transformation of the Full Dataset :

- 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

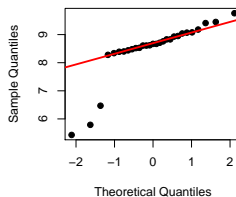
Na Glass Type 1



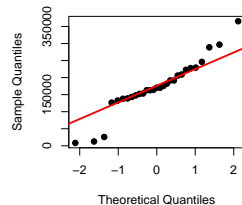
Na Glass Type 1 transformed



Ca Glass Type 7



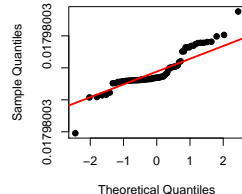
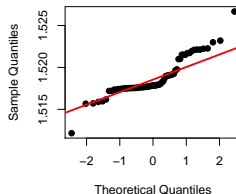
Ca Glass Type 7 transformed



Results of the Transformation of the Subdatasets :

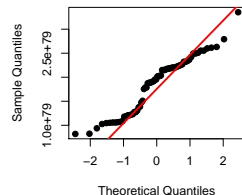
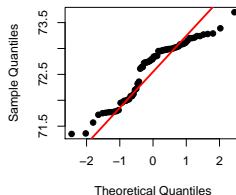
- For unimodal cases the transformation shapes the distribution closer to normality
- For non-unimodal cases the transformation does not show significant improvements towards normality

RI Glass Type 1 transformed



Si Glass Type 1

Si Glass Type 1 transformed



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
 \implies 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

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

After the Transformation :

The null hypothesis can be rejected for the four transformed variables

⇒ Possible

Explanation:

Combination of different distributions in the different glass types

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

⇒ Apparently 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

Graphical Methods for Normality Testing

Chi-Square Plot

Quantitative Methods for Normality Testing

Pearson's Chi-Squared Test

Quantitative Methods for Normality Testing

Kolmogorov-Smirnov Test

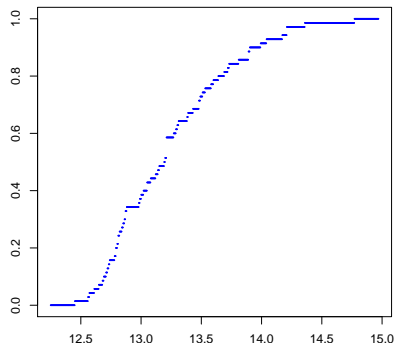
Let $x = (x_1, x_2, \dots, x_n)$ be a sample of unknown distribution \mathbb{P} .

Definition

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

- **empirical** c. d. f. , where

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



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

Kolmogorov-Smirnov Test

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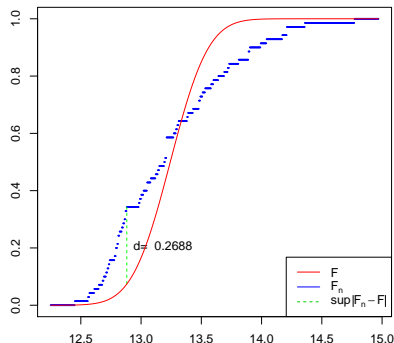
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$F(x)$ - theoretical normal c. d. f.

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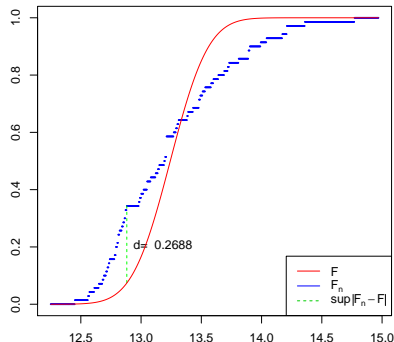
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$$d = \sup_{x \in \mathbb{R}} |F_n(x) - F(x)|$$

- distance between them.



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

Kolmogorov-Smirnov Test

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$$H_0 : \mathbb{P} = \mathbb{P}_0,$$

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 \implies **tabulated**
- $\forall t > 0 :$

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

Quantitative Methods for Normality Testing

Kolmogorov-Smirnov Test

The KS test uses the decision rule

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

where c - critical value

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where c - critical value that
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$$\implies c \approx H_{1-\alpha}$$

Quantitative Methods for Normality Testing

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

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

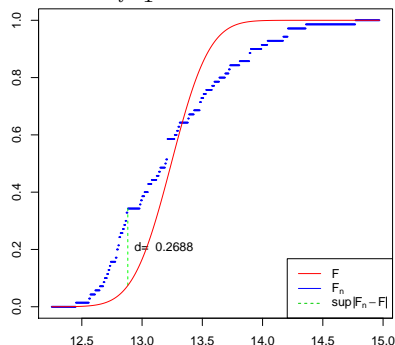
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Example:



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

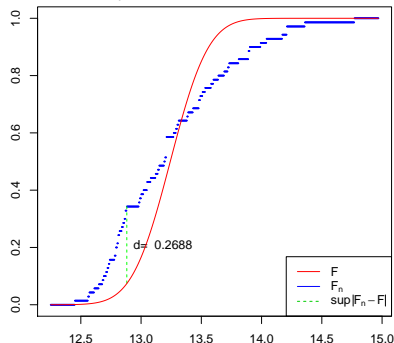
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Example:

• $n = 70$



Glass Type 1, Natrium (Na)

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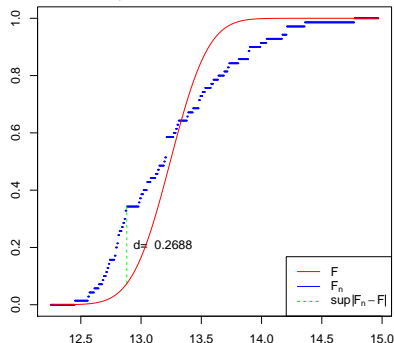
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Example:

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



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

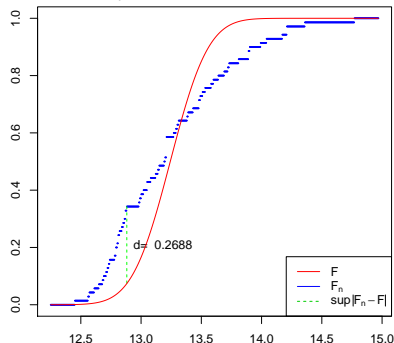
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Example:

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



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

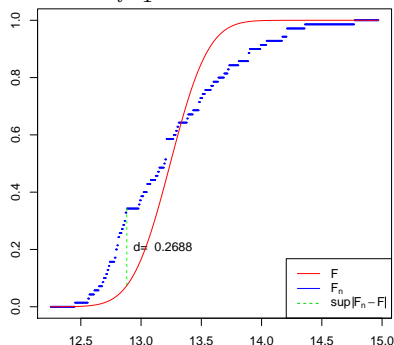
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Example:

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



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

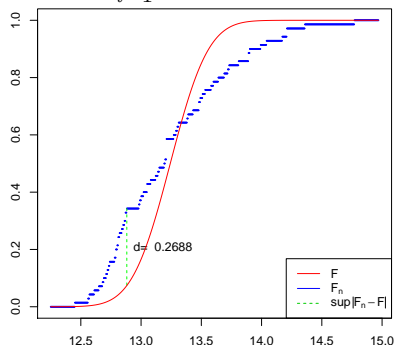
Kolmogorov-Smirnov Test

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

Example:

- $n = 70$
- $D_n = \sqrt{n} \sup |F_n - F| = 2.2493$
- $\alpha = 0.01$
 $\implies c = H_{1-\alpha} = 1.6276$
- $D_n > c \implies H_0$ **rejected**
- $\implies \mathbb{P} \neq \mathbb{P}_0$



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

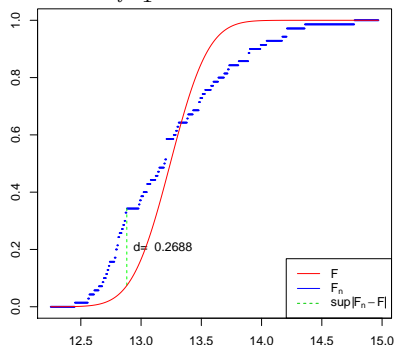
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- $D_n > c \implies H_0$ **rejected**
- $\implies \mathbb{P} \neq \mathbb{P}_0$
- \Rightarrow **data not normally distributed!!!**



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

Improved Kolmogorov-Smirnov Test

KS test is improved by solving the following optimization problem

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

R code used:

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R code used:

```
c(mean(dat), var(dat))
```

```
[1] 13.2422857 0.2493019
```

```
#optim is a predefined R function in stats package
```

```
#default 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
```

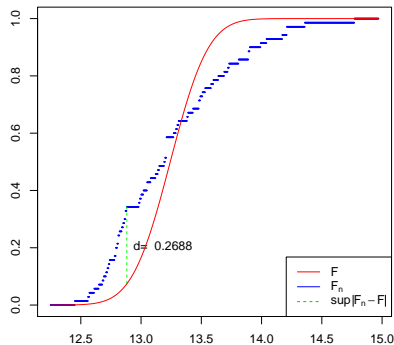

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- Initial vector of parameters
 $\mu = 13.2423, \quad \sigma^2 = 0.2493$
- Optimized vector of parameters
 $\hat{\mu} = 13.1770, \quad \hat{\sigma}^2 = 0.4682$



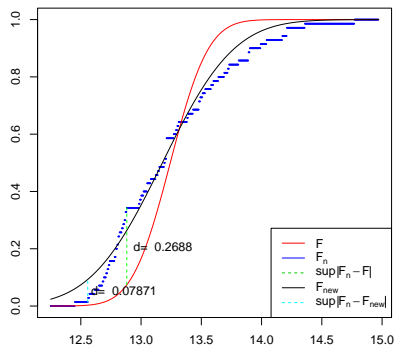
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Glass Type 1, Natrium (Na)

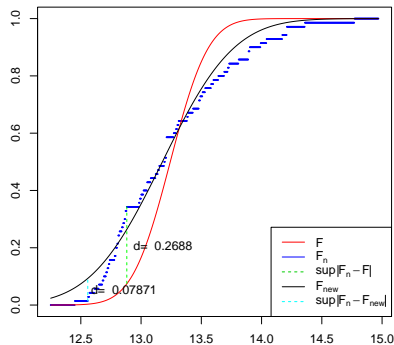
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- $D_n = \sqrt{n} \sup |F_n - F_{new}| = 0.6585$



Glass Type 1, Natrium (Na)

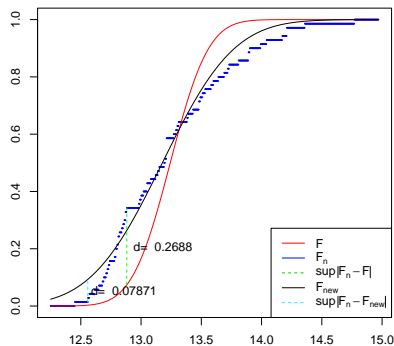
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 $\hat{\mu} = 13.1770, \quad \hat{\sigma}^2 = 0.4682$
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- $c = 1.6276$



Glass Type 1, Natrium (Na)

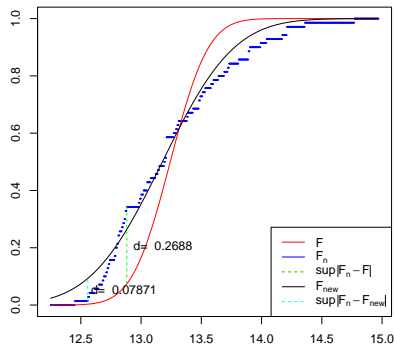
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- $D_n < c \implies H_0$ **accepted**



Glass Type 1, Natrium (Na)

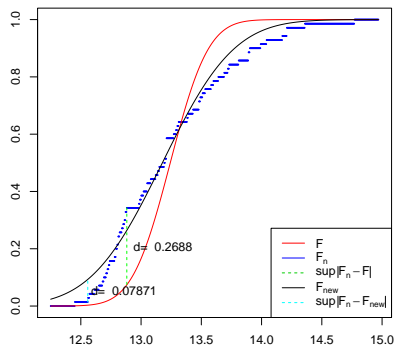
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- $\implies \mathbb{P} = \mathbb{P}_0$



Glass Type 1, Natrium (Na)

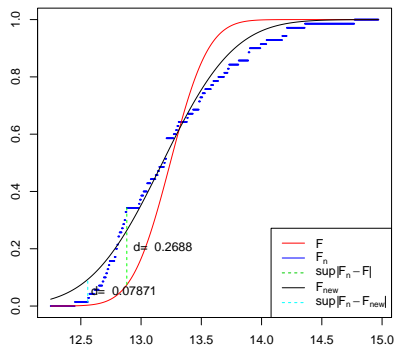
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- $c = 1.6276$
- $D_n < c \implies H_0$ **accepted**
- $\implies \mathbb{P} = \mathbb{P}_0$
- \implies **data normally distributed!**



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

Improved Kolmogorov-Smirnov Test Results

Results of Improved KS 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

Quantitative Methods for Normality Testing

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Fe	4.68	0.01	1.63	< 1.0e-15	yes

- 5 variables are normaly distributed (RI,Na,Al,Si,Ca)

Quantitative Methods for Normality Testing

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Fe	4.68	0.01	1.63	< 1.0e-15	yes

- 5 variables are normally distributed (RI,Na,Al,Si,Ca)
- 4 variables are not (Mg,K,Ba,Fe)

Quantitative Methods for Normality Testing

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Fe	4.68	0.01	1.63	< 1.0e-15	yes

- 5 variables are normally distributed (RI,Na,Al,Si,Ca)
- 4 variables are not (Mg,K,Ba,Fe)
- The best statistics test value for Al

Quantitative Methods for Normality Testing

Improved Kolmogorov-Smirnov Test Results

Results of Improved KS 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
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Fe	4.68	0.01	1.63	< 1.0e-15	yes

- 5 variables are normally distributed (RI,Na,Al,Si,Ca)
- 4 variables are not (Mg,K,Ba,Fe)
- The best statistics test value for Al
- The worst statistic test value for Fe

Quantitative Methods for Normality Testing

Test Results:

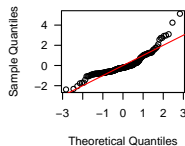
variable	rejected
RI	no
Na	no
Mg	yes
Al	no
Si	no
K	yes
Ca	no
Ba	yes
Fe	yes

Quantitative Methods for Normality Testing

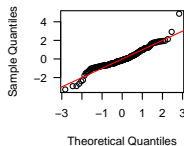
Test Results:

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

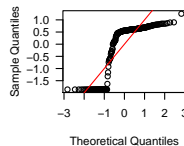
QQ-Plot of RI



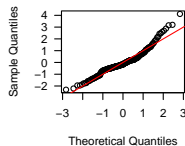
QQ-Plot of Na



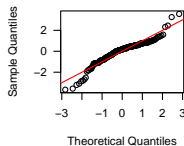
QQ-Plot of Mg



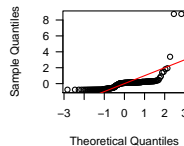
QQ-Plot of Al



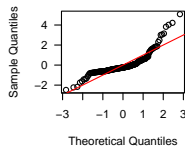
QQ-Plot of Si



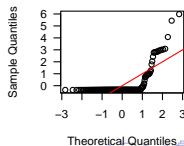
QQ-Plot of K



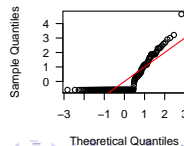
QQ-Plot of Ca



QQ-Plot of Ba



QQ-Plot of Fe



Outline

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- Normality as a requirement for statistical methods
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② Normality Testing

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 - Shapiro-Wilk Test
 - Pearson's Chi-Squared Test
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③ Transformation to Normality

- Box-Cox Transformation
- Transformation Results Testing

④ Summary

Box-Cox Transformation

Transformation Results Testing

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