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

Data Set Overview

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Q-Q-Plots

Sample:

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

Empirical quantiles:

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

Theoretical quantiles:

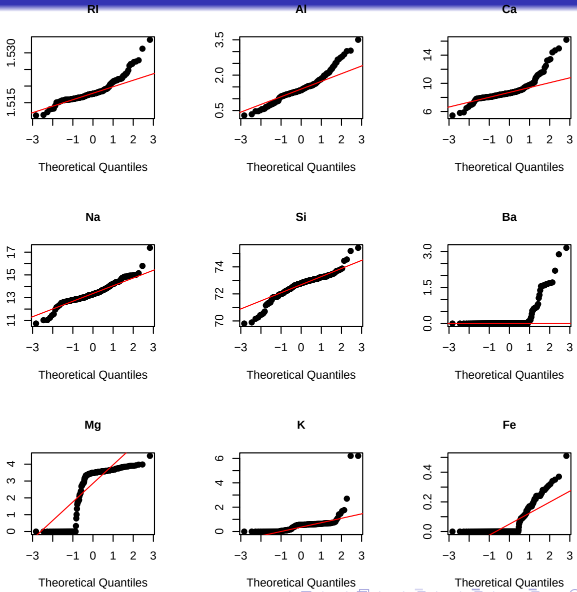
$$q_{(j)} = \Phi^{-1}(p_{(j)}),$$

where

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

Φ - $N(0,1)$ c. d. f. .

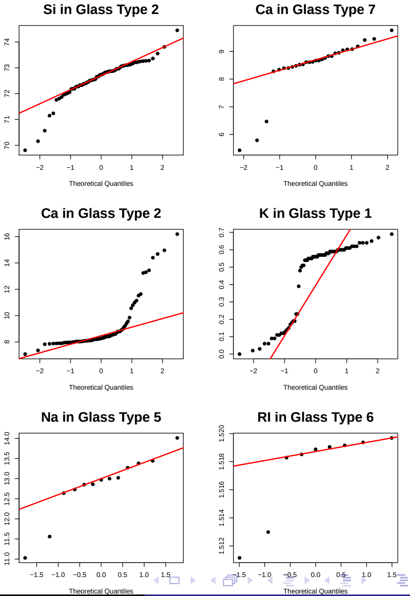
$\Longrightarrow$ Plot $x_{(i)}$ against $q_{(i)}$



Q-Q-Plots

QQ-Plots of the subdatasets:

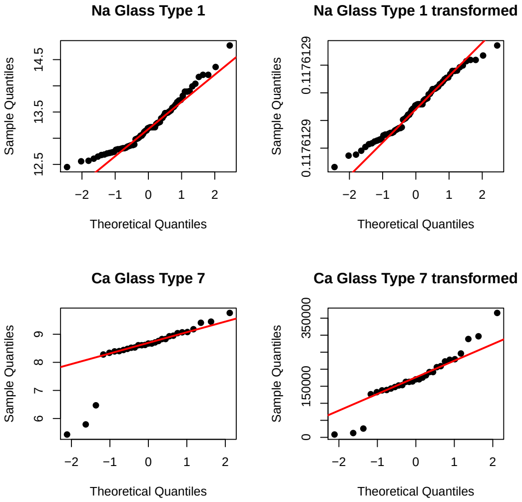
- Variables could be normally distributed within the subclasses
- For some cases there appear to be a linear relationships
- For other cases a linear relationship is questionable
- In some subdatasets a linear relationship seems plausible, however n is very small



Q-Q-Plots

Results of the Transformation of the Full Dataset :

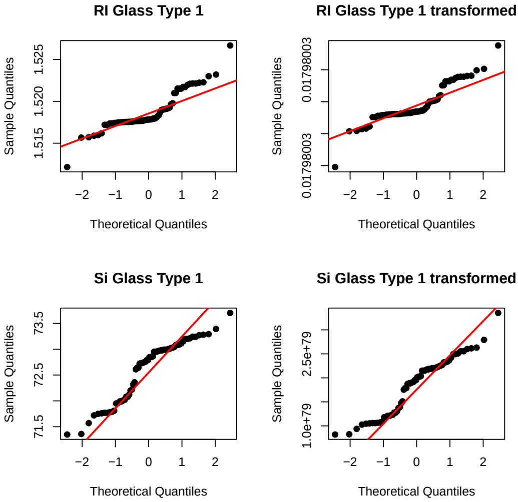
- For some of the cases there seems to be a slight improvement
- For non-unimodal cases the transformation does not show significant improvements towards normality



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
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Graphical Methods for Normality Testing
Chi-Square Plot

Quantitative Methods for Normality Testing

Pearson's Chi-Squared Test

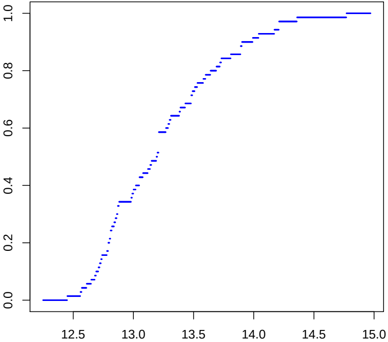
Quantitative Methods for Normality Testing
Kolmogorov-Smirnov Test

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

Definition

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

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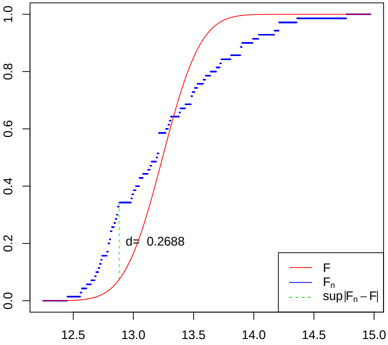
$F(x)$ - theoretical normal c. d. f. with

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



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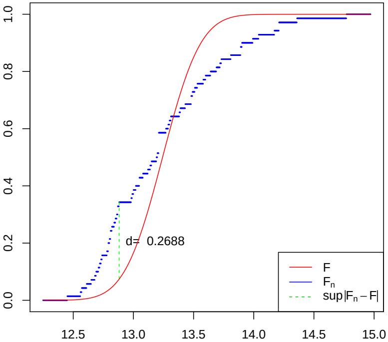
$$d = \sup_{x \in \mathbb{R}} |F_n(x) - F(x)|$$

- distance between them.



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KS test statistics:

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

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

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- $\forall t > 0 :$

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

Quantitative Methods for Normality Testing

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

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

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

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

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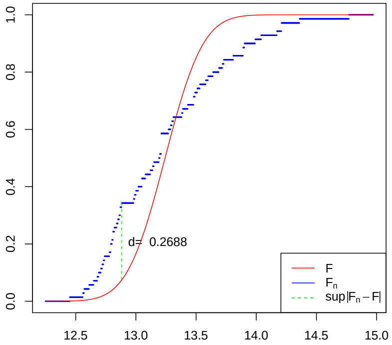
Example:



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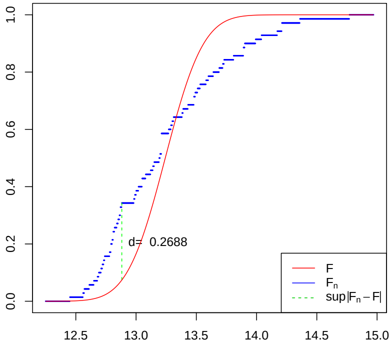
Example:

- $n = 70$



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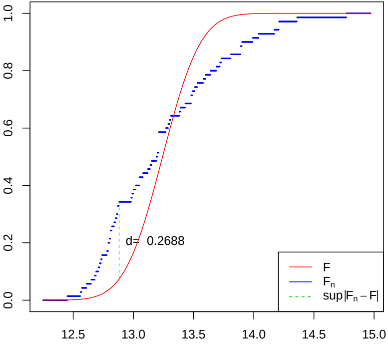

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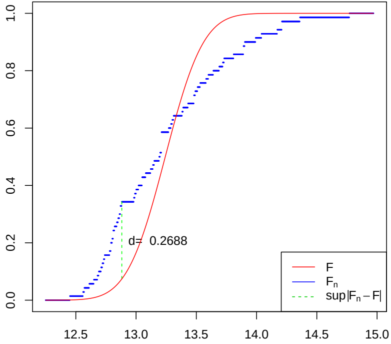
- $\alpha = 0.01$

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



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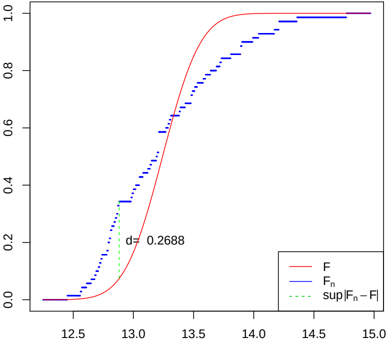
  $\implies c = H_{1-\alpha} = 1.6276$
- $D_n > c \implies H_0$ rejected



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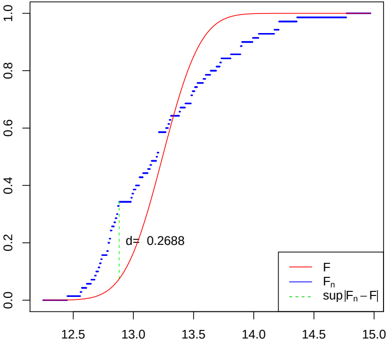
- $\implies \mathbb{P} \neq \mathbb{P}_0$



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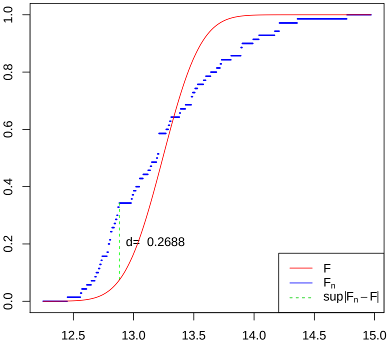
- $\implies \mathbb{P} \neq \mathbb{P}_0$
- $\not\Rightarrow$ data not normally distributed!!!



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Quantitative Methods for Normality Testing

Improved Kolmogorov-Smirnov Test

KS test is improved by solving the following optimization problem

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

R code used:

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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
```

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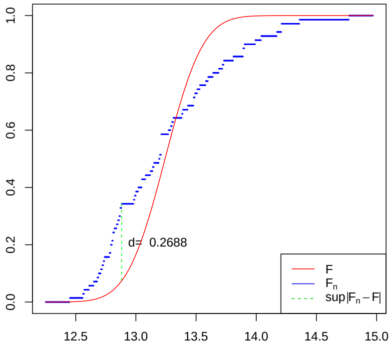
- Initial vector of parameters
  $\mu = 13.2423, \quad \sigma^2 = 0.2493$
- Optimized vector of parameters
  $\hat{\mu} = 13.1770, \quad \hat{\sigma}^2 = 0.4682$



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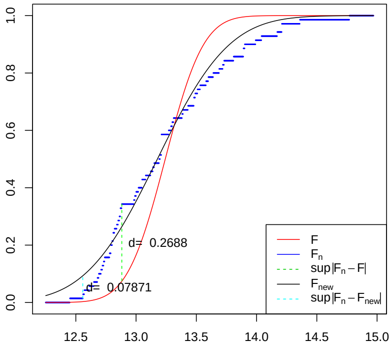


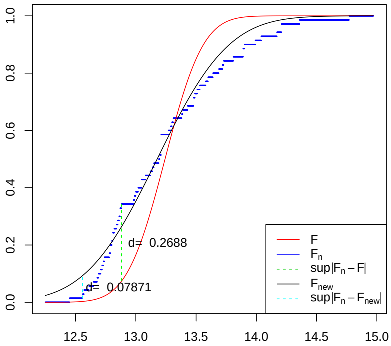
Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing
Improved Kolmogorov-Smirnov Test

KS test is improved by solving the following optimization problem

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

- Initial vector of parameters
  $\mu = 13.2423, \quad \sigma^2 = 0.2493$
- Optimized vector of parameters
  $\hat{\mu} = 13.1770, \quad \hat{\sigma}^2 = 0.4682$
- $D_n = \sqrt{n} \sup |F_n - F_{new}| = 0.6585$



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing
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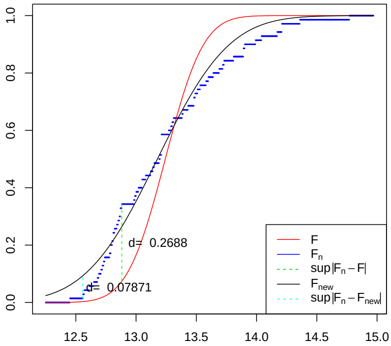
- $c = 1.6276$



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

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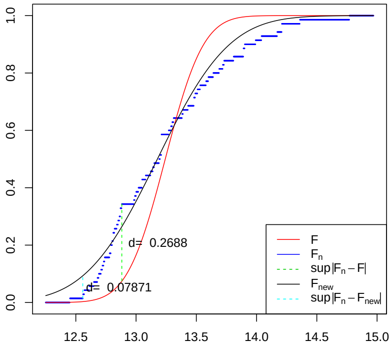
- $c = 1.6276$
- $D_n < c \implies H_0$ accepted



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

Improved Kolmogorov-Smirnov Test

KS test is improved by solving the following optimization problem

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

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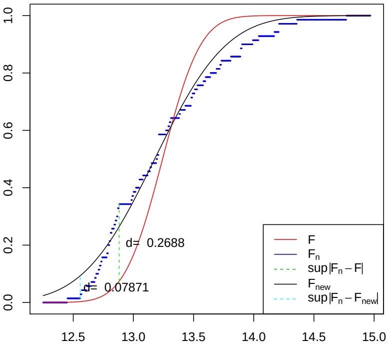
- $\implies \mathbb{P} = \mathbb{P}_0$



Glass Type 1, Natrium (Na)

Quantitative Methods for Normality Testing

Improved Kolmogorov-Smirnov Test

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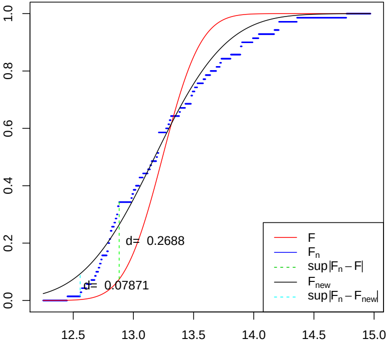
- $c = 1.6276$
- $D_n < c \implies H_0$ accepted
- $\implies \mathbb{P} = \mathbb{P}_0$
- $\implies$ data normally distributed!



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

Quantitative Methods for Normality Testing

Improved Kolmogorov-Smirnov Test Results

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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)
- 4 variables are not (Mg,K,Ba,Fe)

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
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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)
- 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 normaly 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

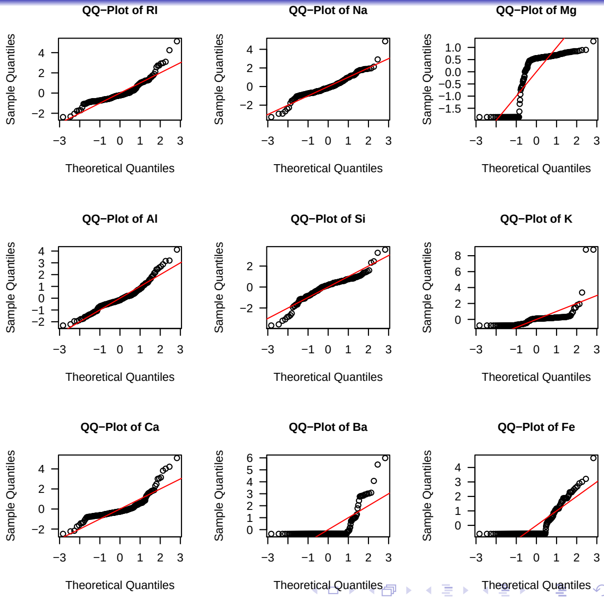
Test Results:

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



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   - 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

Box-Cox Transformation

Transformation Results Testing

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