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BOOTSTRAPPING TECHNIQUE AND CONFIDENCE INTERVALS

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Abstract: This article evaluates methods of computing confidence intervals and values of descriptive statistics, capability and performance indexes with the help of conventional procedures, statistical SW, and the method of generating random subgroups. Comparison of different methods has shown that there are differences between the results obtained by SW and those obtained by manual computing. Alternative estimation of values and confidence intervals by means of bootstrapping technique is discussed.

Keywords: confidence interval, bootstrapping technique, performance index.

1. INTRODUCTION

The distribution of measured data is only a sample distribution, which should represent an overall population. It is, therefore, necessary to complete the calculations from the sample distribution with confidence intervals. The width of a confidence interval characterizes the accuracy of the estimate. A wide confidence interval indicates that the estimate is not accurate.

In this article we briefly describe confidence intervals of basic estimates for the mean, median and standard deviations that are valid if the distribution is well known. Alternatively, a principle of naïve bootstrapping is introduced as a random resampling technique. The results of estimates of calculation and resampling are compared. Because of good correspondence of the results, bootstrapping is then used for estimating of confidences for Ppk (critical performance index) that cannot be calculated directly. The basic concept of SPC (Statistical Process Control) is introduced. The level of quality is evaluated with the help of capability and performance indexes. The correct estimate of these indexes and confidences strongly depends on the correct estimate of the standard deviation. Two types of variability are discussed and their impact on results in process capability analysis is demonstrated.

For precise evaluation it is possible to use many mathematical or statistical tools in available SW. The data user receives the required result very quickly, but cannot be sure if it is correct.

In this project, results from statistical SW and manual computation of the mean, median, standard deviation, capability and performance indexes and confidence intervals are compared. For computation, the valid formulas, available statistical SW and slightly unusual procedure of random resampling called bootstrapping technique were used. The bootstrapping technique was created in the C++ programming language considering no limits for data size.

Statistical software computes the required statistics with no respect to the basic presumptions of normality, stability, homogeneity, symmetry, etc. The result may be incorrect. In one statistical SW fundamental discrepancy between evaluating long and short-term capability was found. Various computation methods are used in different kinds of SW, confidence intervals are missing, numerical results are not exactly the same and the interpretation of results depends only on the data user and his expertise.

Data analysis must be completed with graphical output, the applied procedure must be mentioned and with the respect to differences in the results obtained by SW, the applied type and version of statistical SW must be declared.

2. PURPOSE

As it is shown in Tab. 1, the output from the analysis of process performance for the same data set is not the same in one type of statistical SW. The difference is significant.

Tab. 1 Calculation of Performance Index (for the same example)

SW	Pp
MS Excel	1,00132
QC.Expert 2.5	1,64862
STATISTICA 6.0	1,00132

SW STATISTICA 6.0 does not compute the confidence intervals. SW QC.Expert 2.5 presents a very high value of Pp because of the different type of estimated variability. The manual computation in MS Excel is quite difficult and it is possible to make mistakes. If the distribution is skewed, the confidence intervals are not symmetric and the traditional approach fails. The simple example shows that it is not possible to rely on the results of statistical SW without any risk. As an alternative procedure for the computation of performance index, critical performance index and their confidence intervals, the bootstrapping technique was used and the results were compared in examples with several shapes of distributions.

3. METHODS

Because the distribution from input data is only a sample distribution, the estimate of any statistic should be completed with confidence intervals. The result with the confidences tells us that our estimate is correct with high probability in a small area.

Fig. 1 shows PDF (Probability Density Function). The shape in this example corresponds with the Laplace-Gauss (Normal) distribution. For a simple estimate of the basic statistics obtained by conventional procedures the sample distribution estimated from the measured data should be similar. The best estimate for the mean of distribution is the arithmetic average, which is the same as the median and modus if the data are normally distributed. The position of these statistics is situated on the peak of the bell curve (see Fig. 1 N(0; 1)).

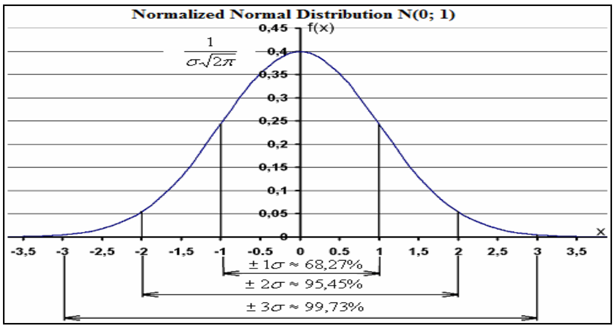

Fig. 1 Normalized Normal Distribution N(0; 1)

The formula for the two-side confidence interval of the mean (if the variability is unknown):

$$\bar{x} - s\frac{t_{1-\alpha/2;(n-1)}}{\sqrt{n}} \leq \mu \leq \bar{x} + s\frac{t_{1-\alpha/2;(n-1)}}{\sqrt{n}} \qquad (1)$$

$\bar{x}$ … Arithmetic average

s … Estimated sample standard deviation

n … Number of sample data

μ … Unknown central value

α … The level of confidence

$t_{1-\alpha/2;(n-1)}$ … Probability points of t-distribution

The estimate of median confidence interval is quite difficult. Formula (2) is one possible nonparametric estimate [3]:

$$\tilde{x} - s_{\tilde{x}}.t_{1-\alpha/2,(n-1)} \leq \tilde{x} \leq \tilde{x} + s_{\tilde{x}}.t_{1-\alpha/2,(n-1)} \qquad (2)$$

$$s_{\tilde{x}} = \frac{\tilde{x}_{(n-k+1)} - \tilde{x}_{(k)}}{2.u_{\alpha/2}}$$

$$k = \frac{n+1}{2} - |u_{\alpha/2}|.\sqrt{\frac{n}{4}}$$

$\tilde{x}$ … Median

$u_{\alpha/2}$ … Probability points of normalized Normal distribution

For the estimate of data variability, standard deviation is used. This characteristic tells us what amount of data is concentrated in proportional interval; see Fig (1). It is not possible to use the confidences of standard deviation (3) if normality is rejected.

$$\left[\frac{(n-1)s^2}{\chi^2_{\alpha/2;n-1}}\right]^{1/2} \leq \sigma \leq \left[\frac{(n-1)s^2}{\chi^2_{(1-\alpha/2);n-1}}\right]^{1/2} \qquad (3)$$

Of course similar procedures for the estimate of other statistics have been described in available literature [1], [3], [5]. Each estimate depends on the shape of the source distribution.

The main idea of the bootstrapping technique [1], [7] is based on random resampling of the source data set. The random samples are generated from the measured data and these samples are situated in subgroups, see Tab. 2.

The basic idea is to get more information from the source data set after resampling with replacement. Tab. 2 shows the concept of resampling with replacement (naïve bootstrapping). For simplicity the input data are only figures from 1 to 5.

Tab. 2 Illustration of Bootstrapping (n=5)

Input data	1	2	3	4	5	Mean	Sorted Mena
1st subgroup	1	3	2	1	5	2,4	2,2
2nd subgroup	5	2	2	4	3	3,2	2,4
3rd subgroup	4	1	3	1	2	2,2	3,2
etc.	.	.	.	.	.	.	.

Each sample contains only input data. Some figures are repeated in one subgroup, some are omitted in another. From each subgroup the desired statistics (e.g. mean, critical performance index, standard deviation etc.) are computed. Then these results are ranked. For 30000 subgroups there are 30000 ranked statistics. If the resampling is correct, the 90% confidence interval of the desired statistic is result value of ranges from 1500 to 28500, for the 95% confidence interval ranges from 750 to 29250.

Fig. 2 shows the estimated distribution (histograms) from the first nine unsorted subgroups (*n = 20; B = 800*).

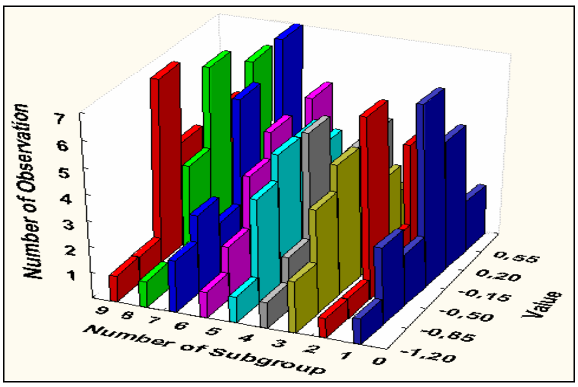

Fig. 2 Histograms from Bootstrap Subgroups

Fig. 3 shows upper part of distribution from averages (negative-exponential smoothing) of unsorted subgroups in other example ($n = 100; B = 1200$).

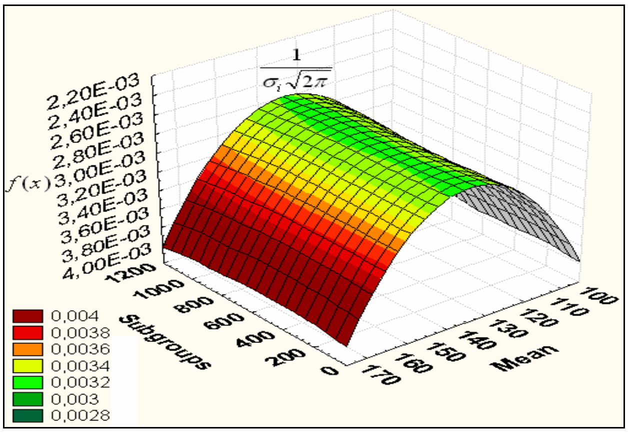

Fig. 3 Upper Part of Estimated Distribution (STATISTICA 6.0)

The number of figures n in each subgroup usually equals the number of figures in source data. The number of simulated subgroups B depends on the number of source data. A simple estimate for sufficient number of subgroups is given by next formula [7]:

$$B = 40.n \tag{4}$$

B … Number of subgroups (bootstrap simulations)
n … Number of input data

The error of the bootstrapping technique is the difference between the real and estimated distribution. It consists of two factors. The first one is a statistical error that depends on the number of source data and, of course, on data correctness. This type of error cannot be eliminated by the bootstrapping technique. The second one is the simulation error (insufficient randomness or scarcity of bootstrap subgroups). This type of error can be reduced by increasing the number of subgroups. Formula (4) is optimal recommendation with respect to the number of computation and related computing demands (time, computer performance, etc.). The final number of bootstrap subgroups B depends on the operator's choice and it can be higher. We used 30000 bootstrap subgroups for all computations. The results of estimated statistics from each bootstrap subgroup are sorted. Then it is possible to determine the confidence intervals (as shown in the Fig. 4, Fig. 5 and Fig. 6) that are valid for symmetrical PDF. Fig. 4 shows the sorted results from the estimate of the mean and its confidences. The result has a very good correspondence with the manual calculation (see Results). Fig. 5 shows the output from the estimate of the median and its confidences. The output is accurate again. In Fig. 6 the bootstrap simulation of sample standard deviation is shown. If the PDF is systematically skewed, the better estimate of central value is the median which is resistant to outliers and is robust to disturbance of normality. The parametric bootstrap provides a more precise estimate of the central value for the asymmetric shape of distributions [7]. For our purpose naïve bootstrapping is sufficient.

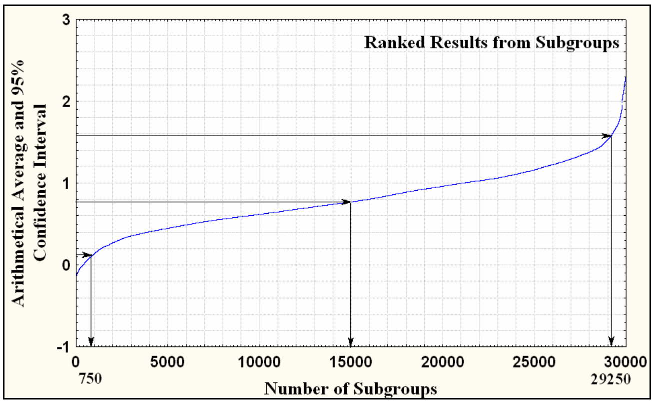

Fig. 4 Result Curve from 30000 Simulated Subgroups (Mean)

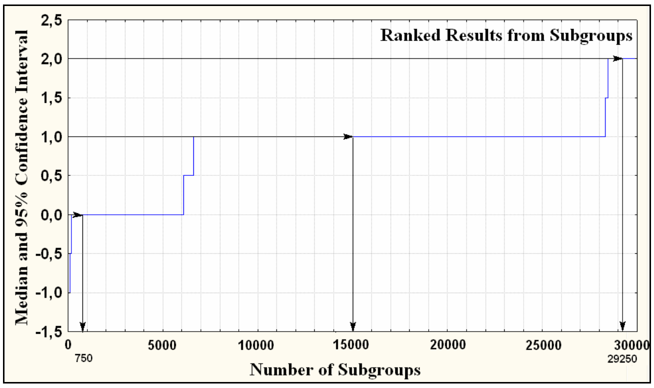

Fig. 5 Result Curve from 30000 Simulated Subgroups (Median)

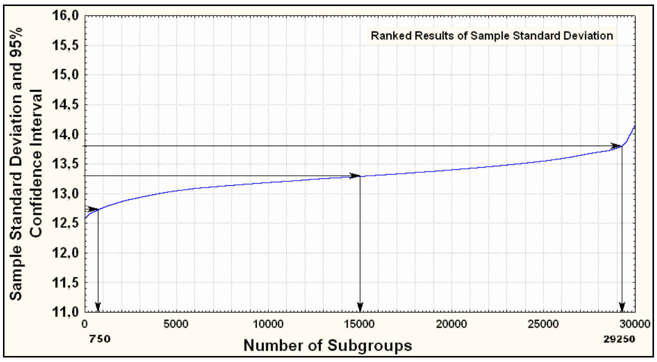

Fig. 6 Result Curve from 30000 Simulated Subgroups (St. Dev.)

In SPC the process characterized by measured data needs to be stable and predictable. Corrective actions are accepted for the stability and predictability of measured data. This means that the process is adjusted so that the data are centered between the upper and lower specification limits (USL, LSL). The input data should correspond to normality, homogeneity, etc. There are eight conditions called assignable causes [1], [6] for the stable and predictable process. Breaking any of these conditions indicates that something highly improbable has happened. The process becomes unstable and unpredictable. How well the data meet the specifications is expressed with the help of process capability and performance indexes (Cp, Pp). In addition to Cp and Pp the critical values (Cpk, Ppk) indicate how well the process of measured data is centered. For higher values of the indexes, reduction of variability is very important. Variability can be understood as a metric of quality and standard deviation as a metric of variability. It means the metric of process capability or product character. With respect to the measured data we distinguish the short-term variability (inherent or within sample variability) and long-term variability (overall or between samples variability). The first one is estimated from a short period of time and includes a minimal amount of noises and process changes. The second one covers the whole process of measuring with all changes and shifts. The capability index is correctly determined from short-term variability. The performance index is determined from overall variability. Both indexes compare the defined and real standard deviation. It stands to reason that the capability index is greater than or equal to the performance index. So the capability index represents potential capability if the process does not contain shifts of central value (centralized process). It takes into account keeping the limits of specifications. The Cp controls the variation or difference in series of measured data. If, for instance, a significant autocorrelation is present, the performance index will be low. The Cp depicts how the process could perform relative to the specification if shifts are eliminated. The Pp depicts how the process is actually performing relative to the specifications. It is estimated only from the standard or sample standard deviation. A significant difference between Cp and Pp indicates that the process is out of control or the source of variability is not covered by short-term (within) variability. The process is not under control with respect to the specifications if Cp or Pp is lower than 1. Minimal requirement for capable process is usually 1.33. The following figures show the difference between classical and critical indexes.

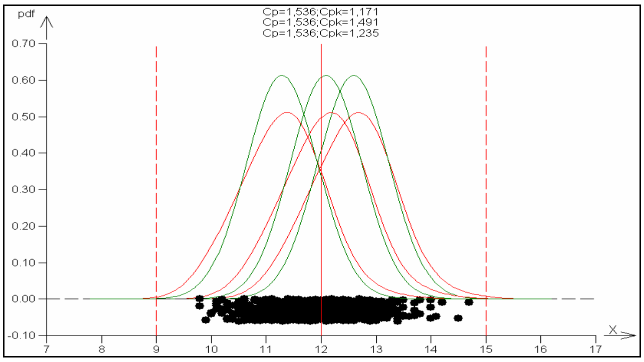

Fig. 7 Three Different Processes with the Same Cp (QC.Expert 2.5)

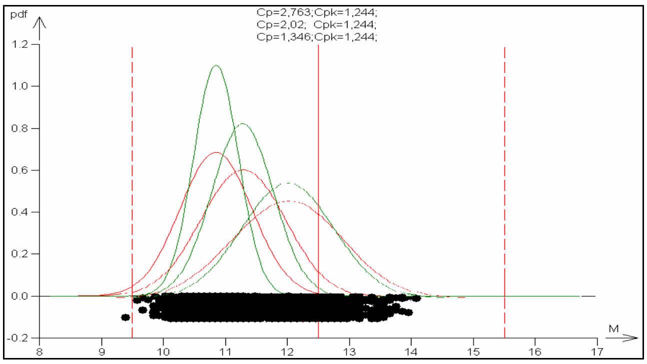

Fig. 8 Three Different Processes with the Same Cpk (QC.Expert 2.5)

The green lines are the Gaussian PDF, the red lines depict an estimates of PDF from measured data. It is obvious that if the process is not centered, the value of Cpk declines. If the measured data are outside specification limits, Cpk can be negative. If the process is centered, Cp and Cpk are equal. The Cp and Cpk have higher value if the process has low variability (it can be proved by higher kurtosis). In the same way, it is possible to explain and interpret the performance index and its critical values. Fig. 7 and Fig. 8 were created in QC.Expert 2.5.

The following formulas characterize the estimate of variability in the sequence of measured data. Its correct type is essential for the computing capability or performance indexes. These types of standard deviation (within variability) are valid for the estimate of the process capability index [1].

$$s_{(within)} = 1{,}047.\tilde{R} \tag{5}$$

$\tilde{R}$ ... Median of moving averages

$$s_{(within)} = \frac{\overline{MR}}{d_2} = \frac{\overline{MR}}{1{,}128} \tag{6}$$

$\overline{MR}$ ... Moving average between two consecutive measured data

d_2 ... Tabulated value 1.128 in ČSN ISO 8258 for subgroup of 2

The calculations of standard deviations in formulas (5) and (6) are only valid for a sequence of measured data. Other procedures are valid for data organized in subgroups. As is clear from the previous formulas, within variability strongly depends on the sequence of measured data (it uses moving averages). If the characteristic sequence is broken, the moving averages are entirely different. Resampling with replacement breaks the characteristic sequence and changes short-term variability. The naïve bootstrapping provides incorrect estimates of Cp, Cpk and their confidence intervals in this example. In this case it is possible to use "subsampling", which solves the problem with data sequence [7]. Nevertheless, the naïve bootstrapping provides a reliable estimate of overall variability, performance index Pp and critical Ppk and their confidences. The sample standard deviation (7) is used for the estimate of overall variability. It is used for the estimate of the performance index. This index takes into consideration the periodicity of the process that is caused for instance by tool abrasion.

$$s_{(between)} = \sqrt{\sum_{i=1}^{n} \frac{(x_i - \bar{x})^2}{n-1}} \tag{7}$$

The performance index and confidence interval are computed from the following formulas [1], [3].

$$Cp = \frac{USL - LSL}{6.s_{(within)}}; \qquad Pp = \frac{USL - LSL}{6.s_{(between)}} \tag{8}$$

$$\hat{P}p\sqrt{\frac{\chi^2_{1-\alpha/2;n-1}}{n-1}} \leq Pp \leq \hat{P}p\sqrt{\frac{\chi^2_{\alpha/2;n-1}}{n-1}} \qquad (9)$$

But this index does not take into account the process position. To achieve this, it is necessary to determine critical index (10). The interpretation of Pp and Ppk corresponds with Figs.7 and 8.

$$P_{pk} = \min\left[\frac{USL-\mu}{3\sigma};\frac{\mu-LSL}{3\sigma}\right] \qquad (10)$$

The estimate of the confidence interval for Ppk is quite difficult. It is not possible to use any time valid procedure directly. Some approximations by Kushler, Hurley, Franklin or Wasserman are mentioned in [3]. In this case the bootstrapping is very simple and suitable technique. It provides stable and relevant estimates for values and confidences of mean, median, standard deviation and performance indexes as is proved in the next section.

The bias occurred in the results of the Pp or Ppk estimate from bootstrapping. For correcting the bias it is necessary to use bias correction. In this project Efron´s bias correction presented in [1] was used. Because the central value of the estimated characteristic is not situated in the middle of the sorted results from bootstrapping, the correction shifts the value and both confidence intervals. The computation is performed with the help of Z_0-values in Standardized Normal distribution, the 95% confidence interval was used in all computations.

4. RESULTS

The first experiment with the bootstrapping technique was done to estimate the value and confidence intervals for the mean, median and standard deviation. The source data set contained 1000 data. The ranked results of the arithmetical averages from 30000 generated subgroups are shown in Fig. 4, the ranked results of the medians are shown in Fig. 5, results of the sample standard deviation are shown in Fig. 6. The values marked by arrows in the pictures displayed a good correspondence to manual calculations and conventional estimation for input data. Tab. 3 represents the output of data analysis and bootstrap simulations of the same data. The data were normally distributed (proved by histogram, Chi-square test, Kolmogorov-Smirnov one-sample test for normality, skewness and kurtosis).

Tab. 3 Estimates of the Mean, Median and Standard Deviation

	SW Calculations			Bootstrapping		
Parameter	Value	Lower	Upper	Value	Lower	Upper
Mean	0,799	0,026	1,624	0,798	0,073	1,602
Median	1,000	-0,001	2,001	1,000	0,000	2,000
St. Dev.	13,290	12,732	13,900	13,298	12,725	13,812

The other results were obtained from capability analysis in SPC. As was already mentioned, this type of analysis is frequently used in quality control. Fig. 9 shows the control charts X-individual and R (Ranges) from the process of measured data. The red lines represent upper and lower control limits. In this example there was a lack of data. For only 20 data it is not possible to reliably check all eight out-of-control conditions. Question was whether the results of bootstrapping and of conventional computation would be significantly different. Tab. 4 shows results from the estimate of the central value, lower and upper confidence limit for the above mentioned characteristics. Estimates of simulations were done with Efron’s bias correction.

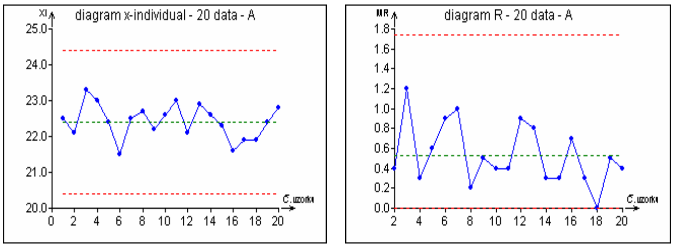

Fig. 9 SPC – Control Chart X-individual and R (QC.Expert 2.5)

Only 20 data were available for the estimate of process quality level. But the results of computations and bootstrapping presented in Tab. 4 correspond well.

Tab. 4 Comparative Results from Calculations and Bootstrapping

Calc. of Descriptive Statistics			
Char.	Value	Lower	Upper
Mean	22,4150	22,1922	22,6378
Median	22,4500	22,1955	22,7045
St.dev	0,4760	0,3620	0,6953
Pp	1,4005	0,9589	1,8415
Ppk	1,3900	0,9480	1,8319

Estimates from Simulations			
Char.	Value	Lower	Upper
Mean	22,4350	22,2300	22,6300
Median	22,5000	22,2000	22,7000
St.dev	0,4568	0,3253	0,5799
Pp	1,4005	1,0897	1,8191
Ppk	1,3900	1,0907	1,9148

The bias correction presented in [1] is necessary for estimate of the confidence interval for performance indexes. In Fig. 10 the ranked results of the performance index without bias correction are shown. The same results after bias correction are presented in Fig. 11. Figures were created in MS.Excel. Horizontal blue lines represent the values of the performance index, upper and lower limits calculated in QC.Expert and MS.Excel (preset $\alpha = 5\%$).

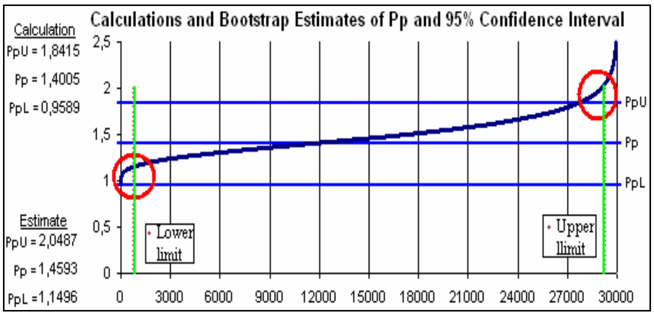

Fig. 10 Pp and Confidence Interval without Bias Correction

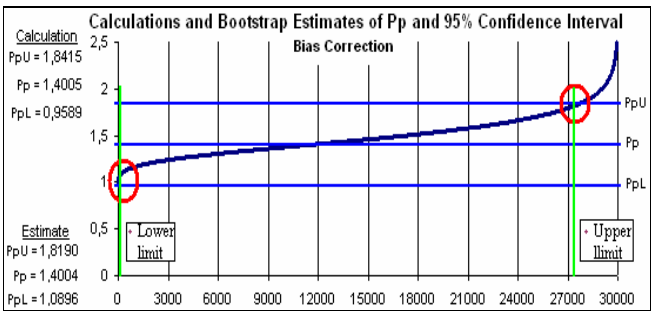

Fig. 11 Pp and Confidence Interval after Bias Correction

The concave-convex curve represents the results from bootstrapping. The vertical green lines enclose the 95% confidence interval. It is clear from the pictures that, after bias correction, the curves of bootstrapping and confidence limits intersect approximately only at one point. This indicates conformity of results from computations and bootstrapping. As was already mentioned, the 95% confidence interval from 30000 simulations in bootstrapping is in the range from 750 to 29250. The bias correction changes this interval. The new range for the 95% confidence interval of Pp was obtained from the sorted simulation number of 153 to 27358.

The central values and the width of bootstrap confidence intervals were compared with the results from calculations in simulated examples. There were 50 examples in the first project. Each example contained only 30 data with approximately Gaussian distribution N(0; 1). The following figures show how the results of two methods are differed. The black curves represent the bootstrapping estimates, the other colors represent the results of calculations. We compared the basic statistics (mean, median, standard deviation) and the performance indexes (Pp, Ppk) after Efron's bias correction. As is obvious, there is a strong correlation and a good correspondence between the results.

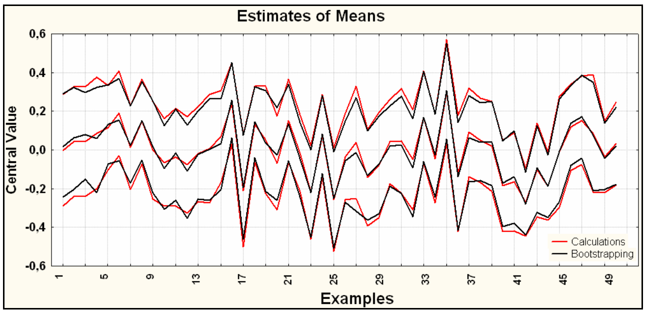

Fig. 12 Estimates of Means and Confidences

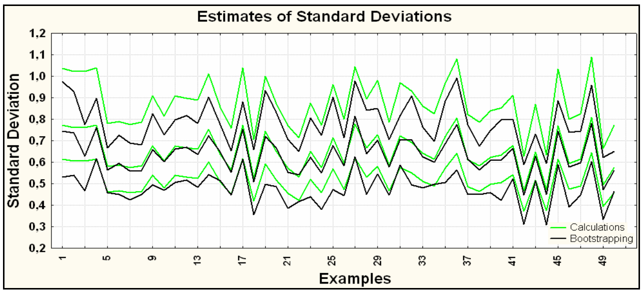

Fig. 13 Estimates of Standard Deviations and Confidences

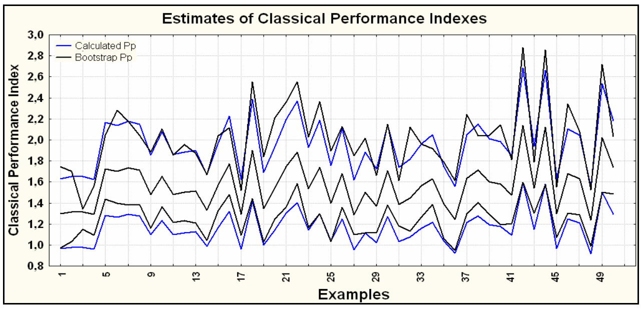

Fig. 14 Estimates of the Performance Indexes and Confidences

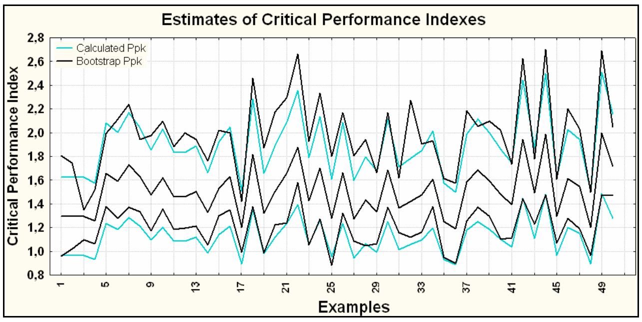

Fig. 15 Estimates of Critical Performance Indexes and Confidences

Figs. 16 and 17 show the estimates of central values and confidence intervals of log-normal distribution LN(20; 2) in the second project. As was mentioned, the median provides a better estimate of central values of skewed distributions. The results of simulations (medians) were compared with the estimates of Box-Cox and exponential transformations. A good correspondence of results exists in the central value estimates (Fig. 12), but the comparison of the confidence intervals (Fig. 13) shows that there is a significant difference. In this case the parametric bootstrapping provides better results [7]. Each example contained 60 data.

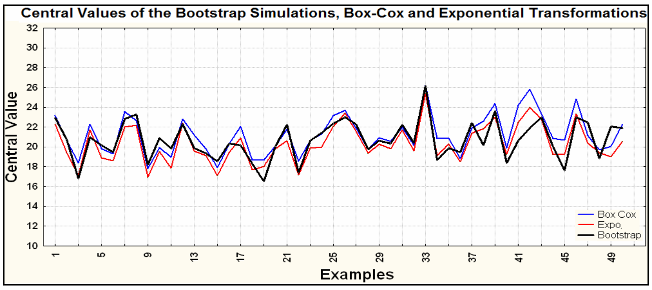

Fig. 16 The Estimates of Central Value in 50 Examples of Log-normal Distribution (bootstrapping, Box-Cox and exponential transformation)

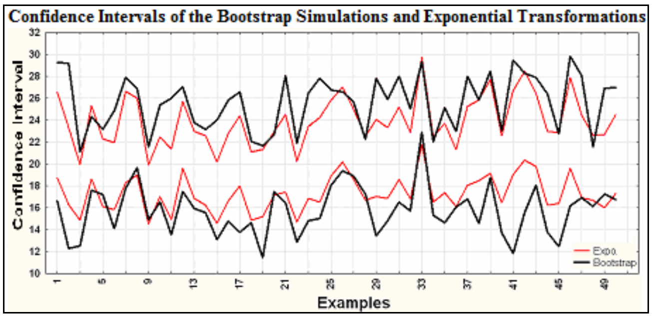

Fig. 17 The Estimates of Confidence Intervals (the same examples)

The difference between the bootstrap estimates and calculations of confidence intervals is strongly influenced by the kurtosis of input data. This result was discovered by significant correlation coefficients r ($\alpha = 5\%$) (Tab. 5).

Tab. 5 Kurtosis and Its Influence on Differences of Results

Difference between simulations and computations	r=f(Kurt.)
PpkU (Bootstrap) - PpkU (Computation)	0,86
PpkU (Corrected Bootstrap) - PpkU (Computation)	0,72
PpkL (Corrected Bootstrap) - PpkL (Computation)	-0,85
PpkL (Bootstrap) - PkpL (Computation)	-0,67

The difference between upper confidence limits increases with higher kurtosis of input data. The difference between lower confidence limits decreases with higher kurtosis of input data.

5. DISCUSSION

The size of subgroups is very important. The same size of subgroup as is the number of figures in the source data set was proved as the best size selection. The number of simulations (the number of subgroups) is optional, but the choice depends on the input data size. Resampling with replacement is a simple method that provides reliable results of estimates of basic descriptive statistics (controlled were the mean, median and standard deviation) and the estimates of performance and critical performance indexes that are determined with the help of long-term variability. The naïve bootstrapping is not suitable for the estimate of short-term variability. In this case it strongly depends on the data sequence and the calculation is based on moving averages. If the data set is resampled, the result is incorrect. The time needed for thousands of simulations may be quite long. Bootstrap is suitable for the estimation of long-term capability (performance index), especially for its lower confidence limit, which is more important. For a greater number of generated subgroups, the results are generally more accurate because the error of insufficient randomness is eliminated. The bias correction eliminates inaccuracies in bootstrap estimates of performance indexes. The confidence interval of the sorted results is adjusted.

If the input data do not fit the Normal distribution, the naïve bootstrapping provides only raw estimates. The results of resampling are influenced by the kurtosis and the number of input data. Bootstrapping technique is not resistant to outliers.

In SPC it is very important to control the confidence intervals of estimated statistics. If someone needs to be sure that the level of quality is not lower than required 1.33, it is necessary to produce quality where the lower confidence interval is greater than established 1.33. The required level 1.33 is only an estimate of central statistics. If this level is to be maintained, the lower limit of the confidence interval should be controlled.

As was mentioned earlier, the required level of process capability is not lower than 1.33. This value varies with time and depends on the type of process which the data come from. Some companies have reached process quality level more than 2.

The concept of long and short-term variability is not unified. As was already shown, it is possible that some kinds of SW compute quality characteristics in a different way. Later it was proved that the new version of QC.Expert 3.0 accepts the above mentioned approach in long-term and short-term variability and the estimated capability and performance indexes correspond to the conventional manual computations.

Results of any data analysis have to be completed with a graphical report; numerical results alone cannot provide a sufficient overview of all process characteristics. In SPC the capability and performance indexes need to be completed with control charts. One figure alone cannot tell us everything about the controlled process, the shape of distribution, trends, heteroscedasticity, outliers, etc. Simultaneously applied methods or procedures should be presented and the specific version and type of SW should be referenced. Statistical software doesn't complete the results with the confidence intervals in all estimates. No essential preliminary analysis is recommended. The bootstrapping technique is a potentially automatic procedure that helps in examples where the basic presumptions do not applied. Nevertheless, the data analysis (in general) and interpretation of results are not automatic processes.

6. CONCLUSION

No commercial bootstrapping technique was used. Original program was created in the C++ programming language. The random numbers (white noise) for random resampling were taken from SW STATISTICA 6.0. The random number generators in STATISTICA 6.0 were verified using the DIEHARD suite of tests, and they passed all the test criteria.

For correct process capability and process performance analysis it is necessary to keep the correct procedures of calculation and estimates and use correct statistics. Firstly the test of normality should be done. If the normality is rejected, it is possible to use transformation (specification limits are transformed too). Procedures introduced in (1), (3), (5-10) are not correct if the normality is rejected. It is not necessary to have an accurate estimate of the index and its confidence interval, but in process capability analysis the biggest emphasis should be placed on the lower confidence limit. The bootstrapping technique provides estimates that are very close to the results of calculations and presents narrower confidences in most of the results.

Because long and short-term variability is not unified in national norms or standards, it depends on the agreement of the parties concerned, which type of variability or which type of procedure will be used for the estimate of the capability or performance index. Both indexes depend on the number of data. With the higher amount of data is better information about the process and its character, but consequently, variability increases.

As was proved in many examples, the bootstrapping technique provides stable results that are not based on normal theory [1]. It is possible to estimate confidence intervals of many statistics even if the source data do not fit normal distribution. Of course, the precision of results depends on the precision of the source data.

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