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Concerns about Least Squares Estimation for the Three-Parameter Weibull Distribution: Case Study of Statistical Software

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Abstract

Least Squares estimation of the 2-parameter Weibull distribution is straightforward; however, there are concerns for the estimation of the 3-parameter Weibull. The third parameter for the 3-parameter Weibull distribution shifts the origin from 0 to some generally positive value sometimes called the location, threshold, or minimum life. The different methods used by the packages sometimes result in fairly major differences in the estimated parameters between the statistical packages. This may have implications for those needing to estimate or apply the results of a 3-parameter Weibull distribution that is used frequently in practice. The results are analyzed based on an experimental design using pseudo-random Weibull data sets.

Key Words: Reliability, Least squares parameter estimation, Weibull

1. Introduction

When performing a statistical test or building a statistical model the analyst generally expects the key statistical results to be the same from different software packages. For example, in linear regression one anticipates obtaining the same equation independent of the software package. Options may vary from one package to another, such as for regression diagnostics and graphics. Similarly, when doing estimation of a distribution's parameters, one might find different goodness of fit tests (e.g., chi-square, Kolmogorov-Smirnov, Cramer von-Mises, Anderson-Darling), and graphical output (e.g., probability plots, empirical distribution functions, P-P plots, Q-Q plots). But one expects the same parameter estimates within rounding.

This expectation is not met for estimation of the 3-parameter Weibull. The 3-parameter Weibull has been documented in the past as a challenge when finding maximum likelihood estimates (MLEs) though such studies were not based on modern statistical software packages until recently. Harper, Eschenbach, and James (2011) highlight fairly major differences in estimated parameters between the statistical packages when maximum likelihood is used. This new article examines the use of least squares (LS) approaches in three statistical packages. Such differences are important as the 3-parameter Weibull distribution is widely used in practice and least squares estimation is the recommended approach under various circumstances in engineering distribution fitting software.

This research began with the use of Minitab for distribution fitting related to oil spill data in the Gulf of Mexico as documented in Eschenbach, Harper (2006) and Eschenbach, Harper, Anderson, Prentki (2010). In using additional statistical software packages, it was noted that the MLEs varied more than anticipated. This led to a literature search as well as the use of multiple software packages. The results of the investigation are documented in

Harper et al (2011). This new article partially follows their MLE work but with LS methods. The MLE article was ambitious in that it compared 10 MLE methods; whereas, only 3 LS alternatives are compared in this article.

2. 3-Parameter Weibull Distribution

This section briefly summarizes the 3-parameter Weibull literature found to be germane to the Weibull differences encountered across statistical packages. One of the challenges of a literature search is keeping track of both the Weibull parameter notation and the terminology. Below are the pdf and cdf used in this article.

$$\begin{aligned} \text{pdf, } f(x) &= \beta \alpha^{-\beta} (x - \gamma)^{\beta-1} e^{-((x-\gamma)/\alpha)^\beta} \text{ for } x > \gamma; \text{ 0 otherwise.} \\ \text{cdf, } F(x) &= 1 - e^{-((x-\gamma)/\alpha)^\beta} \end{aligned}$$

In this notation γ , the 3rd Weibull parameter goes by a variety of names such as location, minimum life, threshold, origin, guaranteed minimum life, guaranteed life, and shift. α is generally called the scale and β is either shape or slope (typically in probability paper or rank regression based approaches). Estimation of the standard 2-parameter Weibull where $\gamma = 0$ is straightforward and comparable results are found across statistical packages. However, the 3-parameter Weibull estimates are problematic.

The American Statistician has published articles over the last 20 years involving the Weibull distribution including Haughton (1997), Perry (1998), Owen, Sinha, and Capozzoli (2000), and Hilbe (2007). *The American Statistician* has also documented other estimation problems in articles including Haughton (1997), Altman (2002), Hilbe (2002), Langohr and Gomez (2005), and Oster and Hilbe (2008). Yalta (2007) also documents other statistical distribution estimation problems in one software package.

We found comments in Oster and Hilbe (2008) and Hilbe (2008) to be very meaningful. Oster and Hilbe (2008) identify that "... maximum likelihood inference (unconditional or conditional) may provide incorrect results, or may fail to provide any results at all, ...". While their comment deals with maximum likelihood it is not limited to just that estimation technique as this paper illustrates with least squares estimation. Hilbe (2008) nicely states the following two items which we have come to appreciate much more as a result of our investigation:

- "But not all statistical applications have the same capabilities, nor the same reliability."
- "At other times, of course, we discover a host of difficulties, or major inadequacies."

3. Software Packages Analysed

Some statistical packages offer only maximum likelihood estimates for Weibull distribution fitting. Maximum likelihood generally has much to offer (consistency, asymptotic normality, and asymptotic efficiency) but such properties are based on large samples. In practice large samples may not be available and thus the often stated advantages of maximum likelihood estimation may not be applicable to moderate sized samples. In some engineering oriented reliability packages and associated documentation the recommended procedure is to use a least squares approach in numerous circumstances

to estimate the Weibull distribution for both the two and three parameter Weibull distribution fitting. This paper examines three packages for the 3-parameter Weibull based on least squares estimation. A subsequent paper is planned comparing both least squares and maximum likelihood estimation based on commercial statistical packages.

Minitab 17 is a general purpose statistical package. Weibull++9 is developed by ReliaSoft and has a book (ReliaSoft, 2005) available for either purchase in hard copy or downloadable free from the web. Weibull++9 is part of a suite of reliability based software. SuperSMITH Weibull (version 5.0CH) is a statistical reliability package (Fulton Findings, LLC) featured in *The New Weibull Handbook* (Abernethy, 2006). These are the three packages compared for least squares fitting of the three parameter Weibull distribution.

3.1 Plotting Positions

Each observation has both an X and Y value. The X value is typically the failure time in reliability data. For this paper it is the pseudo-random three-parameter Weibull values generated. The Y value is an estimate of the cumulative proportion of observations that have “failed” by the “time” of the X value where failed and time is used to give a common instance for the Weibull distribution. There are multiple ways to obtain this Y value but this paper will focus on the two most common median rank based approaches used for Weibull distributions. For the Weibull distribution both SuperSmith and Weibull++9 use the exact median rank approach while Minitab uses Bernard’s approximation for median ranks. Both of these are explained further below.

3.2 Median Ranks

The Median Ranks method is used to obtain an estimate of the probability of failure (or unreliability as sometimes called in engineering texts) for each of the units. The median rank is the value that the probability of failure should have at the jth failure out of a sample of N units. The median rank is obtained by solving this equation for Z at P=0.50:

$$0.50 = \sum_{k=j}^N \binom{N}{k} Z^k (1-Z)^{N-k}$$

For example, if N = 4 and we have four failures, we would solve the median rank equation for the value of Z four times; once for each failure with j = 1, 2, 3 and 4. This result can then be used as the unreliability estimate for each failure or the y plotting position.

3.3 Exact Beta and F Distributions Approach (Weibull++, SuperSmith)

A more straightforward and easier method of estimating median ranks is by applying two transformations to the cumulative binomial equation, first to the beta distribution and then to the F distribution, resulting in the below where $m=2(N-j+1)$, $n = 2j$, and $F_{0.50}$; m ; n denotes the F distribution at the 0.50th percentile (median), with m and n degrees of freedom, for failure j out of N units.

$$MR = \frac{1}{1 + \frac{N - j + 1}{j} F_{0.50; m; n}}$$

3.4 Benard's Approximation for Median Ranks (Minitab)

A quick approximation of the median ranks is also given by:

$$MR = \frac{j - 0.3}{N + 0.4}$$

Various studies including Rinne (2009) and Lawless (2003) have shown that the above and other ranking schemes do not have a major impact on the results. This is further supported later when the Minitab and SuperSmith results are often close.

3.5 Least squares estimates versus maximum likelihood estimates

Least squares estimates are calculated by fitting a regression line to the points in a probability plot. The line is formed by regressing time to failure X on the transformed median rank Y . Maximum likelihood estimates are calculated by maximizing the likelihood function. Some of the claimed advantages of each method follow.

3.5.1 Least squares

- Better graphical display to the probability plot because the line is fitted to the points on a probability plot.
- For samples with little censoring, least squares may be more accurate than MLE, especially for small samples.

3.5.2 Maximum likelihood

- Distribution parameter estimates are more precise than least squares especially for large samples.
- For samples with heavy censoring, maximum likelihood is more accurate than least squares.
- Maximum likelihood will work when there are no failures.
- The maximum likelihood estimation method has attractive mathematical qualities.

When possible, both methods might be tried; if the results are consistent, then there is more support for the conclusions. Otherwise, one should consider the advantages of both approaches and make a choice for the particular problem. Minitab does not take a public stance. Below are 5/1/2015 email quotes from Wes Fulton (SuperSmith) and David Groebel (Weibull++) both providing their good advice. Regression as used below is least squares.

James W. (Wes) Fulton of Fulton Findings LLC (SuperSmith): Generally, not for the specific 3parameter solution, I would say that we recommend to start with the graphical method AND then if there is any question about the solution you

should compare it to the likelihood result. For small samples, Dr. Abernethy's reduced bias adjustment "RBA" removes most of the small sample bias in the likelihood solution for the slope. If those two different techniques reasonably agree, then you have a solid solution, otherwise you have useful information. If the graphical slope is significantly higher than the likelihood slope, you probably have a subpopulation that will not fail by the failure mechanism under analysis (we informally call that a "batch" issue). Now for the 3parameter solution, we recommend larger samples only as it is very difficult to find the correct third parameter shift for small samples anyway as you know. So we know there are benefits to using both graphical and likelihood methods, and that is easy to do now in modern software.

David Groebel from ReliaSoft (Weibull++): In general, we do say that with complete data, particularly with small sample sizes, that we recommend regression. Assuming Beta is greater than one, for complete data with sample sizes of 25, 50 and 100 using the 3p-Weibull distribution, I would actually recommend MLE. As you know there will probably not be much of a difference between rank regression and MLE given these sample sizes. Given that, I would recommend MLE since it would probably help out with other statistics, such as confidence bounds, as these are based on MLE theory (Fisher Matrix and Likelihood Ratio). With these samples sizes, there most likely would not be much of a difference. However, as the sample size decreases then yes, I would recommend regression in that case. Bottom line, I do not think there really is a wrong answer in this case.

3.6 Approaches to 3-Parameter Weibull Least Squares Estimates

Two basic approaches were encountered in the software reviewed to develop the least squares estimates for a 3-parameter Weibull. Minitab and SuperSmith both use an iterative trial and error approach to find an optimal threshold γ that maximizes the correlation (or similarly maximizes the R^2) of the γ adjusted x, y values. In this iterative process a search is made using proprietary approaches that assess both the search direction and when to terminate the search. For a given iteration the current γ value is subtracted from the x values and these $(x - \gamma)$ values are regressed on the y values. Weibull++ uses a nonlinear technique based on a Nelder-Mead optimization approach to estimate γ .

4. Experimental Design for Study of 3-Parameter Weibull

Results for four initial real-world data sets (not shown here but in Harper et al, 2011) illustrated the diversity of results that statistical packages might provide, but it is hard to generalize from such results. This section describes the choices for a 3 by 3 experimental design focused on the Weibull shape parameter ($\beta = 0.5, 1.5, \text{ and } 3.5$) and the sample size ($n = 25, 50, \text{ and } 100$) of the generated data sets. Each statistics package is tested on a total of 270 pseudo-random data sets (9 settings with 30 simulated data sets). For each generated pseudo-random data set, the location was set to 10 and the scale to 1. A scale value of 1 is common in the literature simulations. We wanted a location value different than zero to more fully distinguish the data from a 2-parameter Weibull.

The first decision was to focus on the shape parameter β . This is consistent with a broad array of previous work. For example Goode and Kao (1961, 1962) developed reliability

sampling plans for the Department of Defense that are independent of the scale parameter and that describe the location factor as, “However, if γ has some known value other than zero the procedure and tables can be easily and simply modified to allow for this.” Similarly, Rinne (2009, p. 33) (where c is the shape parameter labelled β in this paper) states “As each WEIBULL density can be derived ..., it will be sufficient to study the behavior of this one-parameter case depending on c only.” Some simulation studies (Antle and Bain, 1969; Thoman, Bain, and Antle, 1969 & 1970; Johnson and Haskell, 1983) explicitly address why only the shape parameter must be studied, while others (Cohen and Whitten, 1982) fix the location and scale parameter without stating the reason.

Hirose (1991) states “the shape parameter β lies in an interval $0.5 \leq \beta \leq 3.5$ in almost all cases.” This is partially based on Cohen (1973) which says the values of β are usually “ranging from around 0.5 to perhaps 3.0 or 3.5”. Cohen and Whitten (1982) state “values of δ in excess of 3.22 seldom occur” where δ is the shape in their paper. We conclude based on multiple publications including Rinne (2009), for our purposes the shape parameter space may be collapsed into the following 3 groups (with our chosen values shown):

1. $0 < \text{shape} \leq 1$ (0.5)
2. $1 < \text{shape} \leq 2$ (1.5)
3. $\text{Shape} > 2$ (3.5).

Our choices of 25, 50, and 100 for the sample sizes are consistent with numerous other studies. Thoman, Bain, and Antle (1970) varied n with a max of 100. Johns and Lieberman (1966) varied n with a max of 100. Archer (1980) varies n from 25 to 200 states on page 61 “However, as n increases, the approximations approach the estimated variances until there is very little difference at $n = 100$. Johnson and Haskell (1983) used samples sizes n of 70, 100 and 200. Zanakakis (1977) used $n = 50, 100, 200$. Abernethy (2006) suggests $n \geq 21$ in general for any 3-param Weibull and Meeker and Escobar (1998) suggested wanting $n \geq 100$.

The next choice was for 30 replications at each sample size. Zanakakis (1979) used 3 replications. Qiao, Tsokos (1995) used 50 random samples examining just one specific case. Meeker and Escobar (1998) use 30 simulations for a censored two-parameter Weibull MLE. Zanakakis (1977) used a total of 225 test problems with replacement of ones that did not pass a Kolmogorov-Smirnov goodness of fit test for the 3-parameter Weibull ($\alpha = 0.1$). We did a similar screening (discarding about 10% of the 270 generated sets) with the Anderson-Darling goodness of fit test ($\alpha = 0.10$) to ensure that the pseudo-random data sets are reasonable 3-parameter Weibull distributions.

The next choice was which metrics to use to measure package performance. First, we discuss one that needed some modification to avoid the nonsensical result of a negative number of correct digits. McCullough (1998) and Altman, Gill, and McDonald (2004) discuss the logarithm of the relative error (LRE), which measures the number of correct significant digits. This is defined as $LRE = -\log_{10} \left[|q - c| / c \right]$ where q is the MLE of a parameter and c is the correct answer (in this study the generating value). Separate LRE statistics were computed for each of the three parameters. The above LRE did go negative in the experimental runs, so we first tried a modification based on Kozluk (2002) and then a variation on that by the lead author (Harper et al, 2011). The resulting metric described

below is LRE_{KH} where the K and H represent the last names of the source of the modifications.

$$LRE_{KH} = \begin{cases} \text{if } abs(MLE / \text{Design parameter}) < \frac{1}{2} \text{ or if } abs(MLE / \text{Design parameter}) > \frac{1}{2}, LRE_{KH} = 0 \\ \text{else } LRE_{KH} = \max\{-\log_{10} [|q - c| / c], 0 \} \end{cases}$$

Numerous metrics were computed: the least squares estimates themselves for all 3 parameters, MSE (Mean Squared Error), MAE (Mean absolute error), MAPE (Mean Absolute Percentage Error), and LRE_{KH} for all 3 parameters. This paper will focus on analysis of variance comparisons of the least squares shape parameter β between the three software packages.

5. Least Squares Simulation Results

For each of the nine design conditions a blocking Analysis of Variance (ANOVA) was run using Minitab's General Linear Model procedure including Tukey's post-hoc multiple comparison. The blocking factor in the ANOVA is the replication number representing the particular replication of the 30 random data sets for each design point. The main effect of interest is the program (Minitab 17, SuperSMITH Weibull, ReliaSoft Weibull++). By using a blocking ANOVA the variability due to the 30 different random replications is partitioned out and allows a more sensitive assessment of the main effect program.

For all nine design points Tukey's multiple comparison grouping output is given for a summary overview. Then due to the 15 page JSM proceedings limit, only those design points with shape $\beta = 0.50$ are analyzed in more depth. These are the design points where statistically significant differences are found between the three packages. Each of these three design points has a box plot, a confidence interval plot, and a Tukey's mean difference plot. The box plot and confidence interval plot include a red dotted line at the design point value for the shape β . The confidence interval plot uses a pooled standard deviation across all three packages. The Tukey's mean difference plot is another more visual way to show the results presented in the initial one page of all nine design point multiple comparisons. The output metric of interest is the estimated least squares shape parameter (called Shape OLS). Other metrics may be reported in subsequent papers including a comparison between maximum likelihood and least squares on this same design matrix. In the Tukey output means not sharing a common grouping letter are significantly different from each other at the specified confidence level (95% in this paper).

Table 1: Tukey Multiple Comparison Procedure: (DOE n = 25, DOE Shape = 0.50)

Program	N	Mean	Grouping
SuperSMITH Weibull	30	0.503456	A
Minitab 17	30	0.495514	A
Weibull++	30	0.450659	B

Table 2: Tukey Multiple Comparison Procedure: (DOE n = 50, DOE Shape = 0.50)

Program	N	Mean	Grouping
SuperSMITH Weibull	30	0.518371	A
Minitab 17	30	0.509093	A
Weibull++	30	0.452381	B

Table 3: Tukey Multiple Comparison Procedure (DOE n = 100, DOE Shape = 0.50)

Program	N	Mean	Grouping
SuperSMITH Weibull	30	0.532352	A
Minitab 17	30	0.511819	B
Weibull++	30	0.458617	C

Table 4: Tukey Multiple Comparison Procedure (DOE n = 25, DOE Shape = 1.50)

Program	N	Mean	Grouping
Weibull++	30	2.29712	A
Minitab 17	30	1.86524	A
SuperSMITH Weibull	30	1.86524	A

Table 5: Tukey Multiple Comparison Procedure (DOE n = 50, DOE Shape = 1.50)

Program	N	Mean	Grouping
Minitab 17	30	1.51084	A
SuperSMITH Weibull	30	1.51079	A
Weibull++	30	1.50894	A

Table 6: Tukey Multiple Comparison Procedure (DOE n = 100, DOE Shape = 1.50)

Program	N	Mean	Grouping
Weibull++	30	1.60263	A
SuperSMITH Weibull	30	1.57784	A
Minitab 17	30	1.57781	A

Table 7: Tukey Multiple Comparison Procedure (DOE n = 50, DOE Shape = 3.50)

Program	N	Mean	Grouping
Weibull++	30	4.07236	A
Minitab 17	30	4.06933	A
SuperSMITH Weibull	30	4.06929	A

Table 8: Tukey Multiple Comparison Procedure (DOE n = 25, DOE Shape = 3.50)

Program	N	Mean	Grouping
Weibull++	30	5.32974	A
SuperSMITH Weibull	30	4.32932	A
Minitab 17	30	4.32927	A

Table 9: Tukey Multiple Comparison Procedure (DOE n = 100, DOE Shape = 3.50)

Program	N	Mean	Grouping
Weibull++	30	3.80930	A
SuperSMITH Weibull	30	3.76023	A
Minitab 17	30	3.76013	A

Figures 1-9 that follow are based on the least squares estimates of the Weibull shape parameter β with only the design $\beta = 0.50$. Captains in the picture refer to this as the Shape OLS while the figure titles use the labeling LS β for space purposes. On the box plots as

well as the interval plots the design value β is shown as a red dotted horizontal line that visually aids bias detection.

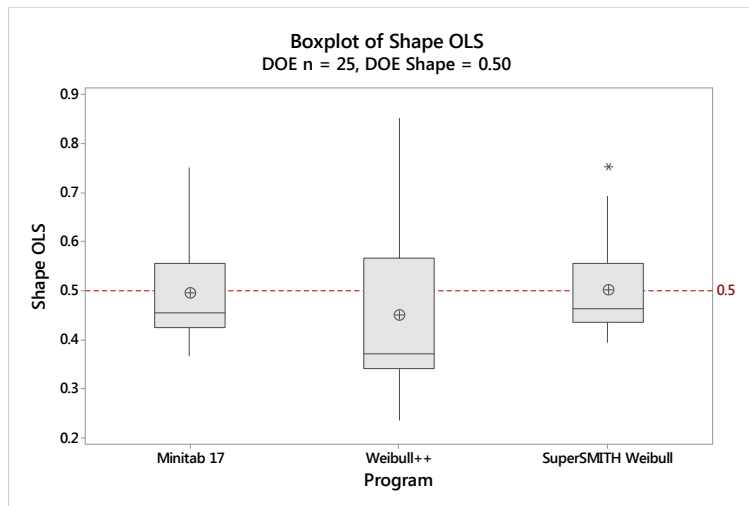


Figure 1: Box plot of LS β for DOE n = 25, DOE Shape = 0.50

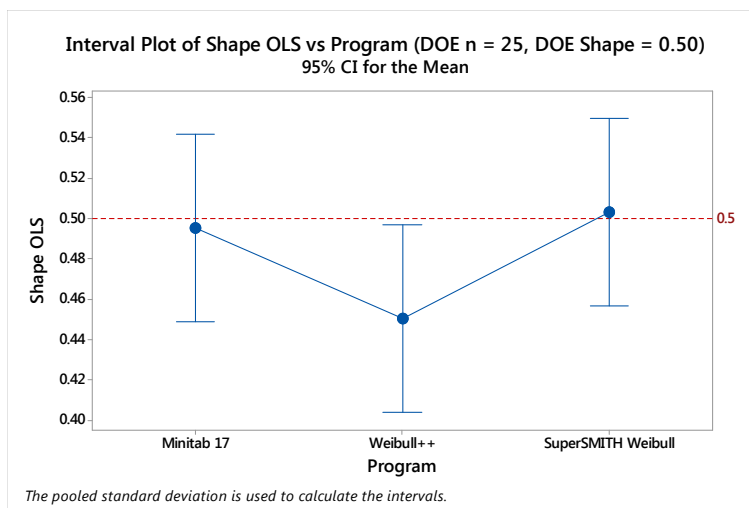


Figure 2: Interval plot of LS β for DOE n = 25, DOE Shape = 0.50

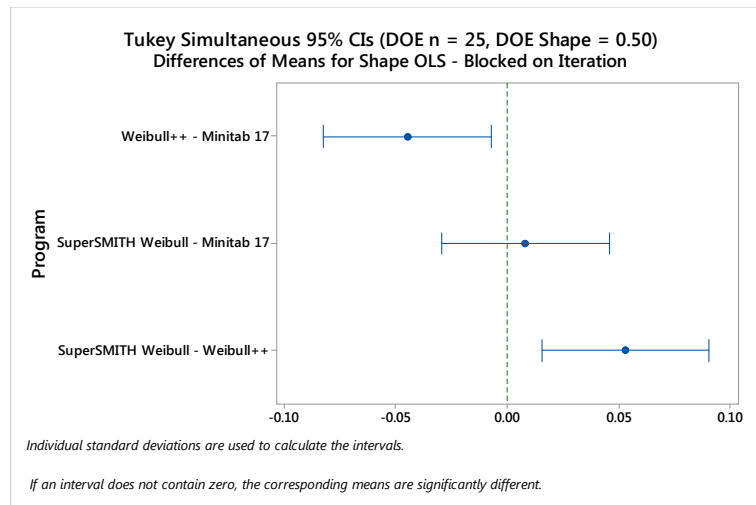


Figure 3: Tukey means plot of LS β for DOE n = 25, DOE Shape = 0.50

Figures 1-3 and the earlier Tukey multiple comparison tabular output indicate there is no statistically significant difference for this design point (n = 25, shape = 0.50) between Minitab 17 and SuperSMITH Weibull at the 95% confidence level; however, both are significantly different from Weibull++. More variability in the Weibull++ output is seen in the box plot plus a possible bias on the low end. Since the ANOVA, Tukey output, and the Confidence Interval plot all used a pooled standard deviation the increased variability of the Weibull++ estimates just contributes to the pooled standard deviation.

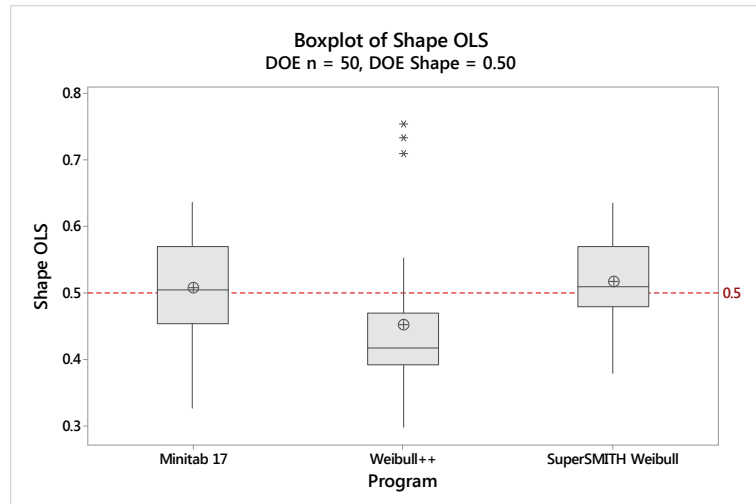


Figure 4: Box plot of LS β for DOE n = 50, DOE Shape = 0.50

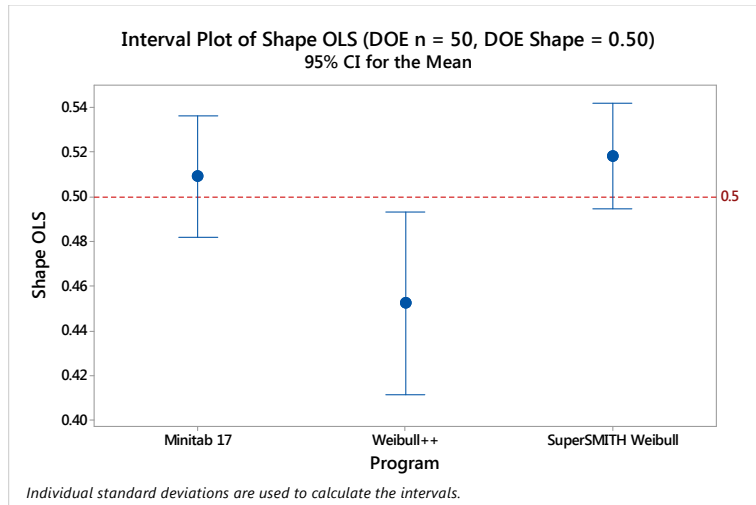


Figure 5: Interval plot of LS β for DOE n = 50, DOE Shape = 0.50

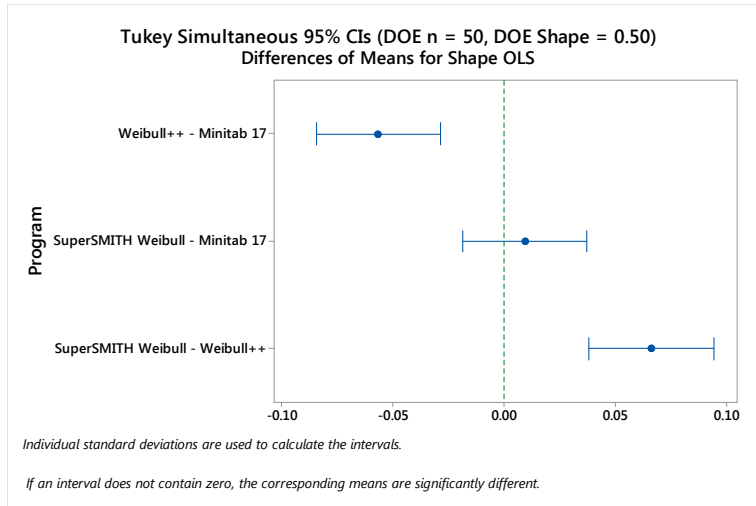


Figure 6: Tukey means plot of LS β for DOE n = 50, DOE Shape = 0.50

Figures 4-6 and the earlier Tukey multiple comparison tabular output indicate there is no statistically significant difference for this design point between Minitab 17 and SuperSMITH Weibull at the 95% confidence level; however, both are significantly different from Weibull++. The Weibull++ estimates also show a possible bias toward lower values.

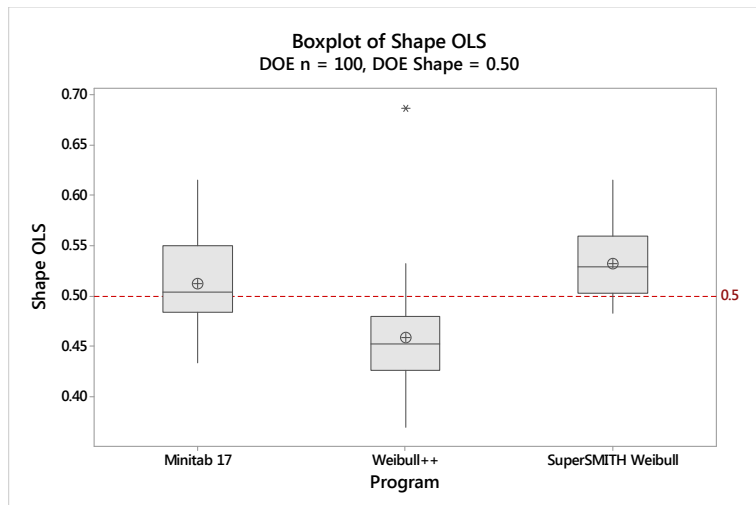


Figure 7: Box plot of LS β for DOE n = 100, DOE Shape = 0.50

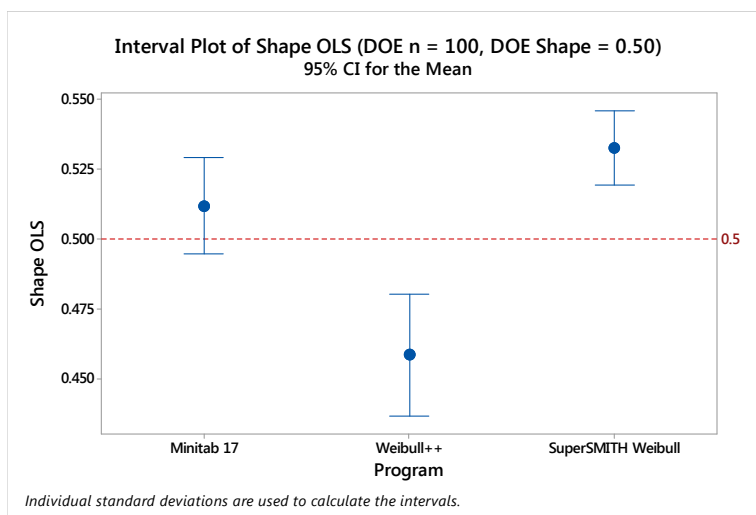


Figure 8: Interval plot of LS β for DOE n = 100, DOE Shape = 0.50

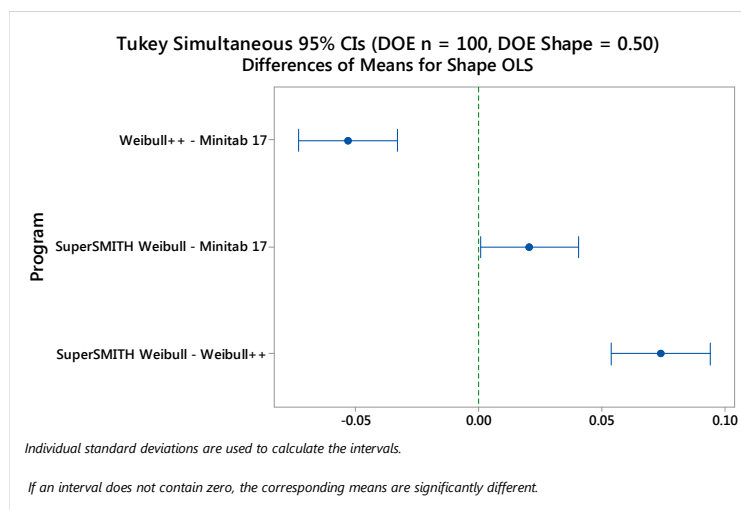


Figure 9: Tukey means plot of LS β for DOE n = 100, DOE Shape = 0.50

Figures 7-9 and the earlier Tukey multiple comparison tabular output indicate there is a statistically significant difference for this design point between all three software package least squares estimates of the shape parameter β . The Weibull++ estimates also show a possible bias toward lower values while SuperSMITH Weibull shows a possible bias toward higher values.

6. Summary

This paper documents modern software issues in the least squares estimation the 3-parameter Weibull distribution shape parameter β . It shows more than expected variability exists in results reported by different statistical packages. These differences may be critical for those who would use the 3-parameter Weibull. In practice it may be advantageous, where possible, to compute both least squares and maximum likelihood estimates using multiple packages and compare the results.

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