Maximum Likelihood and Least Squares Estimation Comparison for the Three-Parameter Weibull Distribution: Case Study of Statistical Software

William V. Harper[1], Thomas R. James[1]
[1]Mathematical Sciences, Otterbein University, One S. Grove Street, Westerville, OH 43081-2006

Abstract
Maximum Likelihood and 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 has been covered previously using modern statistical software separately for maximum likelihood (Harper, Eschenbach, James, 2011) and least squares (Harper, James, 2015). This publication directly compares maximum likelihood and least squares results. The findings 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: Weibull, Reliability, Least squares estimation, Maximum likelihood estimation,

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, Kolmorgov-Smirnoff, 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 in ten different program/methods. Harper and James (2015) examined 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.

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). Harper and James (2015) partially follows their MLE work but with LS methods. The MLE article (Harper et al, 2011) compared 10 MLE methods; whereas, only 3 LS alternatives are compared in Harper et al (2015). This new paper compares MLE to LS using the same experimental design used in the two just mentioned publications.

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.

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

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 Harper and James (2015) illustrated 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 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 briefly shows overall results of ten MLE results and three LS packages for the 3-parameter Weibull. Then a slightly more in-depth analysis is presented comparing MLE and LS for the 3 packages for which both methods were used.

The three packages with a slightly more in-depth MLE versus LS analysis are listed in the paragraph. 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).

Prior to delving into the comparison of the three packages a more cursory showing of MLE versus LS results includes the MLE packages/methods JMP Basic, JMP Reliability, SAS, Palisade's Best-Fit, Statistica, Systat, Stata/IC, Weibull++7 defaults, Weibull++7 True 3 parameter, SuperSmith large bias, SuperSmith small bias; and Minitab. However, it must be stated that their algorithms may have evolved over time. More specifics on the version numbers along with some other packages considered but dropped for various reasons (e.g., SPSS) are found in Harper et al (2011).

4. Least squares estimates versus maximum likelihood estimates in general

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++9) both providing good advice. Regression as used 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++9): 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.

4.1 Approaches to 3-Parameter Weibull Estimates

For LS 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 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. For MLE estimation there are a variety of approaches employed. These are detailed in Harper et al (2011).

5. Experimental Design for Study of 3-Parameter Weibull

Results for initial real-world data (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 (β = 0.5, 1.5, and 3.5) and the sample size (n = 25, 50, 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 $0.5 \le \beta \le 3.5$ 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. $0 <$ shape ≤ 1 (0.5)
2. $1 <$ shape ≤ 2 (1.5)
3. 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. Zanakis (1977) used n = 50, 100, 200. Abernethy (2006) suggests $n \ge 21$ in general for any 3-parm Weibull and Meeker and Escobar (1998) suggested wanting $n \ge 100$.

The next choice was for 30 replications at each sample size. Zanakis (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. Zanakis (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 and replacing about 10% of the initial 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.

Numerous metrics were computed; however, this paper will focus on analysis of variance comparisons of the shape parameter β between the software packages.

6. Least Squares versus Maximum Likelihood 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/method (e.g., Minitab LS). 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 of the three packages that are the major focus of this article. For each design point there are 8 program/method comparisons in each since there are 5 MLE and 3 LS options. The output metric of interest is the estimated shape parameter. Other metrics may be reported in subsequent papers 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, Method	N	Mean	Grouping			
Weibull++7 True 3P MLE	30	0.594733	A			
Minitab 16 MLE	30	0.562369	A	B		
Weibull++7 Default MLE	30	0.526463		B	C	
SuperSmith Large Bias MLE	30	0.517892		B	C	
SuperSMITH LS	30	0.503456			C	D
SuperSmith small bias MLE	30	0.499356			C	D
Minitab 17 LS	30	0.495514			C	D
Weibull++9 LS	30	0.450659				D

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

Program, Method	N	Mean	Grouping		
Weibull++7 True 3P MLE	30	0.623669	A		
Minitab 16 MLE	30	0.530605		B	
SuperSMITH LS	30	0.518371		B	
SuperSmith Large Bias MLE	30	0.516421		B	
Weibull++7 Default MLE	30	0.509207		B	
Minitab 17 LS	30	0.509093		B	
SuperSmith small bias MLE	30	0.507281		B	
Weibull++9 LS	30	0.452381			C

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

Program, Method	N	Mean	Grouping		
Weibull++7 True 3P MLE	30	0.652652	A		
Minitab 16 MLE	30	0.533323		B	
SuperSMITH LS	30	0.532352		B	
SuperSmith Large Bias MLE	30	0.526287		B	
SuperSmith small bias MLE	30	0.521656		B	
Weibull++7 Default MLE	30	0.513106		B	
Minitab 17 LS	30	0.511819		B	
Weibull++9 LS	30	0.458617			C

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

Program, Method	N	Mean	Grouping
Weibull++7 Default MLE	30	2.45812	A
Weibull++9 LS	30	2.29712	A
Minitab 16 MLE	28	1.87972	A
Minitab 17 LS	30	1.86524	A
SuperSMITH LS	30	1.86524	A
Weibull++7 True 3P MLE	29	1.80092	A
SuperSmith Large Bias MLE	30	1.60191	A
SuperSmith small bias MLE	30	1.54457	A

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

Program, Method	N	Mean	Grouping	
Weibull++7 Default MLE	30	1.55783	A	
Weibull++7 True 3P MLE	29	1.55522	A	
Minitab 17 LS	30	1.51084	A	
SuperSMITH LS	30	1.51079	A	
Weibull++9 LS	30	1.50894	A	
Minitab 16 MLE	30	1.42490		B
SuperSmith Large Bias MLE	30	1.42238		B
SuperSmith small bias MLE	30	1.39721		B

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

Program, Method	N	Mean	Grouping		
Weibull++7 Default MLE	30	1.62822	A		
Weibull++9 LS	30	1.60263	A	B	
Weibull++7 True 3P MLE	29	1.59859	A	B	
SuperSMITH LS	30	1.57784		B	
Minitab 17 LS	30	1.57781		B	
Minitab 16 MLE	30	1.52840			C
SuperSmith Large Bias MLE	30	1.52832			C
SuperSmith small bias MLE	30	1.51487			C

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

Program, Method	N	Mean	Grouping	
Weibull++7 Default MLE	30	5.60211	A	
Weibull++9 LS	30	5.32974	A	B
SuperSMITH LS	30	4.32932	A	B
Minitab 17 LS	30	4.32927	A	B
Weibull++7 True 3P MLE	30	3.55496	A	B
Minitab 16 MLE	29	3.53729	A	B
SuperSmith Large Bias MLE	30	3.48390	A	B
SuperSmith small bias MLE	30	3.35920		B

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

Program, Method	N	Mean	Grouping	
Weibull++7 Default MLE	30	4.16101	A	
Weibull++9 LS	30	4.07236	A	
Minitab 17 LS	30	4.06933	A	
SuperSMITH LS	30	4.06929	A	
Weibull++7 True 3P MLE	30	3.51552		B
Minitab 16 MLE	30	3.49931		B
SuperSmith Large Bias MLE	30	3.48958		B
SuperSmith small bias MLE	30	3.42782		B

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

Program, Method	N	Mean	Grouping		
Weibull++7 Default MLE	30	3.88401	A		
Weibull++9 LS	30	3.80930	A		
SuperSMITH LS	30	3.76023	A	B	
Minitab 17 LS	30	3.76013	A	B	
Weibull++7 True 3P MLE	30	3.60633		B	C
SuperSmith Large Bias MLE	30	3.60585		B	C
Minitab 16 MLE	30	3.59929		B	C
SuperSmith small bias MLE	30	3.57412			C

In an endeavor to have a reasonable coverage of the 9 design points given the proceedings 15 page limit the following 3 design points were selected representing in some sense the extremes of and the middle. On the plots the design value β is shown as a red dotted horizontal line that visually aids bias detection.

- β = 0.50, n = 30 - smallest β, n
- β = 1.50, n = 50 – middle β, n
- β = 3.50, n = 100 – largest β, n

Figures 1-3 show the results of all the MLE and LS results from both Harper et al (2011) and Harper et al (2015). Figures 4-9 focus just on the three packages that are the main focus of this paper. For each of the selected 3 design points selected an overall box plot (similar to Figures 1-3) is given followed by a box plot that summarizes LS versus MLE.

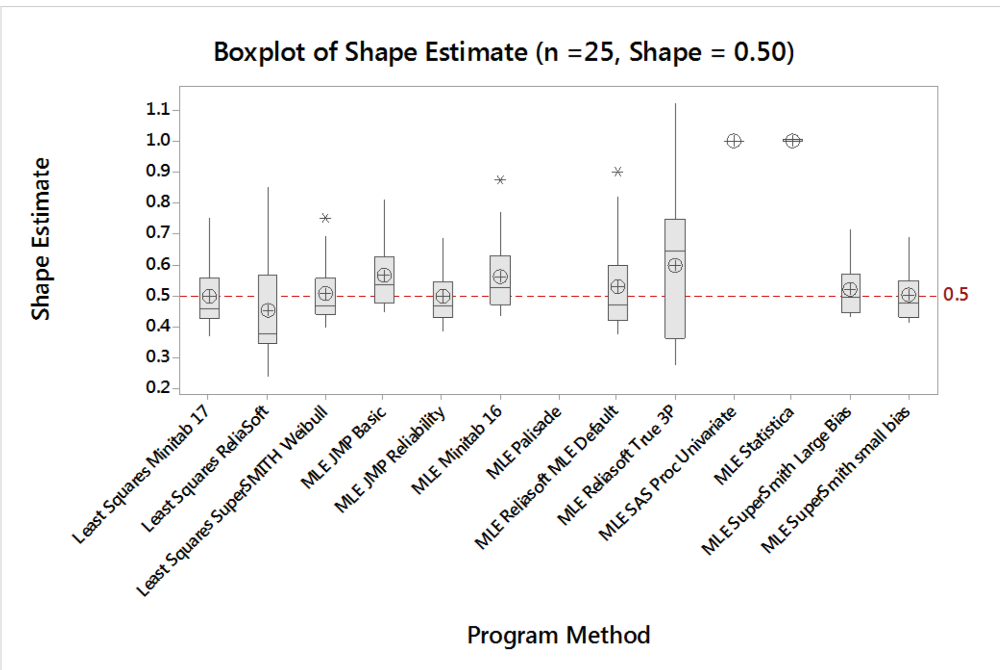

Figure 1. All MLE, LS program/methods for β = 0.50, n = 30

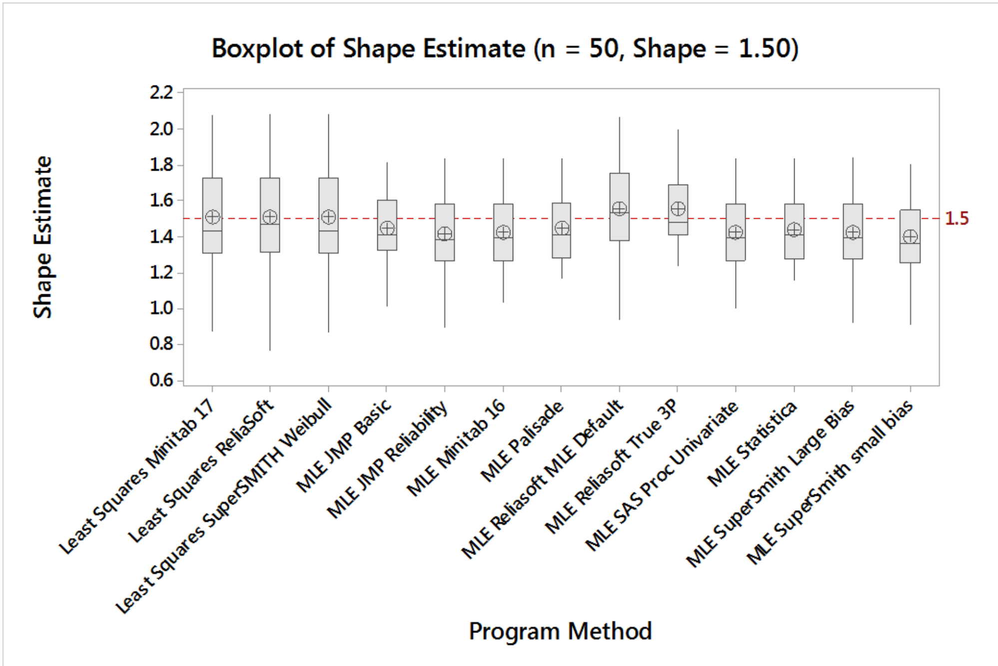

Figure 2. All MLE, LS program/methods for β = 1.50, n = 50

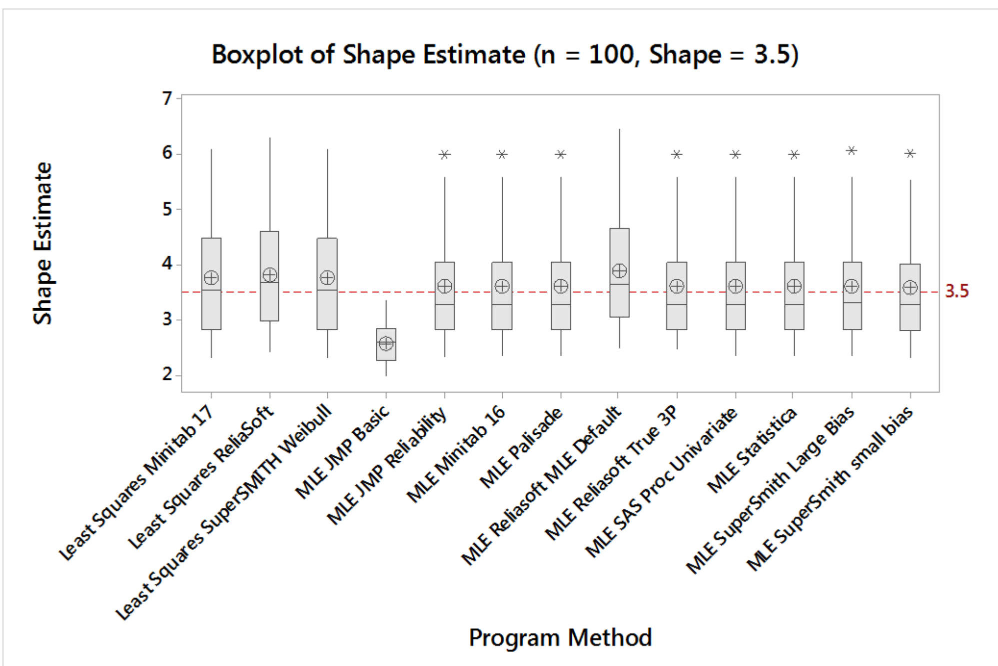

Figure 3. All MLE, LS program/methods for β = 3.50, n = 100

Figures 1-3 showed all LS and MLE comparisons for all packages/methods studied. Software algorithms may have change over time; therefore, one cannot be sure that the same exact results would be found in the most current versions of each package/method. See the earlier Harper et al (2011, 2015) for more detailed results. The main message is that there may be considerable variation of the three-parameter Weibull results across different packages/methods. Figure 4-9 that follow focus just the three software packages

Minitab, SuperSMITH, and Weibull++, but even here the MLE results are older than the LS results. Nonetheless, the comparisons illustrate that both the LS and MLE methods result in differing results depending on the package/method used. The estimation of the three-parameter Weibull is a challenge.

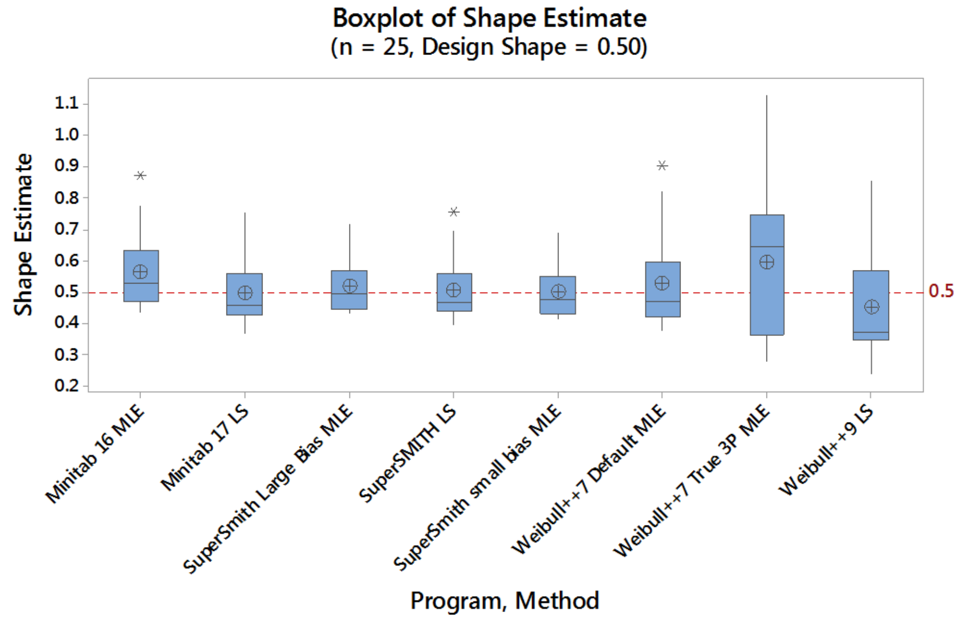

Figure 4. Minitab, SuperSMITH, Weibull++9 MLE, LS results for β = 0.50, n = 30

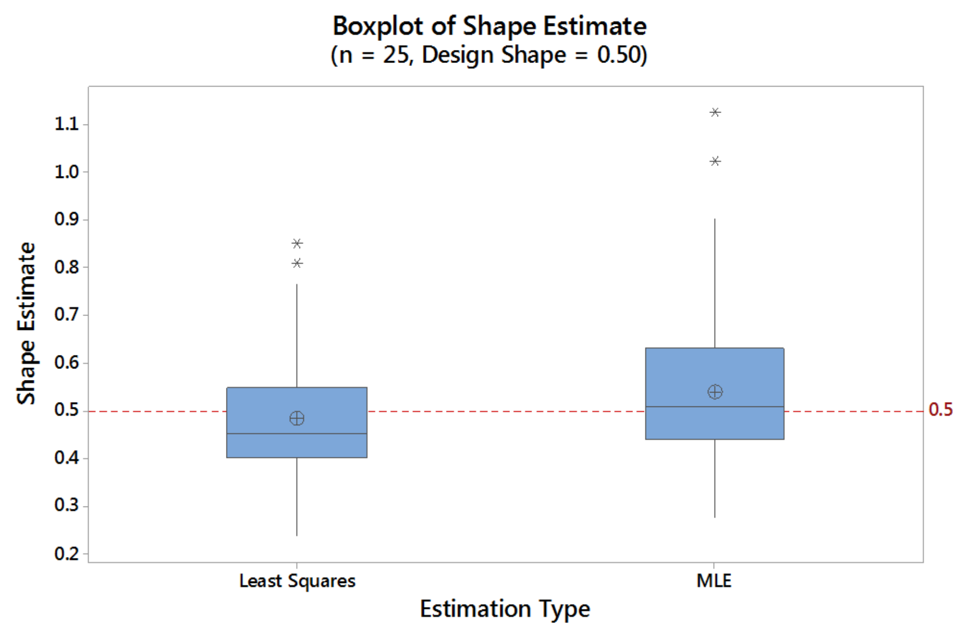

Figure 5. Minitab, SuperSMITH, Weibull++9 MLE, LS summary for β = 0.50, n = 30

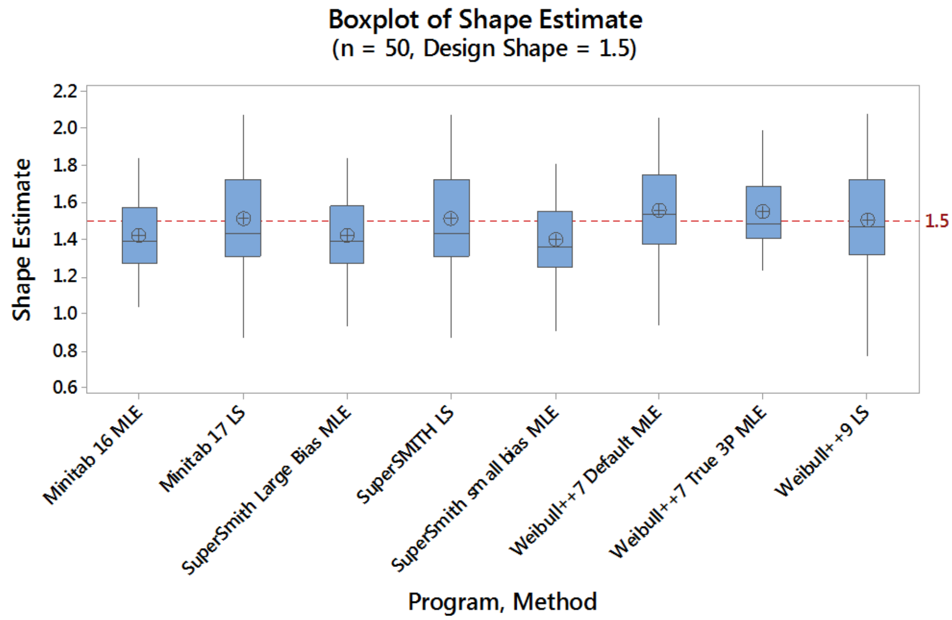

Figure 6. Minitab, SuperSMITH, Weibull++9 MLE, LS results for β = 1.50, n = 50

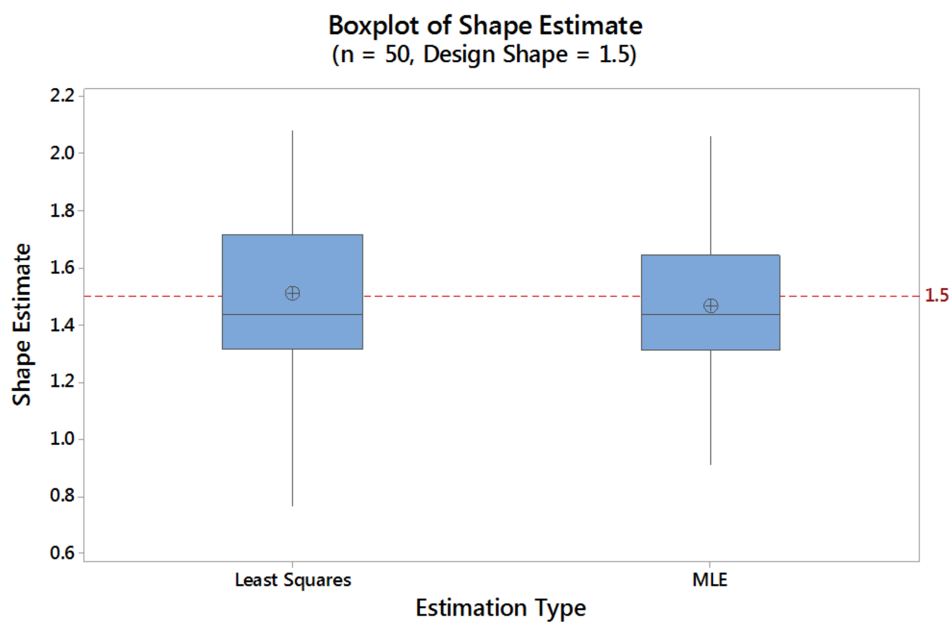

Figure 7. Minitab, SuperSMITH, Weibull++9 MLE, LS summary for β = 1.50, n = 50

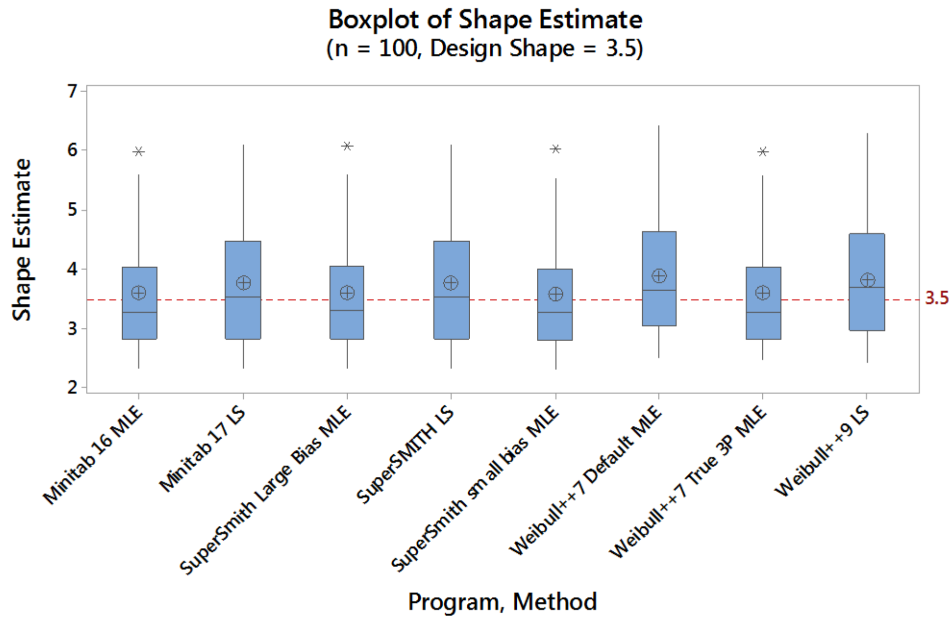

Figure 8. Minitab, SuperSMITH, Weibull++9 MLE, LS results for β = 3.50, n = 100

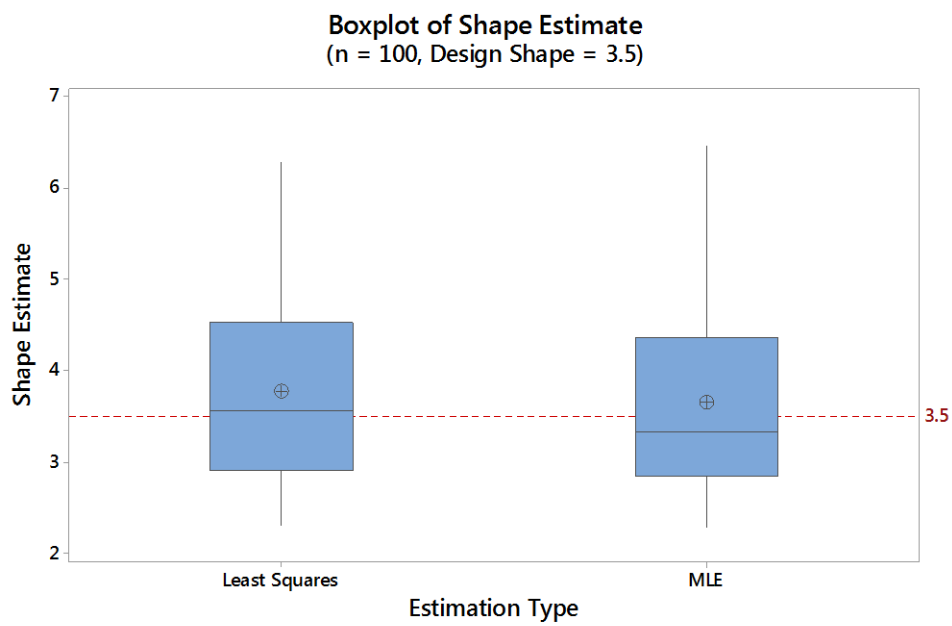

Figure 9. Minitab, SuperSMITH, Weibull++9 MLE, LS summary for β = 3.50, n = 100

7. Summary

This paper documents (primarily through plots) modern software issues in the LS and MLE estimation of 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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