



NUMERICAL EXPERIMENT TO EVALUATING TWO-SIDED TOLERANCE LIMIT FOR SAFETY ANALYSIS

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ABSTRACT

Uncertainty analysis is required to quantify uncertainties in safety evaluation for industrial applications when the best-estimate methodology is employed. The nonparametric order statistics method suggested by the GRS (Gesellschaft für Anlagen-und Reaktorsicherheit) is one of the uncertainty evaluation methodologies to obtain the figure of merits with a probability of 95 % and confidence of 95 %, namely 95/95 value. In this method, the number of repeated calculations with perturbation to acquire the 95/95 value is decided by a formula suggested by Wilks and is dependent on the number of uncertainty parameters. Thus, the method is effective when the reference system has a large number of parameters which bring uncertainty in the analysis. Previous studies indicate that the method can estimate the 95/95 value successfully when the figure of merit has one-sided tolerance limit where either the upper or lower limit exists. However, when it is necessary to cut off the tails of 2.5% evenly in both ends, namely the centered two-sided tolerance limit, the suggested formula results in a lower confidence level. Thus, a modified formula is suggested in this study to account for such characteristics, and, as a result, the number of repeated calculations required to obtain the 95/95 value is calculated. The validity of the formula and the number of repeated calculations are examined using numerical experiments for 21 different distributions. The numerical experiment has been conducted with one to ten million sample sets to estimate the confidence level. The results of the numerical experiments indicate that the 95/95 value is predicted successfully by the repeated calculations decided by the modified formula when the figure of merit has characteristics of the centered two-sided distribution, while the existing formula results in a confidence level of 80%.

Keywords: nonparametric order statistics, wilks' formula, GRS method, best-estimate plus uncertainty, centered two-sided tolerance limit.

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1. INTRODUCTION

Deterministic safety analysis is an important method to demonstrate the safety of industrial applications by comparing the load and capacity of a reference system directly [1]. Traditionally, conservative analysis methodology has been widely used for the deterministic safety analysis. The conservative safety analysis has been conducted by means of conservative computer codes combined with conservative initial and boundary conditions, which postulate the worst accident scenarios. The main idea of this approach is to demonstrate the safety even under the worst conditions and to compensate for uncertainties due to the random nature of system parameters and lack of knowledge. However, as the physical understanding has been developed, the safety analysis has aimed at a more realistic evaluation of the system safety. This is because the previous approach has no choice but to include a large amount of conservatism and, as a result, safety margin which reduce the economy of the industrial applications. With this background, the best-estimate safety analysis has been introduced in order to obtain both the safety and economy of industrial applications. A typical example of the best-estimate methodology in the regulatory framework is given in the regulatory guide 1.157 issued by the United States Nuclear Regulatory Commission in 1989 [2].

In the best-estimate analysis methodology, the deterministic safety analysis is conducted by means of best estimate computer codes with realistic input data. However, the uncertainties induced by the random nature of the system parameters and lack of knowledge could not be considered in the analysis because the physical models in the codes and input data for the analysis are decided as realistically as possible. For example, when the heat transfer coefficient is determined using an empirical correlation, not all of the actual data points used to develop the correlation will be on the line drawn by the correlation. Thus, it is clear that the impact of the uncertainties on the figure of merits should be quantified when the best-estimate analysis is conducted. The best-estimate analysis method with uncertainty quantification is so called as the best-estimate plus uncertainty (BEPU) [3].

In the safety analysis, the uncertainties induced by system and physical parameters will be propagated and combined throughout the calculation. In order to consider the statistical characteristics of the parameters and impact of the characteristics on the figure of merits, a series of calculations by using the sets of the sampled parameters are necessary. One of the uncertainty propagation methods to acquire the figure of merits with a probability of 95% and a confidence level of 95%, namely 95/95 value, is the nonparametric order statistics method based on Wilks' formula [4-5] suggested by the GRS (Gesellschaft für



Anlagen-und Reaktorsicherheit) [6]. This method has a characteristic that the number of the repeated calculations is independent of the number of the uncertainty parameters. Thus, the computational effort could be minimized, especially, compared to the Monte-Carlo method. It was demonstrated successfully that the 95/95 value can be obtained for one-sided tolerance limit, where either upper or lower limit exists, by relatively small number of calculations (practically, less than 200 calculations) [7-8].

The suggested formula is valid when both upper and lower tolerance limits exist. However, the suggested formula results in a lower confidence level when it is necessary to cut off the tails evenly in both ends, namely centered two-sided tolerance limit. It is because the formula, which will be explained in Section 2, considers only the size of the cumulative probability, not the location. Thus, it is necessary to modify the formula for the centered two-sided tolerance limit. In this study, the Wilks' formula has been modified for the centered two-sided tolerance limit. A series of numerical experiments has been conducted in order to investigate the validity of the formula.

2. NONPARAMETRIC ORDER STATISTICS METHOD WITH WILKS' FORMULA

The Wilks' formula is given as follows:

$$1 - \sum_{k=n-p+1}^n {}_n C_k \alpha^k (1 - \alpha)^{n-k} \geq \beta \text{ for one-sided tolerance limit} \quad (1)$$

$$1 - \sum_{k=n-2p+1}^n {}_n C_k \alpha^k (1 - \alpha)^{n-k} \geq \beta \text{ for two-sided tolerance limit} \quad (2)$$

where, n and p denote number of calculations and the order of the formula, respectively. In the formula, α and β mean the cumulative probability and confidence level, respectively.

In the above formula, n could be obtained when the cumulative probability, confidence level, and the order of the formula. Since the 95/95 value of the figure of merits is utilized as a result of the best-estimate safety analysis, α and β should have a value of 0.95. From the order statistics, the order of the formula, p , indicates that p values exist in the upper probability range $(1 - \alpha)$ with a confidence level of β in case of the one-sided tolerance limit. Thus, if the 1st order formula is considered ($p=1$) for one-sided tolerance limit, there is only one value whose probability is greater than 95% with a confidence level of 95% so that this value is considered as the 95/95 value. In this case, equation (1) will be reduced as follows and the solution of equation (3) given as 59:

$$1 - \alpha^n \geq \beta \quad (3)$$

In the same manner, if the 2nd order formula is considered, as given in equation (4), there is two values whose probability is greater than 95% so that the 2nd largest value becomes the 95/95 value. Here, n is decided as 93.

$$1 - \alpha^n - n(1 - \alpha)\alpha^{n-1} \geq \beta \quad (4)$$

For two-sided tolerance limit where both upper and lower limits exist, the Wilks' formula has the same shape as one for the one-sided tolerance limit, except for the order of the formula which is replaced by an even number. Thus, the 1st order formula for the two-sided tolerance limit has exactly the same shape as the 2nd order formula for the one-sided tolerance limit given as equation (4). The statistical meaning of equation (4) is as follows:

$$1 - P(n \text{ values hit } \alpha) - P(n - 1 \text{ values hit } \alpha \text{ and } 1 \text{ value hits } 1 - \alpha) \quad (5)$$

where, P is the probability. Equation (5) indicates that the Wilks' formula considers the cumulative probability only. This reveals that the portion of the truncated probability cannot be considered with the Wilks' formula. For example, when the 95/95 value is estimated for the two-sided tolerance limit by means of the Wilks' formula, the formula gives the number of calculations to obtain the 95/95 value and, in total; a probability of 5% will be truncated. In this case, a probability of 5% is defined just as the sum of the truncated probability beyond both ends. However, considering general industrial applications, if the location of the truncated probability is fixed as 2.5 % evenly for above upper and below lower limits, respectively, it means a peculiar case of the general solution by the Wilks' formula. Therefore, it is obvious that the number of calculation estimated by the Wilks' formula is insufficient to obtain the target confidence level.

3. FORMULA FOR CENTERED TWO-SIDED TOLERANCE LIMIT

A formula has been derived in order to obtain the number of simulations for applications where the upper and lower tolerance limit is located symmetrically, namely centered two-sided tolerance limit, as depicted in Figure-1. The 1st order formula when the lower and upper limits are equally distributed as equally $\frac{1-\alpha}{2}$ and $\frac{1+\alpha}{2}$, respectively, was suggested by Hong and Connolly [9] as follows:

$$1 + \alpha^n - 2\alpha^n \sum_{k=0}^n {}_n C_k \left(\frac{1-\alpha}{2}\right)^k \geq \beta \quad (6)$$

The required number of calculations to obtain the 95/95 value is estimated as 146 from Equation (6) which is larger than the result of the Wilks' formula. This means that more calculations than one estimated by Wilks' formula are necessary to achieve a confidence level of 95% when the centered two-sided tolerance limit is examined, as a fore mentioned.

The generalized formula for the centered two-sided tolerance limit can be derived by means of the order statistics and mathematical induction. The resulted formula is given as follows:



$$1 - \sum_{A=0}^{p-1} [2 \times {}_n C_A \left(\frac{1-\alpha}{2}\right)^A \alpha^{n-A} \sum_{k=A}^{n-A} \{ {}_{n-A} C_k \left(\frac{1-\alpha}{2\alpha}\right)^k \} - {}_n C_A \left(\frac{1-\alpha}{2}\right)^A {}_{n-A} C_A \left(\frac{1-\alpha}{2}\right)^A \alpha^{n-2A}] \geq \beta \quad (7)$$

The number of calculations required to obtain the 95/95 value can be calculated by Equation (7) and the numbers as a function of the order of the formula are summarized in Table-1.

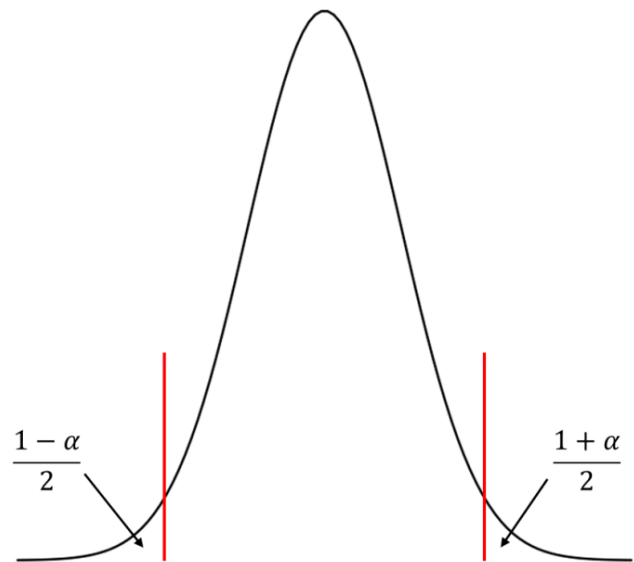


Figure-1. Centered two-sided tolerance limit.

Table-1. Number of calculationstoobtainthe95/95value.

| Limit | Formula | 1 st order | 2 nd order | 3 rd order | 4 th order | 5 th order |
|-----------|----------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| One-sided | Wilks | 59 | 93 | 124 | 153 | 181 |
| Two-sided | Wilks | 93 | 153 | 208 | 260 | 311 |
| | centered | 146 | 221 | 286 | 348 | 406 |

4. NUMERICAL EXPERIMENT WITH VARIOUS TRIAL DISTRIBUTIONS

A series of numerical experiments have been conducted to validate the derived formula for the centered two-sided tolerance limit. The numerical experiment aimed at estimating the confidence of the 95/95 value by the repeated calculations with a large number of sample sets. The number required obtaining the 95/95 value which is the same as the size of each sample set was determined by the Wilks’ formula and the formula derived in this study for the centered two-sided tolerance limit. The characteristics by the orders of the formula were examined for 1stto5th orders and the total numbers of the sample sets were decided as 1million in order to draw a statistical conclusion. Since the formula is based on the principle of the nonparametric order statistics, the confidence level should be independent of the distribution of the figure of merits. In order to investigate the impact of the distribution of the figure of merits, in total, 21 distributions were considered in the numerical experiment as the distributions of the figure of merits. The considered distributions included Normal, Beta, Burr, Birnbaum Saunders, Exponential, Extreme Value, Gamma, Generalized Extreme Value, Generalized Pareto, Inverse Gaussian, Logistic, Loglogistic, Lognormal, Nakagami, Rayleigh, Rician, t Location-Scale, Weibull, Uniform, Triangular, and Piecewise Linear distributions.

The numerical experiment has been conducted by the following steps:

- **Step 1:** The figure of merit was assumed to follow a given trial distribution.
- **Step 2:** Random values which represent arbitrary figure of merits were generated from the given trial distribution. The number of samples is determined by the order of Wilks’ and derived formula.
- **Step 3:** The 95/95 values for each order were estimated.
- **Step 4:** Steps 2 and 3 were repeated for a given number of sets. The number of sets was 1 million.
- **Step 5:** The confidence level of each order was estimated.
- **Step 6:** Steps 2 to 5 were repeated for 21 different trial distributions.

The numerical experiment was conducted by means of MATLAB® R2022b [10].



5. RESULTS AND DISCUSSIONS

Figures 2 and 3 depict the probability density of the 95/95 values for the 21 trial distributions by using the Wilks' formula and the centered two-sided formula. The figures indicate that the distributions of the 95/95 value are independent of the kind of the trial distribution and determined by the order of the formula. The characteristics of the 95/95 value distribution reveals the distribution-free characteristics of the non-parametric order statistics method. In addition, the figures demonstrate that the mean probability density of the 95/95 value moves closer to the upper and lower limits as the order of the formulas increases. This also supports the conclusion drawn by reference [8] for the one-sided tolerance limit that more conservative 95/95 value will be obtained when lower order formula is employed.

Table-2 summarizes the numerical confidence obtained by the numerical experiment. In case of Wilks' formula, the table indicates that the experimental confidence is much lower than the analytical confidence of 0.95, which is expected by the explanation given in Section 2. Thus, it is obvious that the original Wilks' formula is inadequate to estimate the 95/95 value for the centered two-sided tolerance limit. However, the table reveals that the formula of the centered two-sided tolerance limit could achieve a confidence limit of 95% which is the target confidence level. Thus, it can be concluded that the formula derived in this study should be employed in order to estimate the number of simulations to obtain the 95/95 value for the centered two-sided tolerance limit.

Table-2. Analytical and experimental confidences.

| Order | | 1 st | 2 nd | 3 rd | 4 th | 5 th |
|--------------------|-----------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Wilks | Analytical confidence | 0.9500 | 0.9506 | 0.9508 | 0.9502 | 0.9504 |
| | Numerical confidence | 0.8191 | 0.8058 | 0.7991 | 0.7941 | 0.7916 |
| Centered two-sided | Analytical confidence | 0.9509 | 0.9510 | 0.9502 | 0.9507 | 0.9501 |
| | Numerical confidence | 0.9510 | 0.9511 | 0.9503 | 0.9508 | 0.9503 |

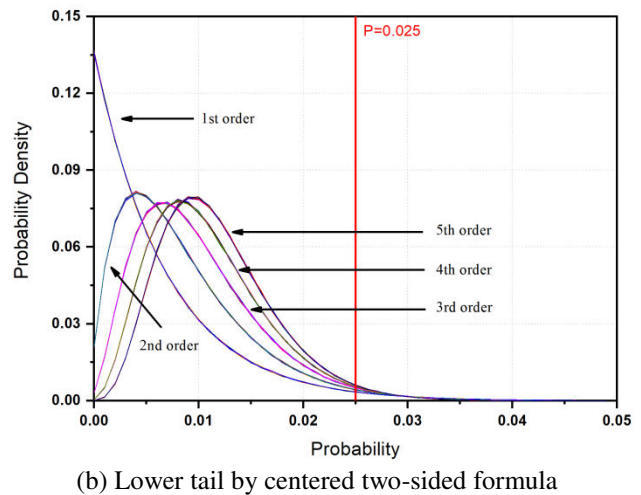
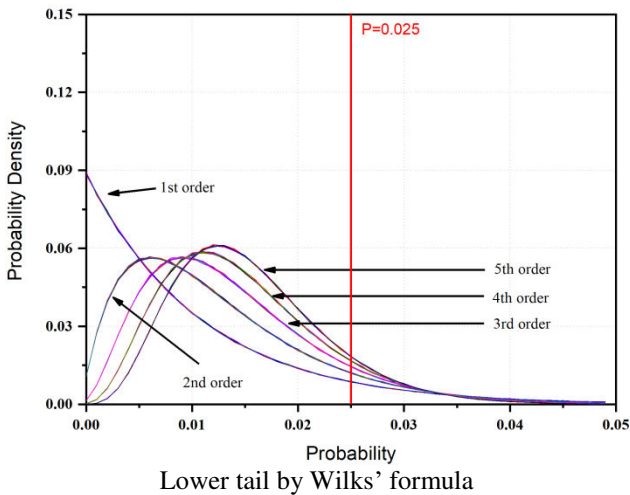


Figure-2. Results of numerical experiment for lower tail.

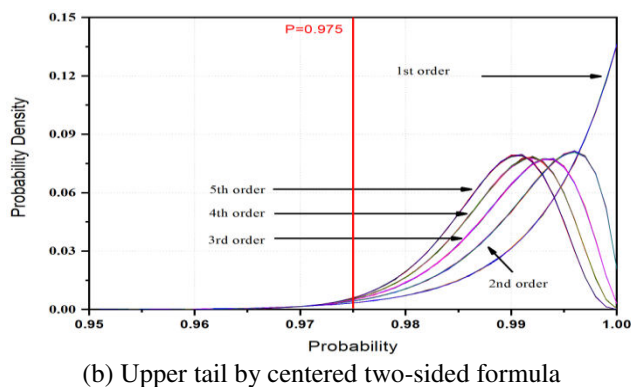
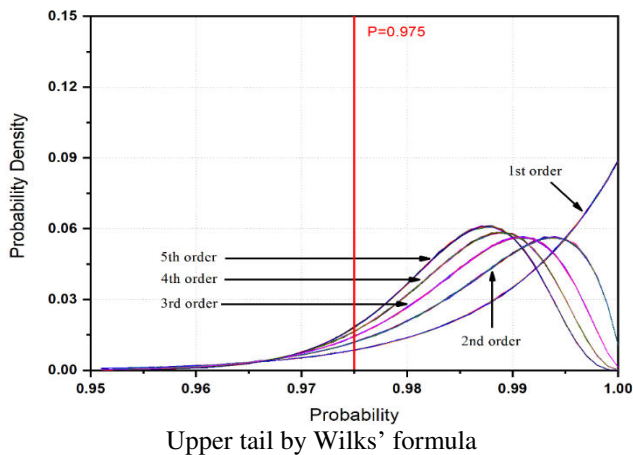


Figure-3. Results of the numerical experiment for the upper tail.

5. CONCLUSIONS

The nonparametric order statistics method has been utilized to evaluate the uncertainty in safety analyses and, in this method, the number of simulations to obtain the 95/95 value is determined by means of the Wilks' formula. However, since the formula does not account for the location of the tolerance limit, it was expected that the number of simulations was insufficient to obtain a confidence of 95% when the centered two-sided tolerance limit was considered. In this study, a new formula has been derived to determine the number of simulations to obtain the 95/95 value for the centered two-sided tolerance limit. The formula indicates that the number of simulations should be larger than that estimated by the Wilks formula. To validate the soundness of the formula, a series of numerical experiments have been conducted with one million sample sets for various order of the formula. In total, 21 trial distribution was considered as distributions for arbitrary output parameters to investigate the distribution-free characteristics of the methodology. The results of the numerical experiment demonstrated the distribution-free characteristics of the methodology and general behavior of the 95/95 value according to the order of the formula. The results also indicated that a confidence level of around 80% was achieved by the Wilks' formula, which is far below than the target confidence of 95%. On the contrary, it was found that the number of simulations

determined by the newly derived formula were appropriate to obtain the target confidence. Therefore, it was concluded that the newly derived formula should be employed to estimate the number of simulations to obtain the 95/95 value for the centered two-sided tolerance limit.

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