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Uncertainty, Sample Size and the 95/95 Tolerance Limit

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Outline

- Study objectives
- Methodology
  - Basic idea and example
  - Wilks' method
- Tolerance limits
- Sample size determination
- Estimation vs. ensuring compliance
- Summary and conclusions

Premise

- The objective of safety analysis is to demonstrate that some important or critical variable (e.g., pressure, temperature, etc.) meets a specified acceptance (i.e., regulatory, safety, etc.) limit
- Monte Carlo simulation is often used to derive the distribution of the critical variable
  - i.e., probabilistic assessment
  - Hence, the limit must be met with <u>high probability</u>
- **Key Question:** How many simulations should be performed to ensure sufficient confidence in the results?
  - Depends on what quantity is being estimated

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Study Objectives

- The objective of this study is to illustrate how an upper bound value (e.g., 95th percentile) can be estimated with high confidence (e.g., the 95/95 value) using a very small number (e.g., 59) of simulation trials
  - Based on the original work by Wilks (1941)
  - The estimation is independent of the underlying probability distribution (i.e., the <u>unknown</u> distribution of the model output from Monte Carlo simulation)
- Key distinction is made between
  - Estimation vs.
  - Ensuring compliance

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Wilks’ Method

- The uncertainty or confidence associated with upper (or lower) bound estimates was first rigorously derived by **Wilks** in 1941
  - Often referred to as the Wilks’ method (or formula)
- The original derivation is quite tedious and mathematically intensive
- Our paper provides a simpler derivation based on the concept of order statistics and the Binomial distribution
  - Please refer to our paper in the conference proceedings for more details…

Basic Idea

- In a random sample of 100 values, the 95th percentile value can be estimated as the 95th highest value (in the sorted list)
  - Need to consider ordering, or **order statistics**
- Consider a random sample of only four different values x_1, x_2, x_3, x_4 from some continuous distribution
- **Question:** What is the probability that the third highest value (i.e., next to largest order statistic) will be less than, say 1?
  - <u>At least</u> 3 of the values must be less than 1

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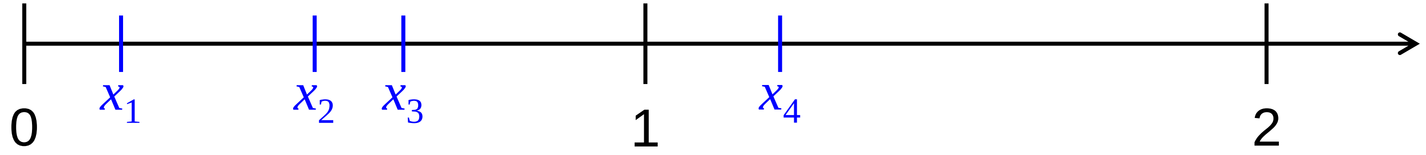
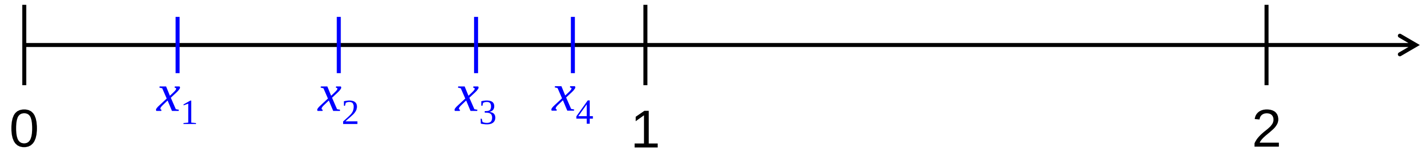
Basic Idea (cont'd)

3 out of 4



OR

All 4



- Note that the **order** of the sample values can change
  - The various combinations of k out of n values can be evaluated using the **Binomial distribution**

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Upper Bound Confidence

- The upper bound $100(1-\alpha)\%$ confidence limit for any percentile π_p can be stated as

$$P(Y_i > \pi_p) = 1 - \sum_{k=i}^{n} \binom{n}{k} p^k (1-p)^{n-k} = 1 - \alpha$$

Probability (or confidence) that a particular i^{th} order statistic (in a sample of size n) is greater than a particular p^{th} percentile value of the distribution

- Unknowns
  - i is the i^{th} order statistic (i.e., i^{th} highest value)
  - n is the sample size
  - p is the percentile value
  - α is the "level of significance" ($(1-\alpha)$ is the confidence)

Upper Tolerance Limit

- The one sided (upper) confidence bound is equivalent to the upper **tolerance limit**

$$P(Y_i > \pi_p) = 1 - \sum_{k=i}^{n} \binom{n}{k} p^k (1-p)^{n-k} = 1 - \alpha$$

- This equation can be used to back-calculate the <u>sample size</u> that would be required to make the probabilistic statement true at a given level of confidence (for a chosen order statistic)
  - This derivation is **independent** of the underlying probability distribution

Maximum (or highest) Value

- The upper confidence limit associated with the n^{th} highest (i.e., **maximum**) value in a sample of n is

$$P(Y_n > \pi_p) = 1 - \sum_{k=n}^{n} \binom{n}{k} p^k (1-p)^{n-k} = 1 - p^n = 1 - \alpha$$

- Solving for the sample size n

$$n = \frac{\ln(\alpha)}{\ln(p)}$$

- For the 95/95 tolerance limit, α is equal to 0.05 and p is 0.95, resulting in n equal to 58.4

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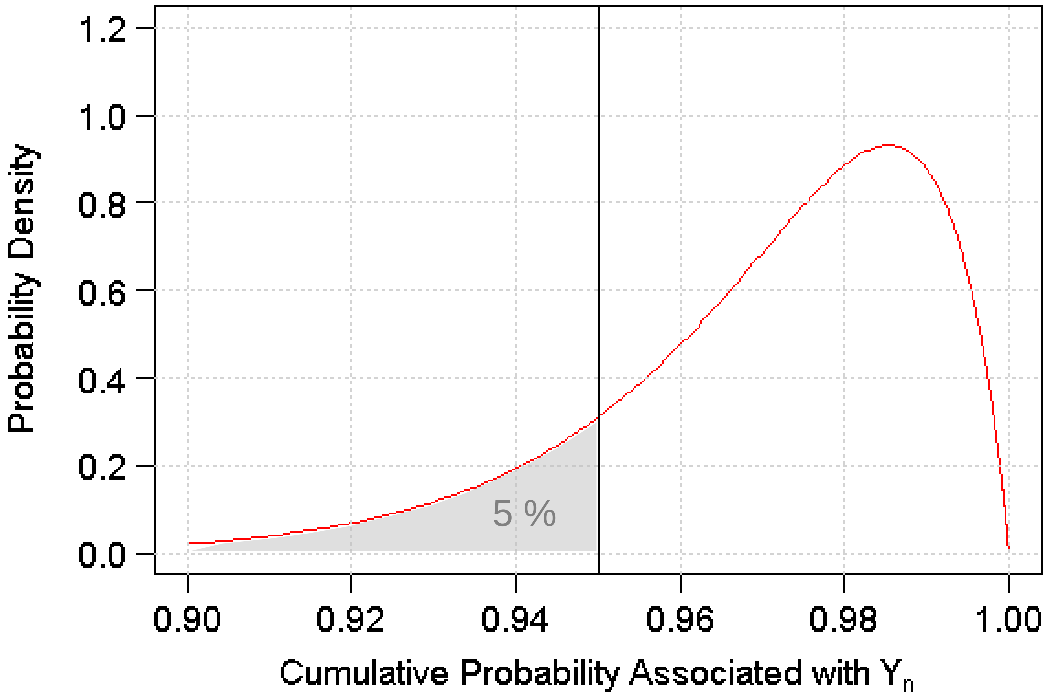
What does this mean?

- Choosing the highest (or maximum) value in a random sample of 59 values (e.g., from Monte Carlo simulation) will satisfy the 95/95 probability/confidence criterion
  - Identical statement can also be made for a lower bound value using the minimum value in the sample
- In other words, 95 % of the time (i.e., 19 times out of 20), the maximum value in a sample of 59 will be greater than the “true” or actual 95th percentile value of the distribution
  - 5 % of the time it will be lower

Distribution of Maximum (n = 59)

- The sampling distribution of the maximum value in a sample of 59



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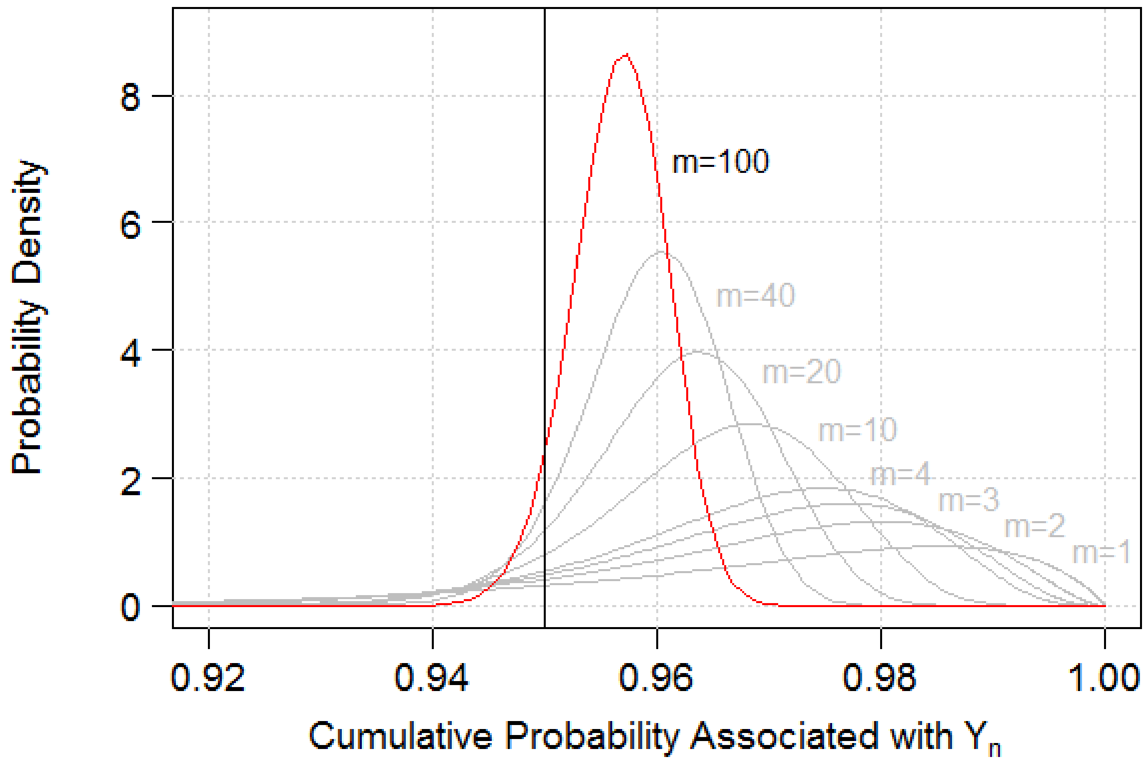
Estimation Problem

- Wilks' formula **guarantees** that 95 % of the time, the maximum value (in a group of 59) will be greater than the true 95th percentile value
- But, there is a high likelihood of getting a value greater than the 98th percentile
- May result in an upper bound **estimate** that is too high or unrealistic
- The estimation can be improved by performing a higher number of simulations
  - i.e., using Wilks' method to find the required sample size for different (lower) order statistics

Sampling Distributions

animation

- Sampling distributions of the m^{th} highest values in a given number of simulation trials



m^{th} Highest Value	Number of Simulations
100	2326
40	1008
20	548
10	311
4	153
3	124
2	93
1	59

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Comments

- In all cases, as before, the estimated value will always be greater than the true 95th percentile with 95 % probability
- However, choosing a higher number of simulations (i.e., lower order statistic in the sample) generally results in a **less conservative** estimate of the upper bound value
  - The estimated value is likely to be closer to the actual true 95th percentile value, rather than some higher percentile

Ensuring Compliance

- Rather than estimation, Wilks' method is highly useful for **demonstrating compliance** with a specified acceptance limit
  - e.g., 2200°F peak cladding temperature of a fuel rod
- The 95/95 rule is met if **none** of the 59 simulated values exceed the critical limit
  - The maximum value would represent the 95th percentile value (likely to be higher)
  - Since the maximum value is less than the acceptance limit, then 95 % of all possible values of the random variable (e.g., simulated peak cladding temperature) should by definition be less than the acceptance limit (this statement is true with 95 % probability)

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Model Uncertainty

- Given the small sample size, this approach naturally raises the key issue of **model uncertainty**
  - e.g., estimating the 95th percentile with 50 % confidence requires only 14 simulations (95/50 rule)
- The model output (i.e., the small number of sample values) depend entirely on the
  - Distributions (i.e., probabilistic models) of the inputs
  - Computational model itself
- Need to perform comprehensive
  - Model validation and verification
  - Sensitivity and uncertainty analysis

Summary and Conclusions

- The origin of Wilks' sample size formula was derived using simple examples
  - Please see actual paper for more details
- The resulting expression can be used to determine the required sample size for <u>any</u> probability and confidence level
  - e.g., 99/99 criterion would require 459 simulations
- Rather than **estimation**, the method is most useful for **ensuring compliance** with a particular acceptance limit

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