Statistical considerations on safety analysis

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Abstract
Alerting experience with a well-acknowledged safety analysis code initiated the authors to pay attention to safety issues of complex systems. Their first concern was the statistical characteristics of such a code. We point out a remarkable weakness of the so called 0.95/0.95 methodology: when repeating the search for the tolerance limit, we get a higher value with non-negligible probability. We propose the sign test as an alternative method. We point out the correct form of Wilks’ formula when the number of parameters subjected to limitation is two or more.

Keywords: safety analysis, 0.95|0.95 methodology, sign test

1 Introduction
Alerting experience with a well-acknowledged safety analysis code [1], [2] which is widely used in the licensing process of nuclear power plants, initiated the authors to pay attention to safety issues of nuclear reactors. Their first concern was the statistical characteristics of such a code. In order to judge if a given nuclear reactor was safe, one had to demonstrate that safety criteria are met with a reasonable probability. But to judge the output of the code, one needed to know the probability distribution of the output.

In a former paper [3] we discussed the handling of statistics of model calculations with several outputs. The present work provides a correct statistical estimation of a quantile and we point out the inadequacy of the
traditional 95% probability limit approach, which seems to be the practice at US Nuclear Regulatory Commission. We advocate the sign test instead.

Let us consider results of $N$ runs of a code modelling the single output variable, which is subjected to limitation. Let the output values be ordered:

$$y(1) < y(2) < \cdots < y(N).$$

We call the ensemble (1) a sample. Let the acceptance range be given as $(-\infty, U_T]$, where $U_T$ is the technological limit for $y$. We assume that the distribution of $y$ is unknown, and are looking for a quantile $Q_\gamma$ such that

$$\int_{-\infty}^{Q_\gamma} dG(y) = \gamma,$$

where $G(y)$ is the unknown cumulative distribution function of output variable $y$. Quantile $Q_\gamma$ is to be derived from measured value, thus, itself is a random variable.

In Section 2, we address the problem of estimating quantile $Q_\gamma$. Two solutions are mentioned: the classical Bayesian solution and a recent solution, which is applicable to several variables. In Section 3, we present an example where the 0.95—0.95 methodology seems to fail and in Section 4, we suggest another methodology based on sign test. Our concluding remarks are summarized in the last Section.

## 2 Estimation for one-tailed quantile

The random interval $(-\infty, y(s)]$ covers a proportion larger than $\gamma$ of the unknown distribution function $G(y)$ with probability $\beta$ when

$$\beta = \mathcal{P}\{y(s) > Q_\gamma\},$$

where $\mathcal{P}\{A\}$ denotes the probability of event $A$. It can be shown [4] that

$$\beta = \sum_{j=0}^{s-1} \binom{N}{j} \gamma^j (1 - \gamma)^{N-j}.$$  

When $s = N$, i.e. the largest element of the sample is chosen as upper limit of the random interval, one obtains the well-known formula:

$$\beta = 1 - \gamma^N.$$  

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Since one finds misinterpretations in the engineering practice it is not superfluous to underline the proven notion of formula (5). $\beta$ is the probability that the largest value $y(N)$ of a sample comprising $N$ observations is greater than the $\gamma$ quantile of the unknown distribution of output variable $y$. Another formulation asserts that $\beta$ is the probability that the interval $(-\infty, y(N)]$ covers a larger than $\gamma$ portion of the unknown distribution $G(y)$ of the output variable $y$.

2.1 Old Bayesian method

If we carry out $N$ runs, i.e., we determine the output variable from $N$ fluctuating inputs, and define a fix acceptance region $\mathcal{H}_a = [L_T, U_T]$. The probability

$$\mathcal{P}\{y \in \mathcal{H}_a\} = \int_{\mathcal{H}_a} g(u) \, du = w$$

Table 1: Number of failures observations $N - k$ at which $w \geq \omega$ holds with probability at least $\alpha$

| $\alpha$ | $\omega$ | $N - k = 0$ | $N - k = 1$ | $N - k = 2$ |
|---|---|---|---|---|
| 0.90 | 0.90 | 21 | 31 | 51 |
| 0.95 | 0.95 | 44 | 75 | 104 |
| 0.99 | 0.99 | 228 | 387 | 530 |
| 0.95 | 0.90 | 27 | 45 | 60 |
| 0.95 | 0.95 | 57 | 92 | 123 |
| 0.99 | 0.99 | 297 | 472 | 626 |
| 0.99 | 0.90 | 43 | 63 | 80 |
| 0.95 | 0.95 | 89 | 129 | 164 |
| 0.99 | 0.99 | 457 | 660 | 836 |

of the output variable $y$ to lay in $\mathcal{H}_a$ is unknown. However, knowing that $k$ elements out of $N$ are in the acceptance interval, we can estimate the probability that the unknown acceptance probability $w$ is greater than a prescribed $\omega$ without knowing the distribution function $g(u)$. The claim is based on Bayes theorem on conditional probabilities and asserts

$$\beta(\omega|N, k) = \sum_{j=0}^{k} \binom{N+1}{j} (1-\omega)^j \omega^{N+1-j}. \quad (6)$$
The proof is available in textbooks. Using (6), we can easily determine the allowed number of rejections in a sample of \( N \) elements to make sure that \( w \geq \omega \) is true with a given \( \beta \geq \alpha \) prescribed probability. In Tab. 1, we have collected a few examples to give an impression how expression (6) works. It is noteworthy that even if \( k = 0 \), i.e. when all outputs are accepted, there is a non-zero probability that outputs will appear which should have been rejected. As we see, no failure out of 21 runs assures the same probability as one failure out of 31 runs or two failures out of 51 runs (cf. the first row of Tab. 1).

\[ \int_{U_1}^{L_1} \cdots \int_{L_n}^{U_n} g(y_1, \ldots, y_n) \, dy_1 \cdots dy_n > \gamma \]

is free of \( g(y_1, \ldots, y_n) \) and is given by

\[
P \left\{ \int_{L_1}^{U_1} \cdots \int_{L_n}^{U_n} g(y_1, \ldots, y_n) \, dy_1 \cdots dy_n > \gamma \right\} = \beta,
\]

were \( 0 < \beta \leq 1 \) is a given number. Details and proof of the statement can be found in [4].

### 2.2 Case of Several Variables

The following statement generalizes the estimate of a quantile to several output variables. In the case of \( n \geq 2 \) output variables with continuous joint distribution function \( G(y_1, \ldots, y_n) \) it is possible to construct \( n \)-pairs of random intervals \([L_j, U_j], \, j = 1, \ldots, n\) such that the probability of the inequality

\[
\int_{L_1}^{U_1} \cdots \int_{L_n}^{U_n} g(y_1, \ldots, y_n) \, dy_1 \cdots dy_n > \gamma
\]

is free of \( g(y_1, \ldots, y_n) \) and is given by

\[
P \left\{ \int_{L_1}^{U_1} \cdots \int_{L_n}^{U_n} g(y_1, \ldots, y_n) \, dy_1 \cdots dy_n > \gamma \right\} = \beta,
\]

were \( 0 < \beta \leq 1 \) is a given number. Details and proof of the statement can be found in [4].

### 3 Challenge of the 0.95|0.95 methodology

In the present section, we consider an example. We assume the single output variable \( y \) to have a lognormal distribution with parameters \( m \) and \( d \). This will be our ”unknown” \( G(y) \) distribution. The density function is

\[
g(y) = \frac{1}{yd\sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\log y - m}{d} \right)^2 \right],
\]

where \( y \geq 0 \).
We use Monte Carlo simulation to generate four samples of size $N = 100$, in the simulation we take $m = 2.5$ and $d = 0.5$. The goal is to get point estimates of $0.95$-quantiles for each sample and to determine the shortest two-tailed confidence intervals which cover with $0.95$ probability the "unknown" quantile $Q_{0.95}$, the reference value is $Q_{0.95} \approx 27.73$. The four samples are labeled as A, B, C, and D, the results of the simulation are summarized in Tab. 2.

|       | $A$    | $B$    | $C$    | $D$    |
|-------|--------|--------|--------|--------|
| $y(r)$| 22.66  | 25.21  | 22.48  | 23.29  |
| $Q_{0.95}$| 27.73  | 27.73  | 27.73  | 27.73  |
| $y(s)$| 33.25  | 38.28  | 35.88  | 53.05  |
| $(r, s)$| (91, 100)| (91, 100)| (91, 100)| (91, 100)|

If the upper limit, determined by the technology would be $U_T=40$, then, cases A, B, and C could be considered only as safe.

Setting $\beta = 0.95$ and $\gamma = 0.95$, from Eq. (4) we get the sample size $N = 58$, i.e. the largest element of a sample having 58 elements should be chosen as $Q_{0.95}$. We performed the following numerical experiment: Generated a sample of 58 elements, that sample is called basic sample, in notation: $y^{(b)}$. Then, we repeat the sample generation $n = 1000$ times, thus obtaining the samples $y^{(1)}, y^{(2)}, \ldots, y^{(1000)}$. The largest elements of those samples can be seen in Fig. 1. The minimum of the values is 22.62, the largest value is 132.27. One can observe that in 224 samples (more than 22% of the one thousand samples) the maximum exceeds the maximum of the basic sample ($y^{(b)}(58) = 45$). Let us check whether that number is reliable or not.

The probability that the largest element in a given sample is greater than $Q_{\gamma}$ is $1 - \gamma^N$. Let $\xi_n(Q_{\gamma})$ stand for the random variable giving the number of maximum elements exceeding $Q_{\gamma}$. The probability distribution of the newly introduced random variable is

$$
\mathcal{P}\{\xi_n(Q_{\gamma}) = k\} = \binom{n}{k} (1 - \gamma^N)^k \gamma^{N(n-k)}.
$$

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1In the practice $N = 59$ is used.
Figure 1: Results of 1000 samples of size $N = 58$. The largest element of the basic sample is $y^{(b)}(58) \approx 45$.

From this expression we obtain the expectation value and the variance as

$$E\{\xi_n(Q_\gamma)\} = n(1 - \gamma^N),$$

$$D^2\{\xi_n(Q_\gamma)\} = n \gamma^N (1 - \gamma^N).$$

When $n$ and $k$ are sufficiently large, the distribution of the random variable

$$\chi_n(Q_\gamma) = \frac{\xi_n(Q_\gamma) - E\{\xi_n(Q_\gamma)\}}{D\{\xi_n(Q_\gamma)\}}$$

is approximately standard normal, hence,

$$E\{\xi_n(Q_\gamma)\} - \lambda D\{\xi_n(Q_\gamma)\} \leq \xi_n(Q_\gamma).$$

$$E\{\xi_n(Q_\gamma)\} + \lambda D\{\xi_n(Q_\gamma)\} \geq \xi_n(Q_\gamma)$$

is valid with probability $w$ and $\lambda$ is the root of

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\lambda} e^{-u^2/2} du = \frac{1 + w}{2}.$$ 

Substituting here $n = 1000$, $N = 58$ and $w = 0.95$, we get $E\{\xi_n(Q_\gamma)\} = 950$, $D\{\xi_n(Q_\gamma)\} \approx 6.96$, $\lambda \approx 1.96$, and the following relationship is fulfilled.
with probability 95%: 936 < \xi_{1000}(Q_{0.95}) < 964. We can not estimate the number of samples, in each of which the maximum exceeds the maximum of the basic sample but we can count the number of maximal values exceeding the known quantile \( Q_{0.95} \), that number is 949, a number witnessing the correctness of the statistics.

In spite of the nice agreement we wish to underline that the \((0.95|0.95)\) safety policy does not exclude rare events such as limit violation when some of the calculated values are over the limit \( U_T \).

Another conclusion is that the maximal element of a single sample of 58 elements would be \( y^{(b)}(58) \) and if we repeat the sampling several times, then in relatively large number of the samples we get a higher than \( y^{(b)}(58) \) value for the maximal element. In the light of this experience one asks: is this the intended outcome of the \( 0.95|0.95 \) methodology? It is clear that a larger safety margin is needed to compensate for the weakness of the \( 0.95|0.95 \) methodology.

One must mention here that the result found in the above presented example is not exceptional but it is a direct consequence of a well-known theorem of mathematical statistics. It is easy to show that if one repeats the sampling from any continuous distribution \((n+1)\) times independently, then the probability that at least \( k \) out of \( n \) maximal sample elements \( y^{(1)}(N), \ldots, y^{(n)}(N) \) will exceed the initial (basic) sample value \( y^{(b)}(N) \), is equal to \( 1 - k/(n+1) \). The proof of the theorem and two important remarks are given in the Appendix.

4 Method based on sign test

The concluding remarks at the end of the previous section are not optimistic. The question is whether one can find a method more suitable for checking, from a computer model, the safety of a large device? Below we propose such a method based on sign test.

Again, we assume the cumulative distribution function \( G(y) \) of the output variable to be continuous but unknown. Let \( S_N = \{y_1, \ldots, y_N\} \) be a sample of \( N \) observations (runs of a computer model). Define the function

\[
\Delta(x) = \begin{cases} 
1, & \text{if } x > 0, \\
0, & \text{if } x < 0,
\end{cases}
\] (15)
and introduce the statistical function
\[
    z_N = \sum_{j=1}^{N} \Delta(U_T - y_j) \tag{16}
\]
which gives the number of sample elements smaller than \( U_T \). Criteria based on statistical function (16) are called sign criterion since \( z_N \) counts the positive \( U_T - y_j \) differences. When \( G(y) \) is continuous, the probability of \( U_T - y = 0 \) is zero.

Obviously, distribution of \( z_N \) is binomial, using the notation
\[
    \mathcal{P}\{ \Delta(U_T - y) = 1 \} = \mathcal{P}\{ y \leq U_T \} = p, \tag{17}
\]
we obtain
\[
    \mathcal{P}\{ z_N = j \} = \binom{N}{j} p^j (1-p)^{N-j}, \quad j = 0, 1, \ldots, N. \tag{18}
\]

Our task is to find a confidence interval \([\gamma_L(k), \gamma_U(k)]\) that covers the value \( p \) with a prescribed probability \( \beta \) provided we have a sample of size \( N \) and in that sample \( z_N = k \leq N \). The probability (17) gives the probability that the output \( y \) is not larger than the technological limit \( U_T \). When the lower level \( \gamma_L(k) \) of the confidence interval is close to unity, we can claim at least with probability \( \beta \) that the chance of finding the output \( y \) smaller than \( U_T \) is also close to unity and the system under consideration can be regarded as safe at the level \([\beta|\gamma_L(k)]\).

If the sample size \( N > 50 \), the random variable
\[
    \frac{k - Np}{\sqrt{Np(1-p)}} = \zeta_k \tag{19}
\]
has approximately normal distribution. Here \( k \) is the number of sample elements not exceeding \( U_T \). Let \( \beta \) denote the confidence level, then
\[
    \mathcal{P}\{ |\zeta_k| \leq u_\beta \} = 2\Phi(u_\beta) - 1 = \beta,
\]
where \( \Phi(x) \) is the standard normal distribution function. This equation can be rewritten in the form
\[
    \mathcal{P}\{ |\zeta_k| \leq u_\beta \} = \mathcal{P}\{ (N + u_\beta^2)(p - \gamma_L)(p - \gamma_U) \leq 0 \} = \beta,
\]
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where

$$\gamma_L = \gamma_L(k, u_\beta) =$$

$$= \frac{1}{N + u_\beta^2} \left[ k + \frac{1}{2} u_\beta^2 - u_\beta \sqrt{k(1 - k/N) + u_\beta^2/4} \right], \quad (20)$$

and

$$\gamma_U = \gamma_U(k, u_\beta) =$$

$$= \frac{1}{N + u_\beta^2} \left[ k + \frac{1}{2} u_\beta^2 + u_\beta \sqrt{k(1 - k/N) + u_\beta^2/4} \right]. \quad (21)$$

Here $u_\beta$ is the root of

$$\Phi(u_\beta) = \frac{1}{2}(1 + \beta).$$

In a number of cases it suffices to know the probability of the event \( \{ \gamma_L(k, u_\beta) \leq p \} \). Since $\zeta_k$ with $k$ fixed is a decreasing function of $p$, the events \( \{ \zeta_k \leq v_\beta \} \) and \( \{ \gamma_L(k, v_\beta) \leq p \} \) are equivalent, hence

$$\mathcal{P}\{ \zeta_k \leq v_\beta \} = \mathcal{P}\{ \gamma_L(k, v_\beta) \leq p \} = \Phi(v_\beta) = \beta.$$

Consequently, the operation of a system can be regarded safe if the parameter $p$ for all output variables is covered by $[\gamma_L(k, v_\beta), 1]$ with a prescribed probability $\beta$, provided that $\gamma_L(k, v_\beta)$ is close to unity.

Table 3: Number of successes $k$ in a sample of size $N$

| $k$  | 99 | 108 | 118 | 128 | 137 | 147 | 157 | 166 | 176 | 185 | 195 |
|------|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| $N$  | 100| 110 | 120 | 130 | 140 | 150 | 160 | 170 | 180 | 190 | 200 |

Table 3 gives the number of successes $k$ in a sample of size $N$ needed for acceptance at the level $\beta = \gamma_L = 0.95$. We utilized approximate formula (20) to derive the entries in Tab. 3.

When the sample size is less than 50, we may not apply the asymptotically valid normal distribution. The below given derivation of the confidence limits
is a modified method proposed by Clopper and Pearson. The probability of at least \( k \) successes from \( N \) observations is given by

\[
S_k^{(N)}(p) = \sum_{j=0}^{k} \binom{N}{j} p^j (1 - p)^{N-j},
\]

where \( p = \mathcal{P}\{y \leq U_T\} \). This formula can be recast as

\[
S_k^{(N)}(p) = \frac{N!}{k! \,(N-k-1)!} \int_0^{1-p} (1 - v)^k \, v^{N-k-1} \, dv,
\]

and it is clear from that expression that \( S_k^{(N)}(p) \) is a monotonously decreasing function of \( p \). Since

\[
S_k^{(N)}(p) = \begin{cases} 
1, & \text{if } p = 0, \\
0, & \text{if } p = 1,
\end{cases}
\]

it assumes an arbitrary value only once in the interval \([0,1]\). Consequently, a \( p = p_\delta \) value exists so that

\[
S_k^{(N)}(p_\delta) = \delta, \quad \forall \, 0 < \delta < 1.
\]

Exploiting the monotony, we can construct a function such that

\[
R_k^{(N)}(p) < R_k^{(N)}(p_\delta) = \delta,
\]

when \( p > p_\delta \). Such a function is

\[
R_k^{(N)}(p) = 1 - S_k^{(N)}(p) = \sum_{j=k}^{N} \binom{N}{j} p^j (1 - p)^{N-j},
\]

Finally, we establish the upper limit \( \gamma_U \) from

\[
S_k^{(N)}(\gamma_U) \leq \frac{1}{2} (1 - \beta),
\]

and the lower limit \( \gamma_L \) from

\[
R_k^{(N)}(\gamma_L) \leq \frac{1}{2} (1 - \beta).
\]

The interval \([\gamma_L, \gamma_U]\) covers the unknown parameter \( p \) with probability \( \beta \). The dependence of \( \gamma_L \) and \( \gamma_U \) are shown in Fig. 2 for a sample of \( N = 100 \) elements, \( cl \) stands for confidence level \( \beta \).
Figure 2: Dependence of $\gamma_L$ and $\gamma_U$ on the number of successes in a sample of $N=100$ elements.

4.1 Several output variables

Now we assume the output to comprise $n$ variables. Let these variables be $y_1, \ldots, y_n$. There are several fairly good tests to prove if they are statistically independent. To independent variables we can apply the considerations above but for dependent variables we need novel considerations. Let

$$S_N = \begin{pmatrix} y_{11} & y_{12} & \cdots & y_{1N} \\ y_{21} & y_{22} & \cdots & y_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ y_{n1} & y_{n2} & \cdots & y_{nN} \end{pmatrix}$$

denote the sample matrix obtained in $N >> 2n$ independent observations. With a computer model, an observation is a run. Introducing the column vector $\vec{y}_k$, the sample matrix is written as

$$S_N = (\vec{y}_1, \ldots, \vec{y}_N).$$

Below we expound the sign test for two output variables $y_1$ and $y_2$ relying on the assumption that their joint distribution function $G(y_1, y_2)$ is unknown but continuous in either variable. The goal of the foregoing analysis is to verify the safety conditions $y_1 < U_T^{(1)}$ and $y_2 < U_T^{(2)}$. When the condition is accomplished with probability $p_{12} = G(U_T^{(1)}, U_T^{(2)}) \approx 1$ we say the system is safe. Here, as before, the limits $U_T^{(1)}$ and $U_T^{(2)}$ are determined by the technology. Since $p_{12}$ is unknown, our job is to construct a confidence
interval $[\gamma_{L}^{(1,2)}$, $\gamma_{U}^{(1,2)}]$ so that it covers $p_{12}$ with probability $\beta_{12}$. In most cases it suffices to calculate solely $\gamma_{L}^{(1,2)}$ and to use the interval $[\gamma_{L}^{(1,2)}$, 1] as confidence interval. Now the column vectors introduced above have two components. In accordance with our assumption, different vectors are statistically independent but the components in a given vector are not necessarily independent. In order to keep the notation as simple as possible, the event \{\(y_{1} < U_{T}^{(1)}\), \(y_{2} < U_{T}^{(2)}\)\} will be called a success. If \(y_{1k} < U_{T}^{(1)}\) and \(y_{2k} < U_{T}^{(2)}\), then
\[
\Delta(U_{T}^{(1)} - y_{1k}) \Delta(U_{T}^{(2)} - y_{2k}) = 1,
\]
while 0 otherwise, and introduce the statistical function
\[
z_{N}^{(1,2)} = \sum_{k=1}^{N} \Delta(U_{T}^{(1)} - y_{1k}) \Delta(U_{T}^{(2)} - y_{2k})
\]
which gives the number of successes in the sample of size $N$. Since the newly introduced random variable is the sum of $N$ independent random variables, assuming values either 1 or 0, its distribution is binomial. Using the notation
\[
P\{\Delta(U_{T}^{(1)} - y_{1}) \Delta(U_{T}^{(2)} - y_{2}) = 1\} = \]
\[
= P\{y_{1} < U_{T}^{(1)}$, \(y_{2} < U_{T}^{(2)}\} = p_{12},
\]
we can write
\[
P\{z_{N}^{(1,2)} = k\} = \binom{N}{k} p_{12}^{k} (1 - p_{12})^{N-k},
\]
for $k = 0, 1, \ldots, N$. At this point we rejoin the thought of line of the previous subsection. Instead of repeating the already familiar argumentation, we amend two trivial although important remarks. Let us define the following two statistical functions:
\[
z_{N}^{(1)} = \sum_{i=1}^{N} \Delta(U_{T}^{(1)} - y_{1i})
\]
and
\[
z_{N}^{(2)} = \sum_{j=1}^{N} \Delta(U_{T}^{(2)} - y_{2j}).
\]
These two functions are not statistically independent, either one is the sum of \( N \) independent random variables with values 1 or 0, therefore, one can write
\[
P\{z_N^{(1)} = i\} = \binom{N}{i} p_1^i (1 - p_1)^{N-i}
\]
and
\[
P\{z_N^{(2)} = j\} = \binom{N}{j} p_2^j (1 - p_2)^{N-j},
\]
\(i, j = 1, \ldots, N,\)
where
\[
p_\ell = P\{y_\ell < U^{(\ell)}_T\} = P\{\Delta(U^{(\ell)}_T - y_\ell) = 1\},
\]
\(\ell = 1, 2,\)
are unknown probabilities. Applying the method used previously, this time separately to the samples
\[
S_{N}^{(1)} = \{y_{1i}, \ i = 1, \ldots, N\}
\]
and
\[
S_{N}^{(2)} = \{y_{2j}, \ j = 1, \ldots, N\}
\]
we construct two random intervals \([\gamma_L^{(1)}, 1]\) and \([\gamma_L^{(2)}, 1]\) covering \(p_1\) and \(p_2\) with probabilities \(\beta_1\) and \(\beta_2\), respectively.

Obviously, it could occur that the levels \((\beta_1|\gamma_L^{(1)})\) and \((\beta_2|\gamma_L^{(2)})\) corroborate the claim that samples \(S_{N}^{(1)}\) and \(S_{N}^{(2)}\) separately comply with safety requirements. This does not mean that we would arrive at the same conclusion from analyzing the two sets jointly. The reason is that \(y_1\) and \(y_2\), the two output random variables are not statistically independent. Hence, we should ascertain whether the interval \([\gamma_L^{(1,2)}, 1]\) covers the probability \(p_{12}\) with the pre-assigned probability \(\beta_{12}\). Since \(\gamma_L^{(1,2)} \leq \min\{\gamma_L^{(1)}, \gamma_L^{(2)}\}\), \(\gamma_L^{(1)}\) and \(\gamma_L^{(2)}\) would not contain information sufficient to declare the system safe. Decision on the safety, when two output variables are subjected to limitations should go as follows. Firstly, we test the hypothesis concerning dependence of the output variables \(y_1\) and \(y_2\). If they are dependent, we should estimate the probability of the event \(\{y_1 < U^{(1)}_T, \ y_2 < U^{(2)}_T\}\). Solely if they are statistically independent should we estimate the probability of events \(\{y_1 < U^{(1)}_T\}, \{y_2 < U^{(2)}_T\}\) independently.
Finally, we mention that the generalization of the sign test to \( n > 2 \) output variables is straightforward, we have to use the statistical function

\[
z_{N}^{(1,\ldots,n)} = \sum_{k=1}^{N} \prod_{j=1}^{n} \Delta(U_{T}^{(j)} - y_{jk})
\]

(22)

\( N \) to evaluate safety based on observation of \( N \) samples of the \( n \) output variables. In this manner we obtain the sum of \( N \) independent random variables in expression (22), and then, the further steps will be the same as at the beginning of the subsection.

![Figure 3: Sample a)](image)

![Figure 4: Sample b)](image)

An example is given below. We have generated two samples a) and b) using Monte Carlo simulation, either sample contains \( N = 100 \) observations.
(or runs) of two output variables. The samples have been generated from a bivariate normal distribution with parameters \( m_1 = m_2 = 0 \) and \( \sigma_1 = \sigma_2 = 1 \) but the correlation coefficient is \( C = 0.1 \), \( C = 0.7 \) in sample a) and b), respectively. The acceptance range is \([-2, 2]\) for both output variables. In sample a) and b) four and one samples lie respectively outside the acceptance range. The results of the simulation can be seen in Fig. 3 and in Fig. 4.

Table 4: Lower confidence limits in a sample of \( N = 100 \), \( k \) is the number of success.

| \( k \) | \( \beta \) | 0.90  | 0.95  | 0.99  |
|-------|--------|------|------|------|
| 90    | 0.8501 | 0.8362 | 0.8086 |
| 91    | 0.8616 | 0.8482 | 0.8212 |
| 92    | 0.8733 | 0.8602 | 0.8340 |
| 93    | 0.8850 | 0.8725 | 0.8471 |
| 94    | 0.8970 | 0.8850 | 0.8604 |
| 95    | 0.9092 | 0.8977 | 0.8741 |
| 96    | 0.9216 | 0.9108 | 0.8882 |
| 97    | 0.9344 | 0.9242 | 0.9030 |
| 98    | 0.9476 | 0.9383 | 0.9185 |
| 99    | 0.9616 | 0.9534 | 0.9354 |
| 100   | 0.9772 | 0.9704 | 0.9549 |

First let us consider sample a). From Tab. 4 one can read that the interval \([0.9108, 1]\) covers the parameter \( p_{12} \) with probability \( \beta_{12} = 0.95 \).

When we assess the output variables one by one, we see that the associated probabilities \( p_1 \) and \( p_2 \) are covered by the interval \([0.9383, 1]\) with probability \( \beta = 0.95 \) in either sample. However tempting is to use 0.9383 as lower bound for the probability to be used in safety analysis, that number has nothing to do with \( p_{12} \) and should not be used in safety analysis.

Now let us pass on to sample b) where we see a strong correlation between \( y_1 \) and \( y_2 \). From Tab. 4 one can read that the confidence interval \([0.9383, 1]\) covers the probability \( \beta_{12} = 0.95 \). From that sample we conclude that the probability of the event \( \{ y_1 < U_T^{(1)}, y_2 < U_T^{(2)} \} \) is at least 0.9383. The single variable parameters \( p_1 \) and \( p_2 \) determined from sample b) are covered by the intervals \([0.9534, 1]\) and \([0.9383, 1]\), respectively on the level \( \beta_1 = \beta_2 = 0.95 \). Again, however favorable these numbers are, they should not be used
in assessing safety. The above discussed simple numerical example clearly indicated the danger awaiting the analyst when his/her judgment is based on tests performed separately on correlated output variables.

5 Concluding remarks

The authors have investigated the statistical methods applied to safety analysis of nuclear reactors and arrived at alarming conclusions: Guba and Trosztel carried out a series of calculations with the generally appreciated safety code ATHLET to ascertain the stability of the results against input uncertainties in a simple experimental situation. Scrutinizing those calculations, we came to the conclusion [3] that the ATHLET results may exhibit irregular behavior. A further conclusion is that the technological limits are incorrectly set [5] when the output variables are correlated. Another formerly unnoticed conclusion of the Guba-Trosztel calculations is that certain innocent looking parameters (like wall roughness factor, the number of bubbles per unit volume, the number of droplets per unit volume) can influence considerably such output parameters as water levels. The authors are concerned with the statistical foundation of present day safety analysis practices and can only hope that their own misjudgment will be dispelled.

Until then, the authors suggest applying correct statistical methods in safety analysis even if it makes the analysis more expensive. It would be desirable to continue exploring the role of internal parameters (wall roughness factor, steam-water surface in thermal hydraulics codes, homogenization methods in neutronics codes) in system safety codes and to study their effects on the analysis.

In the validation and verification process of a code one carries out a series of computations. The input data are not precisely determined because measured data have an error, calculated data are often obtained from a more or less accurate model. Some users of large codes are content with comparing the nominal output obtained from the nominal input, whereas all the possible inputs should be taken into account when judging safety. At the same time, any statement concerning safety must be aleatory, and its merit can be judged only when the probability is known with which the statement is true. In some cases statistical aspects of safety are misused as in [5], where the number of runs for several outputs is correct only for statistically independent outputs, or misinterpreted as in [6].
We do not know the probability distribution of the output variables subjected to safety limitations. At the same time in some asymmetric distributions the 0.95|0.95 methodology simply fails: if we repeat the calculations in many cases we would get a value higher than the basic value, which means the limit violation in the calculation becomes more and more probable in the repeated analysis.

Consequent application of order statistics or the application of the sign test may offer a way out of the present situation. The authors are also convinced that efforts should be made

- to study the statistics of the output variables,
- to study the occurrence of chaos in the analyzed cases.

All these observations should influence, in safety analysis, the application of best estimate methods, and underline the opinion that any realistic modelling and simulation of complex systems must include the probabilistic features of the system and the environment.

### Appendix

Let $\eta$ be a random variable with continuous distribution defined over the real numbers $\mathbb{R}$, and let the distribution function of $\eta$ be

$$P \{ \eta \leq y \} = G(y). \quad (23)$$

We carry out $N$ statistically independent observations of $\eta$. That operation is called $K$. We repeat $K \times n + 1$ times. We group the observed values into the following $(n + 1) \times N$ matrix:

$$
\begin{array}{cccc}
\eta_{01} & \eta_{02} & \cdots & \eta_{0N} \\
\eta_{11} & \eta_{12} & \cdots & \eta_{1N} \\
\cdots & \cdots & \cdots & \cdots \\
\eta_{n1} & \eta_{n2} & \cdots & \eta_{nN}
\end{array}
$$

Let denote $\zeta_j = \max_{1 \leq k \leq N} \eta_{jk}$ the maximum observed in operation $j$.

**Lemma.** Since the probability density function $G(y)$ is monotonously increasing, and continuous, the following equation holds for $0 \leq \gamma \leq 1$:

$$P \left\{ \max_{1 \leq k \leq N} \eta_{jk} > G^{-1}(\gamma) \right\} = P \left\{ \int_{-\infty}^{\zeta_j} dG(y) > \gamma \right\} = 1 - \gamma^N, \quad (25)$$

where $G^{-1}(\gamma) = Q_\gamma$ is the $\gamma$ quantile of the probability density distribution function $G(y)$.

The presented Lemma is well known, we omit its proof. Now we turn to the determination of the probability distribution of the largest sample elements.

**Theorem.** The probability of the event that among the independent random variables $\zeta_1, \ldots, \zeta_N$ there is $k \leq N$ greater than $\zeta_0$ is

$$P_k = 1 - \frac{k}{n+1}. \quad (26)$$

**Proof:** Since $\eta_{jk}, j = 0, 1, \ldots, n; k = 1, \ldots, N$ are independent and identically distributed, we have

$$\mathcal{P} \{\zeta_j \leq z\} = \mathcal{P} \left\{ \max_{1 \leq k \leq N} \eta_{jk} \leq z \right\} = \prod_{k=1}^{N} \mathcal{P} \{\eta_{jk} \leq z\} = H(z). \quad (27)$$

In other words, $H(z)$ is the probability of $\zeta_j$ not being larger than $z \in \mathcal{R}$ for any $j = 0, 1, \ldots, n$. Let $0 \leq \nu_n(z) \leq n$ denote the number of those variables from among $\zeta_1, \ldots, \zeta_n$ which are greater than $z$. Obviously,

$$\mathcal{P} \{\nu_n(z) = \ell\} = J_{\ell}^{(n)}(z) = \binom{n}{\ell} (1 - H(z))^\ell (H(z))^{n-\ell}. \quad (28)$$

Let $P_k$ stand for the probability that from among the random variables $\zeta_1, \ldots, \zeta_n$ at least $k \leq n$ is greater than $\zeta_0$, which may take any number from $\mathcal{R}$. We get

$$P_k = \sum_{\ell=k}^{n} p_\ell = \sum_{\ell=k}^{n} \int_{-\infty}^{+\infty} J_{\ell}^{(n)}(z)dH(z). \quad (29)$$

The determination of probabilities $p_\ell$ is straightforward:

$$p_\ell = \int_{-\infty}^{+\infty} J_{\ell}^{(n)}(z)dH(z) = \binom{n}{\ell} \int_{-\infty}^{+\infty} (1 - H(z))^\ell (H(z))^{n-\ell} dH(z). \quad (30)$$

The integrals are evaluated without difficulties:

$$p_\ell = \binom{n}{\ell} \int_{0}^{1} (1 - u)^\ell u^{n-\ell} du = \frac{1}{n+1}. \quad (31)$$
As we see, $p_\ell$ is independent of $\ell$ and using Eq. (29), we get

$$P_k = \sum_{\ell=k}^{n} \frac{1}{n+1} = \frac{n-k+1}{n+1} = 1 - \frac{k}{n+1}.$$  \hspace{1cm} (32)

Q.E.D.

We add two remarks.

1. **Remark 1.** Whichever we choose from among the random variables $\zeta_0, \zeta_1, \ldots, \zeta_n$, with probability $1/n+1$ we find among the others $\ell$ exceeding the first chosen one. (Since $\zeta_0, \zeta_1, \ldots, \zeta_n$ are continuous random variables, the probability of two values to be identical is zero.)

2. **Remark 2.** Let $\lambda$ be the number of those $\zeta_{j1}, \zeta_{j2}, \ldots, \zeta_{jn}$ variables which are greater than a given $\zeta_{j0}$. Clearly, $\lambda$ is a random variable, its expectation value is

$$E\{\lambda\} = \sum_{\ell=0}^{n} \ell p_\ell = \frac{n}{2},$$ \hspace{1cm} (33)

the variance being

$$D^2\{\lambda\} = \sum_{\ell=0}^{n} (\ell - n/2)^2 p_\ell = \frac{1}{6}n \left(1 + \frac{1}{2}n\right).$$ \hspace{1cm} (34)

References

[1] M.J. Burwell et al.: The Thermohydraulic Code ATHLET for Analysis of PWR and BWT Systems, NURETH-4, Karlsruhe, (1989).

[2] H. Austregesil, H. Dellenbeck: ATHLET Mod 12 Cycle A, Programmers Manual, vol. 1. GRS, March (1998).

[3] A. Guba, M. Makai, L. Pál, Rel. Eng. and Sytem Safety, 80, 217 (2003).

[4] L. Pál, M. Makai, arXiv:physics/0308086.

[5] B. Krzykacz: A Computer Program for the Derivation of Empirical Uncertainty Statements of Results from Large Computer Models, Report GRS-A-1720, Garching, (1990).
[6] B. Wallis, Rel. Eng. and System Safety, 80, 309 (2003).

[7] A. Guba and T. Trosztel: *Uncertainty Analysis of a PMK-2 Pressurizer Surge Line Middle Size Break Experiment*, Report KFKI AEKI, Budapest, 2000.

[8] C.J. Clopper and E.S. Pearson, Biometrica, 26, 404 (1934).