

A step-down test for effects in unreplicated factorial trials

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1 Introduction

Two-level fractional factorial designs are important statistical tools in particular for screening experiments and in situations where the cost of experimentation is high. It is common that no replicates are taken. Also full factorial designs may often be performed without replicates. This means that there does not exist any within series estimate of experimental error variance.

The problem has been overcome in different ways. If the fraction is not too small, the estimates of interactions of some high orders, not aliased with main effects or low order interactions may be used for variance estimation.

A common subjective method is to make a normal or half normal plot of all effect estimates and then select as important (significant) the effects with estimates deviating much from a straight line. This method by Daniel (1959) is commonly adopted in textbooks, e.g. Box et al. (1978) and Montgomery (1984).

There exist also some methods which have a warranted level of significance for declaring effects to be nonzero when they are in fact zero. The most important of those methods is Voss (1999, 1988). He constructs a variance estimate based on the half of the estimates with the smallest moduli.

The aim of the present paper is to present an alternative method with warranted level. It is based on another type of estimate, which makes it flexible with respect to the true number of zero and nonzero effects. Further this type of estimate makes it possible to construct a step-down test with a multiple level of significance. Principles and definitions for step-down test may be found in Hochberg and Tamhane (1987).

2 Coverage bounds

The test method to be presented later is based on coverage bounds for order statistics. In this section we will make a general discussion of coverage bounds in order to prepare for the method presentation in the next section.

Let $X^{(1)}, X^{(2)}, \dots, X^{(n)}$ be order statistics in a sample of size n from a distribution with a cumulative distribution function $F(x)$. A left one-sided coverage band with coverage probability q is a sequence of constants a_1, a_2, \dots, a_n such that $\mathbb{P}\{X^{(k)} \geq a_k \text{ for } k = 1, 2, \dots, n\} = q$. The band is said to be balanced if the individual missing probabilities $\mathbb{P}\{X^{(k)} < a_k\}$ are the same for all $k = 1, 2, \dots, n$. In some application it is reasonable to have a coverage bound, which is balanced, but in others it is more reasonable to have a varying individual coverage probability for the order statistics. A right one-sided balanced coverage band may be defined analogously.

One may also define coverage bounds on both sides simultaneously, which then gives a coverage band. A two-sided coverage band with coverage probability q consists of two sequences of constants a_1, a_2, \dots, a_n and b_1, b_2, \dots, b_n such that $\mathbb{P}\{a_k \leq X^{(k)} \leq b_k \text{ for } k = 1, 2, \dots, n\} = q$. The band is said to be balanced if the individual missing probabilities $\mathbb{P}\{X^{(k)} < a_k\}$ and $\mathbb{P}\{X^{(k)} > b_k\}$ are the same on both sides and for all $k = 1, 2, \dots, n$.

An attempt to use balanced coverage bands for out-lier detection is made by Atkinson (1981). He uses a half normal plot to detect outliers and influential observations. On the normal probability paper is constructed a band and the position of order statistics are compared to that band. The statistics are of a type given by Cook (1977). The band is constructed as an envelop of the order statistics for 20 simulated series of statistics. The reason for having 20 series seems to be related to some idea of standard coverage probability, since for each order the band reaches from the smallest to the largest of corresponding order statistics in the 20 simulated series. The method is further developed by Flack and Flores (1989). They made more

accurate bands by basing it on a larger simulation and they also discussed other similar constructions.

We now consider the calculation of the coverage probability of a left one-sided coverage bound. The calculation can be made for the $U(0, 1)$ distribution by first making the transformation $U_i = F(X_i)$ for $i = 1, 2, \dots, n$ giving the ordered statistics $U^{(1)}, U^{(2)}, \dots, U^{(n)}$. Then $U^{(k)}$ has a Beta distribution with parameters k and $n + 1 - k$. Now let a_1, a_2, \dots, a_n be any constants with the ordering $a_1 < a_2 < \dots < a_n$ for which we want to calculate the probability $\mathbb{P}\{U^{(k)} \geq a_k \text{ for } k = 1, 2, \dots, n\}$.

For each individual order statistic $U^{(k)}$ the probability $\mathbb{P}\{U^{(k)} < a_k\}$ is obtained by the Beta distribution. We introduce events $A_n = \{U^{(n)} < a_n\}$ and $A_k = \{U^{(k)} < a_k \text{ and } U^{(k+1)} \geq a_{k+1}\}$ for $k = 1, 2, \dots, n - 1$, which can be interpreted as a passage over the bound. Further we introduce the events $B_n = A_n$ and $B_k = A_k \cap (\cup_{j=k+1}^n A_j^c)$ for $k = 1, 2, \dots, n - 1$, which can be interpreted as the first passage over the bound when going from above in index. Thus now

$$\mathbb{P}\{U^{(k)} \geq a_k \text{ for } k = 1, 2, \dots, n\} = 1 - \sum_{k=1}^n \mathbb{P}\{B_k\}.$$

The probabilities $\mathbb{P}\{B_k\}$ may be calculated successively with a simple equation system by using conditioning.

Since $A_k = \cup_{j=k}^n \{A_k \cap B_j\}$ we get

$$\mathbb{P}\{B_n\} = \mathbb{P}\{A_n\}, \quad \mathbb{P}\{B_{n-1}\} = \mathbb{P}\{A_{n-1}\}$$

and

$$\begin{aligned} \mathbb{P}\{A_k\} &= \mathbb{P}\{A_k \cap B_k\} + \sum_{j=k+1}^n \mathbb{P}\{A_k \cap B_j\} \\ &= \mathbb{P}\{B_k\} + \sum_{j=k+1}^n \mathbb{P}\{B_j\} \mathbb{P}\{A_k | B_j\} \text{ for } k = 1, 2, \dots, n - 2. \end{aligned}$$

Here

$$\begin{aligned} \mathbb{P}\{A_k\} &= \binom{n}{k} a_k^k (1 - a_{k+1})^{n-k} \text{ and} \\ \mathbb{P}\{A_k | B_j\} &= \binom{j}{k} \frac{a_k^k (a_j - a_{k+1})^{j-k}}{a_j^j} \text{ for } j > k \end{aligned}$$

which is proved in Lemma 1 in the appendix. Thus the equation system for determining $\mathbb{P}\{B_k\}$ is

$$\begin{aligned}\mathbb{P}\{B_n\} &= a_n^n \\ \mathbb{P}\{B_{n-1}\} &= \binom{n}{n-1} a_{n-1}^{n-1} (1 - a_n)^1 \\ \mathbb{P}\{B_k\} &= \binom{n}{k} a_k^k (1 - a_{k+1})^{n-k} \\ &\quad - \sum_{j=k+1}^n \mathbb{P}\{B_j\} \binom{j}{k} \frac{a_k^k (a_j - a_{k+1})^{j-k}}{a_j^j} \text{ for } k = n-2, n-3, \dots, 1\end{aligned}$$

By doing the calculation successively in the indicated order we do not even need to solve an equation system. From this result we can easily get the same type of result for random variables X_1, X_2, \dots, X_n with any continuous cumulative distribution function $F(x)$ by considering the transformation $U_k = F(X_k)$.

If $X^{(1)}, X^{(2)}, \dots, X^{(n)}$ are the order statistics the coverage probability $\mathbb{P}\{X^{(k)} \geq a_k^* \text{ for } k = 1, 2, \dots, n\}$ of a left one-sided coverage band with constants $a_1^*, a_2^*, \dots, a_n^*$ is obtained by using $a_k = F(a_k^*)$ in the above calculation for the $U(0, 1)$ distribution.

For the statistical problems to be treated later we want a reversed calculation. That is, for a given internal relation between the individual coverage probabilities for the different order statistics, we want to determine the absolute size of these probabilities in order to get a given total coverage probability. For instance if we want a balanced coverage bound we use the same individual coverage probability, which should be determined so that the total coverage probability is equal to some given value. In our statistical problems there are reasons for having individual coverage, which increases with the order of the statistic. Using a linear increase the individual probability $\mathbb{P}\{U^{(k)} \leq a_k\}$ is proportional to k . In order to get a given total coverage probability we need to determine this proportionality constant.

The problem of getting a given total coverage probability for a given structure of individual coverage probabilities is easily solved by iteration. From some starting values of the individual coverage probabilities, with the given internal structure, we calculate the constants a_k by the Beta distribution and then calculate the total coverage probability by the equation system for $\mathbb{P}\{B_k\}$. If this total coverage probability is smaller than intended the individual coverage probabilities are increased with the relative sizes preserved

and if the total coverage probability is too big they are decreased. When there are results on both sides of the required total coverage the calculation is iterated in new points estimated linearly from the previous cases most close to the required result. The procedure converges to acceptable approximation in a few steps.

3 Estimation by use of coverage bound

A left coverage bound with a coverage probability of 0.5 is in a sense an estimate of a "natural left tangent" of the empirical cumulative distribution function. This coverage bound is situated in a median position to the left. In particular in one-parameter problems this may be used to get good parameter estimates.

When using the common method by Daniel (1959) one selects intuitively a lower part of the ordered values of the effect estimates to fit a straight line on the half normal plot and then declare as significant those factors whose absolute values of effect estimates deviate much from this line. We will now here use an objective and adaptive method with the same intention. In our method the estimate of the standard deviation is obtained by a scale factor required for aligning the ordered sample to the right of a left coverage bound with coverage probability 50%. In order to get good estimates we will use a coverage bound which has a linearly increasing individual coverage probability. This means that there is greater probability that a great ordered absolute value will be used for the estimate.

We describe the details of the construction in order to be precise. Let a_1, a_2, \dots, a_n be the boundary constants for a left bound with linearly increasing individual coverage probability and total coverage probability 50% for the case of $U(0, 1)$ distribution. Then calculate the boundary constants $a_k^* = \Phi^{-1}((a_k + 1)/2)$ for the distribution of ordered absolute values $X^{(1)}, X^{(2)}, \dots, X^{(n)}$ of observations which are normally distributed with parameters $(0, \sigma)$. Then σ may be estimated by $\hat{\sigma} = \min_{1 \leq k \leq n} (X^{(k)} / a_k^*)$. When using the estimate in a situation with non-replicated factorial design, we have sample sizes of the type $n = 2^m - 1$ and the random variables are the absolute values of the estimates. If there are no true effects the estimate is median unbiased. If there are true effects, there is a tendency that the biggest absolute values deviate more or less to the right and σ is estimated by absolute values of lower order. Then the estimate is no more median un-

k	1	2	3	4	5	6	7
Bound	0.00062	0.0142	0.0452	0.0881	0.1390	0.1950	0.2575
8	9	10	11	12	13	14	15
0.3228	0.3915	0.4632	0.5379	0.6155	0.6966	0.7825	0.8771

Table 1: Bounds for a 50% left coverage bound for order statistics in a series of 15 ordered statistics from a uniform $[0;1]$ distribution.

biased. We will use this type of estimate in the effect testing method in the next section.

In practice one needs to make a minor correction to the method. Since we always work with some rounding off of the observed quantities we might by coincidence get some estimates, which are 0. This numerical problem would completely destroy the estimate and give . It can in practice be avoided by adjusting the fitting with the size of the smallest observable unit. If this is d it means that we use the estimate $\hat{\sigma} = \min_{1 \leq k \leq n} ((X^{(k)} + d)/a_k^*)$. This adjustment gives a minor median bias of the estimate.

4 Testing for effects in nonreplicated factorial designs

A full or fractional two-level experiment has $n = 2^k$ trials for some natural number k . We exemplify the discussion here with $k = 4$ which means 16 trials. In such a trial there is one estimate of the general mean and 15 effect estimates. Our aim is to get a reasonable test for effects which has a required small multiple level of significance $\alpha = 0.05$, i.e. a probability of at most 0.05 for declaring as significantly non-zero any effect which is in fact zero. This should be true for all possible combinations of zero and non-zero effects.

We need the 50% coverage bound constants for 15 ordered observations of absolute values from a $N(0, 1)$ distribution and we can get those for the corresponding constants for the case of $U(0, 1)$ distribution. In the calculation we use linearly increasing individual coverage probabilities. The individual probabilities, which give total coverage 50% are $0.1398 * i/15$. The result of the points a_i are given in Table 1.

By the simple transformation we get the corresponding constants for the

k	1	2	3	4	5	6	7
Bound	0.00078	0.0178	0.0567	0.1106	0.1751	0.2481	0.3285
8	9	10	11	12	13	14	15
0.4163	0.5123	0.6177	0.7353	0.8696	1.029	1.233	1.543

Table 2: Constants for a 50% left coverage bound for ordered absolute values of 15 normal (0;1) random variables.

case of absolute values of normal (0,1) random variables. The result is given in Table 2.

Using the constants in Table 2 and the estimate $\hat{\sigma}$ obtained by aligning the sample of absolute values of estimates to them we may now also make a test for effects. In the subjective method by Daniel (1959) one looks for much deviation among the biggest absolute values of the estimates. We follow the same line of thought in an objective method with prescribed risk of making any false statements on nonzero true effects. This is done by calculating a bound which will act as a rejection boundary, and for all effects with a greater absolute value of the estimate we will declare that there is a true effect.

The test we propose is a step down multiple test with a prescribed multiple level of significance α , which we will now describe in more detail.

Consider first a test of the hypothesis that all random variables are normally distributed with expectation 0 and the same (unknown) variance σ^2 . First the absolute values of the estimates are ordered and then the scale is changed to align the cumulative distribution function with the 50 coverage bound. Next we consider the maximal value of this scale changed series, i.e. the scale changed maximal order statistic, which is used as a test statistic. The distribution of this test statistic under the null hypothesis is rather complicated but a simulation easily gives e.g. the 95% quantile in the distribution, which then serves as a rejection limit.

In order to get a step down test we also study the distribution of the maximal ordered statistic in smaller samples of different sizes m after scale changes to alignment to the m smallest boundary values of the 50% left coverage bound defined above for the full sample. The 95% quantiles in these distributions are used as rejection limits.

In the closed test we may go from above successively and declare effects significant as long as the ordered statistics (absolute values) are above the

k	1	2	3	4	5	6	7
Bound	-	0.021	0.133	0.30	0.49	0.69	0.94
8	9	10	11	12	13	14	15
1.18	1.43	1.71	2.00	2.27	2.60	2.93	3.32

Table 3: Upper bounds for step down test with alignment to a 50% left coverage bound for ordered absolute values of 15 normal random variables. Multiple level of significance is 5%.

corresponding limits. Observe that the procedure has to stop the first time an order statistic is below the corresponding limit. In Theorem 1 in the appendix is proved that this test procedure has a multiple level of significance α .

This type of procedure can easily be constructed for other sample sizes. In two-level factorial designs the cases of 31 and 63 effects are particularly interesting. The very construction with a left coverage band, scale alignment and step down test limits can be used also for other scale families than the normal distribution.

When performing the test in practice we need to consider the rounding off results. Due to rounding there may be a considerable relative variation in the small estimates in practical applications. This extra variation may destroy the estimate of the standard deviation if some estimate just happens to be extremely small. Occasionally an estimate may even get the rounded value 0, which completely destroys the estimate, since it makes it formally equal to 0. A simple way to get rid of the problem in practice is to add the maximal rounding error to the absolute values of the estimates. It is easily seen that this makes the test procedure just slightly more conservative, and it means that the rounding can never decrease the estimate of σ .

5 An application example

As an illustration we use an example from Box et al. (1978). The estimates are given in their table 10.9 on page 331. In this case the measurement values are rounded to 0.25 units and the definition of the effects means that the maximal error in an estimate is 0.125. Thus after taking the absolute values of estimates we add 0.125 before we estimate the standard deviation and normalize the estimates. The estimated standard deviation in this case

1.80, which occurs in the alignment of the ordered absolute value 0.75 number 8 with the alignment value 0.4163.

Comparing the normalized absolute values of estimates with the rejection bound shows that in a multiple test with multiple level of significance 5% we may reject three hypothesis. In notations of Box et al. (1978) we can demonstrate existence of the main effects 2 (with estimate 24.0), 1 (with estimate -8.0) and 4 (with estimate -5.5). The next effect is not significant for the multiple level of significans 0.05.

It may be illustrative to use a half normal plot for the test bounds as well as the normalised estimates. In figure 1 a plot of the data and the rejection bounds are presented.

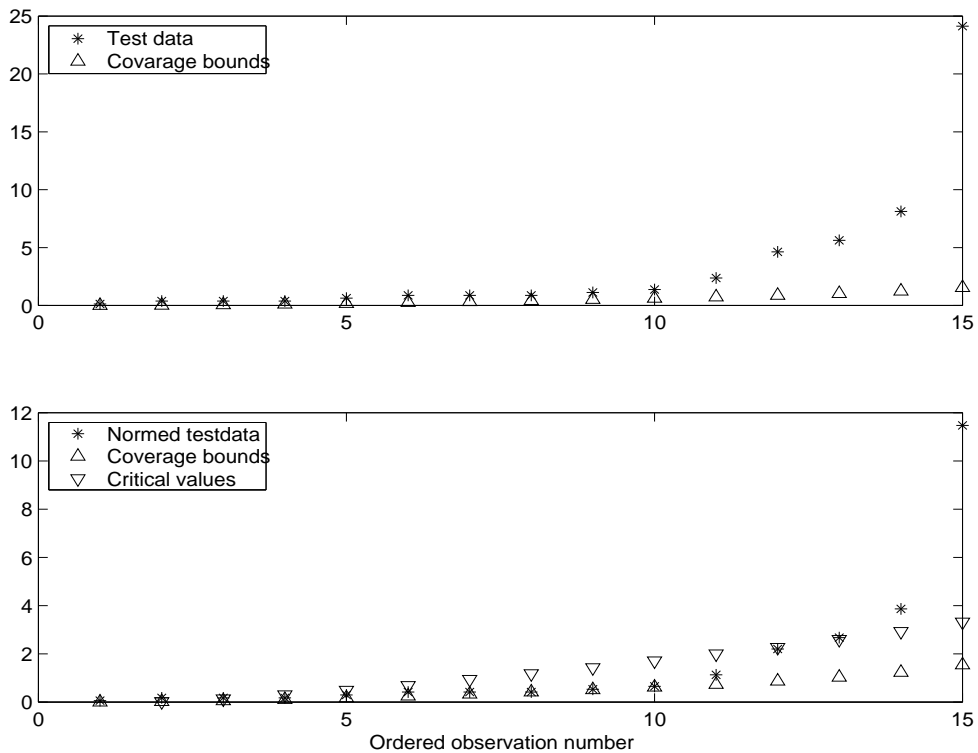


Figure 1: The top plot contains the raw data from Box et al. (1978) page 331 and the 50% coverage bounds. The bottom plot contains the normed data, the coverage bounds, and the rejection bounds

6 Discussion

The statistical problem of determining significant effects in a reduced factorial design without replicates needs some method to obtain an error estimate from the very set of effect estimates we are investigating. The method we used here is based on a kind of tangent estimates, which is rather much related to a subjective technique of looking for a bend in a cumulative absolute normal probability plot.

Of course the technique means using order statistics to get the estimates. Usually order statistics are not the most efficient ones. On the other hand we have here the “sample size adaption” problem which can be suitably handled for order statistics. Further our method is well suited for illustration. The effect estimates can be seen together with the lower fitting boundary and the upper rejection boundary.

As already mentioned the method can be used for other sample sizes after preparation of a table. It can not only be used for reduced factorial designs but also for other problems with independent test statistics and these need not be normally distributed. An example may be some type of life time distributions with scale parameter, where it could be used after preparation of a suitable table. It is to be noted that for the table preparation there is the possibility of simulation beside the analytical calculation.

A Proofs

Lemma 1

$$\begin{aligned}\mathbb{P}\{A_k\} &= \binom{n}{k} a_k^k (1 - a_{k+1})^{n-k} \\ \mathbb{P}\{A_k|B_j\} &= \binom{j}{k} \frac{a_k^k (a_j - a_{k+1})^{j-k}}{a_j^j} \text{ for } j > k\end{aligned}$$

using the notation in section 2.

Proof: In the first equation we have that

$$\begin{aligned}\mathbb{P}\{A_k\} &= \mathbb{P}\{U^{(k)} < a_k \text{ and } U^{(k+1)} \geq a_{k+1}\} \\ &= \mathbb{P}\{k \text{ of the } U_i:s < a_k \text{ and } (n - k) \text{ of the } U_i:s \geq a_{k+1}\} \\ &= \binom{n}{k} a_k^k (1 - a_{k+1})^{n-k}\end{aligned}$$

since the U_i 's are independent $U(0, 1)$. For the second part we notice that

$$\mathbb{P}\{A_k|B_j\} = \mathbb{P}\{A_k|U^{(j)} < a_j\}$$

so that the $U^{(k)}$, $k = 1, \dots, j$ conditioned on B_j are an ordered sample from $U(0, a_j)$. Hence we have

$$\begin{aligned} \mathbb{P}\{A_k|B_j\} &= \binom{j}{k} \left(\frac{a_k}{a_j}\right)^k \left(\frac{a_j - a_k}{a_j}\right)^{j-k} \\ &= \binom{j}{k} \frac{a_k^k (a_j - a_{k+1})^{j-k}}{a_j^j} \end{aligned}$$

Q.E.D.

Theorem 1 *The multiple test procedure described in section 4 has a multiple level of significance α .*

Proof: Denote the set of indices for the true hypotheses by I and the number of true hypotheses by m . Consider the ordered absolute values of the estimates x_i to these hypotheses and denote their maximal absolute value by z .

The proof is to a great extent based on conditioning on this z . Next consider the estimates x_i belonging to the false hypotheses, thus characterized by $\mu_i \neq 0$. Given Z , there is a random number N of the x_i -variables getting outcomes of their absolute values below z . These variables can in principle correspond to any of the $\mu_i \neq 0$.

The test procedure is based on ratios between ordered absolute variables. For the test actually made to reject the hypotheses corresponding to z , the ratio of absolute values of smaller index in the ordered series and z are used. A rejective error can only occur if there is rejection in this step.

Now condition on N as well as z . Decreasing values of the ordered absolute values of x_i with index less than $m + N$ increase the risk of making an error.

There is a stochastic order between the conditional distributions given an upper boundary z for the with $\mu = 0$ and any case with $|\mu| \neq 0$. Cases with $|\mu| \neq 0$ have stochastically greater conditional distributions. See lemma 2. Thus in a conditional calculation the risk is increased if, in the cases of false hypotheses, the distributions are substituted by the distribution of the

true cases. Neither m nor N are known, but the sum $m + N$ appears as the number of remaining variables in the test really done.

Thus we now get an upper estimate of the risk of error by integrating over z in the conditional error obtained for $m + N$ variables with the same distribution. Observe however that the distribution of z is that of a maximal variable among m variables, where m is not known. The final trick is now to make the integration of the distribution of the maximum of the known number of $m + N$ variables (of the type in true hypotheses), which is stochastically larger than that of the unknown number of m variables. This gives again an overestimation of the risk since the conditional distributions are monotonically decreasing in the conditioning value z . See lemma 3.

The table used is based on calculations for this distribution. In order for a rejective error to occur, the procedure must reject in earlier steps and reject in the step corresponding to z . Since the risk in that step is bounded by α , the multiple risk is bounded by α . **Q.E.D.**

Note. There exists cases for which the values of the table are not conservative. If all false hypothesis have expectations μ_i with $|\mu_i|$ approaching ∞ , the risk approaches α .

Lemma 2 *Suppose that U_1 is $N(0, 1)$ distributed and U_2 is $N(\mu, 1)$ distributed where $\mu \neq 0$. Then the distribution of $|U_1|$ given $|U_1| < z$ is stochastically smaller than the distribution of $|U_2|$ given $|U_2| < z$.*

Proof: We make the proof for $\mu > 0$, since the result depends only on the absolute value of μ . The cumulative distribution function of $|U_2|$ is equal to

$$\Phi(x - \mu) - \Phi(-x - \mu)$$

for any μ and all $x > 0$. The cumulative distribution function of $|U_1|$ is obtained as the special case $\mu = 0$. The probability density function in the general case is then

$$\varphi(x - \mu) + \varphi(-x - \mu) = 2\varphi(x) e^{-\mu^2/2} \cosh(\mu x)$$

and for the special case $\mu = 0$, the distribution of $|U_1|$, it is

$$2\varphi(x).$$

In order to prove the lemma we now consider the probabilities of the two intervals $(0, x)$ and (x, z) for the general case. We have for any z and any x ,

$0 < x < z$, and $\mu > 0$

$$\begin{aligned}\mathbb{P}_\mu \{0 < |U_2| < x\} &= \int_0^x 2\varphi(v) e^{-\mu^2/2} \cosh(\mu v) dv \\ &< e^{-\mu^2/2} \cosh(\mu x) \int_0^x 2\varphi(v) dv\end{aligned}$$

and

$$\begin{aligned}\mathbb{P}_\mu \{x < |U_2| < z\} &= \int_x^z 2\varphi(v) e^{-\mu^2/2} \cosh(\mu v) dv \\ &> e^{-\mu^2/2} \cosh(\mu x) \int_0^x 2\varphi(v) dv.\end{aligned}$$

Thus we have

$$\frac{\mathbb{P}_\mu \{0 < |U_2| < x\}}{\mathbb{P}_\mu \{x < |U_2| < z\}} < \frac{\mathbb{P}_0 \{0 < |U_1| < x\}}{\mathbb{P}_0 \{x < |U_1| < z\}}$$

which gives the stochastic ordering requirement

$$\frac{\mathbb{P}_\mu \{0 < |U_2| < x\}}{\mathbb{P}_\mu \{0 < |U_2| < z\}} < \frac{\mathbb{P}_0 \{0 < |U_1| < x\}}{\mathbb{P}_0 \{0 < |U_1| < z\}}.$$

Q.E.D.

Lemma 3 *Conditional distributions of the modulus $V = |U|/v$ of random $N(0, 1)$ variables U , given $|U| \leq v$ is stochastically decreasing in v .*

Proof: Let Φ denote the cumulative distribution function for the $N(0, 1)$ distribution. We have to show that if $v_1 < v_2$ then

$$\frac{\Phi(v_1 x) - 0.5}{\Phi(v_1) - 0.5} < \frac{\Phi(v_2 x) - 0.5}{\Phi(v_2) - 0.5}$$

for all $x, 0 < x < 1$. The left and right member coincide at $x = 0$ and $x = 1$. For any $v > 0$ and any $x, 0 < x < 1$, we have, however,

$$\begin{aligned}\frac{\partial}{\partial v} \frac{\Phi(vx) - 0.5}{\Phi(v) - 0.5} &= \frac{x\varphi(vx)(\Phi(v) - 0.5) - \varphi(v)(\Phi(vx) - 0.5)}{(\Phi(v) - 0.5)^2} \\ &> \frac{x\varphi(vx)(\Phi(v) - 0.5) - \varphi(v)x(\Phi(v) - 0.5)}{(\Phi(v) - 0.5)^2} > 0\end{aligned}$$

since $\Phi(v)$ is concave for $v > 0$ and $\varphi(v)$ is decreasing for $v > 0$. This proves the statement. **Q.E.D.**

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