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**REGULAR ARTICLE** 



# An unbiased rank-based estimator of the Mann–Whitney variance including the case of ties

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#### Abstract

Many estimators of the variance of the well-known unbiased and uniform most powerful estimator of the Mann-Whitney effect, are considered in the literature. Some of these estimators are only valid in cases of no ties or are biased in small sample sizes where the amount of bias is not discussed. Here, we derive an unbiased estimator based on different rankings, the so-called 'placements' (Orban and Wolfe in Commun Stat Theory Methods 9:883–904, 1980), which is therefore easy to compute. This estimator does not require the assumption of continuous distribution functions and is also valid in the case of ties. Moreover, it is shown that this estimator is non-negative and has a sharp upper bound, which may be considered an empirical version of the well-known Birnbaum-Klose inequality. The derivation of this estimator provides an option to compute the biases of some commonly used estimators in the literature. Simulations demonstrate that, for small sample sizes, the biases of these estimators depend on the underlying distribution functions and thus are not under control. This means that in the case of a biased estimator, simulation results for the type-I error of a test or the coverage probability of a confidence interval do not only depend on the quality of the approximation of by a normal distribution but also an additional unknown bias caused by the variance estimator. Finally, it is shown that this estimator is  $L_2$ -consistent.

Keywords Mann–Whitney effect  $\cdot$  Mann–Whitney variance  $\cdot$  Ties  $\cdot$  Birnbaum–Klose inequality

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#### **1** Introduction

The Mann–Whitney effect  $\theta = P(X_1 \le X_2)$  is a common nonparametric effect that is used to describe a treatment effect in a nonparametric setting for two independent random variables  $X_1 \sim F_1(x)$  and  $X_2 \sim F_2(x)$  involving continuous distribution functions. This effect was introduced by Mann and Whitney (1947) for testing the hypothesis  $H_0^F : F_1 = F_2$ . A few years later, Putter (1955) considered the case of ties in some nonparametric tests and derived the consistency region for the Mann–Whitney test in the general case as  $\theta = P(X_1 < X_2) + \frac{1}{2}P(X_1 = X_2) \neq \frac{1}{2}$ . An unbiased and  $L_2$ -consistent estimator  $\hat{\theta}$  of the Mann–Whitney effect  $\theta$  can be obtained from U-statistics theory, and it is well known (see, e.g., Lehmann 1951) that this estimator is the uniform most powerful unbiased estimator of  $\theta$ . Moreover, it can be represented by ranks. To compute confidence intervals for  $\theta$ , the variance  $\sigma_N^2$  of this estimator  $\hat{\theta}$ is required, and it seems to be less straightforward to provide an unbiased estimator of  $\sigma_N^2$  which is also valid in case of ties.

Under the assumption of continuous distribution functions Sen (1967) and Govindarajulu (1968) provided unbiased estimators of  $\sigma_N^2$  but did not discuss whether these estimators could become negative. Hilgers (1981) derived a rank representation of Sen's estimator but did not discuss whether this estimator could become negative. Shirahata (1993) derived an unbiased estimator of the Mann–Whitney variance based on U-statistics, which is only valid if there are no ties. Shirahata mentioned that his estimator is equivalent to Sen's estimator, but he also mentioned that there is a possibility that it might become negative. In his simulations, however, he did not observe negative values. In Sect. 4, it will be shown that this estimator is non-negative in case of no ties - disproving Shirahata's conjecture. But, when in the case of ties, the ranks in Hilgers' estimator are replaced with mid-ranks, it turns out by simple counterexamples that this estimator can become negative. This shows that it is not trivial to derive an unbiased and non-negative estimator of the Mann–Whitney variance.

It seems that Bamber (1975) was the first to provide (without detailed proof) an unbiased estimator, which is also valid in the case of ties. On the one hand, the representation of this estimator is quite involved. It is a linear combination of several positive and negative terms; thus, it is unclear whether this estimator will become negative. This is not discussed in Bamber's paper. Moreover, this estimator is not well recognized in the statistical literature and recent publications (see, e.g., Brunner and Munzel (2000), Perme and Manevski (2019), Gasparyan et al. (2021) mainly use the so-called DeLong-estimator,  $\hat{\sigma}_{DL}^2$  (DeLong et al. 1988) which can conveniently be represented using ranks and is also valid in case of ties. DeLong's estimator is nonnegative since it can be written as a weighted sum of quadratic forms involving only non-negative weights and specific rankings. However,  $\hat{\sigma}_{DL}^2$  can be biased for small sample sizes. Some details on variance estimators from the literature are discussed in Sect. 4.

Therefore, it shall be one of the aims of this paper to provide a simple representation of an unbiased estimator of  $\sigma_N^2$ , which is also valid in the case of ties. Moreover, this estimator's basic properties, such as non-negativity,  $L_2$ -consistency, and an empirical version of the Birnbaum–Klose inequality (1957), will be investigated.

The paper is organized as follows. The statistical model and some basic notations are stated in Sect. 2, where the exact (finite) variance of the Mann–Whitney statistic involving the case of ties is briefly considered to provide the necessary notations. An unbiased estimator of the Mann–Whitney variance is derived in Sect. 3 by deriving the covariance matrix of the placements in both samples, which provides the key to computing the bias of an estimator using Lancaster's theorem. In Sect. 4, some well-known estimators from the literature and their properties are investigated. The proofs of the main results are deferred to the Appendix.

#### 2 Statistical model and notations

#### 2.1 Mann–Whitney estimator and placements

Let  $X_{ik} \sim F_i$ ,  $k = 1, ..., n_i$ ; i = 1, 2, be independent and identically distributed random variables. Let further  $\theta = P(X_{1k} < X_{2r}) + \frac{1}{2}P(X_{1k} = X_{2r}) = \int F_1 dF_2$  denote the Mann–Whitney effect which can equivalently be written as

$$\theta = \int F_1 dF_2 \qquad \text{and } 1 - \theta = \int F_2 dF_1 \qquad (2.1)$$

where  $F_i(x) = \frac{1}{2} \left[ F_i^+(x) + F_i^-(x) \right]$  denotes the so-called normalized version of the distribution function in the sense of Lévy (1925). Here,  $F_i^-(x)$  denotes the left-continuous and  $F_i^+(x)$  the right-continuous version of the distribution function (Ruymgaart 1980). For further explanations regarding this version of the distribution function we refer to Brunner and Puri (2001, Sects.1.2.2 and 1.3.1), Brunner and Puri (2002, Sect.2 and Appendix, Lemma A.1), and Kruskal (1952, Sect.9).

A simple plug-in estimator of  $\theta$  is given by

$$\widehat{\theta} = \int \widehat{F}_1 d\widehat{F}_2 = \frac{1}{n_2} \sum_{k=1}^{n_2} \widehat{F}_1(X_{2k}) = \frac{1}{n_1} \left( \overline{R}_{2\cdot} - \frac{n_2 + 1}{2} \right) = \frac{1}{N} \left( \overline{R}_{2\cdot} - \overline{R}_{1\cdot} \right) + \frac{1}{2}$$
(2.2)

where  $\widehat{F}_i(x)$  denotes the normalized version of the empirical distribution function (see Def.2.1.3 in Brunner et al. 2019) and  $\overline{R}_{i.} = \frac{1}{n_i} \sum_{k=1}^{n_i} R_{ik}$ , i = 1, 2, denotes the mean of the ranks  $R_{ik}$  of  $X_{ik}$  in sample *i* among all  $N = n_1 + n_2$  observations (overall rank). Note that the last step in (2.2) follows from  $R_{1.} + R_{2.} = N(N+1)/2$  (see also Result 3.1 and Exercise/Problem 3.7 in Brunner et al. 2019). It is well-known that  $\widehat{\theta}$  is an unbiased and  $L_2$ -consistent estimator of  $\int F_1 dF_2$ , which can immediately be seen from Theorem 2.1.

Let

$$c(x, y) = \begin{cases} 0 & , x > y \\ \frac{1}{2} & , x = y \\ 1 & , x < y \end{cases}$$
(2.3)

denote the indicator function, called 'counting statistic' (Randles and Wolfe 1979). Then,

$$E(\widehat{\theta}) = E\left(\int \widehat{F}_1 d\widehat{F}_2\right) = E\left(\frac{1}{n_2} \sum_{k=1}^{n_2} \widehat{F}_1(X_{2k})\right)$$
$$= \frac{1}{n_1 n_2} \sum_{r=1}^{n_1} \sum_{k=1}^{n_2} E[c(X_{1r}, X_{2k})] = \int F_1 dF_2$$

(for details, we refer, e.g., to Brunner et al. 2019, Sect. 7.2.3). We note that in most textbooks,  $\hat{\theta}$  is defined as

$$\widehat{\theta} = \frac{1}{n_1 n_2} \sum_{r=1}^{n_1} \sum_{k=1}^{n_2} c(X_{1r}, X_{2k})$$
(2.4)

which is identical to (2.2). We prefer the approach of using the empirical functions, for convenience. The results are identical to those obtained using the indicator function c(x, y). The relation of  $\hat{\theta}$  in (2.4) to (2.2) follows immediately from the definition of the empirical distribution function  $\hat{F}_1(x) = \frac{1}{n_1} \sum_{r=1}^{n_1} c(X_{1r}, x)$  and the relation  $n_1 \hat{F}_1(X_{2k}) = R_{2k} - R_{2k}^{(2)}$ , where  $R_{2k}^{(2)}$  is the rank of  $X_{2k}$  among all  $n_2$  observations within sample 2. In general, the *overall rank*  $R_{ik}$  of an observation  $X_{ik}$ ,  $k = 1, \ldots, n_i$ , i = 1, 2, is defined as  $R_{ik} = \frac{1}{2} + \sum_{j=1}^{2} \sum_{r=1}^{n_j} c(X_{jr}, X_{ik})$  and the *internal rank* of  $X_{ik}$  within sample *i* is defined as  $R_{ik}^{(i)} = \frac{1}{2} + \sum_{r=1}^{n_i} c(X_{ir}, X_{ik})$ . Note that  $\frac{1}{2}$  must be added to the sum of the indicator functions to obtain the intuitive meaning of ranks as place numbers of the observations in the order statistic in case of no ties since the comparison  $c(X_{ik}, X_{ik})$  of the observation  $X_{ik}$  with itself equals  $\frac{1}{2}$ .

The quantities

$$R_{1k}^* = R_{1k} - R_{1k}^{(1)} = n_2 \widehat{F}_2(X_{1k}) = \sum_{\ell=1}^{n_2} c(X_{2\ell}, X_{1k})$$
(2.5)

$$R_{2\ell}^* = R_{2\ell} - R_{2\ell}^{(2)} = n_1 \widehat{F}_1(X_{2\ell}) = \sum_{k=1}^{n_1} c(X_{1k}, X_{2\ell})$$
(2.6)

are called 'placements' (Orban and Wolfe 1980, 1982). The placements  $R_{1k}^*$  and  $R_{2\ell}^*$  are basically the place numbers (ranks) of  $X_{1k}$  within sample 2 and of  $X_{2\ell}$  within sample 1. The formal representations in (2.5) and (2.6) are immediately obvious from

the following considerations. Let  $\widehat{H}(x) = \frac{1}{N} [n_1 \widehat{F}_1(x) + n_2 \widehat{F}_2(x)]$  denote the weighted mean of the empirical distribution functions  $\widehat{F}_1(x)$  and  $\widehat{F}_2(x)$ . Then

$$\underbrace{N\widehat{H}(X_{1k})}_{R_{1k}-\frac{1}{2}} = \sum_{j=1}^{2} \sum_{s=1}^{n_j} c(X_{js}, X_{1k}) = n_1 \widehat{F}_1(X_{1k}) + n_2 \widehat{F}_2(X_{1k})$$
$$= \underbrace{\sum_{s=1}^{n_1} c(X_{1s}, X_{1k})}_{R_{1k}^{(1)}-\frac{1}{2}} + \underbrace{\sum_{s=1}^{n_2} c(X_{2s}, X_{1k})}_{R_{1k}^*}$$

and the expression for  $R_{2\ell}^*$  follows in the same way. Then the mean  $\frac{1}{n_1 n_2} \sum_{\ell=1}^{n_2} R_{2\ell}^* = \frac{1}{n_1} \overline{R}_{2\cdot}^* = \frac{1}{n_1} \overline{R}_{2\cdot} - \frac{n_2+1}{2}$  yields the representation of  $\widehat{\theta}$  in (2.2).

#### 2.2 The variance of the Mann–Whitney estimator

First, we briefly derive the variance  $\sigma_N^2$  of  $\hat{\theta}$ , including the case of discrete distributions since some quantities appearing in this derivation will be used later to derive an unbiased estimator of  $\sigma_N^2$ . We note that the representation of the Mann–Whitney variance  $\sigma_N^2$  presented below is identical to that in Bamber (1975), which extends the representation for continuous distribution functions by Van Dantzig (1951) to the case of ties.

Since  $E(\widehat{\theta}) = \theta$ , the variance is given by  $Var(\widehat{\theta}) = E(\widehat{\theta} - \theta)^2$  and it follows that

$$(\widehat{\theta} - \theta)^2 = \left(\frac{1}{n_2} \sum_{k=1}^{n_2} \widehat{F}_1(X_{2k}) - \theta\right)^2 = \left(\frac{1}{n_2} \sum_{k=1}^{n_2} \left[\widehat{F}_1(X_{2k}) - \theta\right]\right)^2$$
$$= \frac{1}{n_1^2 n_2^2} \sum_{k=1}^{n_2} \sum_{\ell=1}^{n_2} \sum_{r=1}^{n_1} \sum_{s=1}^{n_1} \left[c(X_{1r}, X_{2k}) - \theta\right] \left[c(X_{1s}, X_{2\ell}) - \theta\right] . \quad (2.7)$$

When taking the expectation of  $(\hat{\theta} - \theta)^2$ , four cases in (2.7) must be distinguished. They are given in the following table, where the expectations of the products of the indicator function in (2.7) are listed in the right column and are obtained by computing conditional expectations using routine computations. The numbers of combination cases (left column) are in the middle column.

Combination		Number of Cases	$E\left(\left[c(X_{1r},X_{2k})-\theta\right]\left[c(X_{1s},X_{2\ell})-\theta\right]\right)$
$k = \ell,$ $k = \ell,$ $k \neq \ell,$ $k \neq \ell,$ $k \neq \ell,$	r = s $r \neq s$ r = s $r \neq s$	$n_1n_2 n_1n_2(n_1 - 1) (n_2 - 1)n_1n_2 (n_1 - 1)n_1(n_2 - 1)n_2$	$= \theta(1-\theta) - \frac{1}{4} \int (F_1^+ - F_1^-) dF_2$ = $\int F_1^2 dF_2 - \theta^2 = \sigma_2^2$ = $\int F_2^2 dF_1 - (1-\theta)^2 = \sigma_1^2$ = 0

The result of the summation over all combinations is given in the following theorem. **Theorem 2.1** The variance  $\sigma_N^2$  of  $\hat{\theta}$  is given by

$$\sigma_N^2 = \frac{1}{n_1 n_2} \left[ (n_2 - 1)\sigma_1^2 + (n_1 - 1)\sigma_2^2 + \theta(1 - \theta) - \frac{1}{4}\tau \right],$$
 (2.8)

where

$$\sigma_1^2 = Var\left(F_2(X_{11})\right) = \int F_2^2 dF_1 - (1-\theta)^2, \qquad (2.9)$$

$$\sigma_2^2 = Var(F_1(X_{21})) = \int F_1^2 dF_2 - \theta^2, \qquad (2.10)$$

$$\tau = \int (F_1^+ - F_1^-) dF_2 = \int (F_2^+ - F_2^-) dF_1 = P(X_{11} = X_{21}). \quad (2.11)$$

**Remark 2.1** The quantity  $\tau$  in (2.11) can easily be interpreted as the probability of ties in the overlap region of  $F_1$  and  $F_2$ .

## 3 Derivation of an unbiased estimator of $\sigma_N^2$

In this section, we derive an estimator of  $\sigma_N^2$ , which is unbiased and non-negative for all sample sizes  $n_1, n_2 \ge 2$  and valid in case of ties. Moreover, we give some essential properties of this estimator in Theorem 3.1. First, some notations and relations between sums of count functions and different rankings are considered.

#### 3.1 Notations and basic results

First, we note that

$$c^{2}(x, y) = c(x, y) - \frac{1}{4}[c^{+}(x, y) - c^{-}(x, y)], \qquad (3.12)$$

where  $c^+(\cdot)$  denotes the right-continuous version and  $c^-(\cdot)$  the left-continuous version of the indicator function. In particular,

$$E\left[c^{2}(X_{2\ell}, X_{1k})\right] = \int F_{2}dF_{1} - \frac{1}{4}\tau = 1 - \theta - \frac{1}{4}\tau, \qquad (3.13)$$

where  $\tau$  is defined in (2.11).

Since  $\hat{\theta}$  in (2.1) is the mean of the placements  $R_{2\ell}^*$  as considered in Sect. 2.1, the placements  $R_{1k}^*$  and  $R_{2\ell}^*$  shall be considered in more detail. They are the empirical counterparts of the quantities  $n_2F_2(X_{1k})$  and  $n_1F_1(X_{2\ell})$  and will be used to estimate the variances  $\sigma_1^2$  and  $\sigma_2^2$  in (2.9) and (2.10).

To compute the variance of  $\hat{\theta} = \frac{1}{n_2} \sum_{\ell=1}^{n_2} \widehat{F}_1(X_{2\ell})$ , the covariance matrices of the scaled placement vectors  $\frac{1}{N-n_i} \mathbf{R}_i^* = \frac{1}{N-n_i} (R_{i1}^*, \dots, R_{in_i}^*)', i = 1, 2$ , shall be derived.

Since  $E[c(X_{2\ell}, X_{1r})] = \int F_2 dF_1 = 1 - \theta$  and  $E[c(X_{1k}, X_{2r})] = \int F_1 dF_2 = \theta$ , it follows from (2.5) and (2.6) that the expectations of the placement vectors are  $E(\mathbf{R}_1^*) = n_2(1-\theta)\mathbf{1}_{n_1}$  and  $E(\mathbf{R}_2^*) = n_1\theta\mathbf{1}_{n_2}$ .

The structure of the covariance matrices  $V_i = Cov(\mathbf{R}_i^*)$ , i = 1, 2 follows from the relations in (2.5) and (2.6) by noting that the  $X_{ik}$  are independent and identically distributed within each group *i*, by assumption. Thus, the common distribution function of the  $X_{i1}, \ldots, X_{in_i}$  is invariant under all permutations and the variances of  $\mathbf{R}_{ik}^* =$  $n_r \hat{F}_r(X_{ik})$ ,  $i \neq r = 1, 2$  are all the same,  $s_i^2$ , say. Moreover, all covariances  $\rho_i =$  $Cov(\mathbf{R}_{ik}^*, \mathbf{R}_{i\ell}^*)$  are identical for  $k \neq \ell = 1, \ldots, n_i$ , i = 1, 2, and it follows that  $V_i$ has a consumption symmetry structure,

$$V_i = Cov(\mathbf{R}_i^*) = (s_i^2 - \rho_i) \mathbf{I}_{n_i} + \rho_i \mathbf{J}_{n_i}, \ i = 1, 2,$$
(3.14)

where  $I_{n_i}$  denotes the unit matrix of dimension  $n_i$  and  $J_{n_i} = \mathbf{1}_{n_i} \mathbf{1}'_{n_i}$  denotes the  $(n_i \times n_i)$ -matrix of 1 s.

By the same arguments, the covariances  $Cov(R_{1k}^*, R_{2\ell}^*)$  are all identical,  $\rho_3$ , say, and the total covariance matrix V is given by

$$V = Cov \begin{pmatrix} \mathbf{R}_1^* \\ \cdots \\ \mathbf{R}_2^* \end{pmatrix} = \begin{pmatrix} (s_1^2 - \rho_1) \mathbf{I}_{n_1} + \rho_1 \mathbf{J}_{n_1} & \vdots & \rho_3 \mathbf{J}_{n_1 \times n_2} \\ \cdots & \cdots & \cdots & \cdots \\ \rho_3 \mathbf{J}_{n_2 \times n_1} & \vdots & (s_2^2 - \rho_2) \mathbf{I}_{n_2} + \rho_2 \mathbf{J}_{n_2} \end{pmatrix}$$
$$= \begin{pmatrix} \mathbf{V}_1 & \vdots & \rho_3 \mathbf{J}_{n_1 \times n_2} \\ \cdots & \cdots & \cdots & \cdots \\ \rho_3 \mathbf{J}_{n_2 \times n_1} & \vdots & \mathbf{V}_2 \end{pmatrix}.$$
(3.15)

To derive an unbiased estimator of  $\sigma_N^2$  in (2.8), we consider the quadratic forms

$$Q_i^2 = \sum_{k=1}^{n_i} \left( R_{ik}^* - \overline{R}_{i.}^* \right)^2, \ i = 1, 2$$
(3.16)

of the centered placements  $R_{ik}^* - \overline{R}_{i.}^* = R_{ik} - R_{ik}^{(i)} - \left(\overline{R}_{i.} - \frac{n_i + 1}{2}\right)$ .

**Remark 3.1** 1. Many estimators of  $\sigma_N^2$  from the literature can be written as a function of  $Q_1^2$  and  $Q_2^2$  (for details see Sect. 4, Table 1).

2. In this case, the representation of the covariance matrix of  $\mathbf{R}^* = \begin{pmatrix} \mathbf{R}_1^* \\ \cdots \\ \mathbf{R}_2^* \end{pmatrix}$  enables a simple computation of the expectation of an estimator of  $\sigma_N^2$ .

Let  $\boldsymbol{P}_{n_i} = \boldsymbol{I}_{n_i} - \frac{1}{n_i} \boldsymbol{J}_{n_i}$  denote the  $n_i$ -dimensional centering matrix. Then,  $Q_i^2$  can be written as  $Q_i^2 = (\boldsymbol{R}_i^*)' \boldsymbol{P}_{n_i} \boldsymbol{R}_i^*$  and by Lancaster's theorem,

$$E(Q_i^2) = tr(\boldsymbol{P}_{n_i}\boldsymbol{V}_i) + E\left[(\boldsymbol{R}_i^*)'\right]\boldsymbol{P}_{n_i}E\left[\boldsymbol{R}_i^*\right]$$
  
= tr(\boldsymbol{P}\_{n\_i}\boldsymbol{V}\_i) (3.17)

since  $n_2^2(1-\theta)^2 \mathbf{1}'_{n_1} \boldsymbol{P}_{n_1} \mathbf{1}_{n_1} = 0$  and  $n_1^2 \theta^2 \mathbf{1}'_{n_2} \boldsymbol{P}_{n_2} \mathbf{1}_{n_2} = 0$ .

Note that from (3.14),  $P_{n_i}V_i = [s_i^2 - \rho_i]P_{n_i}$ , since  $P_{n_i}J_{n_i} = 0$ . Then, from  $tr(P_{n_i}) = n_i - 1$ , it follows from (3.14) that

$$tr(\boldsymbol{P}_{n_i}\boldsymbol{V}_i) = (n_i - 1)[s_i^2 - \rho_i]; \ i = 1, 2.$$
(3.18)

Only the coefficients  $s_1^2$ ,  $s_2^2$  and  $\rho_1$ ,  $\rho_2$ , and  $\rho_3$  have to be determined. They are obtained from

$$s_{1}^{2} = Var\left(R_{1k} - R_{1k}^{(1)}\right) = Var\left(\sum_{\ell=1}^{n_{2}} c(X_{2\ell}, X_{1k})\right)$$
$$= E\left[\sum_{\ell=1}^{n_{2}} \sum_{r=1}^{n_{2}} [c(X_{2\ell}, X_{1k}) - (1-\theta)][c(X_{2r}, X_{1k}) - (1-\theta)]\right] \quad (3.19)$$

$$s_{2}^{2} = Var\left(R_{2k} - R_{2k}^{(2)}\right) = Var\left(\sum_{\ell=1}^{n_{1}} c(X_{1\ell}, X_{2k})\right)$$
$$= E\left[\sum_{\ell=1}^{n_{1}} \sum_{r=1}^{n_{1}} [c(X_{1\ell}, X_{2k}) - \theta][c(X_{1r}, X_{2k}) - \theta]\right]$$
(3.20)

$$\rho_{1} = Cov \left( R_{11} - R_{11}^{(1)}, R_{12} - R_{12}^{(1)} \right)$$
$$= E \left[ \sum_{\ell=1}^{n_{2}} \sum_{r=1}^{n_{2}} [c(X_{2\ell}, X_{11}) - \theta] [c(X_{2r}, X_{12}) - \theta] \right]$$
(3.21)

$$\rho_2 = Cov \left( R_{21} - R_{21}^{(2)}, R_{22} - R_{22}^{(2)} \right)$$
  
=  $E \left[ \sum_{\ell=1}^{n_1} \sum_{r=1}^{n_1} [c(X_{1\ell}, X_{21}) - (1 - \theta)][c(X_{1r}, X_{22}) - (1 - \theta)] \right].$  (3.22)

The expectations are obtained from Sect. 2.2 by some routine computations and using (3.12). This leads to

$$s_1^2 = n_2 \left[ (n_2 - 1)\sigma_1^2 + \theta(1 - \theta) - \frac{1}{4}\tau \right]$$
 and  $\rho_1 = n_2 \sigma_2^2$  (3.23)

$$s_2^2 = n_1 \left[ (n_1 - 1)\sigma_2^2 + \theta(1 - \theta) - \frac{1}{4}\tau \right]$$
 and  $\rho_2 = n_1\sigma_1^2$  (3.24)

where  $\tau$  is defined in (2.11). Finally, the expectations of  $Q_1^2$  and  $Q_2^2$  are

$$E(Q_1^2) = (n_1 - 1)n_2 \left[ (n_2 - 1)\sigma_1^2 - \sigma_2^2 + \theta(1 - \theta) - \frac{1}{4}\tau \right], \qquad (3.25)$$

$$E(Q_2^2) = (n_2 - 1)n_1 \left[ (n_1 - 1)\sigma_2^2 - \sigma_1^2 + \theta(1 - \theta) - \frac{1}{4}\tau \right].$$
 (3.26)

Since the expectations of  $Q_1^2$  and  $Q_2^2$  are mixtures of all the quantities  $s_1^2, s_2^2, \rho_1$ , and  $\rho_2$ , it is preferable to consider the expectation of the sum  $Q_1^2 + Q_2^2$ .

Now let  $K(\theta, \tau) = \theta(1 - \theta) - \frac{1}{4}\tau$ , for convenience, and let  $\oplus$  denote the direct sum of matrices and let  $\odot$  denote the Hadamard product of matrices. Then it follows from (3.14) and (3.15) and from V = V' that

$$E(Q_1^2 + Q_2^2) = tr\left[\left(P_{n_1} \oplus P_{n_2}\right)V\right] = \mathbf{1}'_N\left[\left(P_{n_1} \oplus P_{n_2}\right) \odot V\right]\mathbf{1}_N$$
  

$$= \sum_{i=1}^2 \mathbf{1}'_{n_i}(P_{n_i} \odot V_i)\mathbf{1}_{n_i} = \sum_{i=1}^2 (n_i - 1)[s_i^2 - \rho_i]$$
  

$$= (n_1 - 1)n_2\left[(n_2 - 1)\sigma_1^2 - \sigma_2^2 + K(\theta, \tau)\right]$$
  

$$+ (n_2 - 1)n_1\left[(n_1 - 1)\sigma_2^2 - \sigma_1^2 + K(\theta, \tau)\right]$$
  

$$= (n_2 - 1)[n_1n_2 - N]\sigma_1^2 + (n_1 - 1)[n_1n_2 - N]\sigma_2^2$$
  

$$+ [n_1n_2 - N + n_1n_2]K(\theta, \tau)$$
  

$$= (n_1n_2 - N)\underbrace{\left[(n_2 - 1)\sigma_1^2 + (n_1 - 1)\sigma_2^2 + K(\theta, \tau)\right]}_{n_1n_2\sigma_N^2} + n_1n_2K(\theta, \tau)$$

which simplifies to

$$E\left(\frac{1}{n_1n_2}(Q_1^2+Q_2^2)-[\theta(1-\theta)-\frac{1}{4}\tau]\right)=(n_1n_2-N)\sigma_N^2.$$
 (3.27)

Now replacing  $\theta(1-\theta)$  by  $E[\widehat{\theta}(1-\widehat{\theta}) + \sigma_N^2] = \theta(1-\theta)$  finally leads to

$$E\left(\frac{1}{n_1n_2}(Q_1^2+Q_2^2)-\left[\widehat{\theta}(1-\widehat{\theta})-\frac{1}{4}\tau\right]\right) = (n_1n_2-N+1)\sigma_N^2$$
  
=  $(n_1-1)(n_2-1)\sigma_N^2.$  (3.28)

It remains to find an unbiased estimator of  $\tau = P(X_{11} = X_{21})$ . To this end let  $F_1^+(x) = P(X_{11} \le x)$  and  $F_1^-(x) = P(X_{11} < x)$ . Then it holds that  $E[F_1^+(X_{21})] = P(X_{11} \le X_{21})$  and  $E[F_1^-(X_{21})] = P(X_{11} < X_{21})$ . Thus,

$$E\left[F_1^+(X_{21}) - F_1^-(X_{21})\right] = P(X_{11} \le X_{21}) - P(X_{11} < X_{21})$$
$$= P(X_{11} = X_{21}).$$

To estimate these quantities let  $c^+(y, x) = \begin{cases} 1, & y \le x, \\ 0, & y > x \end{cases}$  and  $c^-(y, x) = \begin{cases} 1, & y < x, \\ 0, & y \ge x \end{cases}$  denote the indicator function's right- and left-continuous versions, respectively. Further let  $\widehat{F}_1^+(x) = \frac{1}{n_1} \sum_{r=1}^{n_1} c^+(X_{1r}, x)$  denote the right-continuous version and  $\widehat{F}_1^-(x) = \frac{1}{n_1} \sum_{r=1}^{n_1} c^-(X_{1r}, x)$  the left-continuous version, respectively, of the empirical distribution function of  $F_1$ . Using Relation (2.6) it follows that the plug-in estimator

$$\begin{aligned} \widehat{\tau}_{N} &= \frac{1}{n_{2}} \sum_{\ell=1}^{n_{2}} \left[ \widehat{F}_{1}^{+}(X_{2\ell}) - \widehat{F}_{1}^{-}(X_{2\ell}) \right] \\ &= \frac{1}{n_{2}} \sum_{\ell=1}^{n_{2}} \frac{1}{n_{1}} \left[ \left( R_{2\ell}^{+} - R_{2\ell}^{-} \right) - \left( \overline{R}_{2\ell}^{(2)+} - \overline{R}_{2\ell}^{(2)-} \right) \right] \\ &= \frac{1}{n_{1}} \left[ \overline{R}_{2\cdot}^{+} - \overline{R}_{2\cdot}^{-} - \left( \overline{R}_{2\cdot}^{(2)+} - \overline{R}_{2\cdot}^{(2)-} \right) \right]. \end{aligned}$$
(3.29)

is an unbiased estimator of  $\tau$ . Here,  $R_{2\ell}^+$  and  $R_{2\ell}^-$  denote the maximal and minimal overall ranks of  $X_{2\ell}$ , respectively, and  $R_{2\ell}^{(2)+}$  and  $R_{2\ell}^{(2)-}$  denote the maximal and minimal internal ranks of  $X_{2\ell}$  within sample 2. We refer to Brunner et al. (2019), Sect. 2.3.2, Def. 2.19, for details regarding maximal and minimal ranks. Unbiasedness of  $\hat{\tau}_N$  follows by noting that  $E\left[\widehat{F}_1^+(X_{21})\right] = P(X_{11} \leq X_{21})$  and  $E\left[\widehat{F}_1^-(X_{21})\right] = P(X_{11} < X_{21})$  and in turn  $E\left[\widehat{F}_1^+(X_{21}) - \widehat{F}_1^-(X_{21})\right] = \tau$ .

Replacing  $\tau$  in (3.28) with the unbiased estimator  $\hat{\tau}$  leads to the final result stated in Theorem 3.1 where the preceding derivations are summarized and some other essential properties of the estimator  $\hat{\sigma}_N^2$  in (3.30) are stated.

**Theorem 3.1** Let  $X_{ik} \sim F_i$ ,  $k = 1, ..., n_i$ ; i = 1, 2, be independent and identically distributed random variables, where  $F_i(x) = \frac{1}{2} \left[ F_i^+(x) + F_i^-(x) \right]$  and assume that  $(X_{1k})_{k=1}^{n_1}$  is independent from  $(X_{2\ell})_{\ell=1}^{n_2}$ . Further let  $U_N = \sqrt{N} [(\overline{Y}_2 - \overline{Y}_1) + 1 - 2\theta]$ , where  $\overline{Y}_i = \frac{1}{n_i} \sum_{k=1}^{n_i} Y_{ik}$  and  $Y_{1k} = F_2(X_{1k})$  and  $Y_{2\ell} = F_1(X_{2\ell})$  and let

$$s_N^2 = Var(U_N) = \frac{N}{n_1 n_2} (n_2 \sigma_1^2 + n_1 \sigma_2^2),$$
 (3.30)

where the variances  $\sigma_1^2$  and  $\sigma_2^2$  are defined in (2.9) and (2.10), respectively. Further let  $R_{ik}^* = R_{ik} - R_{ik}^{(i)}$  denote the placements in (2.5) and (2.6) and let  $\overline{R}_{i}^* = \frac{1}{n_i} \sum_{k=1}^{n_i} R_{ik}^*$ , i = 1, 2 denote their means. Finally, let  $\widehat{\tau}_N$  denote the unbiased estimator of  $\tau$  in (3.29). Then, the variance estimator

$$\widehat{\sigma}_{N}^{2} = \frac{1}{(n_{1}-1)(n_{2}-1)} \left( \frac{1}{n_{1}n_{2}} (Q_{1}^{2} + Q_{2}^{2}) - \left[ \widehat{\theta}(1-\widehat{\theta}) - \frac{1}{4}\widehat{\tau}_{N} \right] \right) \quad (3.31)$$

has the following properties

- 1. If  $\sigma_1^2, \sigma_2^2 > 0$  and if  $N/n_i \le N_0 < \infty$ , i = 1, 2, then  $N\widehat{\sigma}_N^2$  is  $L_2$ -consistent for  $s_N^2$  in (3.30) in the sense that  $E(N\widehat{\sigma}_N^2/s_N^2 1)^2 \to 0$ .
- 2. For all samples sizes  $n_1, n_2 \ge 2$  it holds that

  - (a) E(∂<sup>2</sup><sub>N</sub>) = σ<sup>2</sup><sub>N</sub>,
    (b) 0 ≤ ∂<sup>2</sup><sub>N</sub> ≤ θ(1 − θ)/(m − 1), where m = min{n<sub>1</sub>, n<sub>2</sub>}. Both these limits are sharp in the sense that there exist samples X<sub>i1</sub>,..., X<sub>ini</sub>, i = 1, 2, such that either  $\widehat{\sigma}_N^2 = 0$ , or  $\widehat{\sigma}_N^2 = \widehat{\theta}(1 - \widehat{\theta})/(m - 1)$ .

These results are true for data involving ties and for data without ties.

The derivation of Statement 2a is given before Theorem 3.1 while the proofs of the other statements are given in the Appendix. 

- **Remark 3.2** 1. Note that  $\sqrt{N}(\hat{\theta} \theta)$  is asymptotically equivalent to  $U_N = \sqrt{N} \left[ (\overline{Y}_2 \overline{Y}_1) + 1 2\theta \right]$ . This means the asymptotic variances of  $\sqrt{N} \hat{\theta}$  and  $U_N$  are equal. For a formal proof, see, e.g., Brunner et al. (2019), Proposition 7.19, p. 386.
- 2. The result that  $\widehat{\sigma}_N^2 \leq \widehat{\theta}(1-\widehat{\theta})/(m-1)$  may be considered as an empirical version of the Birnbaum-Klose inequality (Birnbaum 1956; Birnbaum and Klose 1957). It is essential, however, to note that this result does not state that it is valid for all estimators of  $\sigma_N^2$  in (2.8). The statement is that it holds for the estimator  $\hat{\sigma}_N^2$  in (3.31). Thus, this may be considered a particular (noteworthy) property of this estimator. Moreover, it is easily seen that  $\hat{\sigma}_N^2 \leq 1/[4(m-1)]$ .
- 3. For continuous distributions it follows that  $\tau = \hat{\tau}_N = 0$  and  $\hat{\sigma}_N^2$  in (3.31) is equivalent to Hilgers' (1981) estimator using ranks or to Shirahata's (1993) estimator using indicator functions. In the case of ties, however, these estimators are negatively biased if the ranks are replaced with the mid-ranks. Moreover, they may become negative in extreme cases. More details regarding comparisons with different variance estimators from the literature are given in the next Section.
- 4. The assumption  $\sigma_1^2, \sigma_2^2 > 0$  implies that  $s_N^2 > 0$  in (3.30) which is needed to derive the  $L_2$ -consistency of  $\hat{\sigma}_N^2$ .

#### 4 Comparison with estimators from the literature

There exist several estimators of  $\sigma_N^2$  in the literature. Some are only valid in the case of no ties or are only asymptotically unbiased. The representation of  $\sigma_N^2 = Var(\hat{\theta})$ 

in case of no ties is known since Van Dantzig (1951) and in case of ties since Bamber (1975).

Here, we review some variance estimators from the literature and discuss their properties. Throughout this section, we will use the following notations for convenience:

- 1.  $d_N = n_1(n_1 1)n_2(n_2 1)$  and  $m = \min\{n_1, n_2\}$ 2.  $Q_i^2 = \sum_{k=1}^{n_i} \left( R_{ik}^* \overline{R}_{i.}^* \right)^2$  as given in (3.16) and  $Q_i^2/(n_i 1)$  are the empirical variances of the placements  $R_{ik}^*$ , i = 1, 2.
- 3.  $\theta$ : Mann–Whitney estimator given in (2.2) and (2.4)
- 4.  $\hat{\tau}_N$ : estimator of the probability of ties in the overlap region of the distributions as given in (3.29).

A brief overview of the following estimators is composed in Table 1 at the end of this section.

#### 4.1 Sen-Hilgers-Shirahata estimator

Estimators of  $\sigma_N^2$  were already suggested by Sen (1967) and Govindarajulu (1968), assuming continuous distribution functions. Later, Hilgers (1981) provided the estimator  $\hat{\sigma}_{SHS}^2$  in Table 1 using ranks also assuming continuous distribution functions and he showed that his estimator is identical to Sen's estimator corrected by  $1/n_i^2$ . Halperin et al. (1987) also mentioned this typo in Sen's estimator in their paper.

Neither Sen nor Hilgers discussed whether this estimator could become negative. Shirahata (1993) briefly discussed this and developed the same estimator based on indicator functions also assuming continuous distribution functions. He mentioned that this estimator,  $\hat{\sigma}_{U}^{2}$  in his notation, could become negative while in his simulations, however, this did not happen. Since the estimators of Sen (1967), Hilgers (1981), and Shirahata (1993) are identical and are special cases of the estimator  $\hat{\sigma}_{N}^{2}$ in (3.31), Theorem 3.1, Statement 2b, shows that Shirahata's conjecture is incorrect and thus,  $\hat{\sigma}_{U}^{2} \geq 0$ . If, however, in the case of ties, the ranks in Hilgers' estimator  $\hat{\sigma}_{SHS}^{2}$ are replaced with mid-ranks, then the resulting estimator (without adding the term  $n_1 n_2 \hat{\tau}_N / 4$ ) is no longer unbiased, and it can become negative as demonstrated by the following counter-example.

Let  $X_{1k} = \{1, 1, 2, 2, 3\}$  and let  $X_{2\ell} = \{3, 4, 4, 4, 5\}$ . Then  $\widehat{\sigma}_N^2 = 0.0004$  while  $\hat{\sigma}_{SHS}^2 = -0.000225$ . Note that  $\hat{\sigma}_N^2$  in (3.31) contains the term  $n_1 n_2 \hat{\tau}_N / 4$ .

This shows that providing an unbiased and non-negative estimator, which is also valid in the case of ties, is not trivial.

#### 4.2 Cliff estimator

Cliff (1993) provides an unbiased estimator of  $\sigma_N^2$ , including the case of ties, similar to Hilgers' estimator. However, this estimator may become negative, as discussed in his paper. He suggested to limit this estimator by  $(1 - \hat{\theta}^2)/(n_1 n_2)$ . But then he mentions that this substitution introduces a bias. Therefore, we do not consider this estimator in detail.

#### 4.3 Bamber estimator

Allowing for ties, Bamber (1975) presented an estimator using some involved explanations without formal proof, stating that his estimator is unbiased. He did not discuss, however, whether this estimator may become negative. Also, formal proof of the consistency is not given. It turns out (for a formal derivation, see Nowak et al. 2022) that Bamber's estimator is equivalent to  $\hat{\sigma}_N^2$  in (3.31). This means that  $\hat{\sigma}_N^2$  in (3.31) provides a convenient rank representation of Bamber's estimator.

It may be noted that none of the subsequent papers by Halperin et al. (1987), Mee (1990), or Shirahata (1993) refers to Bambers's (1975) paper. Hanley and McNeil (1982) refer to Bamber's estimator but assume no ties. Astonishingly, Bamber's unbiased estimator of the Mann–Whitney variance is not broadly perceived in the statistical literature. One reason may be that its representation is quite involved. In this paper, we provide an unbiased estimator in (3.31), which is based on ranks, or more precisely on the placements  $R_{1k}^*$  and  $R_{2\ell}^*$  in (2.5) and (2.6) and thus, has a convenient representation.

#### 4.4 DeLong estimator

(DeLong et al. 1988) refer to Bamber's estimator. But in their paper, they develop an estimator of the covariance matrix in a multivariate model, which reduces to the variance estimator  $\hat{\sigma}_{DL}^2$  in Table 1 in a univariate model.

This estimator is identical to  $\hat{\sigma}_{BF}^2$  derived by Brunner and Munzel (2000) in the nonparametric Behrens–Fisher situation. Brunner and Munzel showed that  $\hat{\sigma}_{BF}^2$  (and in turn  $\hat{\sigma}_{DL}^2$ ) is  $L_2$ -consistent for  $s_N^2$  in the sense that  $E(\hat{\sigma}_{BF}^2/s_N^2 - 1)^2 \rightarrow 0$ , if  $N/n_i \leq N_0 < \infty$ , i = 1, 2.

DeLong's estimator  $\hat{\sigma}_{DL}^2$  in Table 1 may be biased for small sample sizes. This can be easily seen from (3.25) and (3.26) and one obtains

$$E(\hat{\sigma}_{DL}^2) = \sigma_N^2 + \frac{1}{n_1 n_2} \Big[ \underbrace{\theta(1-\theta) - (\sigma_1^2 + \sigma_2^2)}_{\ge 0} - \frac{1}{4} \tau \Big].$$
(4.32)

Then, from van Dantzig's inequality (1951),  $\sigma_1^2 + \sigma_2^2 \leq \theta(1 - \theta)$ , it follows that  $\widehat{\sigma}_{DL}^2$  may be unbiased or biased in both directions depending on ties and whether  $\theta(1-\theta) \neq \sigma_1^2 + \sigma_2^2$ .

#### 4.5 Perme–Manevski estimator

In a quite recent paper, Perme and Manevski (2019) state that the DeLong estimator  $\hat{\sigma}_{DL}^2$  is not 'exact' and that (DeLong et al. 1988) and Bamber (1975) propose an asymptotic non-parametric estimator. They do not mention, however, that Bamber (1975) stated that his estimator is unbiased for all sample sizes  $n_i \ge 2$ . Instead, they propose an alternative estimator  $\hat{\sigma}_{PM}^2$  which they call 'exact.' This estimator is also listed in Table 1. From (3.25) and (3.26) it follows that

$$E(\hat{\sigma}_{PM}^{2}) = \sigma_{N}^{2} + \frac{1}{n_{1}n_{2}} \Big[ \underbrace{2[\theta(1-\theta) - (\sigma_{1}^{2} + \sigma_{2}^{2})]}_{>0} - \frac{1}{4}\tau + O(\frac{1}{N}) \Big]$$

By van Dantzig's inequality, it follows that in case of no ties, the bias may be larger than the one of the DeLong estimator since the non-negative expression  $\theta(1 - \theta) - (\sigma_1^2 + \sigma_2^2)$  is multiplied by 2. It may be unbiased or biased in both directions depending on ties and whether  $\theta(1 - \theta) \neq \sigma_1^2 + \sigma_2^2$ . Perme and Manevski (2019) only consider the case of no ties.

#### 4.6 Hanley–McNeil estimator

Hanley and McNeil (1982) discuss two estimators of  $\hat{\theta}$  in their paper. Regarding the first estimator, they refer to Bamber (1975). However, the estimator given in Eq.(1) in their paper is not Bamber's estimator. It is similar to  $\hat{\sigma}_{PM}^2$  in Table 1 but using different weights for  $Q_i^2$ . Unfortunately, Bamber did neither discuss nor derive the properties of his estimator. Hanley and McNeil intended to provide a conservative estimator when presenting their second estimator. They observed that in the case of exponential distributions, the variance of  $\hat{\theta}$  was larger than for other distributions. As in the case of exponential distributions, the variance of  $\hat{\theta}$  is a function only of  $\theta$  and the sample sizes, they suggested an estimator  $\hat{\sigma}_{HM}^2$  by plugging in  $\hat{\theta}$  for  $\theta$  in the variance representation for  $\hat{\theta}$  assuming of exponential distributions

$$Var_{exp}(\widehat{\theta}) = \frac{1}{n_1 n_2} \,\theta(1-\theta) \,\left[1 + (n_2 - 1)\frac{1-\theta}{2-\theta} + (n_1 - 1)\frac{\theta}{1+\theta}\right].$$

Perme and Manevski (2019) mention that 'there is no theoretical reason for consistency (of this estimator) in case of other distributions'. Moreover, the variance of  $\hat{\theta}$  in the case of exponential distributions is not the maximum possible variance of  $\hat{\theta}$ . In fact,  $\sigma_{\max}^2 = \theta(1-\theta)/m$ , as shown by the Birnbaum and Klose (1957). Because of these flaws, we will not consider  $\hat{\sigma}_{HM}^2$  in more detail. It is somewhat unfortunate that later, Newcombe (2006) recommended a modification of this estimator as a basis for deriving a confidence interval for  $\theta$ .

Some more estimators are considered in the literature for particular models where mainly continuous distribution functions are assumed. As they are more or less similar to the DeLong estimator and are restricted to specific models, we do not consider them here in detail.

There is an uncertainty in the statistical literature as to which variance estimator of  $\hat{\theta}$  should be used.

#### **5** Simulations

## 5.1 Simulated biases of the estimators $\hat{\sigma}_{N}^{2}, \hat{\sigma}_{DL}^{2}$ , and $\hat{\sigma}_{PM}^{2}$

To demonstrate the amount of the different biases and the dependency on the underlying distributions, a simulation study was performed where the following distributions were selected:

- 1. Normal distributions  $N(0, \sigma_1^2)$ ,  $N(\delta, \sigma_2^2)$
- 2.  $D_{\text{max}}$ -distributions generating the maximal variance  $\sigma_{\text{max}}^2 = \theta(1-\theta)/m$  of  $\hat{\theta}$ , where,  $\theta = \int F_1 dF_2$  and

$$F_1(x) = \begin{cases} 0, & x \le 0, \\ \theta x, & 0 < x \le 1, \\ \theta, & 1 < x \le 2, \\ (1-\theta)x + 3\theta - 2, & 2 < x \le 3, \\ 1, & x > 3 \end{cases} \quad F_2(x) = \begin{cases} 0, & x \le 0, \\ x - 1, & 1 < x \le 2, \\ 1, & x > 1. \end{cases}$$

- 3. Poisson distributions  $X_i \sim Po(\lambda_i)$ , i = 1, 2, with parameters  $\lambda_1 = 1$  and  $\lambda_2 = 1, \ldots, 13$
- 4. 5-points ordinal scale distributions for ordered categorical data which are generated by discretizing the observations  $X_i^B \sim \text{Beta}(x|a_i, b_i), i = 1, 2$  from the Beta distributions  $\text{Beta}(x|a_i, b_i)$  such that  $X_i^{ord} = \text{INT}(5X_i^B|a_i, b_i) + 1$ . Here we have selected the Beta(2, 15)-distribution and the Beta( $a_2$ , 15)-distribution for  $a_2 = 2, \ldots, 8$ .

Since all estimators  $\hat{\sigma}_N^2$ ,  $\hat{\sigma}_{DL}^2$ , and  $\hat{\sigma}_{PM}^2$  are asymptotically unbiased, we performed the simulations for the small sample sizes  $n_1 = n_2 = 10$  as an example. Figure 1 shows the biases of the estimators mentioned above. The data were generated by the above listed distribution functions, normal,  $D_{\text{max}}$ , Poisson, and a 5-points ordinal scale distributions. These graphs demonstrate that in a practical data example, the actual type-I error  $\alpha^*$  of a test and for a confidence interval the actual coverage probability  $1 - \alpha^*$  do not only depend on the quality of the approximation of  $\hat{\theta}$  by a normal distribution but also depend on an unknown bias of the variance estimator of  $\hat{\theta}$ . Thus, removing this uncertainty by using an estimator with only a small or even no bias appears advisable.

It shall be noted here that these considerations only matter in small sample sizes where 'small' is a vague expression that depends on the underlying distribution functions and the effect  $\theta$ . For sample sizes  $n_1 = n_2 = 50$ , for example, the ratio  $\hat{\sigma}_{PM}^2/\sigma_N^2 \ge 1.1$  for  $\theta \ge 0.98$  in case of normal distributions or ordinal data on a 5-points scale. Sample sizes of about  $n_1 = n_2 = 500$  are necessary to obtain a similar graph for the same ratio as for  $n_1 = n_2 = 10$  in the case of the  $D_{\text{max}}$ -distributions in Fig. 1 (upper row, right). For discrete distributions, e.g., in case of a 5-points ordinal scale, also for quite a small effect close to  $\theta = 1/2$ , it is possible that the ratio  $\hat{\sigma}_{PM}^2/\sigma_N^2 \approx 1.3$  for  $n_1 = n_2 = 10$  while a samples size of about 100 per group reduces this bias to  $\approx 1.02$ .

Estimator	Properties
Sen = Hilgers = Shirahata $\hat{\sigma}_{SHS}^2 = \frac{1}{d_N} \left[ Q_1^2 + Q_2^2 - n_1 n_2 \hat{\theta} (1 - \hat{\theta}) \right]$	only valid in case of no ties unbiased non-negative.
Bamber $\hat{\sigma}_N^2 = \frac{1}{d_N} \left( Q_1^2 + Q_2^2 - n_1 n_2 \left[ \hat{\theta} (1 - \hat{\theta}) - \frac{1}{4} \hat{\tau}_N \right] \right)$	valid in general unbiased non-negative $\widehat{\sigma}_N^2 \leq \widehat{\theta}(1-\widehat{\theta})/(m-1)$
DeLong-DeLong-Ckarke-Pearson $\hat{\sigma}_{DL}^2 = \frac{1}{d_N} \left[ \left( 1 - \frac{1}{n_2} \right) Q_1^2 + \left( 1 - \frac{1}{n_1} \right) Q_2^2 \right]$	may be unbiased or biased in both directions depending on ties and whether $\theta(1-\theta) > \sigma_1^2 + \sigma_2^2$
Perme-Manevski $\hat{\sigma}_{PM}^{2} = \frac{1}{d_{N}} \left[ \left( 1 - \frac{1}{n_{2}} \right)^{2} Q_{1}^{2} + \left( 1 - \frac{1}{n_{1}} \right)^{2} Q_{2}^{2} + (n_{1} - 1) (n_{2} - 1) \theta(1 - \theta) \right]$	may be unbiased or biased in both directions depending on ties and whether $\theta(1-\theta) > \sigma_1^2 + \sigma_2^2$

**Table 1** List of some estimators of  $\sigma_N^2 = Var(\hat{\theta})$  discussed in the literature

The estimators as functions of  $d_N, m, \hat{\theta}, Q_1^2, Q_2^2, and \hat{\tau}_N$  are listed in the left column, and some properties of the estimators in the right column

This motivates using the unbiased estimator  $\hat{\sigma}_N^2$  in (3.31) first derived by Bamber (1975) and studied in more detail in this paper.

## 5.2 MSE of the estimators $\widehat{\sigma}_{N}^{2}$ , $\widehat{\sigma}_{DL}^{2}$ , and $\widehat{\sigma}_{PM}^{2}$

A summary measure for the quality of an estimator, which includes the bias as well as the variance of the estimator, is the so-called 'means-squared-error' (MSE),

$$MSE(\widehat{\lambda}, \lambda) = Var(\widehat{\lambda}) + \left[E(\widehat{\lambda}) - \lambda\right]^2,$$

where  $\lambda$  denotes the parameter to be estimated,  $\hat{\lambda}$  an estimator of  $\lambda$ , and  $Var(\hat{\lambda})$  the variance of this estimator. As seen from Fig. 1 the biases of the estimators  $\hat{\sigma}_N^2$ ,  $\hat{\sigma}_{DL}^2$ , and  $\hat{\sigma}_{PM}^2$  depend on  $\theta$ . Thus, we consider these biases relative to the quantity it should estimate. Here, the variance  $\sigma_N^2$  in (2.8) shall be estimated, and the relative MSEs are given by

$$\begin{split} q &- \mathrm{MSE}(\widehat{\sigma}_N^2, \sigma_N^2) = \frac{1}{\sigma_N^2} \left( \mathrm{Var}(\widehat{\sigma}_N^2) + \left[ E(\widehat{\sigma}_N^2) - \sigma_N^2 \right]^2 \right) = \frac{1}{\sigma_N^2} \mathrm{Var}(\widehat{\sigma}_N^2) \\ q &- \mathrm{MSE}(\widehat{\sigma}_{DL}^2, \sigma_N^2) = \frac{1}{\sigma_N^2} \left( \mathrm{Var}(\widehat{\sigma}_{DL}^2) + \left[ E(\widehat{\sigma}_{DL}^2) - \sigma_N^2 \right]^2 \right) \\ q &- \mathrm{MSE}(\widehat{\sigma}_{PM}^2, \sigma_N^2) = \frac{1}{\sigma_N^2} \left( \mathrm{Var}(\widehat{\sigma}_{PM}^2) + \left[ E(\widehat{\sigma}_{PM}^2) - \sigma_N^2 \right]^2 \right) \,. \end{split}$$

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**Fig. 1** Biases of the variance estimators  $\widehat{\sigma}_N^2$  (solid),  $\widehat{\sigma}_{DL}^2$  (dashed), and  $\widehat{\sigma}_{PM}^2$  (dotted) displayed in Table 1 for the samples sizes  $n_1 = n_2 = 10$ . The data were generated from normal distributions (upper row, left),  $D_{\text{max}}$ -distributions (upper row, right), Poisson-distributions (lower row, left), and a 5-point ordinal scale (lower row, right)

Basically,  $\sigma_N^2$  is a scaling factor. In our simulations,  $\hat{\sigma}_N^2$  has the smallest q-MSE in all cases. As examples, we display the results for normal distributions, 5-points ordinal scale distributions, exponential distributions, and  $D_{\text{max}}$ -distributions in Fig. 2.

This simulation study concludes that the unbiased estimator  $\hat{\sigma}_N^2$  (Bamber's estimator) can be recommended as a 'good variance estimator' for the Mann–Whitney variance. It outperforms the DeLong- and Perme–Manevski estimators.

#### 6 Discussion

We intended to derive an unbiased variance estimator of the well-known Mann– Whitney variance  $\sigma_N^2$  in (2.8). In the case of continuous distribution functions  $F_1(x)$ and  $F_2(x)$ , the variance representation has been known since Van Dantzig (1951). But it seems that Bamber (1975) was the first to provide a representation of  $\sigma_N^2$ , which is also valid in the case of ties. The representation of Bamber's estimator, however, is quite involved. Moreover, this estimator's basic properties - except unbiasedness - are not discussed in Bamber's paper. In particular, it is necessary that an unbiased variance estimator cannot become negative since, in many applications, the standard



**Fig. 2** Relative q-MSEs of the estimators  $\hat{\sigma}_N^2$  (solid),  $\hat{\sigma}_{DL}^2$  (dashed), and  $\hat{\sigma}_{PM}^2$  (dotted) in [10<sup>5</sup>] simulations runs for each setting for the sample sizes  $n_1 = n_2 = 10$ . The alternatives  $\theta \in [0.5, 0.999]$  are generated from normal distributions (upper row, left), 5-points ordinal scale distributions (upper row, right), exponential distributions (lower row, left), and  $D_{\text{max}}$ -distributions (lower row, right). Note that the scales of the ordinate are different in the upper and lower rows to better demonstrate the differences between the estimators

deviation of this estimator is used. If the estimator is set equal to 0 or negative, then it is no longer unbiased.

To the best of our knowledge, it has not been shown for any unbiased variance estimator of the Mann–Whitney variance, which is also valid for ties that cannot become negative. Bamber (1975) does not discuss this topic, and Cliff (1993) states that the estimator given in Equation (9) in his paper may become negative.

Neither Sen (1967) nor Hilgers (1981) discuss whether their estimators can become negative. Moreover, these estimators are only valid if there are no ties. However, the proposed estimator  $\hat{\sigma}_N^2$  in (3.31) is also valid for ties, and it is shown in the appendix that  $\hat{\sigma}_N^2 \ge 0$ . In addition, the covariance matrices of the placements  $R_{1k}^*$  in (2.5) and  $R_{2\ell}^*$  in (2.6) are derived. Since many variance estimators provided in the literature are based on the quadratic forms  $Q_i^2$  in (3.16) of the centered placements, this derivation enables a simple computation of the bias of the different estimators.

The key point in the derivation of  $\hat{\sigma}_N^2$  is that the covariance matrices of the placement vectors  $\mathbf{R}_1^*$  and  $\mathbf{R}_2^*$  in (3.14) have compound symmetry structures. The expectations of the quadratic forms  $Q_i^2$  in (3.16) based on  $\mathbf{R}_1^*$  and  $\mathbf{R}_2^*$  are not unbiased estimators of  $s_1^2 = Var(\mathbf{R}_{11}^*)$  or  $s_2^2 = Var(\mathbf{R}_{21}^*)$ . Computing the bias by Lancaster's theorem and then appropriately estimating the bias leads to the unbiased estimator  $\hat{\sigma}_N^2$ .

Finally, the behavior of  $\hat{\sigma}_N^2$  compared with competing estimators, the mean-squarederror (MSE), is commonly used. Note that the variance  $\sigma_N^2$  depends on  $\theta$ . However, a 'uniform' superiority of an estimator requires that the MSE of this estimator should be uniformly larger than that of a competing estimator. Then, graphing the MSE over  $\theta$  scaled by  $\sigma_N^2$  can show whether this estimator is uniformly preferable.

The simulation study in Sect. 5.2 shows that  $\hat{\sigma}_N^2$  is preferable to  $\hat{\sigma}_{DL}^2$  and  $\hat{\sigma}_{PM}^2$  for some important classes of distribution functions such as a normal distribution, exponential distribution, and 5-points ordinal distributions. For the extreme case of  $D_{\text{max}}$ -distributions it turns out that  $\hat{\sigma}_N^2$ ,  $\hat{\sigma}_{DL}^2$ , and  $\hat{\sigma}_{PM}^2$  are comparable. We have also investigated some more distributions, such as Laplace-,  $\gamma$ -, and Beta-distributions (not shown here). Also, these examples show that  $\hat{\sigma}_N^2$  is always superior to  $\hat{\sigma}_{DL}^2$  and  $\hat{\sigma}_{PM}^2$  regarding the scaled MSE.

In this paper, Bamber's estimator  $\sigma_N^2$  of the Mann-Whitney variance is studied in detail. On the other hand, a convenient representation using some simple rankings is given. In addition, it is shown that this estimator cannot become negative (disproving Shirahata's conjecture). Moreover, a sharp upper bound of  $\hat{\sigma}_N^2$  is derived, which can be regarded as an empirical version of the well-known Birnbaum-Klose inequality, a noteworthy property of this estimator. Finally, it is demonstrated in a simulation study that this estimator outperforms the commonly used variance estimators  $\hat{\sigma}_{DL}^2$  and  $\hat{\sigma}_{PM}^2$  by a uniformly smaller MSE relative to  $\sigma_N^2$  as graphically shown in Fig. 2.

Unfortunately, the statistical literature poorly perceives Bamber's estimator  $\hat{\sigma}_N^2$ . We hope the properties derived from this paper will contribute to its more considerable popularity and more frequent use. It is easy to compute and has an intuitive representation using rankings; it is unbiased and cannot become negative, and finally outperforms commonly used estimators by a smaller MSE.

#### Apendix A: Proof of Theorem 3.1

### A.1 $L_2$ -consistency of the variance estimator $\hat{\sigma}_N^2$

To show  $L_2$ -consistency of  $\widehat{\sigma}_N^2$  it suffices to show that  $E[N\widehat{\sigma}_N^2 - s_N^2]^2 \to 0$  since  $s_N^2 > 0$  by the assumption that  $\sigma_1^2, \sigma_2^2 > 0$ . Note that  $s_N^2 = N(\sigma_1^2/n_1 + \sigma_2^2/n_2)$  and let

$$\widehat{\sigma}_1^2 = \frac{Q_1^2}{n_2^2(n_1 - 1)}$$
, and  $\widehat{\sigma}_2^2 = \frac{Q_2^2}{n_1^2(n_2 - 1)}$ 

Then straightforward computations show that

$$N\left[\widehat{\sigma}_{N}^{2} - \left(\frac{\sigma_{1}^{2}}{n_{1}} + \frac{\sigma_{2}^{2}}{2_{1}}\right)\right] = N\left[\frac{n_{2}}{n_{1}}\left(\frac{\widehat{\sigma}_{1}^{2}}{n_{2} - 1} - \frac{\sigma_{1}^{2}}{n_{2}}\right) + \frac{n_{1}}{n_{2}}\left(\frac{\widehat{\sigma}_{2}^{2}}{n_{1} - 1} - \frac{\sigma_{2}^{2}}{n_{1}}\right) - \frac{1}{(n_{1} - 1)(n_{2} - 1)}\left[\widehat{\theta}(1 - \widehat{\theta}) - \frac{1}{4}\widehat{\tau}_{N}\right]\right].$$

Now note that  $0 < \sigma_i^2 \le 1, 0 \le \widehat{\sigma}_i^2 \le 1, i = 1, 2$ , and that  $0 \le \widehat{\theta}(1 - \widehat{\theta}) \le \frac{1}{4}$  and  $0 \le \widehat{\tau}_N \le 1$ . Then, using Jensen's inequality and taking expectations, it follows from

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the assumption  $N/n_i \leq N_0$  that

$$\begin{split} E\left(N\left[\widehat{\sigma}_{N}^{2}-\left(\frac{\sigma_{1}^{2}}{n_{1}}+\frac{\sigma_{2}^{2}}{2_{1}}\right)\right]\right)^{2} &\leq 6N_{0}^{2}E(\widehat{\sigma}_{1}^{2}-\sigma_{1}^{2})^{2}+O\left(\frac{N_{0}^{2}}{n_{2}^{2}}\right) \\ &+6N_{0}^{2}E(\widehat{\sigma}_{2}^{2}-\sigma_{2}^{2})^{2}+O\left(\frac{N_{0}^{2}}{n_{1}^{2}}\right)+O\left(\frac{N_{0}^{2}}{n_{1}n_{2}}\right) \,. \end{split}$$

Then the result follows by noting that  $E(\hat{\sigma}_i^2 - \sigma_i^2)^2 \to 0$  for  $N \to \infty$ , i = 1, 2, such that  $N/n_i \le N_0$  and if  $\sigma_1^2, \sigma_2^2 > 0$  (for details see Brunner and Munzel 2000).  $\Box$ 

## A.2 Non-negativity of the variance estimator $\widehat{\sigma}_{\scriptscriptstyle N}^2$

It is not straightforward to show that  $\hat{\sigma}_N^2 \ge 0$  using its rank representation in (3.31). Therefore, we re-write  $\hat{\sigma}_N^2$  as sums of squares and products of count functions which, of course, are all non-negative as defined in Sect. 2.1. Let

$$\mathcal{A} = \sum_{k=1}^{n_2} \sum_{r=1}^{n_1} c(X_{1r}, X_{2k})^2, \qquad \qquad \mathcal{B} = \sum_{k=1}^{n_2} \sum_{r \neq r'} c(X_{1r}, X_{2k}) c(X_{1r'}, X_{2k}), 
\mathcal{C} = \sum_{k \neq k'} \sum_{r=1}^{n_1} c(X_{1r}, X_{2k}) c(X_{1r}, X_{2k'}), \qquad \qquad \mathcal{D} = \sum_{k \neq k'} \sum_{r \neq r'} c(X_{1r}, X_{2k}) c(X_{1r'}, X_{2k'}),$$
(A1)

and for convenience let S = A + B + C + D and note that  $S \ge 0$ . Further, note that  $R_{2k}^* = \sum_{r=1}^{n_1} c(X_{1r}, X_{2k})$  by (2.6),  $R_{1r}^* = \sum_{k=1}^{n_2} c(X_{2k}, X_{1r})$  by (2.5), and

$$\widehat{\theta}^2 = \frac{1}{n_1^2 n_2^2} \sum_{r=1}^{n_1} \sum_{r'=1}^{n_1} \sum_{k=1}^{n_2} \sum_{k'=1}^{n_2} c(X_{1r}, X_{2k}) c(X_{1r'}, X_{2k'}) = \frac{1}{n_1^2 n_2^2} \mathcal{S}$$
(A2)

by (2.4). Then,

$$Q_{2}^{2} = \sum_{k=1}^{n_{2}} \left( R_{2k}^{*} - \overline{R}_{2}^{*} \right)^{2} = \sum_{k=1}^{n_{2}} \left( R_{2k}^{*} \right)^{2} - n_{2} \left( \overline{R}_{2}^{*} \right)^{2}$$
$$= \sum_{k=1}^{n_{2}} \sum_{r \neq r'}^{n_{1}} c(X_{1r}, X_{2k}) c(X_{1r'}, X_{2k}) + \sum_{k=1}^{n_{2}} \sum_{r=1}^{n_{1}} c(X_{1r}, X_{2k})^{2} - n_{1}^{2} n_{2} \widehat{\theta}^{2}$$
$$= \mathcal{A} + \mathcal{B} - \frac{1}{n_{2}} \mathcal{S},$$
(A3)

by (A2) and noting that  $(\overline{R}_{2}^*)^2 = n_1^2 n_2 \widehat{\theta}^2$ . Furthermore, by using the relation  $c(X_{2k}, X_{1r}) = 1 - c(X_{1r}, X_{2k})$ , it follows in a similar way that

$$Q_{1}^{2} = \sum_{r=1}^{n_{1}} \left( R_{1r}^{*} - \overline{R}_{1.} \right)^{2} = \sum_{r=1}^{n_{1}} \sum_{k=1}^{n_{2}} \sum_{k'=1}^{n_{2}} c(X_{2k}, X_{1r}) c(X_{2k'}, X_{1r}) - n_{1} n_{2}^{2} (1 - \widehat{\theta})^{2}$$

$$= \sum_{r=1}^{n_{1}} \sum_{k=1}^{n_{2}} \sum_{k'=1}^{n_{2}} c(X_{1r}, X_{2k}) c(X_{1r'}, X_{2k'}) - n_{1} n_{2}^{2} \widehat{\theta}^{2}$$

$$= \sum_{r=1}^{n_{1}} \sum_{k \neq k'} c(X_{1r}, X_{2k}) c(X_{1r'}, X_{2k'}) + \sum_{r=1}^{n_{1}} \sum_{k=1}^{n_{2}} c(X_{1r}, X_{2k})^{2} - n_{1} n_{2}^{2} \widehat{\theta}^{2}$$

$$= \mathcal{C} + \mathcal{A} - \frac{1}{n_{1}} \mathcal{S}.$$
(A4)

Finally let  $Q_3^2 = n_1 n_2 \left[ (\widehat{\theta}(1 - \widehat{\theta}) - \frac{1}{4}\widehat{\tau}_N) \right]$ . Then, by noting that  $c^2(X_{1r}, X_{2k}) = c(X_{1r}, X_{2k}) - \frac{1}{4}\widehat{\tau}_N$  by (3.12), the quantity  $Q_3^2$  can be written as

$$Q_{3}^{2} = \sum_{k=1}^{n_{2}} \sum_{r=1}^{n_{1}} \left( c(X_{1r}, X_{2k}) - \widehat{\theta} \right)^{2} = \sum_{k=1}^{n_{2}} \sum_{r=1}^{n_{1}} c^{2}(X_{1r}, X_{2k}) - n_{1}n_{2}\widehat{\theta}^{2}$$
$$= \mathcal{A} - \frac{1}{n_{1}n_{2}} \mathcal{S}$$
(A5)

by using (A2).

Now let  $\widetilde{N} = n_1(n_1-1)n_2(n_2-1)$ . Then  $\widetilde{N}\widehat{\sigma}_N^2 = Q_1^2 + Q_2^2 - Q_3^2$  and by combining the results in (A1), (A2), (A4), (A3), and (A5) it follows that

$$\widetilde{N}\widehat{\sigma}_{N}^{2} = \mathcal{A} + \mathcal{B} - \frac{1}{n_{2}}\mathcal{S} + \mathcal{A} + \mathcal{C} - \frac{1}{n_{1}}\mathcal{S} - \mathcal{A} + \frac{1}{n_{1}n_{2}}\mathcal{S}$$

$$= \mathcal{S} - \mathcal{D} - \left(\frac{1}{n_{1}} + \frac{1}{n_{2}} - \frac{1}{n_{1}n_{2}}\right)\mathcal{S}, \text{ respectively}$$

$$\widehat{\sigma}_{N}^{2} = \frac{1}{n_{1}^{2}n_{2}^{2}}\mathcal{S} - \frac{1}{\widetilde{N}}\mathcal{D} = \widehat{\theta}^{2} - \frac{1}{\widetilde{N}}\mathcal{D}$$

$$= \frac{1}{n_{1}^{2}n_{2}^{2}}\left(\mathcal{A} + \mathcal{B} + \mathcal{C} - \frac{N-1}{(n_{1}-1)(n_{2}-1)}\mathcal{D}\right). \quad (A6)$$

Hence, the non-negativity of  $\widehat{\sigma}_N^2$  follows from the relationship between the sums of two count functions  $\mathcal{A}$ ,  $\mathcal{B}$ ,  $\mathcal{C}$  and  $\mathcal{D}$ , respectively. For convenience, we define the additional sums of count functions

$$\mathcal{E} = \sum_{k=1}^{n_2} \sum_{r=1}^{n_1} c(X_{1r}, X_{2k}) \quad \text{and} \quad \mathcal{F} = \sum_{k=1}^{n_2} \sum_{r=1}^{n_1} [c^+(X_{1r}, X_{2k}) - c^-(X_{1r}, X_{2k})],$$
(A7)

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and note that  $n_1 n_2 \hat{\theta} = \mathcal{E}$  and  $n_1 n_2 \hat{\tau}_N = \mathcal{F}$ . By (A2) it follows that

$$\mathcal{A} + \mathcal{B} + \mathcal{C} = n_1^2 n_2^2 \widehat{\theta}^2 - \mathcal{D}.$$

Equivalently, it follows from (A7), that

$$n_1^2 n_2^2 \widehat{\theta}^2 = \mathcal{E}^2 = \left(\mathcal{A} + \frac{1}{4}\mathcal{F}\right)^2$$

and therefore,

$$\mathcal{A} + \mathcal{B} + \mathcal{C} = \left(\mathcal{A} + \frac{1}{4}\mathcal{F}\right)^2 - \mathcal{D}.$$
 (A8)

The latter implies  $\mathcal{D} \leq (\mathcal{A} + \frac{1}{4}\mathcal{F})^2 = \mathcal{A} + \mathcal{B} + \mathcal{C} + \mathcal{D}$ . Indeed, if  $\mathcal{D} > 0$ , then there exist at least two pairs  $(X_{1r}, X_{2k})$  and  $(X_{1r'}, X_{2k'})$ ,  $r \neq r'$  and  $k \neq k'$ , such that  $c(X_{1r}, X_{2k}) \cdot c(X_{1r'}, X_{2k'}) > 0$ . This implies, however, that at least three pairs  $c(X_{1r}, X_{2k}) > 0$ ,  $c(X_{1r'}, X_{2k'}) > 0$ , and either  $c(X_{1r}, X_{2k'}) > 0$  or  $c(X_{1r'}, X_{2k}) > 0$ exist. Hence, whenever  $\mathcal{D} > 0$ , then  $\mathcal{A} > 0$  and  $\mathcal{B} > 0$  or  $\mathcal{C} > 0$  (or both). In particular, there must exist at least one pair  $c(X_{1r}, X_{2k}) = 1$ , otherwise  $\mathcal{D}$  would be 0. Since there are  $n_1n_2$  terms in  $\mathcal{A}, n_2n_1(n_1 - 1)$  in  $\mathcal{B}, n_1n_2(n_2 - 1)$  in  $\mathcal{C}$  and  $n_1(n_1 - 1)n_2(n_2 - 1)$ terms in  $\mathcal{D}$ , it follows from (A8)

$$\mathcal{A} + \mathcal{B} + \mathcal{C} \ge \frac{n_1 n_2 + n_1 n_2 (n_2 - 1) + n_2 n_1 (n_1 - 1)}{n_1 (n_1 - 1) n_2 (n_2 - 1)} \mathcal{D},$$
  
$$= \frac{N - 1}{(n_1 - 1)(n_2 - 1)} \mathcal{D}.$$
 (A9)

Hence, plugging-in (A9) into (A6),  $\widehat{\sigma}_N^2 \ge 0$ . Note that  $\widehat{\sigma}_N^2 = 0$ , if  $\widehat{\theta} = 0$ , since  $\mathcal{A} = \mathcal{B} = \mathcal{C} = \mathcal{D} = 0$ . If  $\widehat{\theta} = 1$ , then  $\mathcal{D} = n_1(n_1 - 1)n_2(n_2 - 1)$ ,  $\mathcal{A} = n_1n_2$ ,  $\mathcal{B} = n_2n_1(n_1 - 1)n_2(n_2 - 1)$ , and  $\mathcal{C} = n_1n_2(n_2 - 1)$  and hence  $\widehat{\sigma}_N^2 = \frac{1}{n_1^2 n_2^2} \left(\mathcal{A} + \mathcal{B} + \mathcal{C} - \frac{N-1}{(n_1 - 1)(n_2 - 1)}\mathcal{D}\right) = 0$ .

#### A.3 Verification of the upper bound

The computation of the upper bound  $\frac{\hat{\theta}(1-\hat{\theta})}{\min(n_1,n_2)-1}$  of  $\hat{\sigma}_N^2$  is – as the verification of the non-negativity of  $\hat{\sigma}_N^2$  – a very challenging task using its rank-based version. We therefore use its representation with the sums of products of the count functions  $\mathcal{A}, \mathcal{B}, \mathcal{C}$ , and  $\mathcal{D}$ , given in (A1), respectively. In particular, we use the representation

$$\widehat{\sigma}_N^2 = \widehat{\theta}^2 - \frac{1}{\widetilde{N}}\mathcal{D}$$

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as given in the line above (A6). In the following, let  $m = \min(n_1, n_2) - 1$  and let w.l.o.g. be  $n_1 \le n_2$ . The upper bound can now be verified in a few steps:

$$\begin{aligned} & \frac{\widehat{\theta}(1-\widehat{\theta})}{m} - \widehat{\sigma}_N^2 = \frac{\widehat{\theta}(1-\widehat{\theta})}{m} - \widehat{\theta}^2 + \frac{1}{\widetilde{N}}\mathcal{D} = \frac{1}{m}\widehat{\theta} - \frac{m+1}{m}\widehat{\theta}^2 + \frac{1}{\widetilde{N}}\mathcal{D} \\ &= \frac{1}{n_1 - 1}\widehat{\theta} - \frac{n_1}{n_1 - 1}\widehat{\theta}^2 + \frac{1}{\widetilde{N}}\mathcal{D} = \frac{1}{n_1 - 1}\left(\widehat{\theta} - n_1\widehat{\theta}^2\right) \\ &+ \frac{1}{n_1(n_1 - 1)n_2(n_2 - 1)}\mathcal{D} \\ &= \frac{1}{n_1 - 1}\left[\frac{1}{n_1n_2}\sum_{k=1}^{n_2}\sum_{r=1}^{n_1}c(X_{1r}, X_{2k}) - n_1\widehat{\theta}^2\right] + \frac{1}{n_1(n_1 - 1)n_2(n_2 - 1)}\mathcal{D} \\ &= \frac{1}{(n_1 - 1)n_1n_2}\left[\underbrace{\mathcal{E} - \frac{1}{n_2}\left(\mathcal{A} + \mathcal{B} + \mathcal{C} + \mathcal{D}\right) + \frac{1}{(n_2 - 1)}\mathcal{D}}_{\ge 0}\right] \ge 0 \\ &\ge 0 \end{aligned}$$

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