EFFICIENT COMPUTATION OF THE BERGSMAN-DASSIOS SIGN COVARIANCE

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ABSTRACT. In an extension of Kendall’s $\tau$, Bergsma and Dassios (2014) introduced a covariance measure $\tau^*$ for two ordinal random variables that vanishes if and only if the two variables are independent. For a sample of size $n$, a direct computation of $\tau^*$, the empirical version of $\tau^*$, requires $O(n^4)$ operations. We derive an algorithm that computes the statistic using only $O(n^2 \log(n))$ operations.

1. Introduction

Kendall’s $\tau$ (Kendall, 1938) and Spearman’s $\rho$ (Spearman, 1904) are popular measures of dependence between two random variables $X$ and $Y$. However, both have the undesirable property that they may be equal to zero even when $X$ and $Y$ are not independent. Addressing this weakness, Bergsma and Dassios (2014) have defined a new coefficient, $\tau^*$, which, under mild conditions on the joint distribution of $(X,Y)$, is zero if and only if $X$ and $Y$ are independent. However, a computational price is to be paid for this property as a naïve computation of $\tau^*$, the empirical version of $\tau^*$, requires $O(n^4)$ time for a sample of size $n$.

In this paper we present an algorithm which computes $\tau^*$ in $O(n^2 \log(n))$ time, inspired by a similar improvement for computing (the empirical version of) Kendall’s $\tau$. Indeed, by leveraging binary tree algorithms and observing that Kendall’s statistic depends only on the relative order of data points, Christensen (2005) showed that Kendall’s $\tau$ could be computed in $O(n \log(n))$ time rather than $O(n^2)$. We follow a similar strategy by exploiting the fact that computing $\tau^*$ relies only on the relative ordering of quadruples of points. Due to excessive time requirements, Bergsma and Dassios limit their computational examples to sample sizes with $n \leq 50$ and suggest approximating $\tau^*$ by random subsampling for larger samples. As will be shown in Section 4, our algorithm computes $\tau^*$ exactly in less than a second for sample sizes in the thousands.

1.1. Background and Setup. Given a sample $(x_1, y_1), \ldots, (x_n, y_n)$ of points in $\mathbb{R}^2$, define the statistic

$$t^* := \frac{(n-4)!}{n!} \sum_{\substack{1 \leq i,j,k,l \leq n \\ i,j,k,l \text{ distinct}}} a(x_i, x_j, x_k, x_l) a(y_i, y_j, y_k, y_l)$$

where $a(x, y) = 1$ if $x > y$ and $a(x, y) = 0$ otherwise.

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Figure 1. Relative position of points within quadrants does not matter, only that they remain in their respective quadrants

where

$$a(z_1, z_2, z_3, z_4) := \text{sign}(|z_1 - z_2| + |z_3 - z_4| - |z_1 - z_3| - |z_2 - z_4|).$$

This definition of $t^*$ is in the form of a U-statistic whereas Bergsma and Dassios (2014) introduce it as a V-statistic. We consider the U-statistic as it simplifies some of the computations in Sections 2 and 3. We do, however, present modifications to our algorithm that allow one to compute the V-statistic in Appendix A.

As noted by Bergsma and Dassios (2014), we may rewrite the function $a$ as

$$a(z_1, z_2, z_3, z_4) = I(z_1, z_3 < z_2, z_4) + I(z_1, z_3 > z_2, z_4)$$

$$- I(z_1, z_2 < z_3, z_4) - I(z_1, z_2 > z_3, z_4)$$

(1.2)

where $I(z_1, z_2 < z_3, z_4)$ is the indicator of the event $\max(z_1, z_2) < \min(z_3, z_4)$. After rewriting $a$ in this way we see that computation of the $t^*$ statistic requires only knowledge of the relative positioning of the observations for which we make the following definitions. Let $(x_1, y_1), \ldots, (x_4, y_4)$ be four points relabelled so that $x_1 \leq x_2 \leq x_3 \leq x_4$. We then say that the points are

- **inseparable** if $x_2 = x_3$ or there exists a permutation $\pi$ of $\{1, 2, 3, 4\}$ so that $y_{\pi(1)} \leq y_{\pi(2)} = y_{\pi(3)} \leq y_{\pi(4)}$,

and if they are not inseparable, then we call them

- **concordant** if $\max(y_1, y_2) < \min(y_3, y_4)$ or $\max(y_3, y_4) < \min(y_1, y_2)$,

- **discordant** if $\max(y_1, y_2) > \min(y_3, y_4)$ and $\max(y_3, y_4) > \min(y_1, y_2)$.

These definitions categorize all quadruples of points, that is, any quadruple of points must be exactly one of inseparable, concordant, or discordant. Moreover, when all coordinates are distinct any collection of four points will be either concordant or discordant, see Figure 1. We motivate calling points inseparable by noting that, in the $x_2 = x_3$ case, we cannot draw a line parallel to the $y$-axis that separates the $x$ values into two groups. Similarly in the $y_{\pi(1)} \leq y_{\pi(2)} = y_{\pi(3)} \leq y_{\pi(4)}$ case there exists no such line parallel to the $x$-axis that separates the $y$ values into two groups.

We will derive two algorithms for the computation of $t^*$, the first works only in the case that the data contains no ties, that is all $x_1, \ldots, x_n$ are distinct and similarly for $y_1, \ldots, y_n$, and the second works for all data. While the second algorithm is strictly more general than the first it is also substantially complicated by the need to
consider the case of inseparable points. We present the algorithm for data without ties in Section 2 and give the general algorithm in Section 3.

1.2. A Preliminary Lemma. Before moving on it will be useful to rewrite \( t^* \) to capture a certain permutation invariance and state a basic, but very useful, lemma. Let \( C(n, 4) = \{\{i, j, k, l\} : 1 \leq i < j < k < l \leq n\} \) and \( S_4 \) be the set of permutations on 4 elements. For ease of notation, for any \( \pi \in S_4 \) and \( (z_1, z_2, z_3, z_4) \in \mathbb{R}^4 \) we define \( z_{\pi(1),\ldots,\pi(4)} := (z_{\pi(1)}, \ldots, z_{\pi(4)}) \). We may then rewrite (1.1) as

\[
\begin{align*}
t^* &= \frac{(n - 4)!}{n!} \sum_{\{i, j, k, l\} \in C(n, 4)} \sum_{\pi \in S_4} a(x_{\pi(i, j, k, l)}) a(y_{\pi(i, j, k, l)}) \\
&= \frac{(n - 4)!}{n!} \sum_{\{i, j, k, l\} \in C(n, 4)} b_{ijkl},
\end{align*}
\]

where

\[
b_{ijkl} := \sum_{\pi \in S_4(i, j, k, l)} a(x_{\pi(i, j, k, l)}) a(y_{\pi(i, j, k, l)})
\]

is clearly invariant to any permutation of \( i, j, k, l \).

We now characterize the possible values \( b_{ijkl} \) may take.

**Lemma 1.1.** Let \( A = \{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4)\} \subset \mathbb{R}^2 \). Then

\[
b_{1234} = \begin{cases} 
16 & \text{if the points in } A \text{ are concordant} \\
-8 & \text{if the points in } A \text{ are discordant} \\
0 & \text{if the points in } A \text{ are inseparable}
\end{cases}
\]

The proof of Lemma 1.1 is a straightforward but lengthy case-by-case analysis and we defer it to Appendix B.

2. The Algorithm for Data Without Ties

Throughout this section we assume that \( (x_1, y_1), \ldots, (x_n, y_n) \) contain no ties, that is, \( x_1, \ldots, x_n \) are pairwise distinct and so are \( y_1, \ldots, y_n \). As there are no ties, every quadruple of points is either concordant or discordant. It follows from Equation (1.3) and Lemma 1.1 that

\[
\begin{align*}
t^* &= \frac{(n - 4)!}{n!} \sum_{\{i, j, k, l\} \in C(n, 4)} b_{ijkl} \\
&= \frac{(n - 4)!}{n!} \sum_{\{i, j, k, l\} \in C(n, 4)} \left[ 16 \cdot I(\{(x_i, y_i), \ldots, (x_l, y_l)\} \text{ are concordant}) \\
&\quad - 8 \cdot I(\{(x_i, y_i), \ldots, (x_l, y_l)\} \text{ are discordant}) \right] \\
&= \frac{(n - 4)!}{n!} (16 \cdot N_c - 8 \cdot N_d) \\
&= \frac{(n - 4)!}{n!} (24 \cdot N_c) - \frac{1}{3},
\end{align*}
\]

where \( N_c \) and \( N_d \) are the numbers of concordant and discordant quadruples in \( (x_1, y_1), \ldots, (x_n, y_n) \), respectively, and the last equality holds since every quadruple of points is either concordant or discordant implying that \( \binom{n}{4} = N_d + N_c \). Thus
computing $t^*$ requires only computing the number of concordant quadruples of points. We now show that this can be done efficiently.

Suppose we have relabeled the points so that $x_1 < x_2 < \ldots < x_n$. Rewriting sums we have that

$$N_c = \sum_{1 \leq i < j < k < l \leq n} I((x_i, y_i), (x_j, y_j), (x_k, y_k), (x_l, y_l) \text{ are concordant})$$

$$= \sum_{3 \leq k \leq n-1} \sum_{1 \leq i < j < k} I((x_i, y_i), (x_j, y_j), (x_k, y_k), (x_i, y_i) \text{ are concordant})$$

$$= \sum_{3 \leq k \leq n-1} \sum_{1 \leq i < j < k} I(y_i, y_j < y_k, y_l) + I(y_k, y_l < y_i, y_j)$$

$$= \sum_{3 \leq k \leq n-1} \sum_{1 \leq i < j < k} \left( M_<(k, l) \right) + \left( M_>(k, l) \right)$$

where we define

$$M_<(k, l) := |\{ i : 1 \leq i < k, y_i < \min(y_k, y_l) \}|,$$

$$M_>(k, l) := |\{ i : 1 \leq i < k, y_i > \max(y_k, y_l) \}|.$$

The last line in the above summation is, effectively, the algorithm. Note that the summation is over $O(n^2)$ terms and, consequently, if we can find $M_<(k, l)$ and $M_>(k, l)$ in $O(\log(n))$ time then we have found an algorithm for computing $N_c$ in $O(n^2 \log(n))$ time. To find $M_<(k, l)$ and $M_>(k, l)$ in $O(\log(n))$ time we use a binary tree data structure with an appropriate balancing algorithm to ensure that inserts and searching can be done in $O(\log(n))$ time. One example of this type of data structure are the so-called red-black trees (Guibas and Sedgewick, 1978). In particular, given that we have inserted the values $y_1, y_2, \ldots, y_{k-1}$ into a red-black tree we may insert another $y_k$ into the tree in $O(\log(k))$ time and a simple extension of the traditional red-black framework allows one, for any $y$, to find $|\{ 1 \leq i \leq k-1 : y_i < y \}|$ and $|\{ 1 \leq i \leq k-1 : y_i > y \}|$ in $O(\log(k))$ time.

Combining the above observations, Algorithm 1 gives an $O(n^2 \log(n))$ procedure for finding the number of concordant quadruples which is easily extended to a computation of $t^*$ via Equation (2.1). Note that in Algorithm 1 there is a preprocessing step in which we sort the $x_1, \ldots, x_n$ values in ascending order and then reorder the $y_i$ to match this new order. Since this preprocessing can be done in worst case $O(n \log(n))$ time with a number of algorithms, merge-sort for example, it is not a significant component of the overall asymptotic run time analysis.

3. The General Algorithm

Now suppose that there are no restrictions on the values of $(x_1, y_1), \ldots, (x_n, y_n)$ and that we have reordered the points so that $x_1 \leq \ldots \leq x_n$. For any $3 \leq k \leq l \leq n$, let

(3.1) $top(k, l) = |\{ 1 \leq i < k : x_i \neq x_k \text{ and } y_i > \max(y_k, y_l) \}|,$

(3.2) $mid(k, l) = |\{ 1 \leq i < k : x_i \neq x_k \text{ and } \min(y_k, y_l) < y_i < \max(y_k, y_l) \}|,$

(3.3) $bot(k, l) = |\{ 1 \leq i < k : x_i \neq x_k \text{ and } y_i < \min(y_k, y_l) \}|,$

(3.4) $eqMin(k, l) = |\{ 1 \leq i < k : x_i \neq x_k \text{ and } y_i = \min(y_k, y_l) \}|,$

(3.5) $eqMax(k, l) = |\{ 1 \leq i < k : x_i \neq x_k \text{ and } y_i = \max(y_k, y_l) \}|.$
Algorithm 1

1: procedure NumConcordant((x1, y1),..., (xn, yn))
2: \( x \leftarrow (x_1, \ldots, x_n) \)
3: \( y \leftarrow (y_1, \ldots, y_n) \)
4: Sort \( x \) in ascending order and relabel \( y \) to match this new order
5: \( rbTree \leftarrow \) empty red-black tree
6: \( totalConcordant \leftarrow 0 \)
7: for \( k = 1, \ldots, n-1 \) do
8: \( \quad \) for \( \ell = k + 1, \ldots, n \) do
9: \( \quad \quad \) \( minY \leftarrow \min(y_k, y_\ell) \)
10: \( \quad \quad \) \( maxY \leftarrow \max(y_k, y_\ell) \)
11: \( \quad \quad \) \( numLess \leftarrow \) number of elements \( < minY \) in \( rbTree \)
12: \( \quad \quad \) \( numGreater \leftarrow \) number of elements \( > maxY \) in \( rbTree \)
13: \( \quad \quad \) \( totalConcordant = totalConcordant + (numLess^2) + (numGreater^2) \)
14: \( \quad \) Insert \( y_k \) into \( rbTree \)
15: \( \) return \( totalConcordant \)

Figure 2. Partitioning of the points with \( x \) value strictly less than two given points. Solid lines correspond to \( eqMax \) and \( eqMin \), the points whose \( y \)-values equal the maximum or minimum of the \( y \) values of the two given points, respectively.

These quantities correspond to a partitioning of the points \((x_i, y_i)\) with \( i < k \) and \( x_i \neq x_k \). We illustrate this partitioning in Figure 2. For fixed \( 3 \leq k < l \leq n \) we have, by Lemma 1.1 and since \( x_1 \leq \ldots \leq x_n \),

\[
\sum_{1 \leq i < j < k} b_{ijkl} = 16 \cdot |\{1 \leq i < j < k : i, j, k, l \text{ correspond to concordant points}\}| \\
= 16 \cdot N_{con}(k, l) - 8 \cdot N_{dis}(k, l).
\]

Hence, similarly as in the case without ties, we may write

\[
\sum_{(i,j,k,l) \in C(n,4)} b_{ijkl} = \sum_{3 \leq k \leq n-1} \sum_{k < j \leq n} \sum_{1 \leq i < j < k} b_{ijkl}
\]
where

\[
= \sum_{3 \leq k \leq n-1} \sum_{k < l \leq n} 16 \cdot N_{\text{con}}(k, l) - 8 \cdot N_{\text{dis}}(k, l).
\]

Again the last line of the above summation is effectively the algorithm. Since the sums are over \(O(n^2)\) terms, if we can show that \(N_{\text{con}}(k, l)\) and \(N_{\text{dis}}(k, l)\) can be computed in \(O(\log(n))\) time then we have obtained an \(O(n^2 \log(n))\) algorithm for computing \(t^*\). We show next that this is indeed possible, beginning with the observation that

\[
N_{\text{con}}(k, l) = \left(\frac{\text{top}(k, l)}{2}\right) + \left(\frac{\text{bot}(k, l)}{2}\right),
\]

if \(y_k = y_l\) then

\[
N_{\text{dis}}(k, l) = 0,
\]

and if \(y_k \neq y_l\) then

\[
N_{\text{dis}}(k, l) = \text{top}(k, l) \cdot (\text{mid}(k, l) + \text{eqMin}(k, l) + \text{bot}(k, l))
+ \text{bot}(k, l) \cdot (\text{mid}(k, l) + \text{eqMax}(k, l))
+ \text{eqMin}(k, l) \cdot (\text{mid}(k, l) + \text{eqMax}(k, l))
+ \text{eqMax}(k, l) \cdot \text{mid}(k, l)

+ \left(\frac{\text{mid}(k, l)}{2}\right) - \sum_{y \in \text{unique}(k, l)} \left(\frac{|\{1 \leq i < k : x_k \neq x_i \text{ and } y_i = y\}|}{2}\right)
\]

where

\[
\text{unique}(k, l) := \{y_i : 1 \leq i < k \text{ and } x_i \neq x_k \text{ and } \min(y_k, y_i) < y_i < \max(y_k, y_i)\}.
\]

Suppose we have a red-black tree into which we have inserted all \(y_i\) with \(1 \leq i < k\) and \(x_i \neq x_k\). Then it is clear that the quantities in Equations (3.1)-(3.5) can each be computed in \(O(\log(k))\) time. Note that, unlike in the untied case, we require that the red-black tree not include any \(y_i\) values corresponding to \(x_i = x_k\); accomplishing this algorithmically is very simple: as we iterate across the \(x_k\) values we delay inserting their associated \(y_k\) values into the red-black tree until we reach a \(x_i\) with \(x_i \neq x_{i-1}\), upon reaching such an \(x_i\) we insert all postponed \(y\) values into the red-black tree and then restart the postponing of \(y\) values starting with \(y_i\).

We see that, as in the discussion of Algorithm 1, we can progressively compute almost all of the quantities in Equations (3.6) and (3.8) with each iteration taking \(O(\log(n))\) time. The only complication is the computation of

\[
\sum_{y \in \text{unique}(k, l)} \left(\frac{|\{1 \leq i < k : x_k \neq x_i \text{ and } y_i = y\}|}{2}\right)
\]

which corresponds to all quadruples of points \((x_i, y_i), (x_j, y_j), (x_k, y_k), (x_l, y_l)\) for which \(\min(y_k, y_l) < y_i = y_j < \max(y_k, y_l)\). These are inseparable and are being over-counted by \((\frac{\text{mid}(k, l)}{2})\). Note that this summation is in the reverse order of what we would like in order to simply generalize Algorithm 1. In particular, there is a condition on the \(y\) values corresponding to \(i\) and \(j\) which is suppressed by the aggregate counts available from a query on a red-black tree.
Table 1. Run times of the naïve algorithm and Algorithm 2 for various sample sizes (in seconds and averaged over 10 samples)

| Sample Size | 100    | 150    | 200    | 250    | 300    |
|-------------|--------|--------|--------|--------|--------|
| Algorithm 2 | 0.0009 | 0.0023 | 0.0043 | 0.0072 | 0.01   |
| Naïve Algorithm | 0.287  | 1.55   | 5.58   | 14.34  | 28.95  |

Table 2. Run times of Algorithm 2 for larger sample sizes (in seconds and averaged over 10 samples)

| Sample Size | 1000   | 3250   | 5500   | 7750   | 10000  |
|-------------|--------|--------|--------|--------|--------|
| Algorithm 2 | 0.0618 | 0.777  | 2.58   | 5.89   | 10.98  |

We have, however, already established a methodology to count values such as (3.9). In particular note that

$$\sum_{3 \leq k < l \leq n} \sum_{y \in \text{unique}(k,l)} \left( \left\{ \{1 \leq i < k : x_k \neq x_i \text{ and } y_i = y \} \right\} \right)$$

$$= \sum_{1 \leq i < j < k < l \leq n} I(\{x_k \neq x_j \text{ and } y_i = y_j \text{ and } \min(y_k, y_l) < y_i < \max(y_k, y_l)\})$$

$$= \sum_{1 \leq i < j \leq n-2} I(\{y_i = y_j\}) \cdot \left| \{k : j < k \leq n \text{ and } x_k \neq x_j \text{ and } y_j < y_k\} \right|$$

$$:= \text{top}^*(j)$$

$$\cdot \left| \{k : j < k \leq n \text{ and } x_k \neq x_j \text{ and } y_j > y_k\} \right|$$

$$:= \text{bot}^*(j)$$

$$\sum_{j \in \{n-2, n-1, \ldots, 2\}} \sum_{i \in \{j-1, j-2, \ldots, 1\}} I(\{y_i = y_j\}) \cdot \text{top}^*(j) \cdot \text{bot}^*(j).$$

(3.10)

It follows that all that is needed to compute the total contribution of the term in Equation (3.9) to $t^*$ is to run a modified version of Algorithm 1 across the data in reverse order. Our algorithm becomes the following:

1. Perform a first pass across the data where we ignore the effect of (3.9) and count all other quantities.
2. Perform a second pass across the data in reverse order to compute (3.10).
3. Appropriately combine the results of (1) and (2) to obtain $t^*$.

This amounts to over-counting discordant quadruples on a first pass and then undoing this over-counting on a second pass. Since both of these passes over the data require $O(n^2 \log(n))$ time, our general Algorithm 2, which leverages the above observations, computes $t^*$ in $O(n^2 \log(n))$ time.

4. Simulations

We test the run times of Algorithm 2 and a naïve implementation, both written in C++, for sample sizes $n$ ranging from 100 to 300. The results of these simulations are presented in Table 1. As the table shows, the $O(n^4)$ running time of the naïve algorithm becomes already a practical concern for sample sizes in the hundreds while Algorithm 2 is essentially instant for such sample sizes. Table 2 provides a perspective on the run time of Algorithm 2 for substantially larger samples.
Algorithm 2

1: procedure $t^*([(x_1, y_1), ...(x_n, y_n)])$
2: $x \leftarrow (x_1, ..., x_n)$
3: $y \leftarrow (y_1, ..., y_n)$
4: Sort $x$ in ascending order and relabel $y$ to match this new order
5: $rbTree \leftarrow$ empty red-black tree $\triangleright$ Used in first pass through data
6: $revRbTree \leftarrow$ empty red-black tree $\triangleright$ Used in second pass through data
7: $\triangleright$ The following is a list that will be used to store $y$ values
8: $\triangleright$ whose insertion into the red-black tree has been delayed
9: $savedYValues \leftarrow$ empty list
10: $totalConcordant \leftarrow 0 \triangleright$ Total concordant quadruples counted so far
11: $totalDiscordant \leftarrow 0 \triangleright$ Total discordant quadruples counted so far
12: for $k = 1, ..., n - 1$ do
13: $\triangleright$ If $k == 1$ or $x_k \neq x_{k-1}$ insert all delayed $y$ values
14: $\triangleright$ into the red-black tree. Also save $y_k$ to potentially be inserted
15: $\triangleright$ in the tree on the next iteration in any case.
16: if $k == 1$ or $x_{k-1} \neq x_k$ then
17: for $yVal$ in $savedYValues$ do
18: Insert $yVal$ into $rbTree$
19: Empty the list $savedYValues$
20: Loop over $\ell > k$ and use equations (3.6), (3.7), (3.8)
21: $\triangleright$ while ignoring contributions of (3.9)
22: for $\ell = k + 1, ..., n$ do
23: $minY \leftarrow \min(y_k, y_\ell)$
24: $maxY \leftarrow \max(y_k, y_\ell)$
25: $top \leftarrow$ number of elements $> maxY$ in $rbTree$
26: $mid \leftarrow$ number of elements $< maxY$ and $> minY$ in $rbTree$
27: $bot \leftarrow$ number of elements $< minY$ in $rbTree$
28: $eqMax \leftarrow$ number of elements equal to $maxY$ in $rbTree$
29: $eqMin \leftarrow$ number of elements equal to $minY$ in $rbTree$
30: $totalConcordant \leftarrow totalConcordant + (\binom{\text{top}}{2}) + (\binom{\text{bot}}{2})$
31: if $minY \neq maxY$ then
32: $totalDiscordant \leftarrow totalDiscordant + (\binom{\text{mid}}{2}) + \text{top} \cdot \text{mid} + \text{top} \cdot \text{bot} + \text{mid} \cdot \text{bot} + \text{eqMin} \cdot (\text{top} + \text{mid} + \text{eqMax}) + \text{eqMax} \cdot (\text{mid} + \text{bot})$
33: $\triangleright$ Now run along the data in reverse to undo the over-counting
34: $\triangleright$ resulting from ignoring the contribution of (3.9)
35: Empty the list $savedYValues$
36: for $j = n, ..., 2$ do
37: if $j == n$ or $x_{j+1} \neq x_j$ then
38: $\triangleright$ Inserting the delayed values
39: for $yVal$ in $savedYValues$ do
40: Insert $yVal$ into $revRbTree$
41: Empty the list $savedYValues$
Append y_j to savedYValues

▷ Use (3.10) to compute the number of over counts

for i = j - 1, ..., 1 do

   \( \min Y \leftarrow \min(y_i, y_j) \)

   \( \max Y \leftarrow \max(y_i, y_j) \)

   \( \text{top} \leftarrow \text{number of elements} > \max Y \text{ in } \text{revRbTree} \)

   \( \text{bot} \leftarrow \text{number of elements} < \min Y \text{ in } \text{revRbTree} \)

if \( \min Y == \max Y \) then

   \( \text{totalDiscordant} \leftarrow \text{totalDiscordant} - \text{top} \cdot \text{bot} \)

return \( \frac{1}{n(n-1)(n-2)(n-3)} (16 \cdot \text{totalConcordant} - 8 \cdot \text{totalDiscordant}) \)

5. Conclusion

We have presented an algorithm which computes the \( U \)-statistic \( t^* \) corresponding to the \( \tau^* \) sign covariance of Bergsma and Dassios (2014) in \( O(n^2 \log(n)) \) time, substantially outperforming a naïve implementation. The computational savings in our algorithm are driven by the use of binary trees and the permutation invariance inherent in \( t^* \) (recall Lemma 1.1).

Appendix A. Modifications for the V-Statistic

This section provides an overview of necessary modifications to Algorithm 2 in order to compute the V-statistic version of \( t^* \). Suppose, as usual, that we have reordered the \((x_1, y_1), ..., (x_n, y_n)\) so that \( x_1 \leq x_2 \leq ... \leq x_n \). Then the V-statistic for \( \tau^* \) is

\[
\begin{align*}
t^*_V &= \frac{1}{n^2} \sum_{1 \leq i,j,k,l \leq n} a(x_i, x_j, x_k, x_l) a(y_i, y_j, y_k, y_l) \\
      &= \frac{1}{n^2} \left( \sum_{1 \leq i < j < k < l \leq n} b_{ijkl} + \sum_{1 \leq i < j < k \leq n} b_{ijkk} + \frac{b_{iikk}}{2} + \sum_{1 \leq i < k \leq n} \frac{b_{iikk}}{4} \right) \\
      &= \frac{1}{n^2} \left( \sum_{1 \leq i < j < k < l \leq n} b_{ijkl} + \sum_{1 \leq i < j < k \leq n} \frac{b_{ijkk} + b_{iikk}}{2} + \sum_{1 \leq i < k \leq n} \frac{b_{iikk}}{4} \right).
\end{align*}
\]

Here, the second equality holds since \( a(x_i, x_j, x_k, x_l) a(y_i, y_j, y_k, y_l) = 0 \) if any three of \( i, j, k, l \) are equal. The third equality holds because \( b_{ijjk} = 0 \) for all \( i < j < k \); indeed, \( x_i \leq x_j \leq x_k \) implies that \( b_{ijjk} \) corresponds to an inseparable collection of points. Note that, in the above equations, we have coefficients of \( \frac{1}{2} \) on \( b_{ijkk}, b_{iikk} \) and \( \frac{1}{4} \) on \( b_{iikk} \), these are corrective factors to account for the fact that the number of permutations of four elements where exactly two are equal is \( |S_4|/2 \) while the number of permutations where exactly two pairs of two are equal is \( |S_4|/4 \). Now we may continue to rewrite \( t^*_V \) as

\[
\begin{align*}
t^*_V &= \frac{1}{n^2} \sum_{1 \leq i < j < k < l \leq n} b_{ijkl} + \sum_{1 \leq i < j < k \leq n} \frac{b_{ijkk} + b_{iikk}}{2} + \sum_{1 \leq i < k \leq n} \frac{b_{iikk}}{4} 
\end{align*}
\]
\[
\frac{1}{n^4} \left( \sum_{1 \leq i < j < k < l \leq n} b_{ijkl} + \sum_{1 \leq i < j < k \leq n} \frac{b_{ijkk}}{2} + \sum_{1 \leq i < k < l \leq n} \frac{b_{iikl}}{2} + \sum_{1 \leq i < k \leq n} \frac{b_{iikk}}{4} \right) = \frac{1}{n^4} \sum_{3 \leq k \leq n} \left( \sum_{k \leq l \leq n} \left( \sum_{1 \leq i < j < k} b_{ijkl} + \sum_{1 \leq i < k} \frac{b_{iikl}}{2} \right) + \sum_{1 \leq i < j < k} \frac{b_{ijkk}}{2} + \sum_{1 \leq i < k} \frac{b_{iikk}}{4} \right) + \frac{1}{n^4} \sum_{3 \leq k \leq n} \left( \sum_{k \leq l \leq n} \left( \sum_{1 \leq i < j < k} b_{ijkl} + \sum_{1 \leq i < k} \frac{b_{iikl}}{2} \right) + \sum_{1 \leq i < j < k} \frac{b_{ijkk}}{2} + \sum_{1 \leq i < k} \frac{b_{iikk}}{4} \right).
\]

Here if \( k = n \) then \( \sum_{k < l \leq n} \) is the empty sum which we define to equal 0. For a fixed \( k < l \) we know already, from Section 3, how to compute \( \sum_{1 \leq i < j < k} b_{ijkl} \) efficiently using a red-black tree and since \( b_{iikl}, b_{ijkk}, \) and \( b_{iikk} \) can only correspond to inseparable or concordant quadruples it is easy to see that

\begin{align}
(A.1) & \quad \sum_{1 \leq i < k} \frac{1}{2} b_{iikl} = 8 \cdot (\text{top}(k, l) + \text{bot}(k, l)) \\
(A.2) & \quad \sum_{1 \leq i < j < k} \frac{1}{2} b_{ijkk} = 8 \cdot \left( \left( \frac{\text{top}(k, k)}{2} \right) + \left( \frac{\text{bot}(k, k)}{2} \right) \right) \\
(A.3) & \quad \sum_{1 \leq i < k} \frac{1}{4} b_{iikk} = 4 \cdot (\text{top}(k, k) + \text{bot}(k, k))
\end{align}

Thus we may compute \( t^*_V \) by running Algorithm 2 with the following modifications:

1. Change line 12 to
   \begin{verbatim}
   for k = 1, ..., n do
   \end{verbatim}
   This corresponds to the outer sum of \( t^*_V \).

2. After line 22 add the lines:
   \begin{verbatim}
   top ← number of elements > y_k in rbTree
   bot ← number of elements < y_k in rbTree
   totalConcordant ← totalConcordant + \frac{1}{2} \left( \left( \frac{\text{top}}{2} \right) + \left( \frac{\text{bot}}{2} \right) \right) + \frac{1}{4}(\text{top} + \text{bot})
   \end{verbatim}
   This accounts for the effect of (A.2) and (A.3).

3. Change line 31 to
   \begin{verbatim}
   totalConcordant ← totalConcordant + \left( \frac{\text{top}}{2} \right) + \left( \frac{\text{bot}}{2} \right) + \frac{1}{2}(\text{top} + \text{bot})
   \end{verbatim}
   This corresponds to (A.1).

4. Change line 52 to
   \begin{verbatim}
   return \frac{1}{n^4}(16 \cdot \text{totalConcordant} - 8 \cdot \text{totalDiscordant})
   \end{verbatim}
   Finally, note that this Algorithm for computing \( t^*_V \) clearly remains \( O(n^2 \log(n)) \).

Appendix B. Proof of Lemma 1.1

By permutation invariance, suppose we have relabeled so that \( x_1 \leq x_2 \leq x_3 \leq x_4 \). We have 3 cases:

1. \textbf{The points in} \( A \) \textbf{are inseparable}. We have that \( b_{1234} = 0 \) as an immediate consequence of Equation (1.2).

2. \textbf{The points in} \( A \) \textbf{are concordant}. In this case we must have that \( x_3 < x_2 \) and either \( \max(y_1, y_2) < \min(y_3, y_4) \) or \( \min(y_1, y_2) > \max(y_3, y_4) \). By symmetry we need only consider the case when \( \max(y_1, y_2) < \min(y_3, y_4) \). By Equation
(1.2) it follows, with some thought, that \( a(x_{\pi(1,2,3,4)}) = a(y_{\pi(1,2,3,4)}) \) for all permutations \( \pi \in S_4 \) and thus, for any \( \pi \in S_4 \) we have \( a(x_{\pi(1,2,3,4)})a(y_{\pi(1,2,3,4)}) = a(x_{\pi(1,2,3,4)})^2 \) with

\[
a(x_{\pi(1,2,3,4)})^2 = \begin{cases} 
1 & \text{if } \max(x_{\pi(1)}, x_{\pi(2)}) < \min(x_{\pi(3)}, x_{\pi(4)}) \text{ or } \\
\min(x_{\pi(1)}, x_{\pi(2)}) > \max(x_{\pi(3)}, x_{\pi(4)}) \text{ or } \\
\max(x_{\pi(1)}, x_{\pi(3)}) < \min(x_{\pi(2)}, x_{\pi(4)}) \text{ or } \\
\min(x_{\pi(1)}, x_{\pi(3)}) > \max(x_{\pi(2)}, x_{\pi(4)}) \\
0 & \text{otherwise.}
\end{cases}
\]

But since \( x_1 \leq x_2 < x_3 \leq x_4 \) we have that \( a(x_{\pi(1,2,3,4)})a(y_{\pi(1,2,3,4)}) = 1 \) if and only if \( \{\pi(1), \pi(2)\} \in \{\{1, 2\}, \{3, 4\}\} \) or \( \{\pi(1), \pi(3)\} \in \{\{1, 2\}, \{3, 4\}\} \). There are exactly \( 2^4 = 16 \) such permutations and thus \( b_{1234} = 16 \).

(3) The points in \( A \) are discordant. Once again we must have that \( x_2 < x_3 \). It then follows, by the definition of discordant, that \( y_1 \neq y_2 \) and \( y_3 \neq y_4 \). We prove an intermediary lemma:

**Lemma B.1.** Suppose that \((x_1, y_1), ..., (x_4, y_4)\) are discordant and \( x_1 \leq x_2 < x_3 \leq x_4 \). Let

\[
(x_5, y_5) = (x_1, y_2) \\
(x_6, y_6) = (x_2, y_1) \\
(x_7, y_7) = (x_3, y_3) \\
(x_8, y_8) = (x_4, y_4)
\]

so that \((x_5, y_5), ..., (x_8, y_8)\) are simply \((x_1, y_1), ..., (x_4, y_4)\) with \( y_1, y_2 \) switched. Then we have that \( b_{1234} = b_{5678} \). Moreover the same result is true if we flipped \( y_3, y_4 \) instead of \( y_1, y_2 \).

**Proof.** First note that, trivially, \( a(x_{\pi(1,2,3,4)}) = a(x_{\pi(5,6,7,8)}) \) for any \( \pi \in S_4 \). Let \( \pi \) be any permutation so that \( a(x_{\pi(1,2,3,4)})^2 = 1 \). From case (2) we know that we must have \( \{\pi(1), \pi(2)\} \in \{\{1, 2\}, \{3, 4\}\} \) or \( \{\pi(1), \pi(3)\} \in \{\{1, 2\}, \{3, 4\}\} \). Suppose that \( \{\pi(1), \pi(2)\} = \{1, 2\} \), and let \( \pi' \in S_4 \) be the permutation where

\[
\pi'(1) = \pi(2), \quad \pi'(2) = \pi(1), \quad \pi'(3) = \pi(3), \quad \pi'(4) = \pi(4).
\]

Then clearly

\[
a(x_{\pi(1,2,3,4)}) = a(x_{\pi'(1,2,3,4)}) = a(x_{\pi(5,6,7,8)}) = a(x_{\pi'(5,6,7,8)})
\]

but

\[
a(y_{\pi(1,2,3,4)}) = a(y_{\pi'(5,6,7,8)})
\]

and thus

\[
a(x_{\pi(1,2,3,4)})a(x_{\pi(1,2,3,4)}) + a(x_{\pi'(1,2,3,4)})a(x_{\pi'(1,2,3,4)})
= a(x_{\pi(5,6,7,8)})a(x_{\pi(5,6,7,8)}) + a(x_{\pi'(5,6,7,8)})a(x_{\pi'(5,6,7,8)}).
\]

Since we may perform a similar procedure to all permutations \( \pi \in S_4 \) with \( a(x_{\pi(1,2,3,4)})^2 = 1 \) (changing the choice of \( \pi' \)), we see that \( b_{1234} = b_{5678} \) as claimed.
Finally, pairing \( \pi \) with \( \pi' \) given by
\[
\pi'(1) = \pi(1), \quad \pi'(2) = \pi(2), \quad \pi'(3) = \pi(4), \quad \pi'(4) = \pi(3)
\]
shows that this result still holds if we had flipped \( y_3, y_4 \) instead of \( y_1, y_2 \). □

By Lemma B.1, we may assume that \( x_1 \leq x_2 < x_3 \leq x_4 \) and \( y_1 < y_2 \) and \( y_3 < y_4 \). Note that, by the definition of discordant, we must have that \( y_2 > y_3 \) and \( y_1 < y_4 \). From case (2) we know that there are only 16 permutations \( \pi \) for which \( a(x_{\pi(1,2,3,4)}) \neq 0 \) and they satisfy
\[
\{\pi(1), \pi(2)\} \in \{\{1, 2\}, \{3, 4\}\} \text{ or } \{\pi(1), \pi(3)\} \in \{\{1, 2\}, \{3, 4\}\}.
\]
If \( \{\pi(1), \pi(2)\} \in \{\{1, 2\}, \{3, 4\}\} \) then if \( \{\pi(1), \pi(3)\} \in \{\{1, 4\}, \{2, 3\}\} \) we have \( a(y_{\pi(1,2,3,4)}) = 0 \). Similarly, \( a(y_{\pi(1,2,3,4)}) = 0 \) if \( \{\pi(1), \pi(3)\} \in \{\{1, 2\}, \{3, 4\}\} \) and \( \{\pi(1), \pi(2)\} \in \{\{1, 4\}, \{2, 3\}\} \). This leaves only 8 permutations \( \pi \in S_4 \) for which \( a(x_{\pi(1,2,3,4)})a(y_{\pi(1,2,3,4)}) \) may be non-zero, and we check these explicitly:
\[
a(x_{1,2,3,4})a(y_{1,2,3,4}) = -1 \cdot 1 = -1, \quad a(x_{2,1,4,3})a(y_{2,1,4,3}) = -1 \cdot 1 = -1, \\
a(x_{3,4,1,2})a(y_{3,4,1,2}) = -1 \cdot 1 = -1, \quad a(x_{4,3,2,1})a(y_{4,3,2,1}) = -1 \cdot 1 = -1, \\
a(x_{1,3,2,4})a(y_{1,3,2,4}) = 1 \cdot -1 = -1, \quad a(x_{2,4,1,3})a(y_{2,4,1,3}) = 1 \cdot -1 = -1, \\
a(x_{3,1,4,2})a(y_{3,1,4,2}) = 1 \cdot -1 = -1, \quad a(x_{4,2,3,1})a(y_{4,2,3,1}) = 1 \cdot -1 = -1.
\]
Hence, we have that \( b_{1234} = -8 \) as claimed.

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