Generalized permutation tests

Rina Foygel Barber*, Emmanuel J. Candès†, Aaditya Ramdas‡, Ryan J. Tibshirani‡

May 6, 2022

Abstract

Permutation tests are an immensely popular statistical tool, used for testing hypotheses of independence between variables and other common inferential questions. When the number of observations is large, it is computationally infeasible to consider every possible permutation of the data, and it is typical to either take a random draw of permutations, or to restrict to a subgroup or subset of permutations. In this work, we extend beyond these possibilities to show how such tests can be run using any distribution over any subset of permutations, with all the previous options as a special case.

1 Introduction

Suppose we observe data $X_1, \ldots, X_n \in \mathcal{X}$, and would like to test the null hypothesis

$$H_0 : X_1, \ldots, X_n \text{ are exchangeable.}$$

(Note that the hypothesis that the $X_i$’s are i.i.d., is a special case of this null.) We assume that we have a pre-specified test statistic, which is a function $T : \mathcal{X}^n \to \mathbb{R}$, where, without loss of generality, we let larger values of $T(X) = T(X_1, \ldots, X_n)$ indicate evidence in favor of an alternative hypothesis.

Since the null distribution of the $X_i$’s is not specified exactly, we usually do not know the null distribution of $T(X)$. The permutation test avoids this difficulty by comparing $T(X)$ against the same function applied to permutations of the data. Specifically, writing $\mathcal{S}_n$ to denote the set of all permutations on $[n] := \{1, \ldots, n\}$, we can compute a p-value

$$P = \frac{\sum_{\sigma \in \mathcal{S}_n} \mathbb{1}\{T(X_{\sigma}) \geq T(X)\}}{n!},$$

where for any $x \in \mathcal{X}^n$ and any $\sigma \in \mathcal{S}_n$, $x_{\sigma} := (x_{\sigma(1)}, \ldots, x_{\sigma(n)})$.

*Department of Statistics, University of Chicago
†Departments of Statistics and Mathematics, Stanford University
‡Departments of Statistics and Machine Learning, Carnegie Mellon University
As an example, suppose that the observed data set actually consists of pairs \((X_i, Y_i)\), which are assumed to be i.i.d. from some joint distribution. If we are interested in testing whether \(X \perp \perp Y\), we can reframe this question as testing whether \(X_1, \ldots, X_n\) are i.i.d. conditional on \(Y_1, \ldots, Y_n\). Our test statistic \(T\) might be chosen as

\[
T(X) = |\text{Corr}((X_1, \ldots, X_n), (Y_1, \ldots, Y_n))|
\]

to see whether the observed correlation is sufficiently large to be statistically significant, we would compare against the correlations computed on the permuted data,

\[
T(X_\sigma) = |\text{Corr}((X_{\sigma(1)}, \ldots, X_{\sigma(n)}), (Y_1, \ldots, Y_n))|
\]

In addition to testing independence, permutation tests are also commonly used for testing other hypotheses such as whether two samples follow the same distribution. Permutation tests are a special case of the more general methodology of invariance based testing (see Lehmann et al. [2005, Chapter 6] for additional background).

Our main contributions are organized in Section 3, where we present a few new generalizations of the standard permutation test. These, for example, yield valid p-values even when we sample permutations—with or without replacement—from a non-uniform distribution over all permutations or from an arbitrary subset of permutations. In particular, Theorems 5 and 6 generalize all earlier results that we are aware of.

The rest of the paper is organized as follows. For the unfamiliar reader, we recap some existing nontrivial results about permutation tests in Section 2 along with a few extensions. Our main results appear in Section 3. Section 4 mentions some broader connections to the literature on MCMC and randomization tests, before we conclude in Section 5.

## 2 Permutation tests with subgroups, subsets, and more

The p-value \(P\) computed in (1) requires computing \(T(X_\sigma)\) for every \(\sigma \in S_n\). We may be interested in reducing the computational cost of this procedure, since computing \(T(X_\sigma)\) for \(|S_n| = n!\) many permutation may be computationally prohibitive for even moderately large \(n\)—can we instead compute \(T(X_\sigma)\) for only a subset of all possible permutations, chosen either deterministically or randomly? We might also be interested in reducing the set of permutations \(\sigma\) for other reasons, for instance, if we believe that certain types of permutations are more informative for distinguishing between the null and alternative hypothesis.

In this section, we cover some well known (and some not so well known) results about the validity of variants of the permutation test when using subgroups and other subsets of the entire permutation group. Of particular interest is a simple example of the failure of the naive permutation test when using a non-subgroup, and a simple fix. The intuitions developed below will be helpful later in the paper, but readers who are familiar with these facts may directly jump to Section 3 where we present a handful of results that generalize all the results stated in this section.
2.1 Permutation tests with subgroups

One alternative is to use only a subgroup of $S_n$. Specifically, let $G \subseteq S_n$ be any subgroup, and define

$$P = \frac{\sum_{\sigma \in G} \mathbb{1}\{T(X_{\sigma}) \geq T(X)\}}{|G|},$$

(2)

where $|G|$ is the cardinality of $G$. This subgroup may be chosen strategically to balance between computational efficiency and the power of the test (see, e.g., Hemerik and Goeman [2018], Koning and Hemerik [2022]).

Theorem 1. If $G \subseteq S_n$ is a subgroup, then the value $P$ defined in (2) is a valid p-value, i.e., $\mathbb{P}_{H_0}\{P \leq \alpha\} \leq \alpha$ for all $\alpha \in [0, 1]$.

In this theorem, validity is retained when conditioning on the order statistics of the data, meaning that $\mathbb{P}_{H_0}\{P \leq \alpha \mid X_{(1)}, \ldots, X_{(n)}\} \leq \alpha$, where $X_{(1)} \leq \cdots \leq X_{(n)}$ are the order statistics of $X = (X_1, \ldots, X_n)$. The reason that this holds is simply because $H_0$ remains true even conditional on the order statistics—that is, if $X$ is exchangeable, then $X \mid (X_{(1)}, \ldots, X_{(n)})$ is again exchangeable. The same conditional validity holds for all results to follow, as well.

Theorem 1 is a well known result has multiple possible proofs; see Hemerik and Goeman [2018, Theorem 1] for a recent example. To help build intuition for our forthcoming results, we offer one style of proof.

Proof. For brevity, we represent $\mathbb{P}_{H_0}\{\cdot\}$ as $\mathbb{P}\{\cdot\}$ throughout this work. First, for all $\sigma' \in G$, we have

$$\mathbb{P}\left\{ \frac{\sum_{\sigma \in G} \mathbb{1}\{(X_{\sigma'})_{\sigma} \geq T(X_{\sigma'})\}}{|G|} \leq \alpha \right\} = \mathbb{P}\left\{ \sum_{\sigma \in G} \mathbb{1}\{T(X_{\sigma}) \geq T(X)\} \leq \alpha \right\},$$

(3)

since $X \overset{d}{=} X_{\sigma'}$ under $H_0$. Next, for any $\sigma' \in G$, we also have

$$\sum_{\sigma \in G} \mathbb{1}\{T((X_{\sigma'})_{\sigma}) \geq T(X_{\sigma'})\} = \sum_{\sigma \in G} \mathbb{1}\{T(X_{\sigma}) \geq T(X_{\sigma'})\}.$$  

(4)

This is because

$$\{\sigma \circ \sigma' : \sigma \in G\} = G$$  

for any $\sigma' \in G$,  

(5)

since $G$ is a subgroup. Combining (3) with (4), we obtain

$$\mathbb{P}\{P \leq \alpha\} = \mathbb{P}\left\{ \sum_{\sigma \in G} \mathbb{1}\{T(X_{\sigma}) \geq T(X)\} \leq \alpha \right\}$$

$$= \frac{1}{|G|} \sum_{\sigma' \in G} \mathbb{P}\left\{ \sum_{\sigma \in G} \mathbb{1}\{(X_{\sigma'})_{\sigma} \geq T(X_{\sigma'})\} \leq \alpha \right\}$$

$$= \frac{1}{|G|} \sum_{\sigma' \in G} \mathbb{P}\left\{ \sum_{\sigma \in G} \mathbb{1}\{T(X_{\sigma}) \geq T(X_{\sigma'})\} \leq \alpha \right\}.  \hspace{1cm} (6)$$
Finally, it holds deterministically that

\[
\sum_{\sigma \in G} 1 \left\{ \frac{\sum_{\sigma' \in G} \mathbb{1} \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|G|} \leq \alpha \right\} \leq |\alpha|G|].
\]  

(7)

To see this, let \( T(1) \leq \ldots \leq T(|G|) \) be the order statistics of \( \{ T(X_{\sigma}) : \sigma \in G \} \). Then for any fixed \( \sigma' \in G \), the event \( \sum_{\sigma \in G} \mathbb{1} \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \} \leq \alpha \) holds if and only if \( T(X_{\sigma'}) > T(|(1-\alpha)|G|) \), which by definition of the order statistics can only hold for at most \( |G| - \lceil (1-\alpha)|G| \rceil = \lfloor \alpha|G| \rfloor \) many permutations \( \sigma' \in G \).

Combining (6) with (7), we obtain

\[
P \{ P \leq \alpha \} = \frac{1}{|G|} \sum_{\sigma' \in G} \mathbb{P} \left\{ \frac{\sum_{\sigma \in G} \mathbb{1} \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|G|} \leq \alpha \right\}
\]

\[
= \frac{1}{|G|} \mathbb{E} \left[ \sum_{\sigma' \in G} 1 \left\{ \frac{\sum_{\sigma \in G} \mathbb{1} \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|G|} \leq \alpha \right\} \right] \leq \frac{1}{|G|} \mathbb{E} \left[ \alpha|G| \right] \leq \alpha,
\]

completing the proof.

2.2 Randomly sampling permutations from a subgroup

If working with the full set of permutations to compute the p-value in (1) is computationally infeasible, instead of restricting to a subgroup \( G \subseteq S_n \), we might instead choose to randomly sample from \( S_n \) —indeed, this is by far the most common approach. This practice can also be extended to sampling from a subgroup, as is also well known (see, e.g., Hemerik and Goeman [2018, Theorem 2]):

**Theorem 2.** Let \( G \subseteq S_n \) be a subgroup, and sample \( \sigma_1, \ldots, \sigma_M \overset{iid}{\sim} \text{Unif}(G) \). Then

\[
P = 1 + \sum_{m=1}^{M} \mathbb{1} \{ T(X_{\sigma_m}) \geq T(X) \} \]

\[
1 + M
\]

(8)

is a valid p-value, i.e., \( \mathbb{P}_{H_0} \{ P \leq \alpha \} \leq \alpha \) for all \( \alpha \in [0, 1] \).

If we take \( G = S_n \) to be the full set of possible permutations, then this method reduces to the usual random sampling permutation test.

2.3 Subsets of permutations

In Theorem 1 we saw that it is valid to run a permutation test using a subgroup \( G \subseteq S_n \) of permutations, or a random sample from a subgroup. If we want to use a fixed, rather than random, set of permutations, are we restricted to using a subgroup \( G \), or can an arbitrary subset be used? Consider defining

\[
P = \sum_{\sigma \in S} \mathbb{1} \{ T(X_{\sigma}) \geq T(X) \} \]

\[
|S|
\]

(9)
where $S \subseteq S_n$ is an arbitrary fixed subset.

The subgroup assumption is actually critical—in the proof of Theorem 1, we can see that the step (5) would not hold for a set $S$ that is not a subgroup (this problem remains even if we require the set to contain the identity permutation, $\text{Id} \in S$). The problem is not simply theoretical—it can cause large issues in practice, as has been frequently emphasized. For example, consider the tool of balanced permutations—in the setting of testing whether a randomly assigned treatment has a zero or nonzero effect, this method has been proposed as a variant of the permutation test in this setting, where the subset $S$ consists of all permutations such that the permuted treatment group contains exactly half of the original treatment group, and half of the original control group. Southworth et al. [2009] show that the quantity $P$ computed in (9) for this choice of subset $S$ can be substantially anti-conservative, i.e., $P \{ P \leq \alpha \} > \alpha$, particularly for low significance levels $\alpha$. (See also Hemerik and Goeman [2018] for additional discussion of this issue.)

We now give a simple example to illustrate this point.

**Example 1.** Let $n = 4$, and consider the set

$$S = \{ \text{Id}, \sigma_{1\leftrightarrow 3,2\leftrightarrow 4}, \sigma_{1\leftrightarrow 4,2\leftrightarrow 3} \},$$

where, e.g., $\sigma_{1\leftrightarrow 3,2\leftrightarrow 4}$ is the permutation swapping entries 1 and 3 and also swapping 2 and 4. Let $X_1, X_2, X_3, X_4 \overset{iid}{\sim} \mathcal{N}(0, 1)$ be standard normal random variables, and set $T(X) = X_1 + X_2$. Then the quantity $P$ defined in (9) is equal to

$$P = \frac{1}{3} \{ T(X_{\text{Id}}) \geq T(X) \} + \frac{1}{3} \{ T(X_{\sigma_{1\leftrightarrow 3,2\leftrightarrow 4}}) \geq T(X) \} + \frac{1}{3} \{ T(X_{\sigma_{1\leftrightarrow 4,2\leftrightarrow 3}}) \geq T(X) \}.$$

This gives

$$P = \begin{cases} \frac{1+0+0}{3} = \frac{1}{3}, & \text{if } X_3 + X_4 < X_1 + X_2, \\ \frac{1+1+1}{3} = 1, & \text{otherwise} \end{cases}$$

and, therefore,

$$P = \begin{cases} \frac{1}{3}, & \text{with probability } \frac{1}{2}, \\ 1, & \text{with probability } \frac{1}{2}. \end{cases}$$

We can see that $P$ is anti-conservative at the threshold $\alpha = \frac{1}{3}$.

As we see in the example above, naively applying a permutation test using a subset $S$ of permutations that is not a subgroup, can lead to large problems with the resulting p-value $P$. Hemerik and Goeman [2018] propose a simple correction to the procedure, which restores the validity of the p-value.

**Theorem 3 [Hemerik and Goeman 2018, Section 3.3].** Let $S \subseteq S_n$ be an arbitrary nonempty subset. Let $\sigma_0 \sim \text{Unif}(S)$ be a permutation chosen at random from $S$, and define

$$P = \frac{\sum_{\sigma \in S} \mathbb{1} \{ T(X_{\sigma_0\sigma^{-1}}) \geq T(X) \}}{|S|},$$

(10)

Then $P$ is a valid p-value, i.e., $\mathbb{P}_{H_0} \{ P \leq \alpha \} \leq \alpha$ for all $\alpha \in [0, 1]$. 

5
We remark that, in the special case that \(S = G\) is a subgroup, then adding this modification will not change the procedure—that is, if \(S\) is a subgroup then the p-value from \((10)\) is exactly equal to the quantity \(P\) defined in \((9)\). This is because a subgroup \(G\) is closed under inverses and multiplication, so \(\{\sigma \circ \sigma^{-1} : \sigma \in G\} = G\) for any \(\sigma_0 \in G\). For a subset \(S\) that is not a subgroup, however, these two definitions of \(P\) are not the same.

For completeness, we give a proof of Hemerik and Goeman [2018]'s result.

**Proof.** The proof will follow essentially the same steps as for the subgroup setting studied in Theorem 1. First, for all \(\sigma' \in S\), we have

\[
\mathbb{P}\left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|S|} \leq \alpha \right\} = \mathbb{P}\left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma'\sigma^{-1}}) \geq T(X) \}}{|S|} \leq \alpha \right\}
\]

because \(X \overset{d}{=} X_{\sigma'}\) under \(H_0\) (and note that \((X_{\sigma'})_{\sigma'\sigma^{-1}} = X_{\sigma}\)). Therefore, we have

\[
\mathbb{P}\{ P \leq \alpha \} = \mathbb{P}\left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma'\sigma^{-1}}) \geq T(X) \}}{|S|} \leq \alpha \right\}
\]

\[
= \sum_{\sigma' \in S} \mathbb{P}\left\{ \sigma_0 = \sigma' \text{ and } \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma'\sigma^{-1}}) \geq T(X) \}}{|S|} \leq \alpha \right\}
\]

\[
= \frac{1}{|S|} \sum_{\sigma' \in S} \mathbb{P}\left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma'\sigma^{-1}}) \geq T(X) \}}{|S|} \leq \alpha \right\}
\]

\[
= \frac{1}{|S|} \sum_{\sigma' \in S} \mathbb{P}\left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|S|} \leq \alpha \right\}, \tag{11}
\]

where the next-to-last equality holds since \(\sigma_0\) is drawn uniformly at random from \(S\) (and is independent of the data \(X\)). Finally, it holds deterministically that

\[
\sum_{\sigma' \in S} 1 \left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|S|} \leq \alpha \right\} \leq |\alpha| |S|, \tag{12}
\]

exactly as in \((7)\) for the subgroup case. Combining \((11)\) with \((12)\), we obtain

\[
\mathbb{P}\{ P \leq \alpha \} = \frac{1}{|S|} \sum_{\sigma' \in S} \mathbb{P}\left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|S|} \leq \alpha \right\}
\]

\[
= \frac{1}{|S|} \mathbb{E}\left[ \sum_{\sigma' \in S} 1 \left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|S|} \leq \alpha \right\} \right] \leq \frac{1}{|S|} \mathbb{E}[|\alpha||S|] \leq \alpha,
\]

completing the proof. \(\square\)

We see in the proof that the validity of this p-value does not rely, even implicitly, on any subgroup-based arguments (and indeed, the set \(\{\sigma \circ \sigma^{-1} : \sigma, \sigma^{-1} \in S\}\) of permutations that might appear in \(P\) is in general not a subgroup).

It is particularly important to note that the p-value \(P\) is valid on average over the random draw of \(\sigma_0\), and in general would not be valid if we condition on \(\sigma_0\). For example, by taking the fixed value \(\sigma_0 = \text{Id}\) (the identity permutation), we would return to our previous incorrect p-value calculation in \((9)\), which we know to be invalid from our earlier example.
2.4 Fixing the failure example

To see how Theorem 3 [Hemerik and Goeman, 2018] fixes the failure of Example 1, let $P_\sigma$ denote the p-value calculated conditional on the random $\sigma^*$ being equal to $\sigma$, so that

$$P = \begin{cases} P_{id}, & \text{w.p. } 1/3, \\ P_{\sigma_1 \leftrightarrow 3, \sigma_2 \leftrightarrow 4}, & \text{w.p. } 1/3, \\ P_{\sigma_1 \leftrightarrow 3, \sigma_2 \leftrightarrow 4}, & \text{w.p. } 1/3. \end{cases}$$

Then, the calculation that was previously performed effectively shows that

$$P_{id} = \begin{cases} 1/3, & \text{if } X_3 + X_4 < X_1 + X_2, \\ 1, & \text{otherwise.} \end{cases}$$

A similar straightforward calculation then yields

$$P_{\sigma_1 \leftrightarrow 3, \sigma_2 \leftrightarrow 4} = P_{\sigma_1 \leftrightarrow 3, \sigma_2 \leftrightarrow 4} = \begin{cases} 2/3, & \text{if } X_3 + X_4 < X_1 + X_2, \\ 1, & \text{otherwise.} \end{cases}$$

Put together, we obtain

$$P = \begin{cases} 1/3, & \text{w.p. } 1/6, \\ 2/3, & \text{w.p. } 1/3, \\ 1, & \text{w.p. } 1/2. \end{cases} \quad (13)$$

This is indeed stochastically larger than uniform, as claimed by Theorem 3 [Hemerik and Goeman, 2018].

2.5 Randomly sampling permutations from a subset

If $S$ is large, calculating the p-value $P$ given in (10) may be tedious. Hence we provide the following randomized variant, which is new to our knowledge. (We will see shortly that this theorem is a special case of a more general result, and so we defer the proof for now.)

**Theorem 4.** Let $S \subseteq S_n$ be any fixed subset of permutations. Sample $\sigma_0, \sigma_1, \ldots, \sigma_M \overset{iid}{\sim} \text{Unif}(S)$. Then

$$P = \frac{1 + \sum_{m=1}^{M} 1 \{T(X_{\sigma_m \circ \sigma_0^{-1}}) \geq T(X)\}}{1 + M}$$

is a valid p-value, i.e., $P_{H_0} \{P \leq \alpha\} \leq \alpha$ for all $\alpha \in [0, 1]$.

We can compare this result to Theorem 2 which instead takes random samples from a subgroup $G$—in that theorem, the p-value was defined as $P = \frac{1 + \sum_{m=1}^{M} 1 \{T(X_{\sigma_m}) \geq T(X)\}}{1 + M}$, which initially appears different. However, for $\sigma_0, \sigma_1, \ldots, \sigma_M$ drawn i.i.d. uniformly from $G$, we can observe that $(\sigma_1, \ldots, \sigma_M)$ is equal in distribution to $(\sigma_1 \circ \sigma_0^{-1}, \ldots, \sigma_M \circ \sigma_0^{-1})$, by the assumption that $G$ is a subgroup. Therefore, Theorem 2 can be viewed as a special case of this new result.

As a variant, the same result holds if we instead draw permutations without replacement.
Corollary 1. Let \( S \subseteq S_n \) be any fixed subset of permutations. Sample \( \sigma_0, \sigma_1, \ldots, \sigma_M \) uniformly without replacement from \( S \). Then
\[
P = \frac{1 + \sum_{m=1}^{M} 1 \{ T(X_{\sigma_m \circ \sigma_0^{-1}}) \geq T(X) \}}{1 + M}
\]
is a valid p-value, i.e., \( \mathbb{P}_{H_0} \{ P \leq \alpha \} \leq \alpha \) for all \( \alpha \in [0, 1] \).

Proof. Let \( S' \subseteq S \) be a subset of size \( M + 1 \) chosen uniformly at random. Let \( \sigma_0, \sigma_1, \ldots, \sigma_M \) be a random ordering of \( S' \)—in particular, this means that \( \sigma_0 \) is drawn uniformly from \( S' \). Then by Theorem 3 applied with \( S' \) in place of \( S \), \( P \) is a valid p-value. \( \square \)

If \( S = G \) is a subgroup, then this result provides a version of Theorem 2.

Corollary 2. Let \( G \subseteq S_n \) be any fixed subgroup of permutations. Sample \( \sigma_1, \ldots, \sigma_M \) uniformly without replacement from \( G \). Then
\[
P = \frac{1 + \sum_{m=1}^{M} 1 \{ T(X_{\sigma_m}) \geq T(X) \}}{1 + M}
\]
is a valid p-value, i.e., \( \mathbb{P}_{H_0} \{ P \leq \alpha \} \leq \alpha \) for all \( \alpha \in [0, 1] \).

Proof. Suppose \( \sigma_0, \sigma_1, \ldots, \sigma_M \) are sampled without replacement from \( G \). Then by Corollary 1, \( P \) is a valid p-value. However, since \( G \) is a subgroup, we can observe that \( (\sigma_1 \circ \sigma_0^{-1}, \ldots, \sigma_M \circ \sigma_0^{-1}) \overset{d}{=} (\sigma_1, \ldots, \sigma_M) \), which completes the proof. \( \square \)

3 A generalized permutation test

We now present a generalized version of the permutation test, using an arbitrary distribution \( q \) over \( S_n \) in place of a fixed subgroup or subset. These results will generalize all the existing tests we have seen so far.

3.1 Testing with an arbitrary distribution

Theorem 5. Let \( q \) be any distribution over \( \sigma \in S_n \). Let \( \sigma_0 \sim q \) be a random draw, and define
\[
P = \sum_{\sigma \in S_n} q(\sigma) \cdot 1 \{ T(X_{\sigma \circ \sigma_0^{-1}}) \geq T(X) \}.
\]
Then \( P \) is a valid p-value, i.e., \( \mathbb{P}_{H_0} \{ P \leq \alpha \} \leq \alpha \) for all \( \alpha \in [0, 1] \).

Proof. First, for any fixed \( \sigma' \in S_n \), we have
\[
\mathbb{P} \left\{ \sum_{\sigma \in S_n} q(\sigma) \cdot 1 \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \} \leq \alpha \right\} = \mathbb{P} \left\{ \sum_{\sigma \in S_n} q(\sigma) \cdot 1 \{ T(X_{\sigma \circ \sigma_0^{-1}}) \geq T(X) \} \leq \alpha \right\}
\]
because $X \overset{d}{=} X_{\sigma'}$ under $H_0$ (and note that $(X_{\sigma'})_{\sigma \sigma^{-1}} = X_\sigma$). Next, we will apply a deterministic inequality by Harrison [2012]: for all $t_1, \ldots, t_N \in [-\infty, \infty]$ and all $\alpha, w_1, \ldots, w_N \in [0, \infty]$,
\[
\sum_{k=1}^N w_k \mathbb{1} \left\{ \sum_{i=1}^N w_i \mathbb{1} \{ t_i \geq t_k \} \leq \alpha \right\} \leq \alpha.
\]
Applying this bound with $q(\sigma')$'s in place of the $w_i$'s, and $T(X_\sigma)$'s in place of the $t_i$'s, we obtain
\[
\sum_{\sigma' \in S_n} q(\sigma') \cdot \mathbb{P} \left\{ \sum_{\sigma \in S_n} q(\sigma) \cdot \mathbb{1} \{ T(X_\sigma) \geq T(X_{\sigma'}) \} \leq \alpha \right\} = \mathbb{E} \left[ \sum_{\sigma' \in S_n} q(\sigma') \cdot \mathbb{1} \left\{ \sum_{\sigma \in S_n} q(\sigma) \cdot \mathbb{1} \{ T(X_\sigma) \geq T(X_{\sigma'}) \} \leq \alpha \right\} \right] \leq \alpha. \tag{19}
\]
Finally, we have
\[
\mathbb{P} \{ P \leq \alpha \} = \mathbb{P} \left\{ \sum_{\sigma \in S_n} q(\sigma) \cdot \mathbb{1} \{ T(X_{\sigma \sigma_0^{-1}}) \geq T(X) \} \leq \alpha \right\} = \sum_{\sigma' \in S_n} \mathbb{P} \left\{ \sigma_0 = \sigma' \text{ and } \sum_{\sigma \in S_n} q(\sigma) \cdot \mathbb{1} \{ T(X_{\sigma \sigma_0^{-1}}) \geq T(X) \} \leq \alpha \right\} = \sum_{\sigma' \in S_n} q(\sigma') \cdot \mathbb{P} \left\{ \sum_{\sigma \in S_n} q(\sigma) \cdot \mathbb{1} \{ T(X_\sigma) \geq T(X_{\sigma'}) \} \leq \alpha \right\} \leq \alpha,
\]
where the third step holds since $\sigma_0 \sim q$ is drawn independently of the data $X$, while the last two steps apply (18) and (19).

To see how several of the previous results are special cases of this more general formulation, we can recover the subset based test in Theorem 3 [Hemerik and Goeman, 2018, Section 3.3] by taking $q$ to be the distribution on $S_n$ given by
\[
q(\sigma) = \frac{\mathbb{1}_{\sigma \in S}}{|S|}.
\]
Of course, the subgroup test given in Theorem 4 is simply a special case by taking $S = G$.

### 3.2 Random samples from an arbitrary distribution

Next, if we instead choose to randomly sample permutations from a subgroup $G$ (as in Theorem 2) or from a subset $S$ (as in Theorem 3), these two tests can be viewed as a special case of the following general result.
Theorem 6. Let \( q \) be any distribution over \( \sigma \in S_n \). Let \( \sigma_0, \sigma_1, \ldots, \sigma_M \overset{\text{iid}}{\sim} q \), and define
\[
P = \frac{1 + \sum_{m=1}^{M} 1 \left\{ T(X_{\sigma_m \circ \sigma_0^{-1}}) \geq T(X) \right\}}{1 + M}.
\]
Then \( P \) is a valid p-value, i.e., \( \mathbb{P}_{H_0} \{ P \leq \alpha \} \leq \alpha \) for all \( \alpha \in [0, 1] \).

Proof. This result follows from Besag and Clifford [1989]'s well known construction for obtaining exchangeable samples from Markov chain Monte Carlo (MCMC) sampling—the details are deferred to Section 4.2 below. \( \square \)

3.3 Connecting Theorems 5 and 6

Interestingly, Theorems 5 and 6 can be derived from each other. We now show an alternative proof for each result, to show the connection. With these proofs in place, Figure 1 summarizes the connections between all the results presented thus far in the paper.

Alternative proof of Theorem 5 (via Theorem 6). Let \( \sigma_0, \sigma_1, \ldots, \sigma_M \overset{\text{iid}}{\sim} q \), and for any fixed \( M \), define
\[
P_M = \frac{1 + \sum_{m=0}^{M} 1 \left\{ T(X_{\sigma_m \circ \sigma_0^{-1}}) \geq T(X) \right\}}{1 + M} = \frac{\sum_{m=0}^{M} 1 \left\{ T(X_{\sigma_m \circ \sigma_0^{-1}}) \geq T(X) \right\}}{1 + M}.
\]
By the Law of Large Numbers, we see that \( \frac{\sum_{m=0}^{M} 1 \left\{ \sigma_m = \sigma \right\}}{1 + M} \rightarrow q(\sigma) \) almost surely for all \( \sigma \in S_n \), and therefore, \( P_M \rightarrow P \) almost surely, where \( P \) is the p-value defined in (17). In particular, this implies that \( P_M \) converges to \( P \) in distribution, and therefore
\[
\mathbb{P} \{ P \leq \alpha \} = \lim_{M \rightarrow \infty} \mathbb{P} \{ P_M \leq \alpha \} \leq \alpha,
\]
where the last step holds since, for every \( M \geq 1 \), \( P_M \) is a valid p-value by Theorem 6. \( \square \)

Alternative proof of Theorem 6 (via Theorem 5). Let \( \sigma_0, \sigma_1, \ldots, \sigma_M \overset{\text{iid}}{\sim} q \), and define the empirical distribution
\[
\hat{q} = \frac{1}{M + 1} \sum_{m=0}^{M} \delta_{\sigma_m}
\]
where \( \delta_\sigma \) is the point mass at \( \sigma \). Now we treat \( \hat{q} \) as fixed. Let \( k \) be drawn uniformly from \( \{0, \ldots, M\} \) (that is, \( \sigma_k \) is drawn at random from \( \hat{q} \)). Applying Theorem 5 with \( \hat{q} \) in place of \( q \), we then see that
\[
P = \sum_{\sigma \in S_n} \hat{q}(\sigma) \cdot 1 \left\{ T(X_{\sigma \circ \sigma_k^{-1}}) \geq T(X) \right\} = \frac{\sum_{m=0}^{M} 1 \left\{ T(X_{\sigma_m \circ \sigma_k^{-1}}) \geq T(X) \right\}}{1 + M}.
\]
Figure 1: A flowchart to illustrate the connections between (most of) the results presented in this paper. Arrows point from more general results to their special cases.

is a valid p-value conditional on $\hat{\theta}$, and therefore also valid after marginalizing over $\hat{\theta}$. Since $\sigma_0, \ldots, \sigma_M$ are drawn i.i.d. and are therefore in a random order, we see that

$$P = \frac{\sum_{m=0}^{M} \mathbbm{1}\{T(X_{\sigma_m \sigma_0^{-1}}) \geq T(X)\}}{1 + M} \overset{d}{=} \frac{\sum_{m=0}^{M} \mathbbm{1}\{T(X_{\sigma_m \sigma_0^{-1}}) \geq T(X)\}}{1 + M}$$

$$= \frac{1 + \sum_{m=1}^{M} \mathbbm{1}\{T(X_{\sigma_m \sigma_0^{-1}}) \geq T(X)\}}{1 + M},$$

which is the desired p-value.

3.4 Another perspective: exchangeable permutations

Many of the results described above can be viewed through the lens of exchangeability—not on the data $X$ (which we assume to be exchangeable under the null hypothesis $H_0$), but on the collection of permutations used to define the p-value $P$.

**Theorem 7.** Let $\sigma_0, \sigma_1, \ldots, \sigma_M \in S_n$ be a random set of permutations, which are exchangeable, i.e.,

$$(\sigma_0, \sigma_1, \ldots, \sigma_M) \overset{d}{=} (\sigma_{\pi(0)}, \sigma_{\pi(1)}, \ldots, \sigma_{\pi(M)})$$

for any fixed permutation $\pi$ on $\{0, \ldots, M\}$. Then

$$P = \frac{\sum_{m=0}^{M} \mathbbm{1}\{T(X_{\sigma_m \sigma_0^{-1}}) \geq T(X)\}}{1 + M}$$

is a valid p-value, i.e., $\mathbb{P}_{H_0}\{P \leq \alpha\} \leq \alpha$ for all $\alpha \in [0, 1]$.

Many of the results stated earlier can be viewed as special cases—in particular, the results for a subgroup $G$ (Theorems 1 and 2 and Corollary 2), or for a subset $S$ (Theorems 3 and 4).
and Corollary 1, as well as our more general result Theorem 6 for permutations drawn i.i.d. from $q$.

This theorem is essentially just a new perspective on our previous results, and can be proved as a corollary to Theorem 5:

**Proof.** This result follows immediately from Theorem 5. To see why, let $\sigma_0, \ldots, \sigma_M$ be exchangeable, and let $\hat{q} = \frac{1}{M+1} \sum_{m=0}^{M} \delta_{\sigma_m}$ be the empirical distribution induced by the unordered set of permutations drawn. Then since $\sigma_0, \ldots, \sigma_M$ is exchangeable, conditional on $\hat{q}$ it holds that $\sigma_0$ is a random draw from $\hat{q}$. Then applying Theorem 5 with $\hat{q}$ in place of $q$ yields the desired result.

However, we can also prove this result in a more intuitive way, using the framework of exchangeability:

**Alternative proof of Theorem 7.** Since $\sigma_0, \sigma_1, \ldots, \sigma_M$ exchangeable, this means that the sequence

$$T(X_{\sigma_0}), T(X_{\sigma_1}), \ldots, T(X_{\sigma_M})$$

is exchangeable conditional on $X$, and therefore is still exchangeable after marginalizing over $X$. Therefore, under the null hypothesis $H_0$, the test statistic values

$$T(X_{\sigma_0 \circ \sigma_0^{-1}}), T(X_{\sigma_1 \circ \sigma_0^{-1}}), \ldots, T(X_{\sigma_M \circ \sigma_0^{-1}})$$

are also exchangeable—this follows immediately from the previous line because $X \overset{d}{=} X_{\sigma_0}$ under $H_0$. This immediately implies that the p-value $P$ defined in (23) is valid.

### 3.5 Averaging to reduce variance

The p-value $P$ defined in (17) can equivalently be written as

$$P = \mathbb{P}_{\sigma \sim q} \left\{ T(X_{\sigma_0^{-1}}) \geq T(X) \mid X, \sigma_0 \right\}.$$  

With this new notation, it is clear to see that $P$ is random even if we condition on the observed data $X$, because it has additional randomness due to $\sigma_0$. As a result, in some settings we may have high variability of $P$ even conditional on the data $X$, which may be an undesirable property.

To address this, we can also consider averaging over $\sigma_0$ (in addition to averaging over $\sigma$) in the calculation of $P$. This alternative definition is now a deterministic function of the observed data $X$, but may no longer be a valid p-value. Nonetheless, the following theorem shows a bound on the Type I error.

**Theorem 8.** Let $q$ be any distribution over $\sigma \in S_n$. Define

$$P = \sum_{\sigma, \sigma_0 \in S_n} q(\sigma) q(\sigma_0) \cdot 1 \left\{ T(X_{\sigma_0^{-1}}) \geq T(X) \right\},$$

or equivalently,

$$P = \mathbb{P}_{\sigma, \sigma_0 \sim q} \left\{ T(X_{\sigma \circ \sigma_0^{-1}}) \geq T(X) \mid X \right\}.$$  

Then $P$ is a valid p-value up to a factor of 2, i.e., $\mathbb{P}_{H_0} \left\{ P \leq \alpha \right\} \leq 2\alpha$ for all $\alpha \in [0, 1]$.  

Proof. Draw \( \sigma_0^{(1)}, \sigma_0^{(2)}, \ldots \text{ i.i.d. } \sim q \). Let
\[
P_m = \sum_{\sigma \in S_n} q(\sigma) \cdot 1 \left\{ T(X_{\sigma m}) \geq T(X) \right\},
\]
for each \( m \geq 1 \). Then by Theorem 5, each \( P_m \) is a valid p-value. It is known [Rüschendorf, 1982, Vovk and Wang, 2020] that the average of valid p-values is a valid up to a factor of 2, i.e., for any \( M \geq 1 \) the average \( \overline{P}_M = \frac{1}{M} \sum_{m=1}^M P_m \) satisfies \( \mathbb{P} \{ \overline{P}_M \leq \alpha \} \leq 2\alpha \) for all \( \alpha \in [0, 1] \). We can equivalently write
\[
\overline{P}_M = \sum_{\sigma' \in S_n} \frac{\sum_{m=1}^M 1 \left\{ \sigma_0^{(m)} = \sigma' \right\}}{M} \cdot \sum_{\sigma \in S_n} q(\sigma) \cdot 1 \left\{ T(X_{\sigma \sigma'^{-1}}) \geq T(X) \right\}.
\]
By the Law of Large Numbers, \( \overline{P}_M \) converges almost surely to the p-value \( \overline{P} \) defined in (22), which completes the proof.

Returning to Section 2.4 where we fixed Example 1, we see that while \( P \) was a mixture of \( P_{id}, P_{\sigma_1 \leftrightarrow 4, 2 \leftrightarrow 3}, P_{\sigma_1 \leftrightarrow 3, 2 \leftrightarrow 4} \), we now have that \( \overline{P} \) is an average of these, meaning \( \overline{P} = \frac{1}{3} (P_{id} + P_{\sigma_1 \leftrightarrow 4, 2 \leftrightarrow 3} + P_{\sigma_1 \leftrightarrow 3, 2 \leftrightarrow 4}) \). Simplifying, we get
\[
\overline{P} = \begin{cases} 
\frac{5}{9}, & \text{w.p. } 1/2, \\
1, & \text{w.p. } 1/2.
\end{cases}
\]
It is worth noting that this new quantity \( \overline{P} \) is neither more conservative nor more anti-conservative than the p-value \( P \) from earlier. This is perhaps a more general phenomenon: the average of p-values need not in general be anti-conservative, and indeed it could often be more conservative, than the original p-values.

Analogously, the p-value in Theorem 6, computed via random samples from \( q \), can also be averaged to reduce variance.

Theorem 9. Let \( q \) be any distribution over \( \sigma \in S_n \). Let \( \sigma_0, \sigma_1, \ldots, \sigma_M \text{ i.i.d. } \sim q \), and define
\[
\overline{P} = \frac{\sum_{m=0}^M \sum_{m'=0}^M 1 \left\{ T(X_{\sigma m \sigma^{-1} m'}) \geq T(X) \right\}}{(1 + M)^2}.
\]
Then \( \overline{P} \) is a valid p-value up to a factor of 2, i.e., \( \mathbb{P}_{H_0} \{ \overline{P} \leq \alpha \} \leq 2\alpha \) for all \( \alpha \in [0, 1] \).

The proof is similar to that of Theorem 8 and so we omit it for brevity.

4 Connections to the literature

We next mention a few connections to the broader literature.
4.1 Permutation tests vs randomization tests

Hemerik and Goeman [2021] describe the difference between two testing frameworks, permutation tests (as studied in our present work) versus randomization tests. The difference is subtle, because randomization tests may still use permutations. Specifically, Hemerik and Goeman [2021] explain that an important difference in mathematical reasoning between these classes: a permutation test fundamentally requires that the set of permutations has a group structure, in the algebraic sense; the reasoning behind a randomization test is not based on such a group structure, and it is possible to use an experimental design that does not correspond to a group.

To better understand this distinction, we can consider a scenario where a fixed subset $S \subseteq S_n$, which is not a subgroup, is used for a randomization test rather than a permutation test. Consider a study comparing a treatment versus a placebo, with $n/2$ many subjects assigned to each of the two groups. We can use a permutation $\sigma$ to denote the treatment assignments, with $\sigma(i) \leq n/2$ indicating that subject $i$ receives the treatment, and $\sigma(i) > n/2$ indicating that subject $i$ receives the placebo. Now we switch notation, to be able to compare to permutation tests more directly—writing $X = (1, \ldots, 1, 0, \ldots, 0)$, suppose that we will assign treatments via the permuted vector $X_\sigma$, i.e., for each subject $i = 1, \ldots, n$, under this permutation $\sigma$ the $i$th subject will receive the treatment if $X_\sigma(i) = 1$, or the placebo if $X_\sigma(i) = 0$.

Now suppose that we draw a random treatment assignment $\sigma_{\text{asgn}} \sim \text{Unif}(S)$, from a fixed subset $S \subseteq S_n$ (for example, $S$ may be chosen to restrict to treatment assignments that are equally balanced across certain subpopulations). After the treatments are administered, the measured response variable is given by $Y = (Y_1, \ldots, Y_n)$. Fix any test statistic $T(X) = T(X,Y)$ (we will implicitly condition on $Y$), and compute

$$P = \frac{\sum_{\sigma \in S} 1\{T(X_\sigma) \geq T(X_{\sigma_{\text{asgn}}})\}}{|S|}. \quad (24)$$

Since $\sigma_{\text{asgn}}$ was drawn uniformly from $S$, this quantity $P$ is a valid p-value. In the terminology of Hemerik and Goeman [2021], this test is a randomization test, not a permutation test. While the set of possible treatment assignments $\{X_\sigma : \sigma \in S\}$ happens to be indexed by permutations $\sigma$, the group structure of permutations is not used in any way, and we do not rely on any invariance properties.

Comparing to the invalid p-value $P = \frac{\sum_{\sigma \in S} 1\{T(X_\sigma) \geq T(X)\}}{|S|}$ considered in (9), we can easily see the distinction: for a randomization test, the observed statistic is $T(X_{\sigma_{\text{asgn}}})$ for a randomly drawn $\sigma_{\text{asgn}} \sim \text{Unif}(S)$, while in the permutation test in (9), the observed statistic is $T(X)$ (i.e., using the fixed permutation Id in place of a randomly drawn $\sigma_{\text{asgn}}$). For this reason, the randomization test p-value in (24) is valid, while the permutation test calculation in (9) is not valid in general.

Now we again consider Hemerik and Goeman [2018]’s method using a fixed subset, given in (10). This test is a permutation test, not a randomization test—the observed data $X$, and its corresponding statistic $T(X)$, do not arise from a random treatment assignment.
More generally, our proposed test (17) using an arbitrary distribution \( q \) on \( S_n \) is again a permutation test rather than a randomization test—that is, the observed data is given by \( X \) itself, not by a randomly chosen treatment assignment \( X_{\sigma_{\text{asgn}}} \) for \( \sigma_{\text{asgn}} \sim q \). Nonetheless, we are able to produce a valid p-value without assuming an underlying group structure on the permutations considered by the test.

### 4.2 Exchangeable MCMC

The result of Theorem 6, which allows for random samples drawn from an arbitrary distribution \( q \) on \( S_n \), is in fact a special case of Besag and Clifford \[1989\]'s well known construction for obtaining exchangeable samples from Markov chain Monte Carlo (MCMC) sampling.

Consider a distribution \( Q_0 \) on \( Z \), and suppose we want to test \( H_0 : Z \sim Q_0 \) with some test statistic \( T(Z) \). To find a significance threshold for \( T(Z) \), we would ideally like to draw from the null distribution, i.e., compare \( T(Z) \) against \( T(Z_1), \ldots, T(Z_M) \) for \( Z_m \overset{iid}{\sim} Q_0 \). However, in many settings, sampling directly from \( Q_0 \) is impossible, but we instead have access to a Markov chain whose stationary distribution is \( Q_0 \). If we run the Markov chain initialized at \( Z \) to obtain draws \( Z_1, \ldots, Z_M \) (say, running the Markov chain for some fixed number of steps \( s \) between each draw), then dependence among these sequentially drawn samples means that \( Z, Z_1, \ldots, Z_M \) are not i.i.d., and are not even exchangeable. Therefore, without studying the mixing properties of the Markov chain, we cannot determine how large the number of steps needs to be for the dependence to become negligible. Instead, Besag and Clifford \[1989\] propose a construction where the samples are drawn in parallel (rather than sequentially), which ensures exchangeability:

**Theorem 10** (Besag and Clifford \[1989\], Section 2). Let \( Q_0 \) be any distribution on a probability space \( Z \). Construct a Markov chain on \( Z \) with stationary distribution \( Q_0 \), whose forward and backward transition distributions (initialized at \( z \in Z \)) are denoted by \( Q_{\rightarrow}(\cdot | z) \) and \( Q_{\leftarrow}(\cdot | z) \). Let \( Q_{\rightarrow}^{s}(\cdot | z) \) and \( Q_{\leftarrow}^{s}(\cdot | z) \) denote the forward and backward transition distributions after running \( s \) steps of the Markov chain, for some fixed \( s \geq 1 \). Given an initialization \( Z \), suppose we generate data as follows:

\[
\begin{align*}
\text{Conditional on } Z, & \text{ draw } Z_\ast \sim Q_{\leftarrow}^{s}(\cdot | Z); \\
\text{Conditional on } Z, Z_\ast, & \text{ draw } Z_1, \ldots, Z_M \overset{iid}{\sim} Q_{\rightarrow}^{s}(\cdot | Z_\ast).
\end{align*}
\]

If it holds marginally that \( Z \sim Q_0 \), then the draws \( Z, Z_1, \ldots, Z_M \) are exchangeable.

Given this exchangeability property, the quantity \( P = \frac{1 + \sum_{m=1}^{M} \mathbb{1}_{T(Z_1) \geq T(Z)}}{1 + M} \) is then a valid p-value for testing \( H_0 : Z \sim Q_0 \); and this holds regardless of whether \( Q_0 \) is the unique stationary distribution for the Markov chain. The procedure is illustrated on the left-hand side of Figure 2.

Now we will see how Theorem 6 is related to this result. Let \( Z = X^n \), and let \( Q_0 \) be any exchangeable distribution. In the setting of this paper, we do not know \( Q_0 \) precisely, which makes it a bit different from a typical setting where Besag and Clifford \[1989\]'s method is
applied. However, we will work with a Markov chain for which any exchangeable distribution $Q_0$ is stationary, and thus can still apply their method.

Consider the Markov chain given by applying a randomly chosen permutation $\sigma \sim q$, that is, for $x = (x_1, \ldots, x_n)$,

$$Q \rightarrow (\cdot | x) = \sum_{\sigma \in S} q(\sigma) \cdot \delta_{x_{\sigma}},$$

where $\delta_{x_{\sigma}}$ is the point mass at $x_{\sigma}$, while the backward transition probabilities are given by

$$Q \leftarrow (\cdot | x) = \sum_{\sigma \in S} q(\sigma) \cdot \delta_{x_{\sigma^{-1}}}. $$

Then, to implement the test described in Theorem 6, we run Besag and Clifford's [1989] method (with $s = 1$): we define $X^* = X_{\sigma_0^{-1}}$, and then define $X_m = (X^*_m)_{\sigma_m} = X_{\sigma_m \circ \sigma_0}$ for $m = 1, \ldots, M$. This is illustrated on the right-hand side of Figure 2. If $X$ is exchangeable (that is, it is drawn from some exchangeable $Q_0$), then the exchangeability of $X, X_1, \ldots, X_M$ follows, and this verifies that $P$ is a valid p-value, thus completing the proof of Theorem 6.

Of course, we have only written out our method for the $s = 1$ case (where $s$ is the number of steps of the Markov chain). New variants of our method can be constructed by taking $s > 1$ backward steps to the hidden node, and the same number of forward steps to the permuted data. All of these are valid for the same reason as the $s = 1$ case.

### 4.3 E-values vs p-values

In multiple testing, where permutation p-values are frequently employed, handling arbitrary dependence between the p-values can require conservative corrections, for example, for the Benjamini-Hochberg (BH) procedure. In such settings, it may be useful to construct permutation e-values instead, since the corresponding e-BH procedure [Wang and Ramdas, 2022a] requires no additional corrections for dependence. Following [Wang and Ramdas, 2022b], we present an e-value that one can construct in the context of this paper.
Theorem 11. Let $\sigma_0, \sigma_1, \ldots, \sigma_M \in S_n$ be a set of exchangeable permutations as in Theorem 7. Define
\[ E = \frac{M + 1}{\sum_{m=0}^{M} \exp(T(X_{\sigma_m \circ \sigma_0}) - T(X))}. \] (25)

Then $E$ is a valid e-value, i.e., $E$ is nonnegative and $\mathbb{E}_{H_0}[E] \leq 1$.

As mentioned after Theorem 7, the above theorem captures many settings of sampling with or without replacement from non-uniform distributions over subgroups $G$ or subsets $S$ of all permutations. The proof follows Wang and Ramdas [2022] and is an easy consequence of exchangeability of (21) under the null. In particular, the aforementioned exchangeability even holds conditional on $\sum_{m=0}^{M} \exp(T(X_{\sigma_m \circ \sigma_0}))$. Thus,
\[ \mathbb{E}_{H_0} \left[ \exp(T(X)) \left| \sum_{m=0}^{M} \exp(T(X_{\sigma_m \circ \sigma_0})) \right. \right] = \frac{\sum_{m=0}^{M} \exp(T(X_{\sigma_m \circ \sigma_0}))}{M + 1}. \]

Rearranging, and then marginalizing over $\sum_{m=0}^{M} \exp(T(X_{\sigma_m \circ \sigma_0}))$, yields the result. We note that there is no particular utility of $E$ for a single hypothesis test, since it may be verified that $1/E$ is a p-value, but $P \leq 1/E$ for the p-value $P$ from (7).

5 Conclusion

We proposed a new method for permutation testing that generalizes previous methods. This idea naturally opens up new lines of theoretical and practical enquiry. In this work, we have focused on validity, but it is of course also important to examine the consistency and power of such methods—in particular, understanding the power of using only a subset $S \subseteq S_n$ or a nonuniform distribution over $S_n$, as compared to using the full permutation group $S_n$ as studied by Dobriban [2021], Kim et al. [2021, 2022]. In addition, the theoretical guarantees for all the permutation tests considered here ensure a p-value $P$ that is valid in the sense of satisfying $\mathbb{P}_{H_0} \{ P \leq \alpha \} \leq \alpha$, which means that $P$ could potentially be quite conservative under the null (for instance, we see this behavior in the example described in Section 2.4). It would also be interesting to understand which types of tests reduce overly conservative outcomes.

In conclusion, it is perhaps remarkable that one can still gain new understanding about classical permutation methods. In turn, this enhanced understanding can inform other areas of inference. As an example, the results from this paper were motivated by questions in conformal prediction [Vovk et al., 2005], a method for distribution-free predictive inference. Classically, conformal prediction has relied on exchangeability of data points (e.g., training and test data are drawn i.i.d. from the same unknown distribution), and thus the joint distribution of the data (including both training samples and a test point) is invariant under an arbitrary permutation. In contrast, in our recent work [Barber et al., 2022], we studied the problem of constructing prediction intervals when the data do not satisfy exchangeability; for instance, the distribution of observations may simply drift over time in an unknown fashion. Thus the data is no longer invariant under an arbitrary permutation, and so we instead restrict attention to a weighted distribution over simple permutations that only
swap the test point with a random training point, which at least approximately preserve the distribution of the data. These swaps clearly do not form a subgroup of permutations, and are weighted non-uniformly; understanding how permutation tests operate in this setting, as in Theorem 5 is key to the findings in our aforementioned work.

Acknowledgments

The authors thank Nick Koning and Ilmun Kim for helpful feedback on an early preprint. The authors also thank the SQUARE program run by the American Institute of Mathematics, where our collaboration started. R.F.B. was supported by the National Science Foundation via grants DMS-1654076 and DMS-2023109, and by the Office of Naval Research via grant N00014-20-1-2337. E.J.C. was supported by the Office of Naval Research grant N00014-20-1-2157, the National Science Foundation grant DMS-2032014, the Simons Foundation under award 814641, and the ARO grant 2003514594. R.J.T. was supported by ONR grant N00014-20-1-2787.

References

Rina Foygel Barber, Emmanuel J Candès, Aaditya Ramdas, and Ryan J Tibshirani. Conformal prediction beyond exchangeability. arXiv preprint arXiv:2202.13415, 2022.

Julian Besag and Peter Clifford. Generalized Monte Carlo significance tests. Biometrika, 76(4):633–642, 1989.

Edgar Dobriban. Consistency of invariance-based randomization tests. arXiv preprint arXiv:2104.12260, 2021.

Matthew T Harrison. Conservative hypothesis tests and confidence intervals using importance sampling. Biometrika, 99(1):57–69, 2012.

Jesse Hemerik and Jelle Goeman. Exact testing with random permutations. Test, 27(4):811–825, 2018.

Jesse Hemerik and Jelle J Goeman. Another look at the lady tasting tea and differences between permutation tests and randomisation tests. International Statistical Review, 89(2):367–381, 2021.

Ilmun Kim, Aaditya Ramdas, Aarti Singh, and Larry Wasserman. Classification accuracy as a proxy for two-sample testing. The Annals of Statistics, 49(1):411–434, 2021.

Ilmun Kim, Sivaraman Balakrishnan, and Larry Wasserman. Minimax optimality of permutation tests. The Annals of Statistics, 50(1):225–251, 2022.

Nick W Koning and Jesse Hemerik. Faster exact permutation testing: Using a representative subgroup. arXiv preprint arXiv:2202.00967, 2022.

Erich Leo Lehmann, Joseph P Romano, and George Casella. Testing statistical hypotheses, volume 3. Springer, 2005.
Ludger Rüschendorf. Random variables with maximum sums. *Advances in Applied Probability*, 14(3):623–632, 1982.

Lucinda K Southworth, Stuart K Kim, and Art B Owen. Properties of balanced permutations. *Journal of Computational Biology*, 16(4):625–638, 2009.

Vladimir Vovk and Ruodu Wang. Combining p-values via averaging. *Biometrika*, 107(4):791–808, 2020.

Vladimir Vovk, Alex Gammerman, and Glenn Shafer. *Algorithmic learning in a random world*. Springer Science & Business Media, 2005.

Ruodu Wang and Aaditya Ramdas. False discovery rate control with e-values. *Journal of the Royal Statistical Society, Series B*, 2022a.

Ruodu Wang and Aaditya Ramdas. E-values as unnormalized weights in multiple testing. *arXiv preprint arXiv:2204.12447*, 2022b.