Permutation tests without subgroups

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

April 29, 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 of permutations. In this work, we extend beyond these possibilities to show how such tests can be run using any fixed subset of permutations.

1 Introduction

Suppose we observe data $X_1, \ldots, X_n \in \mathcal{X}$, and would like to test the null hypothesis $H_0: X_1, \ldots, X_n$ 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 $T(X_1, \ldots, X_n)$. 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

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

(1)

∗Department of Statistics, University of Chicago
†Departments of Statistics and Mathematics, Stanford University
‡Departments of Statistics and Machine Learning, Carnegie Mellon University
where for any \( x \in X^n \) and any \( \sigma \in S_n, x_{\sigma} := (x_{\sigma(1)}, \ldots, x_{\sigma(n)}) \).

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

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

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

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

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).

### 1.1 Background: permutation tests with subgroups

The p-value \( P \) computed in (1) requires computing \( T(X_{\sigma(1)}, \ldots, X_{\sigma(n)}) \) for every \( \sigma \in S_n \), which may be computationally prohibitive if \( n \) is large. 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 \( \alpha \in [0, 1] \).

This 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 \( \mathbb{P} \{ \cdot \} \). We begin by noting three facts. First, for all \( \sigma' \in G \), we have

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

(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
\[
\{ \sigma \circ \sigma' : \sigma \in G \} = G \text{ for any } \sigma' \in G,
\]
(5)

since $G$ is a subgroup. Finally, it holds deterministically that
\[
\sum_{\sigma' \in G} \mathbb{1} \left\{ \frac{\sum_{\sigma \in G} \mathbb{1} \{ T(x_{\sigma}) \geq T(x_{\sigma'}) \}}{|G|} \leq \alpha \right\} \leq |\alpha|G|.
\]
(6)

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

Putting these three facts together gives
\[
\mathbb{P} \{ P \leq \alpha \} = \mathbb{P} \left\{ \sum_{\sigma \in G} \mathbb{1} \left\{ \frac{T(X_{\sigma}) \geq T(X)}{|G|} \leq \alpha \right\} \right\}
\]
by \ref{eq:4}
\[
= \frac{1}{|G|} \sum_{\sigma' \in G} \mathbb{P} \left\{ \sum_{\sigma \in G} \mathbb{1} \left\{ \frac{T((X_{\sigma'})_{\sigma}) \geq T(X_{\sigma'})}{|G|} \leq \alpha \right\} \right\}
\]
by \ref{eq:4}
\[
= \frac{1}{|G|} \mathbb{E} \left[ \sum_{\sigma' \in G} \mathbb{1} \left\{ \sum_{\sigma \in G} \mathbb{1} \left\{ \frac{T(X_{\sigma}) \geq T(X_{\sigma'})}{|G|} \leq \alpha \right\} \right\} \right]
\]
by \ref{eq:4}
\[
\leq \frac{1}{|G|} \mathbb{E} \left[ \lfloor |\alpha|G| \rfloor \right] = \frac{|\alpha|G|}{|G|} \leq \alpha,
\]

completing the proof.

\[ \square \]

1.2 Background: randomly sampling permutations

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 permutations from $S_n$—indeed, this is by far the most common approach. This practice can also be extended to sampling from a subgroup:

**Theorem 2.** Let $G \subseteq S_n$ be a subgroup, and sample $\sigma_1, \ldots, \sigma_M \overset{\text{iid}}{\sim} \text{Unif}(G)$. Then
\[
P = \frac{1 + \sum_{m=1}^{M} \mathbb{1} \{ T(X_{\sigma_m}) \geq T(X) \}}{1 + M}
\]
is a valid p-value, i.e., $\mathbb{P}_{H_0} \{ P \leq \alpha \} \leq \alpha$ for all $\alpha \in [0, 1]$.
This result is also well known; see Hemerik and Goeman [2018, Theorem 2] for a recent treatment. If we take $G = \mathcal{S}_n$ to be the full set of possible permutations, then this method reduces to the usual random sampling permutation test.

### 1.3 Our contribution

We make a simple change to the aforementioned permutation tests that completely avoids the use of subgroups, and works for arbitrary sets of permutations. Our modification is simple to implement, and requires only elementary arguments to prove correctness; however, to the best of our knowledge, our method has not been explicitly proposed before, and indeed, recent papers and textbooks dealing with this topic routinely emphasize the necessity of subgroups for permutation testing.

### 2 Beyond subgroups

In the previous section, we saw that it is valid to run a permutation test using a subgroup $G \subseteq \mathcal{S}_n$ of permutations (or alternatively, we may use a random sample of permutations from either $\mathcal{S}_n$ or from a subgroup $G$, with the +1 correction in the calculation of the p-value). 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

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

where $S \subseteq \mathcal{S}_n$ 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 (8) for this choice of subset $S$ can be substantially anti-conservative, i.e., $\mathbb{P}\{P < \alpha\} > \alpha$, particularly for low significance levels $\alpha$. (See also Hemerik and Goeman [2018] for additional discussion of this issue.)

We now give a simple example (which we revisit later) to illustrate this point.

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

$$S = \{\text{Id}, \sigma_{1\leftrightarrow3,2\leftrightarrow4}, \sigma_{1\leftrightarrow4,2\leftrightarrow3}\},$$

(9)
where, e.g., $\sigma_{1\leftrightarrow3,2\leftrightarrow4}$ 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 (8) is equal to

$$P = \frac{1}{3} \{ T(X_\text{id}) \geq T(X) \} + \frac{1}{3} \{ T(X_{\sigma_{1\leftrightarrow3,2\leftrightarrow4}}) \geq T(X) \} + \frac{1}{3} \{ T(X_{\sigma_{1\leftrightarrow4,2\leftrightarrow3}}) \geq T(X) \}.$$

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 $\alpha = \frac{1}{3}$.

### 2.1 Main result: using an extra random permutation

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 $P$. Here we present a simple correction to the procedure, which restores the validity of the p-value.

**Theorem 3.** Let $S \subseteq S_n$ be an arbitrary nonempty subset. Let $\sigma_* \sim \text{Unif}(S)$ be a permutation chosen at random from $S$, and define

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

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

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 (8). This is because a subgroup $G$ is closed under inverses and multiplication, so $\{ \sigma \circ \sigma_*^{-1} : \sigma \in G \} = G$ for any $\sigma_* \in G$.

For a subset $S$ that is not a subgroup, however, these two definitions of $P$ are not the same. We will 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).

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

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

5
because $X \overset{d}{=} X_{\sigma'}$ under $H_0$ (and note that $(X_{\sigma'})_{\sigma'\sigma^{-1}} = X_{\sigma}$). Next, we have

$$
\frac{1}{|S|} \sum_{\sigma' \in S} \mathbb{P}\left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|S|} \leq \alpha \right\}
= \mathbb{E}\left[ \sum_{\sigma' \in S} \frac{1}{|S|} \mathbb{P}\left\{ \frac{\sum_{\sigma \in S} 1 \{ T(X_{\sigma}) \geq T(X_{\sigma'}) \}}{|S|} \leq \alpha \right\} \right] \leq \frac{|\alpha| |S|}{|S|} \leq \alpha, \quad (12)
$$

where the inequality holds exactly as for the bound (6). Finally, we have

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

where the last equality holds since $\sigma_*$ is drawn uniformly at random from $S$ (and is independent of the data $X$), while the final step holds by combining (11) and (12).

It is particularly important to note that the p-value $P$ is valid on average over the random draw of $\sigma_*$, and in general would not be valid if we condition on $\sigma_*$. Indeed, our theorem can be viewed as stemming from the following key property:

When $\sigma_*$ is chosen uniformly at random from $S$, the test statistics $\{ T(X_{\sigma'\sigma^{-1}}) \}_{\sigma \in S}$ form an exchangeable set, and $T(X)$ is an unknown element within this set.

Figure 1 illustrates this intuition. This property holds only on average over $\sigma_* \sim \text{Unif}(S)$, and would no longer be true if $\sigma_*$ is fixed. In particular, by taking the fixed value $\sigma_* = \text{Id}$ (the identity permutation), we would return to our previous incorrect p-value calculation in (8), which we know to be invalid from our earlier example.

### 2.2 Fixing the failure example

To see how our Theorem 3 fixes the failure in the earlier example, let $P_{\sigma}$ denote the p-value calculated conditional on the random $\sigma^*$ being equal to $\sigma$, so that

$$
P = \begin{cases} 
P_{\text{Id}}, & \text{w.p. } 1/3, \\
P_{\sigma_{1\leftrightarrow4,2\leftrightarrow3}}, & \text{w.p. } 1/3, \\
P_{\sigma_{1\leftrightarrow3,2\leftrightarrow4}}, & \text{w.p. } 1/3. 
\end{cases}
$$

Then, the calculation that was previously performed effectively shows that

$$
P_{\text{Id}} = \begin{cases} 
\frac{1}{3}, & \text{if } X_3 + X_4 < X_1 + X_2, \\
1, & \text{otherwise.}
\end{cases}
$$
Figure 1: A hub-and-spoke visual representation of the method described in Theorem 3. The center “hub” $X_{\sigma^{-1}}$ is a randomly permuted version of the original data, which is not used in the test. From that hub node, we now apply each $\sigma \in S$ to obtain $X_{\sigma \circ \sigma^{-1}}$, obtaining $|S|$ many “spokes”. One of these permuted observations happens to be equal to the original data $X$ (i.e., the one obtained at $\sigma = \sigma_\ast$). These $|S|$ many permuted datasets (of which $X$ is one) are exchangeable, and thus the resulting test statistics $T(X_{\sigma \circ \sigma^{-1}})$ are as well, which leads to validity of the p-value $P$ computed in (10).

A similar straightforward calculation then yields

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

Put together, we obtain

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

This is indeed stochastically larger than uniform, as claimed by Theorem 3.

### 2.3 Random permutations from a fixed subset

If $S$ is large, calculation (10) may be tedious. Hence we provide the following randomized variant (we can compare to Theorem 2 which instead takes random samples from a subgroup $G$).

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

$$P = \frac{1 + \sum_{m=1}^{M} I \{T(X_{\sigma_m \circ \sigma^{-1}}) \geq T(X)\}}{1 + M} \quad (13)$$
is a valid p-value, i.e., \( P_{H_0} \{ P \leq \alpha \} \leq \alpha \) for all \( \alpha \in [0, 1] \).

This theorem may be proved as an application of Besag and Clifford’s construction for exchangeable draws from MCMC sampling, as we describe in Section 3.2.

### 2.4 Non-uniform distributions over permutations

We finally extend our results and show that Theorems 3 and 4 can both be viewed as special cases of the following statement:

**Theorem 5.** Let \( q \) be any distribution over \( \sigma \in S_n \). Let \( \sigma^* \sim q \) be a random draw, and define

\[
P = \sum_{\sigma \in S_n} q(\sigma) \cdot 1 \left\{ T(X_{\sigma^* \sigma^{-1}}) \geq T(X) \right\}.
\]

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

The proof follows similar arguments as that of Theorem 3. A key step is to replace the uniform weighting in (12) using weights given by \( q(\sigma) \). This employs a deterministic inequality by Harrison [2012], which we state here for completeness: for all \( t_1, \ldots, t_N \in [-\infty, \infty] \) and all \( \alpha, w_1, \ldots, w_N \in [0, \infty] \), we have

\[
\sum_{k=1}^{N} w_k 1 \left\{ \sum_{i=1}^{N} w_i 1 \left\{ t_i \geq t_k \right\} \leq \alpha \right\} \leq \alpha.
\]

We omit the other steps of the proof since they are as before.

To see how the previous results are special cases of this more general formulation, we can recover Theorem 3 by taking \( q \) to be the distribution on \( S_n \) given by

\[
q(\sigma) = \frac{1_{\sigma \in S}}{|S|},
\]

and we can recover Theorem 4 by taking

\[
q(\sigma) = \frac{1_{\sigma = \sigma^*} + \sum_{m=1}^{M} 1_{\sigma = \sigma_m}}{1 + M}.
\]

In this latter case, \( \sigma^* \) can be viewed as a random draw from \( q \); this is because we can run the procedure of Theorem 4 by first drawing \( M + 1 \) many unlabeled permutations from \( S \), which determines the distribution \( q \), and then randomly labeling these \( M + 1 \) permutations as \( \sigma^*, \sigma_1, \ldots, \sigma_M \), which means that \( \sigma^* \) is a random draw from \( q \).

### 3 Connections to the literature

The main contributions of our paper are complete, but we contextualize our work in the broader literature by mentioning a few connections.
3.1 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

\[
P = \frac{\sum_{\sigma \in S} \mathbb{1} \{ T(X_\sigma) \geq T(X_{\sigma_{\text{asgn}}}) \}}{|S|}. \tag{15}
\]

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 \( P = \frac{\sum_{\sigma \in S} \mathbb{1} \{ T(X_\sigma) \geq T(X) \}}{|S|} \) considered in (8), 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 (8), the observed statistic is \( T(X) \) (i.e., using the fixed permutation \( \text{Id} \) in place of a randomly drawn \( \sigma_{\text{asgn}} \)). For this reason, the randomization test p-value in (15) is valid, while the permutation test calculation in (8) is not valid in general.
Now we again consider our new proposed method, given in (10). This proposed 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. Nonetheless, we are able to produce a valid p-value without assuming an underlying group structure for the subset $S \subseteq S_n$ of permutations considered by the test.

3.2 Exchangeable MCMC

Our last result, Theorem 4, which allows for random samples drawn from an arbitrary fixed subset $S \subseteq S_n$, 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 $\mathcal{Z}$, 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 6 [Besag and Clifford 1989, Section 2]).** Let $Q_0$ be any distribution on a probability space $\mathcal{Z}$. Construct a Markov chain on $\mathcal{Z}$ with stationary distribution $Q_0$, whose forward and backward transition distributions (initialized at $z \in \mathcal{Z}$) are denoted by $Q_\rightarrow(\cdot|z)$ and $Q_\leftarrow(\cdot|z)$. Let $Q^*_\rightarrow(\cdot|z)$ and $Q^*_\leftarrow(\cdot|z)$ 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:

\[
\begin{aligned}
&\left\{\begin{array}{l}
\text{Conditional on } Z, \text{ draw } Z_1, \ldots, Z_M | Z, Z_* \sim Q^*_\rightarrow(\cdot|Z).
\end{array}\right.
\end{aligned}
\]

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 $P = \frac{1 + \sum_{m=1}^M 1\{T(Z_m)\geq T(Z)\}}{1 + M}$ 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 4 is related to this result. Let $Z = \mathcal{X}^n$, 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 $\sigma \in S$, that is, for $x = (x_1, \ldots, x_n)$,

$$Q_\rightarrow(x|\cdot) = \frac{1}{|S|} \sum_{\sigma \in S} \delta_{x_\sigma},$$

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

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

Then using the description in Theorem 4, run Besag and Clifford [1989]'s method (with $s = 1$), we define $X_\sigma = X_{\sigma^{-1}}$, and then define $X_m = (X_\sigma)_{\sigma_m} = X_{\sigma_m \sigma_{m-1}}$ 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.

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 Conclusion

We proposed a new method for permutation testing that does not utilize a subgroup of permutations. 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 $S \subseteq S_n$ as compared to using the full permutation group $S_n$ as studied by Dobriban [2021], Kim et al. [2021, 2022]. Exploring new applications of these ideas, beyond the conformal prediction setting mentioned above, would also be a fruitful direction.

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 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 understanding how permutation tests operate in this non-subgroup setting is key to the findings in our aforementioned work.

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.

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