Supplementary Material

To

Null-Free False Discovery Rate Control

Using Decoy Permutations

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S1 Proof of Theorem 1

Proof. Case 1: permutations sampled with replacement. Our proof is divided into four steps. In the first three steps, we concentrate on the j'-th test (before sorting the tests) where $1 \leq j' \leq m$ and the j'-th null hypothesis is true. For simplicity, we will omit the index j' in these three steps if there is no confusing. For example, $\overrightarrow{X}$ is short for $\overrightarrow{X_{j'}} = [X_{j',1}, X_{j',2}, \cdots, X_{j',n}]$,

$x_1, x_2, \cdots, x_n$ are short for $x_{j',1}, x_{j',2}, \cdots, x_{j',n}$ and $\vec{x}$ is short for $\overrightarrow{x_{j'}} = [x_1, x_2, \cdots, x_n]$.

Step 1. Analysis of the permutation subroutine of each test.

In our proof, we will use pdf to denote the probability density function of continuous random variable and the probability mass function of discrete random variable. Firstly, we define some random variables used in our proof.

If the j'-th null hypothesis is true, the joint distribution of $\vec{X} = [X_{j',1}, X_{j',2}, \cdots, X_{j',n}]$ is symmetric. Therefore, for any permutation π_n of n elements and any $\vec{x} = [x_1, x_2, \cdots, x_n]$, we have the pdf $f_{\vec{X}}$ of $\vec{X}$ satisfies that $f_{\vec{X}}(\vec{x}) = f_{\vec{X}}(\pi_n(\vec{x}))$.

For any fixed $\vec{x}$, let $\vec{y}$ be the result obtained by sorting $\vec{x}$ in descending order. Let $\widetilde{\pi}_n^0$ be the random variable of permutation such that $\vec{x} = \widetilde{\pi}_n^0[\vec{y}]$. If there is more than one permutation meeting the condition, $\widetilde{\pi}_n^0$ is set as one of these permutations randomly with equal probability. Similarly, for random variable $\vec{X}$, let $\vec{Y}$ be the result obtained by sorting $\vec{X}$ in descending order and Π_n^0 be the permutation such that $\vec{X} = \Pi_n^0[\vec{Y}]$.

Let the $t-1$ random permutations for the j'-th test are $\hat{\pi}_n^1, \hat{\pi}_n^2, \cdots, \hat{\pi}_n^{t-1}$ and corresponding decoy scores are $S_{j'}^{D_1}, S_{j'}^{D_2}, \cdots, S_{j'}^{D_{t-1}}$. Let $\overrightarrow{\Pi_n}$ denote

$\Pi_n^0, \Pi_n^1 = \hat{\pi}_n^1 \Pi_n^0, \cdots, \Pi_n^{t-1} = \hat{\pi}_n^{t-1} \Pi_n^0$.

Note that there are three kinds of randomnesses here. The first one is the randomness of $\overrightarrow{X}$, the second one is the randomness introduced in Step 1 of the simplified target-decoy procedure for permuting case and control status, and the last one is the random choice of multiple possible permutations for recovering $\overrightarrow{x}$ from $\overrightarrow{y}$. In our definition, $\hat{\pi}_n^1, \hat{\pi}_n^2, \cdots, \hat{\pi}_n^{t-1}$ only involve the second kind of randomness, $\widetilde{\pi}_n^0$ only involves the third kind of randomness, Π_n^0 involves the first and third kind of randomness and $\Pi_n^1, \Pi_n^2, \cdots, \Pi_n^{t-1}$ involve all of the three kinds of randomnesses.

For any possible π_n^0 and $\overrightarrow{y} = [y_1, y_2, \cdots, y_n]$ where $y_1 \geq y_2 \geq \cdots \geq y_n$, the pdf $f_{\Pi_n^0, \overrightarrow{Y}}$ of $\Pi_n^0, \overrightarrow{Y}$ satisfies

$$f_{\Pi_n^0, \overrightarrow{Y}}(\pi_n^0, \overrightarrow{y}) = \frac{f_{\overrightarrow{X}}(\pi_n^0[\overrightarrow{y}])}{\left|\{\pi_n \middle| \pi_n[\overrightarrow{y}] = \pi_n^0[\overrightarrow{y}]\}\right|}.$$

For any possible $\overrightarrow{y}$ and $\overrightarrow{\pi_n} = \pi_n^0, \pi_n^1\pi_n^0, \cdots, \pi_n^{t-1}\pi_n^0$, we have the pdf $f_{\overrightarrow{\Pi_n}, \overrightarrow{Y}}$ of $\overrightarrow{\Pi_n}, \overrightarrow{Y}$ satisfies that

$$f_{\overrightarrow{\Pi_n}, \overrightarrow{Y}}(\overrightarrow{\pi_n}, \overrightarrow{y}) = \binom{n}{n_1}^{1-t} f_{\Pi_n^0, \overrightarrow{Y}}(\pi_n^0, \overrightarrow{y}) = \binom{n}{n_1}^{1-t} \frac{f_{\overrightarrow{X}}(\pi_n^0[\overrightarrow{y}])}{\left|\{\pi_n \middle| \pi_n[\overrightarrow{y}] = \pi_n^0[\overrightarrow{y}]\}\right|}, \tag{S1.1}$$

because the probability that the randomly chosen $t-1$ random permutations are exactly $\pi_n^1, \cdots, \pi_n^{t-1}$ is $\binom{n}{n_1}^{1-t}$. For any permutation π_t of t elements and any possible $\overrightarrow{\pi_n}$, let $(\pi_t\overrightarrow{\pi_n})_i$ denote the i-th element of

$\pi_t\overrightarrow{\pi_n} = \pi_t[\pi_n^0, \pi_n^1\pi_n^0, \cdots, \pi_n^{t-1}\pi_n^0]$. We also have

$$f_{\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t\overrightarrow{\pi_n}, \overrightarrow{y}) = \binom{n}{n_1}^{1-t} \frac{f_{\overrightarrow{X}}((\pi_t\overrightarrow{\pi_n})_1[\overrightarrow{y}])}{\left|\{\pi_n \middle| \pi_n[\overrightarrow{y}] = (\pi_t\overrightarrow{\pi_n})_1[\overrightarrow{y}]\}\right|}. \tag{S1.2}$$

Because $f_{\overrightarrow{X}}$ is symmetric, we have for permutation π_n^0 and $(\pi_t\overrightarrow{\pi_n})_1$,

$$f_{\overrightarrow{X}}(\pi_n^0[\overrightarrow{y}]) = f_{\overrightarrow{X}}((\pi_t\overrightarrow{\pi_n})_1[\overrightarrow{y}]). \tag{S1.3}$$

Moreover, note that $\left|\{\pi_n \middle| \pi_n[\overrightarrow{y}] = \pi_n^0[\overrightarrow{y}]\}\right| = \left|\{\pi_n \middle| \pi_n[\overrightarrow{y}] = (\pi_t\overrightarrow{\pi_n})_1[\overrightarrow{y}]\}\right|$, because for every permutation $\pi_n^{'}$, $\left|\{\pi_n \middle| \pi_n[\overrightarrow{y}] = \pi_n^{'}[\overrightarrow{y}]\}\right|$ is the same since it is determined by the multiplicities of elements in multiset $y_1, y_2, \cdots, y_n$. Therefore, from equations (S1.1) (S1.2) and (S1.3) we have for any π_t,

$$f_{\overrightarrow{\Pi_n},\overrightarrow{Y}}(\overrightarrow{\pi_n}, \overrightarrow{y}) = f_{\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t\overrightarrow{\pi_n}, \overrightarrow{y}). \tag{S1.4}$$

Step 2: Analysis of the sorting subroutine of each test.

Note that the simplified target-decoy procedure sorts $S_{j'}^T, S_{j'}^{D_1}, \cdots, S_{j'}^{D_{t-1}}$ in descending order and sorts equal scores randomly. Let Π_t denote the used permutation for sorting $S_{j'}^T, S_{j'}^{D_1}, \cdots, S_{j'}^{D_{t-1}}$ in the procedure. Thus, Π_t involves three kinds of randomnesses, i.e., the randomness of $\overrightarrow{X}$, the randomness for permuting case and control status, and the randomness for sorting equal scores. For any possible $\overrightarrow{Y}$ and $\overrightarrow{\pi_n}$, Π_t can only take values in $\mathcal{A}(\overrightarrow{\pi_n}, \overrightarrow{y}) = \{\pi_t \middle| \pi_t[S(\pi_n^0[\overrightarrow{y}]), S(\pi_n^1\pi_n^0[\overrightarrow{y}]), \cdots, S(\pi_n^{t-1}\pi_n^0[\overrightarrow{y}])]$ is in descending order$\}$ if $\overrightarrow{\Pi_n} = \overrightarrow{\pi_n}$ and $\overrightarrow{Y} = \overrightarrow{y}$. Thus, for any fixed π_t in $\mathcal{A}(\overrightarrow{\pi_n}, \overrightarrow{y})$, we have the pdf $f_{\Pi_t,\overrightarrow{\Pi_n},\overrightarrow{Y}}$ of $\Pi_t, \overrightarrow{\Pi_n}, \overrightarrow{Y}$ satisfies that

$$f_{\Pi_t,\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t, \overrightarrow{\pi_n}, \overrightarrow{y}) = \frac{f_{\overrightarrow{\Pi_n},\overrightarrow{Y}}(\overrightarrow{\pi_n}, \overrightarrow{y})}{|\mathcal{A}(\overrightarrow{\pi_n}, \overrightarrow{y})|}, \tag{S1.5}$$

because Π_t sorts equal scores randomly and all permutations in $\mathcal{A}(\overrightarrow{\pi_n}, \overrightarrow{y})$ can sort $S(\pi_n^0[\overrightarrow{y}]), S(\pi_n^1\pi_n^0[\overrightarrow{y}]), \cdots, S(\pi_n^{t-1}\pi_n^0[\overrightarrow{y}])$ in descending order. From $\pi_t \in \mathcal{A}(\overrightarrow{\pi_n}, \overrightarrow{y})$, we have $\pi_t(\pi_t^1)^{-1} \in \mathcal{A}(\pi_t^1\overrightarrow{\pi_n}, \overrightarrow{y})$ for any fixed π_t^1. Therefore, from equation (S1.5) we have for any possible π_t and any fixed π_t^1,

$$\begin{aligned} f_{\Pi_t,\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t(\pi_t^1)^{-1}, \pi_t^1\overrightarrow{\pi_n}, \overrightarrow{y}) &= \frac{f_{\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t^1\overrightarrow{\pi_n}, \overrightarrow{y})}{|\mathcal{A}(\pi_t^1\overrightarrow{\pi_n}, \overrightarrow{y})|} = \frac{f_{\overrightarrow{\Pi_n},\overrightarrow{Y}}(\overrightarrow{\pi_n}, \overrightarrow{y})}{|\mathcal{A}(\overrightarrow{\pi_n}, \overrightarrow{y})|} \\ &= f_{\Pi_t,\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t, \overrightarrow{\pi_n}, \overrightarrow{y}). \end{aligned} \tag{S1.6}$$

The second equality is from equation (S1.4) and $|\{\mathcal{A}(\overrightarrow{\pi_n}, \overrightarrow{y})\}| = |\{\mathcal{A}(\pi_t^1\overrightarrow{\pi_n}, \overrightarrow{y})\}|$, because for every permutation π_t', $\left|\{\mathcal{A}(\pi_t'\overrightarrow{\pi_n}, \overrightarrow{y})\}\right|$ is the same since it is determined by the multiplicities of elements in multiset $\{S(\pi_n^0[\overrightarrow{y}]), S(\pi_n^1\pi_n^0[\overrightarrow{y}]), \cdots, S(\pi_n^{t-1}\pi_n^0[\overrightarrow{y}])\}$. Therefore, from equation (S1.6) we have for any possible $\pi_t, \overrightarrow{\pi_n}$ and any fixed π_t^1,

$$\begin{aligned} \sum_{\pi_t'} f_{\Pi_t,\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t, \pi_t'\overrightarrow{\pi_n}, \overrightarrow{y}) &= \sum_{\pi_t'} f_{\Pi_t,\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t(\pi_t^1)^{-1}, \pi_t^1\pi_t'\overrightarrow{\pi_n}, \overrightarrow{y}) \\ &= \sum_{\pi_t^1\pi_t'} f_{\Pi_t,\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t(\pi_t^1)^{-1}, \pi_t^1\pi_t'\overrightarrow{\pi_n}, \overrightarrow{y}) \\ &= \sum_{\pi_t'} f_{\Pi_t,\overrightarrow{\Pi_n},\overrightarrow{Y}}(\pi_t^2, \pi_t'\overrightarrow{\pi_n}, \overrightarrow{y}), \end{aligned} \tag{S1.7}$$

where $\pi_t^2 = \pi_t(\pi_t^1)^{-1}$ and π_t' takes values in all possible permutations of t elements. The last equality is obtained by substituting $\pi_t^1\pi_t'$ and $\pi_t(\pi_t^1)^{-1}$

with $\pi_t^{'}$ and π_t^2, respectively. Since π_t^1 can be any permutation of t elements for every fixed π_t, we have π_t^2 can also be any permutation.

Step 3: Analysis of the labeling subroutine of each test.

Let $[\pi_t]_{i_1} = i_2$ denote that the original i_2-th element is the i_1-th element after permutation π_t. Consider all permutations $\{\pi_t\}$ of t elements, we have for any i_1,

$$\left|\{\pi_t \big| [\pi_t]_{i_1} = 1\}\right| = \frac{|\{\pi_t\}|}{t} = (t-1)!. \tag{S1.8}$$

Note that the original first element is the $[(\Pi_t)^{-1}]_1$-th element after permutation Π_t, because $[\Pi_t]_i = 1$ is equivalent to $[(\Pi_t)^{-1}]_1 = i$. Thus, for any fixed permutation π_t^2, the pdf $f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \overrightarrow{Y}}$ of $[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \overrightarrow{Y}$ satisfies that

$$\begin{aligned}
\sum_{\pi_t^{'}} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \overrightarrow{Y}}(i_1, \pi_t^{'}\overrightarrow{\pi_n}, \overrightarrow{y}) &= \sum_{[\pi_t]_{i_1}=1} \sum_{\pi_t^{'}} f_{\Pi_t, \overrightarrow{\Pi_n}, \overrightarrow{Y}}(\pi_t, \pi_t^{'}\overrightarrow{\pi_n}, \overrightarrow{y}) \\
&= \sum_{[\pi_t]_{i_1}=1} \sum_{\pi_t^{'}} f_{\Pi_t, \overrightarrow{\Pi_n}, \overrightarrow{Y}}(\pi_t^2, \pi_t^{'}\overrightarrow{\pi_n}, \overrightarrow{y}) \\
&= (t-1)! \sum_{\pi_t^{'}} f_{\Pi_t, \overrightarrow{\Pi_n}, \overrightarrow{Y}}(\pi_t^2, \pi_t^{'}\overrightarrow{\pi_n}, \overrightarrow{y}),
\end{aligned} \tag{S1.9}$$

The penultimate equality is due to equation (S1.7) and the last equality is due to equation (S1.8). From equation (S1.9) we have for any $i_1, i_2 \in$

$\{1, \cdots, t\}$,

$$\sum_{\pi_t'} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}}(i_1, \pi_t' \overrightarrow{\pi_n}, \vec{y}) = (t-1)! \sum_{\pi_t'} f_{\Pi_t, \overrightarrow{\Pi_n}, \vec{Y}}(\pi_t^2, \pi_t' \overrightarrow{\pi_n}, \vec{y}) \\ = \sum_{\pi_t'} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}}(i_2, \pi_t' \overrightarrow{\pi_n}, \vec{y}). \tag{S1.10}$$

Thus, we have for any positive integer $i < \frac{t+1}{2}$,

$$\sum_{\pi_t'} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}}(i, \pi_t' \overrightarrow{\pi_n}, \vec{y}) = \sum_{\pi_t'} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}}(i + \left\lceil \frac{t}{2} \right\rceil, \pi_t' \overrightarrow{\pi_n}, \vec{y})$$

Therefore, the pdf $f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}, S_{j'}}$ of $[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}, S_{j'}$ satisfies that

$$\sum_{\pi_t'} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}, S_{j'}}(i, \pi_t' \overrightarrow{\pi_n}, \vec{y}, s_{j'}) \\ = \sum_{\pi_t'} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}, S_{j'}}(i + \left\lceil \frac{t}{2} \right\rceil, \pi_t' \overrightarrow{\pi_n}, \vec{y}, s_{j'}),$$

because for any possible $\vec{y}, \overrightarrow{\pi_n}, i < \frac{t+1}{2}$ and any fixed π_t', $S_{j'}$ is set as the score ranking i-th in $S((\pi_t' \overrightarrow{\pi_n})_1[\vec{y}]), \cdots, S((\pi_t' \overrightarrow{\pi_n})_t[\vec{y}])$ no matter $[(\Pi_t)^{-1}]_1 = i$ or $i + \lceil \frac{t}{2} \rceil$. Thus, by the above equality we have

$$\sum_{i \leq \frac{t}{2}} \sum_{\pi_t'} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}, S_{j'}}(i, \pi_t' \overrightarrow{\pi_n}, \vec{y}, s_{j'}) \\ = \sum_{i \geq \frac{t}{2}+1} \sum_{\pi_t'} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}, S_{j'}}(i, \pi_t' \overrightarrow{\pi_n}, \vec{y}, s_{j'}),$$

Meanwhile, from Step 2 of the simplified target-decoy procedure, we have the pdf $f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}$ of $L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}$ satisfies that

$$\begin{aligned}\sum_{\pi_t^{'}} f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(T,\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'}) = &\sum_{i\le\frac{t}{2}}\sum_{\pi_t^{'}} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(i,\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'}) \\ &+\frac{1}{2}\sum_{\pi_t^{'}} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(\frac{t+1}{2},\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'})\end{aligned}$$

Note that if t is odd, $f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(\frac{t+1}{2},\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'})$ is zero for any $\pi_t^{'}$ in the above equation. Similarly, we also have

$$\begin{aligned}\sum_{\pi_t^{'}} f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(D,\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'}) = &\sum_{i\ge\frac{t}{2}+1}\sum_{\pi_t^{'}} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(i,\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'}) \\ &+\frac{1}{2}\sum_{\pi_t^{'}} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(\frac{t+1}{2},\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'})\end{aligned}$$

Therefore, by combining the above three equalities, we have

$$\sum_{\pi_t^{'}} f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(T,\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'}) = \sum_{\pi_t^{'}} f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(D,\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'}) \tag{S1.11}$$

From equation (S1.11), we have the pdf $f_{L_{j'},S_{j'}}$ of $L_{j'},S_{j'}$ satisfies that

$$\begin{aligned}f_{L_{j'},S_{j'}}(T,s_{j'}) &= \int\sum_{\overrightarrow{\pi_n}} f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(T,\overrightarrow{\pi_n},\vec{y},s_{j'})\mathrm{d}y \\ &= \int\frac{\sum_{\overrightarrow{\pi_n}}\sum_{\pi_t^{'}} f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(T,\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'})}{t!}\mathrm{d}y \\ &= \int\frac{\sum_{\overrightarrow{\pi_n}}\sum_{\pi_t^{'}} f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(D,\pi_t^{'}\overrightarrow{\pi_n},\vec{y},s_{j'})}{t!}\mathrm{d}y \\ &= f_{L_{j'},S_{j'}}(D,s_{j'}).\end{aligned} \tag{S1.12}$$

The second equality is due to that for any given $\overrightarrow{\pi_n}$, there are $t!$ pairs $\{\pi_t^{'},\overrightarrow{\pi_n}'\}$ such that $\pi_t^{'}\overrightarrow{\pi_n}' = \overrightarrow{\pi_n}$ where $\overrightarrow{\pi_n}' = (\pi_t^{'})^{-1}\overrightarrow{\pi_n}$. Therefore, $f_{L_j,\overrightarrow{\Pi_n},\vec{Y},S_j}(T,$

$\overrightarrow{\pi_n}, \vec{y}, s_j)$ is counted for $t!$ times. From equation (S1.12) we have for any j' where $H_{j'} = 0$ and any possible $s_{j'}$,

$$\Pr(L_{j'} = T \big| S_{j'} = s_{j'}) = \Pr(L_{j'} = D \big| S_{j'} = s_{j'}). \qquad \text{(S1.13)}$$

Step 4: Analysis of the sorting subroutine for all the m tests.

Let Π_m denote the permutation for sorting $\vec{S}$. Let $[\Pi_m]_j = j^{'}$ denote that the original $j^{'}$-th element is the j-th element after sorting with permutation Π_m, i.e., $S_{(j)}$ is from $S_{j^{'}}$. Let $A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)$ denote the event $\overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}, [\Pi_m]_j = j^{'}$.

Note that whether $A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)$ happens is fully determined by $\vec{S}, \overrightarrow{L_{\neq j'}}$ and the randomness introduced by Step 3 of the simplified target-decoy procedure for sorting equal scores. Because Π_m is determined given $\vec{S} = \vec{s}$ and the random choice of permutations which sort $\vec{s}$ in descending order. Therefore, whether $\overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, [\Pi_m]_j = j^{'}$ holds is determined. For any fixed π_m where $[\pi_m]_j = j^{'}$, whether $\overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}$ holds only depends on $\overrightarrow{L_{\neq j'}}$ if $\Pi_m = \pi_m$. Since $\overrightarrow{Z_{(\neq j)}}$ is determined by $\overrightarrow{L_{\neq j'}}$ and $\overrightarrow{H_{\neq j'}}$ for the fixed π_m, and $\overrightarrow{H_{\neq j'}}$ is a constant vector.

Because $\overrightarrow{S_{\neq j'}}, \overrightarrow{L_{\neq j'}}$ and the randomness for sorting equal scores are independent of $L_{j'}$, we have that $\vec{S}, \overrightarrow{L_{\neq j'}}$ and the randomness are independent of $L_{j'}$ given $S_{j'} = s_{j'}$. Then, whether the event $A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}}, j^{'}\big)$ happens is also independent of $L_{j'}$ given $S_{j'} = s_{j'}$. Thus, we have for any possible $j^{'}$,

$$\begin{aligned}
&\Pr\left(L_{j'} = T \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big), S_{j'} = s_{j'}\right) \Pr\left(A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big) \middle| S_{j'} = s_{j'}\right) \\
&= \Pr\left(L_{j'} = T, A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big) \middle| S_{j'} = s_{j'}\right) \\
&= \Pr\left(L_{j'} = T \middle| S_{j'} = s_{j'}\right) \Pr\left(A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big) \middle| S_{j'} = s_{j'}\right).
\end{aligned} \tag{S1.14}$$

The first equality is due to the chain rule and the second equality is due to the independence. From equation (S1.14) we have

$$\Pr\left(L_{j'} = T \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big), S_{j'} = s_{j'}\right) = \Pr\left(L_{j'} = T \middle| S_{j'} = s_{j'}\right). \tag{S1.15}$$

From the definition of $A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)$, we have

$$\Pr\left(L_{j'} = T \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big), S_{j'} = s_{j'}\right) = \Pr\left(L_{j'} = T \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)\right) \tag{S1.16}$$

Thus, from equations (S1.15) and (S1.16) we have

$$\Pr\left(L_{j'} = T \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)\right) = \Pr\left(L_{j'} = T \middle| S_{j'} = s_{j'}\right). \tag{S1.17}$$

Similarly, we can also prove

$$\Pr\left(L_{j'} = D \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)\right) = \Pr\left(L_{j'} = D \middle| S_{j'} = s_{j'}\right). \tag{S1.18}$$

Thus, from equations (S1.13), (S1.17) and (S1.18) we have

$$\Pr\left(L_{j'} = T \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)\right) = \Pr\left(L_{j'} = D \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)\right). \tag{S1.19}$$

Note that

$$
\begin{aligned}
&\Pr\left(Z_{(j)} = 1 \middle| \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \Pr\left(\overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \\
&= \Pr\left(Z_{(j)} = 1, \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \\
&= \Pr\left(L_{(j)} = T, H_{(j)} = 0, \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \\
&= \sum_{j^{'}: H_{j'} = 0} \Pr\left(L_{j'} = T, [\Pi_m]_j = j^{'}, \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \\
&= \sum_{j^{'}: H_{j'} = 0} \Pr\left(L_{j'} = T \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)\right) \Pr\left(A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)\right),
\end{aligned}
\tag{S1.20}
$$

where the last equality is due to the definition of $A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)$ and the chain rule. Similarly, we also have

$$
\begin{aligned}
&\Pr\left(Z_{(j)} = -1 \middle| \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \Pr\left(\overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \\
&= \sum_{j^{'}: H_{j'} = 0} \Pr\left(L_{j'} = D \middle| A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)\right) \Pr\left(A\big(\overrightarrow{s_{(\cdot)}}, \overrightarrow{z_{(\neq j)}}, j^{'}\big)\right).
\end{aligned}
\tag{S1.21}
$$

Thus, from equations (S1.19), (S1.20) and (S1.21) we have for any fixed $1 \leq j \leq m$,

$$
\begin{aligned}
&\Pr\left(Z_{(j)} = 1 \middle| \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \\
&= \Pr\left(Z_{(j)} = -1 \middle| \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right).
\end{aligned}
$$

Case 2: permutations sampled without replacement. The idea is similar to the proof for the case with replacement. Only the following two differences merit attention. Firstly, the permutations $\pi_n^1, \cdots, \pi_n^{t-1}$ should be different and cannot be the identical permutation which does not exchange any element. Secondly, the term $\binom{n}{n_1}^{1-t}$ in equations (S1.1) and (S1.2) should be replaced with $\left(\Pi_{i=1}^{t-1}\left(\binom{n}{n_1}-i\right)\right)^{-1}$. Because the probability that the randomly chosen $t-1$ permutations are exactly $\pi_n^1, \cdots, \pi_n^{t-1}$, which are different and are not the identical permutation, is $\left(\Pi_{i=1}^{t-1}\left(\binom{n}{n_1}-i\right)\right)^{-1}$. $\square$

S2 Proof of Theorem 2

Proof. Case 1: permutations sampled with replacement. The proof is similar to that of Theorem 1. It is not difficult to verify that all the proof of Theorem 1 up to equation (S1.10) also holds.

According to Step 2 of the target-decoy procedure, we have $\Lambda_{j'} = i - P_{j'} \leq \frac{t}{2r}$ if and only if $i \leq \lceil \frac{t}{2r} \rceil$ and $P_{j'} \geq \max(i - \frac{t}{2r}, 0)$. Therefore, for any $\pi_t^{'}$ and any fixed $i' \in [\lceil \frac{t}{2r} \rceil]$, the pdf $f_{\overrightarrow{\Pi_n}, Y, \Lambda_{j'}}$ of $\overrightarrow{\Pi_n}, Y, \Lambda_{j'}$ satisfies that

$$
\begin{aligned}
&\int_{i'-1}^{\min(i', \frac{t}{2r})} f_{\overrightarrow{\Pi_n}, \vec{Y}, \Lambda_{j'}}(\pi_t^{'}\overrightarrow{\pi_n}, \vec{y}, \lambda_{j'}) \mathrm{d}\lambda_{j'} \\
&= \int_{\max(i' - \frac{t}{2r}, 0)}^{1} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}, P_{j'}}(i', \pi_t^{'}\overrightarrow{\pi_n}, \vec{y}, p_{j'}) \mathrm{d}p_{j'} \qquad \text{(S2.22)} \\
&= \min\left(1, \frac{t}{2r} - i' + 1\right) f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}}(i', \pi_t^{'}\overrightarrow{\pi_n}, \vec{y}).
\end{aligned}
$$

The last equality is due to that $P_{j'}$ is independent of the joint distribution of $[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}$. Similarly, we also have $\frac{t}{2} < \Lambda_{j'} \leq t$ if and only if $\lceil \frac{t}{2} \rceil \leq i \leq t$ and $P_{j'} \in \left[0, \min\left(i - \frac{t}{2}, 1\right)\right)$. Therefore,

$$
\begin{aligned}
&\int_{\frac{t}{2}}^{t} f_{\overrightarrow{\Pi_n}, \vec{Y}, \Lambda_{j'}}(\pi_t^{'}\overrightarrow{\pi_n}, \vec{y}, \lambda_{j'}) \mathrm{d}\lambda_{j'} \\
&= \sum_{i''=\lceil \frac{t}{2} \rceil}^{t} \int_0^{\min\left(i'' - \frac{t}{2}, 1\right)} f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}, P_{j'}}(i'', \pi_t^{'}\overrightarrow{\pi_n}, \vec{y}, p_{j'}) \mathrm{d}p_{j'} \qquad \text{(S2.23)} \\
&= \sum_{i''=\lceil \frac{t}{2} \rceil}^{t} \min\left(i'' - \frac{t}{2}, 1\right) f_{[(\Pi_t)^{-1}]_1, \overrightarrow{\Pi_n}, \vec{Y}}(i'', \pi_t^{'}\overrightarrow{\pi_n}, \vec{y}).
\end{aligned}
$$

From equations (S1.10) and (S2.23), we have for any fixed $1 \le i^{'} \le t$,

$$
\begin{aligned}
&\sum_{\pi_t^{'}} \int_{\frac{t}{2}}^{t} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}}(\pi_t^{'}\overrightarrow{\pi_n},\vec{y},\lambda_{j'})\mathrm{d}\lambda_{j'} \\
=&\sum_{i''=\lceil \frac{t}{2}\rceil}^{t} \min\big(i''-\frac{t}{2},1\big) \sum_{\pi_t^{'}} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y}}(i'',\pi_t^{'}\overrightarrow{\pi_n},\vec{y}) \\
=&\sum_{i''=\lceil \frac{t}{2}\rceil}^{t} \min\big(i''-\frac{t}{2},1\big) \sum_{\pi_t^{'}} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y}}(i^{'},\pi_t^{'}\overrightarrow{\pi_n},\vec{y}) \qquad \text{(S2.24)} \\
=&\big(t-\frac{t}{2}\big) \sum_{\pi_t^{'}} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y}}(i^{'},\pi_t^{'}\overrightarrow{\pi_n},\vec{y}) \\
=&\frac{t}{2} \sum_{\pi_t^{'}} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y}}(i^{'},\pi_t^{'}\overrightarrow{\pi_n},\vec{y}).
\end{aligned}
$$

In Step 2 of the target-decoy procedure, $\Lambda_{j'}^{'}$ is defined if and only if $\Lambda_{j'} \in \big(\frac{t}{2},t\big]$. Here we let $\Lambda_{j'}^{'}=t$ if $\Lambda_{j'} \notin \big(\frac{t}{2},t\big]$. Thus, we have for any possible $\overrightarrow{\pi_n},\vec{y}$ and fixed $\pi_t^{'}$, $\Pr\Big(0 < \Lambda_{j'}^{'} \le \frac{t}{2r}\Big|\overrightarrow{\Pi_n}=\pi_t^{'}\overrightarrow{\pi_n},\vec{Y}=\vec{y}\Big) = \Pr(\frac{t}{2} < \Lambda_{j'} \le t\Big|\overrightarrow{\Pi_n}=\pi_t^{'}\overrightarrow{\pi_n},\vec{Y}=\vec{y})$ always holds. Therefore, we have the pdf $f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}^{'}}$ of $\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}^{'}$ satisfies that

$$
\int_0^{\frac{t}{2r}} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}^{'}}(\pi_t^{'}\overrightarrow{\pi_n},\vec{y},\lambda_{j'}^{'})\mathrm{d}\lambda_{j'}^{'} = \int_{\frac{t}{2}}^{t} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}}(\pi_t^{'}\overrightarrow{\pi_n},\vec{y},\lambda_{j'})\mathrm{d}\lambda_{j'}. \qquad \text{(S2.25)}
$$

Because $\Lambda_{j'}^{'}$ follows uniform$\big(0,\frac{t}{2r}\big]$ distribution if $\frac{t}{2} < \Lambda_{j'} \le t$, we have for any fixed $i^{'} \le \lceil \frac{t}{2r} \rceil$,

$$
\begin{aligned}
&\int_{i^{'}-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_j^{'}}(\pi_t^{'}\overrightarrow{\pi_n},\vec{y},\lambda_j^{'})\mathrm{d}\lambda_j^{'} \\
=&\frac{2r\min\big(1,\frac{t}{2r}-i'+1\big)}{t} \int_0^{\frac{t}{2r}} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_j^{'}}(\pi_t^{'}\overrightarrow{\pi_n},\vec{y},\lambda_j^{'})\mathrm{d}\lambda_j^{'}.
\end{aligned} \qquad \text{(S2.26)}
$$

From equations (S2.25) and (S2.26), we have

$$
\begin{aligned}
&\int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda'_j}(\pi'_t\overrightarrow{\pi_n},\vec{y},\lambda'_j)\mathrm{d}\lambda'_j\\
=&\frac{2r\min\left(1,\frac{t}{2r}-i'+1\right)}{t}\int_{\frac{t}{2}}^{t} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}}(\pi'_t\overrightarrow{\pi_n},\vec{y},\lambda_{j'})\mathrm{d}\lambda_{j'}.
\end{aligned}
\tag{S2.27}
$$

Thus, from equations (S2.24) and (S2.27) we have for any fixed $i' \le \lceil \frac{t}{2} \rceil$,

$$
\begin{aligned}
&\sum_{\pi'_t}\int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda'_{j'}}(\pi'_t\overrightarrow{\pi_n},\vec{y},\lambda'_{j'})\mathrm{d}\lambda'_{j'}\\
=&\frac{2r\min\left(1,\frac{t}{2r}-i'+1\right)}{t}\sum_{\pi'_t}\int_{\frac{t}{2}}^{t} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}}(\pi'_t\overrightarrow{\pi_n},\vec{y},\lambda_{j'})\mathrm{d}\lambda_{j'}\\
=&\frac{2r\min\left(1,\frac{t}{2r}-i'+1\right)}{t}\frac{t}{2}\sum_{\pi'_t} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y}}(i',\pi'_t\overrightarrow{\pi_n},\vec{y})\\
=&\,r\min\left(1,\frac{t}{2r}-i'+1\right)\sum_{\pi'_t} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y}}(i',\pi'_t\overrightarrow{\pi_n},\vec{y}).
\end{aligned}
\tag{S2.28}
$$

By combining equations (S2.22) and (S2.28) we have

$$
\begin{aligned}
&\sum_{\pi'_t}\int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda'_{j'}}(\pi'_t\overrightarrow{\pi_n},\vec{y},\lambda'_{j'})\mathrm{d}\lambda'_{j'}\\
=&\,r\min\left(1,\frac{t}{2r}-i'+1\right)\sum_{\pi'_t} f_{[(\Pi_t)^{-1}]_1,\overrightarrow{\Pi_n},\vec{Y}}(i',\pi'_t\overrightarrow{\pi_n},\vec{y})\\
=&\,r\sum_{\pi'_t}\int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}}(\pi'_t\overrightarrow{\pi_n},\vec{y},\lambda_{j'})\mathrm{d}\lambda_{j'}.
\end{aligned}
$$

Therefore, for any possible $\overrightarrow{\pi_n}, \vec{y}, s_{j'}$, the pdf $f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda'_{j'},S_{j'}}$ of $\overrightarrow{\Pi_n}, \vec{Y}, \Lambda'_{j'}, S_{j'}$

satisfies that

$$\begin{aligned}
&\sum_{\pi_t'} \int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}',S_{j'}}(\pi_t'\overrightarrow{\pi_n},\vec{y},\lambda_{j'}',s_{j'})\mathrm{d}\lambda_{j'}' \\
&= r\sum_{\pi_t'} \int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'},S_{j'}}(\pi_t'\overrightarrow{\pi_n},\vec{y},\lambda_{j'},s_{j'})\mathrm{d}\lambda_{j'},
\end{aligned} \tag{S2.29}$$

because according to Step 2 of the target-decoy procedure, $S_{j'}$ is set as the score ranking i'-th in $S((\pi_t'\overrightarrow{\pi_n})_1[\vec{y}]),\cdots,S((\pi_t'\overrightarrow{\pi_n})_t[\vec{y}])$ no matter $i'-1 < \Lambda_{j'} \leq \min(i',\frac{t}{2r})$ or $i'-1 < \Lambda_{j'}' \leq \min(i',\frac{t}{2r})$ for any fixed $i' \leq \lceil\frac{t}{2r}\rceil$ and π_t'. Therefore, from equation (S2.29) we have the pdf $f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}$ of $L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}$ satisfies that

$$\begin{aligned}
&\sum_{\pi_t'} f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(T,\pi_t'\overrightarrow{\pi_n},\vec{y},s_{j'}) \\
&= \sum_{\pi_t'}\sum_{i'\leq\lceil\frac{t}{2r}\rceil} \int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'},S_{j'}}(\pi_t'\overrightarrow{\pi_n},\vec{y},\lambda_{j'},s_{j'})\mathrm{d}\lambda_{j'} \\
&= \sum_{i'\leq\lceil\frac{t}{2r}\rceil}\sum_{\pi_t'} \int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'},S_{j'}}(\pi_t'\overrightarrow{\pi_n},\vec{y},\lambda_{j'},s_{j'})\mathrm{d}\lambda_{j'} \\
&= \frac{1}{r}\sum_{i'\leq\lceil\frac{t}{2r}\rceil}\sum_{\pi_t'} \int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}',S_{j'}}(\pi_t'\overrightarrow{\pi_n},\vec{y},\lambda_{j'}',s_{j'})\mathrm{d}\lambda_{j'}' \\
&= \frac{1}{r}\sum_{\pi_t'}\sum_{i'\leq\lceil\frac{t}{2r}\rceil} \int_{i'-1}^{\min(i',\frac{t}{2r})} f_{\overrightarrow{\Pi_n},\vec{Y},\Lambda_{j'}',S_{j'}}(\pi_t'\overrightarrow{\pi_n},\vec{y},\lambda_{j'}',s_{j'})\mathrm{d}\lambda_{j'}' \\
&= \frac{1}{r}\sum_{\pi_t'} f_{L_{j'},\overrightarrow{\Pi_n},\vec{Y},S_{j'}}(D,\pi_t'\overrightarrow{\pi_n},\vec{y},s_{j'}).
\end{aligned}$$

The first equality is due to that $L_{j'}=T$ if and only if $\Lambda_{j'} \leq \frac{t}{2r}$ and the last equality is due to that $L_{j'}=D$ if and only if $\Lambda_{j'}' \leq \frac{t}{2r}$. Thus, the pdf

$f_{L_{j'},S_{j'}}$ of $L_{j'}, S_{j'}$ satisfies that

$$\begin{aligned} f_{L_{j'},S_{j'}}(T, s_{j'}) &= \int \sum_{\overrightarrow{\pi_n}} f_{L_{j'},\overrightarrow{\Pi_n},\overrightarrow{Y},S_{j'}}(T, \overrightarrow{\pi_n}, \overrightarrow{y}, s_{j'})\mathrm{d}y \\ &= \int \frac{\sum_{\overrightarrow{\pi_n}} \sum_{\pi_t'} f_{L_{j'},\overrightarrow{\Pi_n},\overrightarrow{Y},S_{j'}}(T, \pi_t'\overrightarrow{\pi_n}, \overrightarrow{y}, s_{j'})}{t!}\mathrm{d}y \\ &= \frac{1}{r}\int \frac{\sum_{\overrightarrow{\pi_n}} \sum_{\pi_t'} f_{L_{j'},\overrightarrow{\Pi_n},\overrightarrow{Y},S_{j'}}(D, \pi_t'\overrightarrow{\pi_n}, \overrightarrow{y}, s_{j'})}{t!}\mathrm{d}y \\ &= \frac{1}{r} f_{L_{j'},S_{j'}}(D, s_{j'}). \end{aligned} \tag{S2.30}$$

The second equality is due to that for any given $\overrightarrow{\pi_n}$, there are $t!$ pairs $\{\pi_t', \overrightarrow{\pi_n}'\}$ such that $\pi_t'\overrightarrow{\pi_n}' = \overrightarrow{\pi_n}$ where $\overrightarrow{\pi_n}' = (\pi_t')^{-1}\overrightarrow{\pi_n}$. Thus, $f_{L_{j'},\overrightarrow{\Pi_n},\overrightarrow{Y},S_{j'}}(T, \overrightarrow{\pi_n}, \overrightarrow{y}, s)$ is counted for $t!$ times. From equation (S2.30) we have for any j' where $H_{j'} = 0$ and any possible $s_{j'}$,

$$\Pr(L_{j'} = T \big| S_{j'} = s_{j'}) = \frac{\Pr(L_{j'} = D \big| S_{j'} = s_{j'})}{r}.$$

Now it is easy to verify that for any fixed $1 \le j \le m$,

$$\begin{aligned} &\Pr\left(Z_{(j)} = -1 \big| \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \\ =& r \Pr\left(Z_{(j)} = 1 \big| \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \end{aligned}$$

holds by following the proof of Theorem 1 after equation (S1.13).

Case 2: permutations sampled without replacement. It is straightforward to get a proof by combining the proof of Theorem 1 for the case without replacement and that of Theorem 2 for the case with replacement. □

S3 Proof of Theorem 3

The proof of Theorem 3 is based on the following three lemmas.

Lemma 1. *Let r be a positive constant and $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$ be independent random variables such that* $\Pr(Z_{(i_j)} = -1) = r/(r+1), \Pr(Z_{(i_j)} = 1) = 1/(r+1)$ *for any fixed* $1 \le j \le m'$. *Let* $L = \max\{j : Z_{(i_1)} = Z_{(i_2)} = \cdots = Z_{(i_j)} = 1\}$ *if* $Z_{(i_1)} = 1$. *Otherwise, let L be 0. Then* $\mathbb{E}(L) < 1/r$.

Proof of Lemma 1. For any $j < m'$, the probability that $Z_{(i_1)} = Z_{(i_2)} = \cdots = Z_{(i_j)} = 1$ and $Z_{(i_{j+1})} = -1$ is $1/(r+1)^j \times r/(r+1)$. The probability that $Z_{(i_1)} = Z_{(i_2)} = \cdots = Z_{(i_{m'})} = 1$ is $1/(r+1)^{m'}$. Then we have

$$\mathbb{E}(L) = \sum_{j=0}^{m'-1} j\left(\frac{1}{r+1}\right)^j \frac{r}{r+1} + m'\left(\frac{1}{r+1}\right)^{m'}.$$

Since

$$\sum_{j=0}^{m'-1} j\left(\frac{1}{r+1}\right)^j = \frac{r+1}{r^2}\left[1 - \frac{m'r+1}{(r+1)^{m'}}\right],$$

we have

$$\mathbb{E}(L) < \frac{r+1}{r^2}\left[1 - \frac{m'r}{(r+1)^{m'}}\right]\frac{r}{r+1} + m'\left(\frac{1}{r+1}\right)^{m'} = \frac{1}{r}.$$

□

Lemma 2. *Let p be a positive constant and $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$ be independent random variables such that* $\Pr(Z_{(i_j)} = -1) = p, \Pr(Z_{(i_j)} = 1) = 1-p$ *for any fixed* $1 \le j \le m'$. *Let* $L = \max\{j : Z_{(i_1)} = Z_{(i_2)} = \cdots = Z_{(i_j)} = 1\}$

if $Z_{(i_1)} = 1$*. Otherwise, let* L *be* 0*. Then for any nonnegative constants* c_1 *and* c_2 *satisfying* $c_1 + c_2 \le m'$*,*

$$\mathbb{E}\big(L \big| \#\{Z_{(i_j)} = 1, j \le c_1 + c_2\} = c_1\big) \ge \frac{c_1}{c_2 + 1}.$$

Proof of Lemma 2. If $c_2 = 0$, the lemma is immediate. Consider the case $c_2 > 0$. Under the condition $\#\{Z_{(i_j)} = 1, j \le c_1 + c_2\} = c_1$, the probabilities for $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{c_1+c_2})}$ being all sequences consisting of c_1 elements equal to 1 and c_2 elements equal to -1 are the same because $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$ are independent and identically distributed. Then the c_2 elements equal to -1 separate the c_1 elements equal to 1 into $c_2 + 1$ intervals, and every element equal to 1 falls into each interval with the same probability. Then the probability is $1/(c_2 + 1)$, and the expected number of elements falling into each interval is $c_1/(c_2 + 1)$. L is the number of elements equal to 1 which fall into the interval before the first -1, then the expectation of L is also $c_1/(c_2 + 1)$. □

Lemma 3. *Let* p *be a positive constant and* $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$ *be random variables taking values in* $\{1, -1\}$*. If for any* $1 \le j \le m'$ *and any possible* $\overrightarrow{z_{(i_{\neq j})}}$*,*

$$\Pr\left(Z_{(i_j)} = 1 \middle| \overrightarrow{Z_{(i_{\neq j})}} = \overrightarrow{z_{(i_{\neq j})}}\right) = p, \tag{S3.31}$$

then $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$ *are independent.*

Proof of Lemma 3. We will prove the following claim: for any integer constant $2 \leq C \leq m'$, any C random variables in $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$ are independent. Lemma 3 is a special case of this claim where $C = m'$. If $c_1 = 2$, the claim is immediate. Now we will prove that the claim holds for $C = c \leq m'$ based on the inductive assumption that any $c-1$ variables in $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$ are independent. From equation (S3.31) we have

$$\begin{aligned}
\Pr\left(Z_{(i_1)} = 1\right) &= \sum_{\overrightarrow{z_{(i_{\neq 1})}}} \Pr\left(Z_{(i_1)} = 1, \overrightarrow{Z_{(i_{\neq 1})}} = \overrightarrow{z_{(i_{\neq 1})}}\right) \\
&= \sum_{\overrightarrow{z_{(i_{\neq 1})}}} \Pr\left(Z_{(i_1)} = 1 \middle| \overrightarrow{Z_{(i_{\neq 1})}} = \overrightarrow{z_{(i_{\neq 1})}}\right) \Pr\left(\overrightarrow{Z_{(i_{\neq 1})}} = \overrightarrow{z_{(i_{\neq 1})}}\right) \\
&= p \sum_{\overrightarrow{z_{(i_{\neq 1})}}} \Pr\left(\overrightarrow{Z_{(i_{\neq 1})}} = \overrightarrow{z_{(i_{\neq 1})}}\right) \\
&= p.
\end{aligned}$$

Similarly, we also have

$$\Pr\left(Z_{(i_1)} = 1 \middle| Z_{(i_2)} = z_{(i_2)}, \cdots, Z_{(i_c)} = z_{(i_c)}\right) = p.$$

Thus,

$$\Pr\left(Z_{(i_1)} = 1 \middle| Z_{(i_2)} = z_{(i_2)}, \cdots, Z_{(i_c)} = z_{(i_c)}\right) = \Pr\left(Z_{(i_1)} = 1\right).$$

Similarly, we also have

$$\Pr\left(Z_{(i_1)} = -1 \middle| Z_{(i_2)} = z_{(i_2)}, \cdots, Z_{(i_c)} = z_{(i_c)}\right) = 1 - p = \Pr\left(Z_{(i_1)} = -1\right).$$

Then, we have

$$\Pr\left(Z_{(i_1)} = z_{(i_1)} \middle| Z_{(i_2)} = z_{(i_2)}, \cdots, Z_{(i_c)} = z_{(i_c)}\right) = \Pr\left(Z_{(i_1)} = z_{(i_1)}\right).$$

Meanwhile, by the inductive assumption that $Z_{i_2}, Z_{i_3}, \cdots, Z_{i_c}$ are independent, we have

$$\Pr\left(Z_{(i_2)} = z_{(i_2)}, \cdots, Z_{(i_c)} = z_{(i_c)}\right) = \prod_{j=2}^{c} \Pr\left(Z_{(i_j)} = z_{(i_j)}\right).$$

Thus, by the above two equalities, we have

$$\begin{aligned}
&\Pr\left(Z_{(i_1)} = z_{(i_1)}, Z_{(i_2)} = z_{(i_2)}, \cdots, Z_{(i_c)} = z_{(i_c)}\right) \\
&= \Pr\left(Z_{(i_1)} = z_{(i_1)}\right) \prod_{j=2}^{c} \Pr\left(Z_{(i_j)} = z_{(i_j)}\right) \\
&= \prod_{j=1}^{c} \Pr\left(Z_{(i_j)} = z_{(i_j)}\right).
\end{aligned}$$

Similarly, we can also prove that all the other c variables in $Z_{i_1}, Z_{i_2}, \cdots, Z_{i_{m'}}$ are independent. □

Proof of Theorem 3. Let $V = \#\{Z_{(j)} = 1, j \leq K\}, \widehat{V} = \#\{Z_{(j)} < 0, j \leq K\}, \widehat{V}' = \#\{Z_{(j)} = -1, j \leq K\}$ and $R = \#\{Z_{(j)} \geq 0, j \leq K\}$. Note that for any $1 \leq j \leq m$, we have $|Z_{(j)}|$ is 0,1 or 2. Let $\overrightarrow{|Z_{(\cdot)}|}$ denote $|Z_{(1)}|, |Z_{(2)}|, \cdots, |Z_{(m)}|$. Let $\vec{a}$ denote $a_1, \cdots, a_m$ where $a_j \in \{0, 1, 2\}$ for any $1 \leq j \leq m$. If for any possible $\vec{a}$ and $\overrightarrow{s_{(\cdot)}}$,

$$\mathbb{E}\left(\frac{V}{R \vee 1} \middle| \overrightarrow{|Z_{(\cdot)}|} = \vec{a}, \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}\right) \leq \alpha, \tag{S3.32}$$

then from the law of total expectation, we have

$$\mathbb{E}\left(\frac{V}{R\vee 1}\right)=\mathbb{E}\left(\mathbb{E}\left(\frac{V}{R\vee 1}\middle|\overrightarrow{|Z_{(\cdot)}|}=\vec{a},\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}}\right)\right)\leq\alpha.$$

Therefore, we only need to prove equation (S3.32) for any possible $\vec{a}$ and $\overrightarrow{s_{(\cdot)}}$.

Let $\overrightarrow{a_{\neq j}}$ denote $a_1,\cdots,a_{j-1},a_{j+1},\cdots,a_m$. For any possible $\vec{a}$, $\overrightarrow{z_{(\neq j)}}$ and $\overrightarrow{s_{(\cdot)}}$ where $\overrightarrow{\left|z_{(\neq j)}\right|}=\overrightarrow{a_{\neq j}}$, if $a_j\neq 1$ we have

$$\begin{aligned}&\Pr\left(Z_{(j)}=-1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}},\overrightarrow{|Z_{(\cdot)}|}=\vec{a}\right)\\=&\,r\Pr\left(Z_{(j)}=1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}},\overrightarrow{|Z_{(\cdot)}|}=\vec{a}\right)=0.\end{aligned}$$

If $a_j=1$, we have

$$\begin{aligned}&\Pr\left(Z_{(j)}=-1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}},\overrightarrow{|Z_{(\cdot)}|}=\vec{a}\right)\\=&\Pr\left(Z_{(j)}=-1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}},\left|Z_{(j)}\right|=1\right)\\=&\frac{\Pr\left(Z_{(j)}=-1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}}\right)}{\Pr\left(\left|Z_{(j)}\right|=1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}}\right)}\\=&\frac{r\Pr\left(Z_{(j)}=1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}}\right)}{\Pr\left(\left|Z_{(j)}\right|=1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}}\right)}\\=&\,r\Pr\left(Z_{(j)}=1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}},\left|Z_{(j)}\right|=1\right)\\=&\,r\Pr\left(Z_{(j)}=1\middle|\overrightarrow{S_{(\cdot)}}=\overrightarrow{s_{(\cdot)}},\overrightarrow{Z_{(\neq j)}}=\overrightarrow{z_{(\neq j)}},\overrightarrow{|Z_{(\cdot)}|}=\vec{a}\right).\end{aligned}$$

The third equality is due to Theorem 2 in the main text. In summary, we have for any fixed $1\leq j\leq m$ and any possible $\vec{a}$, $\overrightarrow{z_{(\neq j)}}$ and $\overrightarrow{s_{(\cdot)}}$ where

$\overrightarrow{\left|z_{(\neq j)}\right|} = \overrightarrow{a_{\neq j}}$,

$$\Pr\left(Z_{(j)} = -1 \middle| \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}, \overrightarrow{|Z_{(\cdot)}|} = \vec{a}\right)$$
$$= r \Pr\left(Z_{(j)} = 1 \middle| \overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}, \overrightarrow{|Z_{(\cdot)}|} = \vec{a}\right)$$

always holds. In other words,

$$\Pr\left(Z_{(j)} = -1 \middle| \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) = r \Pr\left(Z_{(j)} = 1 \middle| \overrightarrow{Z_{(\neq j)}} = \overrightarrow{z_{(\neq j)}}\right) \qquad \text{(S3.33)}$$

holds under the condition $\overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}, \overrightarrow{|Z_{(\cdot)}|} = \vec{a}$.

In the following we will assume that $\overrightarrow{S_{(\cdot)}} = \overrightarrow{s_{(\cdot)}}$ and $\overrightarrow{|Z_{(\cdot)}|} = \vec{a}$ always hold for some fixed $\overrightarrow{s_{(\cdot)}}$ and $\vec{a}$, and omit this condition in equations. Moreover, all the random variables and expectations are considered under this condition. Let $m' = \#\{a_i | a_i = 1\}$. Then there are in total m' elements, $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$, equal to 1 or -1. Note that $i_1, i_2, \cdots, i_{m'}$ are constants because $\overrightarrow{|Z_{(\cdot)}|} = \vec{a}$ for some fixed $\vec{a}$.

For any fixed $1 \leq j \leq m'$ and any possible $\overrightarrow{z_{(i_{\neq j})}}$ where $\left|z_{(i_{j'})}\right| = 1$ for all $j' \in \{1, \cdots, j-1, j, \cdots, m'\}$, from equation (S3.33) we have

$$\Pr\left(Z_{(i_j)} = -1 \middle| \overrightarrow{Z_{(i_{\neq j})}} = \overrightarrow{z_{(i_{\neq j})}}\right) = r \Pr\left(Z_{(i_j)} = 1 \middle| \overrightarrow{Z_{(i_{\neq j})}} = \overrightarrow{z_{(i_{\neq j})}}\right).$$

Because $|Z_{(i_j)}| = 1$, we have

$$\Pr\left(Z_{(i_j)} = 1 \middle| \overrightarrow{Z_{(i_{\neq j})}} = \overrightarrow{z_{(i_{\neq j})}}\right) + \Pr\left(Z_{(i_j)} = -1 \middle| \overrightarrow{Z_{(i_{\neq j})}} = \overrightarrow{z_{(i_{\neq j})}}\right) = 1.$$

Therefore, we have

$$\Pr\left(Z_{(i_j)} = 1 \middle| \overrightarrow{Z_{(i_{\neq j})}} = \overrightarrow{z_{(i_{\neq j})}}\right) = \frac{1}{1+r}.$$

Therefore, from Lemma 3, we have $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$ are independent.

Let $L = \max\{j : Z_{(i_1)} = Z_{(i_2)} = \cdots = Z_{(i_j)} = 1\}$ if $Z_{(i_1)} = 1$. Otherwise, let L be 0. Note that there are V elements equal to 1 and $\widehat{V}'$ elements equal to -1 in $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{V+\widehat{V}'})}$. Therefore,

$$\#\{Z_{i_j} = 1, j \leq V + \widehat{V}'\} = V.$$

By applying Lemma 2 to $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$, we have

$$\mathbb{E}(L \big| V = c_1, \widehat{V}' = c_2) = \mathbb{E}\big(L \big| \#\{Z_{i_j} = 1, j \leq c_1 + c_2\} = c_1\big) \geq \frac{c_1}{c_2 + 1}.$$

Therefore,

$$\begin{aligned}\mathbb{E}(L) &= \sum_{c_1, c_2} \mathbb{E}(L|V = c_1, \widehat{V}' = c_2) \Pr(V = c_1, \widehat{V}' = c_2) \\ &\geq \sum_{c_1, c_2} \frac{c_1}{c_2 + 1} \Pr(V = c_1, \widehat{V}' = c_2) = \mathbb{E}\Big(\frac{V}{\widehat{V}' + 1}\Big).\end{aligned}$$

By applying Lemma 1 to $Z_{(i_1)}, Z_{(i_2)}, \cdots, Z_{(i_{m'})}$, we have $\mathbb{E}(L) < \frac{1}{r}$. Then

$$\mathbb{E}\Big(\frac{V}{\widehat{V}' + 1}\Big) \leq \mathbb{E}(L) < \frac{1}{r}.$$

From the definitions of $\widehat{V}'$ and $\widehat{V}$, we have $\widehat{V}' \leq \widehat{V}$ and

$$\mathbb{E}\Big(\frac{V}{\widehat{V} + 1}\Big) \leq \mathbb{E}\Big(\frac{V}{\widehat{V}' + 1}\Big) < \frac{1}{r}. \tag{S3.34}$$

Recall that $\widehat{V} = \#\{Z_{(j)} < 0, j \leq K\}$ and $R = \#\{Z_{(j)} \geq 0, j \leq K\}$. If $R > 0$, from the definition of K, we have

$$\frac{1}{r} \times \frac{\widehat{V} + 1}{R \vee 1} \leq \alpha.$$

Thus,

$$R \geq \frac{\widehat{V} + 1}{r\alpha},$$

and then

$$\frac{V}{R \vee 1} \leq \frac{r\alpha V}{\widehat{V} + 1}. \tag{S3.35}$$

If $R = 0$, we have $V \leq R = 0$ and $V/(R \vee 1) = 0 = r\alpha V/(\widehat{V} + 1)$. Thus, equation (S3.35) always holds no matter $R > 0$ or $R = 0$. Then from equations (S3.34) and (S3.35) we have

$$\mathbb{E}\left(\frac{V}{R \vee 1}\right) \leq \mathbb{E}\left(\frac{r\alpha V}{\widehat{V} + 1}\right) < r\alpha \times \frac{1}{r} = \alpha.$$

$\square$