Abstract: For the better part of a century, methods have been illustrated for the enumeration of all possible permutations of cases from which an exact characterization of the likelihood of obtaining results as or more extreme as that observed may be determined without having to rely on parametric assumptions or schemes that may be only asymptotically correct. The challenge is the computational intensity associated with these methods, which is largely overcome with the wide availability of inexpensive, powerful computational resources. The algorithm presented here is given in two versions, one a general form that can be adapted to a wide variety of permutation tests and a specialized one that is efficient for the exact analog to the dependent- \( t \) test. The application is illustrated using Charles Darwin's \textit{Zea mays} data, which presents a modest task of accounting for \( 2^{15} = 32,768 \) permutations. The resultant algorithm improves on that of Odiase and Ogbonmwan and is presented in syntax that may be run in R, the open source statistical package.

Keywords: Algorithm, Paired Observations, Permutation, Exact Test, P-Value, R

Introduction

Permutation tests have been explicated for nearly a century, so the premise of being able to escape the bonds of parametric tests that are correct only under strong assumptions-and asymptotically at that-is well-known. The usual arguments against the use of permutation (or "exact") tests are: (a) they are more computationally intensive than ordinary parametric or rank-based nonparametric tests; and (b) they are not always available in standard statistical packages. In the first instance, Fisher (1966) noted that his analysis of Charles Darwin's \textit{Zea mays} data set of 15 paired corn plant heights required \( 2^{15} = 32,768 \) permutations. It has been suggested (Ludbrook and Dudley, 1998) that the effort required may have proved a deterrent to Fisher's further use of permutation tests. That's a conclusion consistent with the first argument. However, since that time, computational power has increased dramatically and large-scale, voluntary operations have been established for tackling massive problem sets, such as the Berkeley Open Infrastructure for Network Computing (BOINC; http://boinc.berkeley.edu/), which currently boasts nearly 300,000 volunteers and exceeds 7.3 peta FLOPS of computing power on a daily average. Even on a modest personal computer, Fisher's analysis can be completed in under 0.2 s, using the R package, which is not uniformly optimized for speed. The availability issue is also fading as an argument.

Towards that end, there have been many publications of algorithms to assist in the computation of permutation tests. As a specific example, Odiase and Ogbonmwan (2007) outlined an algorithm suitable for the matched-pairs case of score comparisons. This article presents an improved algorithm and mildly optimized method for the R statistical package that can be used with data sets of any size.

Permutation Tests

As far back as Pitman (1937a; 1937b), the logic of permutation tests has been well-explicated. More recently, excellent explanations from Edgington and Onghena (2007; Manly, 2007) are available. The basic logic is to compare the observed results ("base") to the sample space of all permissible permutations of the scores-what defines permissible permutations depends on the nature of the test. If the number of permutation instances in which the results are as extreme or more extreme than the base results is a sufficiently small fraction of the sample space (e.g., less than one's
threshold for classifying a result as non-chance), then we characterize the result as statistically significant. If not, then the result is declared non-significant. It is a simple framework that can easily be extended.

For comparisons involving two sets of scores, there are three principal sets of permissible permutations. For an independent groups comparison (analogous to the independent t-test), the population of permissible permutations is “n choose r” (Edgington and Onghena, 2007; Manly, 2007; Pitman, 1937a), in which all possible combinations of \( n_1 \) and \( n_2 \) cases are created from the combined set of scores, \( N \). For a correlation coefficient, the population of permissible permutations is \( n! \) (Pitman, 1937b), in which each “\( x \)” score is systematically paired with a different “\( y \)” score. Finally, for a dependent or matched-pairs design, the population of permissible permutations is \( 2^r \) (Fisher, 1966; Ludbrook and Dudley, 1998). The definition of permissible permutations in some classes of designs, however, may require careful thought (Heyvaert and Onghena, 2014) for the class of designs called single subject design.

Materials and Methods

In this presentation, the goal is to present an improved and general algorithm to serve as the basis for permutation tests. It can be used for either independent or matched pairs (dependent) data sets, though the application presented here is strictly for matched pairs sets. In this section, more detailed information is given about: (a) the algorithm presented; and (b) efficiency considerations for implementation of the algorithm in the circumstance of matched pairs data sets.

Permutation Algorithm

The general form of the algorithm presented below can be used to process cases for the paired cases permutation test, or it can also be easily adapted to independent group tests. The algorithm presented by Odiase and Ogbonmwan (2007) relied on hard coding of for loops, one for each case in the data set. The current algorithm may be applied to any sample size without additional coding and is therefore much more portable. The logic is based on the FORTRAN algorithm AS 88 by Gentleman (1975). The result of a single call to the algorithm is that, internally, all subsets of size \( r \) from the \( N \) cases are generated in lexicographic order (e.g., for “5 choose 3”, the 10 resulting sets of cases would be \{1,2,3\} \{1,2,4\} \{1,2,5\} \{1,3,4\} \{1,3,5\} \{1,4,5\} \{2,3,4\} \{2,3,5\} \{2,4,5\} and \{3,4,5\}). These subsets are not saved in memory; rather, after each is generated, the permuted data set is processed and a running tally of results is updated. Other solutions to enumerating the “\( n \) choose \( r \)” options have also been published (Nijenhuis and Wilf, 1978), though those often must be called once for each permutation cycle. The general form below assumes that: (a) the data vector being processed, \( X_i \), represents the difference scores (\( X_{ri}-X_{3i} \)) for each of the \( N \) pairs of cases, \( i = 1, 2, \ldots, N \) and there are no missing values; (b) for a paired cases (dependent) data set, the algorithm is externally called \( N \) times, for \( r = 1, 2, \ldots, N \) and the results within each cycle recorded appropriately against the base (initially observed) result, which represents the case of \( r = 0 \); and (c) the user accumulates the appropriate computation or outcome for each cycle (represented by “PROCESS DATA” in the algorithm).

Algorithm allnr: n Choose r Function in R Syntax

1. allnr <- function(n, r, x) {  
2.   # n is number of cases; r is number to be permuted;  
3.   x is vector of difference scores  
4.   # initialize local variables (note: “#” signifies a comment in R)  
5.   nmr <- (n-r)# n minus r. R can use either “=” or “<-” for assignment statements  
6.   i <- 1  # index.  
7.   j <- c(1:r)  
8.   # create vector to store the chosen case index numbers for a cycle  
9.   # main loop cycles ‘n choose r’ times  
10.  while (i > 0) {  
11.    # R does not have an increment function like C (e.g., + =)  
12.    for (k in ip1:r) { j[k] <- j[k-1] + 1 }  
13.    }  
14.    # end of if loop  
15.  }  
16.  # PROCESS DATA call or insert the data processing here, on chosen cases j[1],j[2],...,j[r]  
17.  i <- r  
18.  while (j[i] >= nmr + i) {  
19.    if (i == 0) break }  
20.   # exit routine when i reaches 0  
21.   j[i] <- j[i] + 1  
22.   # otherwise, increment the index and continue  
23.  }  
24.  # end of main while loop  
25.  }  
26.  # end of function

Efficiency Considerations for Paired Observations

There are several ways that the generation of a permutation test for paired data may be made more efficient. First, the number of permutation cycles that actually have to be generated is only \( 2^r/2 \), not \( 2^r \). The reason is, in the permutation analog to the paired or dependent t-test, the exchange under investigation for a given case is only considering the second score of a pair to come first for an instance, instead of the first score. So, if a case’s values are exchanged, the resulting difference is the negative of the original difference (e.g.,
A second consideration for efficiency is that, for the permutation analog to the dependent t, the sum of the differences is a sufficient statistic for determining whether the results of a permuted data set would equal, exceed, or be less than the originally observed result for a data set. Thus, all the processing step need involve is computation of the sum of the difference scores for a given permutation. This brings up a third efficiency step. In generating that sum, one can sum the exchanged differences, not the full set. These three considerations have been incorporated into the exact.dep.t function and its corresponding version of function allnr, presented in the Appendix. A sample call, using the Darwin data set, also is included.

```
# Local variables
# i = index
# ip1 = i plus 1
# j = vector to store case number/index of chosen cases (1..r) for a given cycle
# nmr = n minus r
#
# initialize local variables
# outcome[1] = number of instances wherein permuted result = base result
# outcome[2] = number of instances wherein permuted result > base result
# outcome[3] = number of instances wherein permuted result < base result
# outcome[4] = number of permutations generated thus far
# outcome[5] = target number of permutations to generate ( = 1/2 of 2^n)

def allnr(n, r, data, base, outcome):
    # R implementation of Algorithm AS 88 by J.F. Gentleman (1975). Applied Statistics, 24, 374-376.
    #
    # n = number of elements in set
    # r = number of elements to be drawn
    # data = vector of scores from which to draw

    # base = base statistic from data set as recorded
    # outcome[1] = number of instances wherein permuted result = base result
    # outcome[2] = number of instances wherein permuted result > base result
    # outcome[3] = number of instances wherein permuted result < base result
    # outcome[4] = number of permutations generated thus far
    # outcome[5] = target number of permutations to generate ( = 1/2 of 2^n)

    # This procedure generates all subsets of r cases out of the set of n.
    # Current processing is set up for matched pairs permutation test.

    if abs(x - base) < 1.0e-7:
        outcome[1] = outcome[1] + 1
    else:
        if x > base:
            outcome[2] = outcome[2] + 1
        else:
            outcome[3] = outcome[3] + 1

    if (abs(x - base) > 1.0e-7) & (x < base):
        outcome[4] = outcome[4] + 1
        for (k in ip1:r): j[k] <- j[k - 1] + 1

        # for dependent t, sum of difference values is sufficient statistic for magnitude
        x <- base - 2.0 * sum(data[j])

        if (abs(x - base) < 1.0e-7) {
            outcome[1] <- outcome[1] + 1
            # equal to base value
        } else {
            outcome[2] <- outcome[2] + 1
            # more extreme than base

        } # end if

    # reset loop indices
    # i = i plus 1
    # nmr = n minus r
    #
    # more extreme than base
```

A second consideration for efficiency is that, for the permutation analog to the dependent t, the sum of the differences is a sufficient statistic for determining whether the results of a permuted data set would equal, exceed, or be less than the originally observed result for a data set. Thus, all the processing step need involve is computation of the sum of the difference scores for a given permutation. This brings up a third efficiency step. In generating that sum, one can sum the exchanged differences only, then subtract twice that sum from the base sum of differences (e.g., permutation sum of differences = base difference-2*sum of exchanged differences). As an example, let the original differences set be (2, 4, 1.5, 1, 3), summing to 11.5. If we exchange the values for cases # 2 and 5, the resulting differences would be (2, -4, 1.5, 1, -3), summing to -2.5. The shortcut described here is to instead take 11.5-2*(4 + 3) = 11.5-14 = -2.5. In other words, we need only sum the exchanged differences, not the full set. These three considerations have been incorporated into the exact.dep.t function and its corresponding version of function allnr, presented in the Appendix. A sample call, using the Darwin data set, also is included.
else outcome[3] <- outcome[3] + 1
# less extreme than base

# process symmetric case result
x <- -x
if (abs(x-base) < 1.0e-7) {outcome[1] <- outcome[1] + 1
# equal to base value
} else if (x > base) {outcome[2] <- outcome[2] + 1
# more extreme than base
} else outcome[3] <- outcome[3] + 1
# less extreme than base

outcome[4] <- outcome[4] + 1
# increment total 'cycles' processed
if (r == ndiv2)
{if (outcome[4] == outcome[5]) break}
# early exit if half of all permutations done
i = r
while (j[i] >= nmr + i)  { i = i - 1; if (i == 0) break}
# exit main loop when i = 0
j[i] <- j[i] + 1
}
# main loop end

return (outcome)
}

exact.dep.t <- function (data) {

n <- length(data)               # number of cases, no check
base <- sum(data)               # total of difference scores;
used as referent (e.g., r = 0th case)
if (base > 0) {
  outcome <- c(1,0,1,1)         # vector of comparisons.
  [1] = results equal to data obtained (base value)
  } else if (base < 0) {
    # [2] = results more than base
    outcome <- c(-1,0,1,1)        # [3] = results less less
    } else outcome <- c(2,0,0,1)  # [4] = number of
    # extrem.equal and symmetric
    outcome[5] <- sum(choose(n,0:n)) %/% 2 # [5] = half
    of the total possible permutations; this is number needed.

for (i in 1:(n %/% 2))         # lexicographic
  # distribution of outcomes is symmetric; only need to
  # process half
  { outcome <- allnr(n, i, data, base, outcome) } } # cycle
allnr for instances r = 1, 2,...,n (0 is base case)

prob1 <- (outcome[1] + outcome[2]) / total          # 1 tail
prob2 <- 2.0 * prob1                                  # 2 tail

if (prob2 > 1.0) prob2 <- 1.0                       # cap
probability at 1

# output results
print (paste0('Observed mean difference ', base / n))
print (paste0('More extreme instances ', outcome[2]))
print (paste0('Equal instances          ', outcome[1]))
print (paste0('Less extreme instances   ', outcome[3]))
print ()
print (paste0('One-tail probability     ', prob1))
print (paste0('Two-tail probability     ', prob2))
}

# Sample call in R, using Darwin data (diff = vector,
# Cross-fertilized plant height – Self-fertilized height)
diff = c(6.125, -8.375, 1.0, 2.0, 0.75, 2.875, 3.5, 5.125,
1.75, 3.625, 7.0, 3.0, 9.375, 7.5, -6.0)
exact.dep.t(diff)               # diff is a vector of differences
in matched pairs observations

Results

The full implementation of the permutation test was evaluated using the Darwin data on corn plant heights (N = 15). As reported by Odiase and Ongbonmwan (2007), there were 835 permutations in which the results were more extreme than those observed in the original data, 28 permutation trials in which the results were equal to the original data and 31,905 instances in which the results were less than those originally observed. Thus, as a directional (“one-tailed”) probability under the null hypothesis of no difference, the p-value is computed as (28+835)/32,768 = 863/32,768 = 0.026337. The non-directional (“two-tailed”) result would evaluate as a p-value of twice as much, (2 * 863)/32,768 = 0.0526733. These values agree with Odiase and Ongbonmwan, who correctly reported that the dependent t statistic, applied to the same data, yields p-values of 0.02485 and 0.04970, respectively, for the directional and non-directional tests. Thus, the dependent t test tends to be close, but mis-represents the exact test results.

The performance of the R package is reasonably quick for data sets of moderate size. Some examples of processing speed on an ordinary desktop running Windows 7 (64 bit) via an Intel i7 CPU (3.4 Ghz) are: N = 20 (2^20 = 1,048,576), approximately 5.7 s; N = 25 (2^25 = 33,554,432), about 185.8 s (approximately 32.5 times longer, which is consistent with the change in size), which is not unreasonable for an interpreted language
interface, as R is. For data sets that are substantially larger, it would well be worth the effort to convert the provided code into a compiled form, which would execute more quickly. There are also some vectorized function operations available in R that could profitably be applied, but one design consideration was to keep the code snippets as simple to convert to a different language or framework as possible.

Discussion

Whenever an algorithm is presented, a pertinent question is that of whether alternative methods or routines already exist. The R package has a built-in function, combn, which will generate a set of indices (as column vectors) for an “n choose r” problem. For example, the call, “x<-combn(15,5)” would generate a 5x3003 matrix containing the indices of all combinations in lexicographic order (i.e., x[,1] would include 1,2,3,4,5; x[,2] would be 1,2,3,4,6; and x[,3003] would be [11,12,13,14,15]). That function could be used in lieu of the allnr function presented here. However, there must be sufficient memory to hold the resultant array. As N increases, this could become problematic; the allnr implementation minimizes memory requirements. The Coin package in R is a more fully developed set of easily-called routines, but these are all for independent group tests. The StatExact package (Cytel company), available in stand-alone or as an add-on to IBM SPSS and Systat, is well-known, but is costly and has just recently added the permutation test for matched pairs cases.

This algorithm was developed to allow researchers a simple, no-cost method for implementing the permutation test for matched pairs data sets. By choice, the code was developed to run in the R statistical package, an open-source software project. However, it can easily be converted to many other languages or platforms. The algorithm by Odiase and Ogbonmwan (2007) is functionally satisfactory, but must be revised, by adding or deleting for loops for each possible sample size that one would encounter, which is a slight nuisance for users. No such modification is needed for the present algorithm.

Conclusion

The method described herein yields an exact representation of the permutation method for judging the equivalence of matched pairs data sets. The memory requirements are minimal, the method runs in the most widely used open-source statistical package on the planet and can easily be made a bit more efficient, as shown in the implementation presented in the Appendix. Resampling methods, while easier to program and quick to run, will always yield an approximate result to an exact distribution.

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Ethics

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