

centrifugeR: A Tool for the Non-trivial Balance of Centrifuge Rotors

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January 2020

Abstract

`centrifugeR` finds the numbers of tubes that can be loaded in centrifuge rotors and gives the instructions on how to balance these tubes in cases of equal or unequal masses. The non-trivial solutions given by this R package offer users greater flexibility and more safety in centrifuge operation.

Introduction

Centrifuges are essential laboratory devices for particle fractionation. The improper use of centrifuges poses many associated hazards (Clark 2001). To reduce the risks, it is crucial to balance centrifuge rotors before the operation.

For rotors that employ single-tube buckets, common practices are distributing tubes in opposite buckets, adding a blank tube to counterweight if odd numbers of tubes need to be centrifuged, and placing tubes at 120 degrees to each other if the number of tubes is divisible by three (Peil and Hauryliuk 2010). However, the balance of centrifuge rotors can be achieved by a non-trivial method. It has been proved that for a rotor with n buckets, balancing k identical tubes ($0 \leq k \leq n$) is perfectly possible “if and only if both k and $n - k$ are expressible as linear combinations of prime factors of n with nonnegative coefficients” (Sivek 2010). In other words, the distribution of k loaded buckets and $n - k$ empty buckets in a balanced rotor is fundamentally a superposition of individual sets whose number of elements is a prime divisor of n and whose position in the rotor is exclusive (Peil and Hauryliuk 2010).

The non-trivial method allows users more flexibility in operating centrifuges. Given a centrifuge, users should know possible numbers of identical tubes can be balanced at one time of operation and their corresponding positions in the rotor. In practice, tubes are often different in mass so the mass of lighter tubes must be increased. The `centrifugeR` package is developed to minimize user effort in balancing centrifuge rotors.

Availability

The `centrifugeR` package is written in R (R Core Team 2019) and is available on CRAN (<https://CRAN.R-project.org/package=centrifugeR>). You can install `centrifugeR` from your R console, view its help page, and attach the package:

```
install.packages("centrifugeR")
package?centrifugeR
library(centrifugeR)
```

A web application built on `centrifugeR` and `shiny` (Chang et al. 2019) is available at <https://phamdn.shinyapps.io/centrifugeRGUI/>.

Illustrated Example

To demonstrate the functionality of `centrifugeR`, a typical centrifuge rotor with 30 buckets is considered ($n = 30$). Three prime divisors of n are 2, 3, and 5. A certain number of tubes (k) can be loaded in the rotor

if and only if k and $n - k$ are linear combinations of 2, 3, and 5. Function `rotorCheck()` filters k values that meet this condition.

```
rotorCheck(30)
```

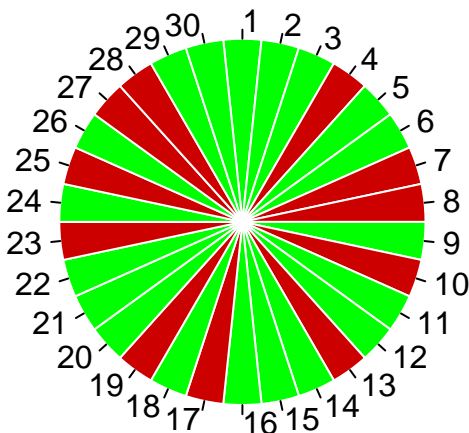
```
## $valid
## [1] 0 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
## [26] 26 27 28 30
##
## $invalid
## [1] 1 29
```

The fact that 1 or 29 tube(s) cannot be loaded in the rotor is obvious. However, some users may find the result surprising as the 30-bucket rotor supports almost all possible numbers of tubes. Users dealing with 19 tubes, for instance, tend to add a blank tube (increase k from 19 to 20) or split tubes into two turns of centrifugation (break k into 16 and 3). Function `rotorEqual()` can find a non-trivial way to balance 19 tubes. There are more than one possibility to express 19 as a linear combination of 2, 3, and 5 (e.g. $19 = 8 \times 2 + 1 \times 3 + 0 \times 5$ and $19 = 2 \times 2 + 0 \times 3 + 3 \times 5$). Not all of them work since the position of individual sets in the rotor must be exclusive. `rotorEqual()` performs random sampling to provide users with a solution (Figure 1).

```
rotorEqual(30, 19)
```

```
## $loaded
## [1] 1 2 3 5 6 9 11 12 14 15 16 18 20 21 22 24 26 29 30
##
## $empty
## [1] 4 7 8 10 13 17 19 23 25 27 28
```

Centrifuge rotor with 30 buckets



19 loaded buckets (in green) and 11 empty buckets (in red)

Figure 1: The distribution of 19 tubes of equal mass in a 30-bucket rotor given by `rotorEqual()`.

In the case of tubes of unequal initial mass, it is not necessary to increase the mass of 18 tubes to the mass of the heaviest tube. The only requirement is that tubes in the same set must have the same mass. Function

rotorUnequal() returns the required masses and the positions of tubes (Figure 2).

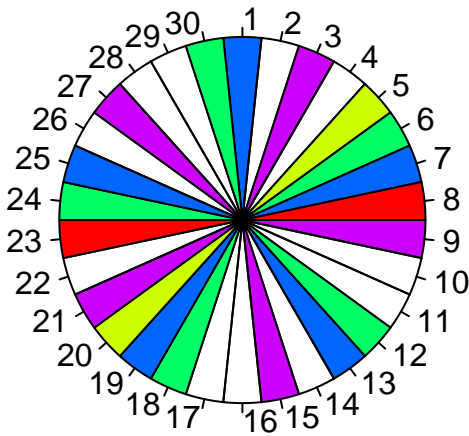
```
samples #mass values of 19 tubes
```

```
## [1] 10.22 9.85 10.10 9.97 9.80 11.51 9.71 11.28 9.88 9.43 10.10 10.30
## [13] 10.17 9.54 9.65 10.50 9.84 9.85 9.76
```

```
rotorUnequal(30, samples)
```

##	initial	required	position
## S10	9.43	9.54	8
## S14	9.54	9.54	23
## S15	9.65	9.71	5
## S7	9.71	9.71	20
## S19	9.76	9.85	6
## S5	9.80	9.85	12
## S17	9.84	9.85	18
## S2	9.85	9.85	24
## S18	9.85	9.85	30
## S9	9.88	10.17	1
## S4	9.97	10.17	7
## S3	10.10	10.17	13
## S11	10.10	10.17	19
## S13	10.17	10.17	25
## S1	10.22	11.51	3
## S12	10.30	11.51	9
## S16	10.50	11.51	15
## S8	11.28	11.51	21
## S6	11.51	11.51	27

Centrifuge rotor with 30 buckets



[2 sets of 2 tubes][3 sets of 5 tubes]

Figure 2: The distribution of 19 tubes of unequal mass in a 30-bucket rotor given by rotorUnequal().

Acknowledgments

The author would like to thank Ms. Martina Schmirl and Dr. Swetlana Herbrandt from the CRAN team for their helpful comments on the package. Thanks to Mr. Tuan-Anh Nguyen for proofreading the package documentation.

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