mRMRe: an R package for parallelized mRMR ensemble feature selection

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1 Introduction

mRMRe is an R package for parallelized mRMR ensemble feature selection.

1.1 Installation and Settings

mRMRe requires that Rcpp is installed. These should be installed automatically when you install mRMRe. Install mRMRe from CRAN or Bioconductor using biocLite function.

```
> install.packages("mRMRe")
```

Load mRMRe into your current workspace:

> library(mRMRe)

The mRMRe package allows its users to set the number of threads it will use for computations. One should may consider the following method to avoid crowding computing clusters, or fully utilize them.

```
> set.thread.count(2)
```

Load the example dataset *cgps* into your current workspace:

```
> data(cgps)
> data.annot <- data.frame(cgps.annot)
> data.cgps <- data.frame(cgps.ic50, cgps.ge)</pre>
```

1.2 Requirements

mRMRe has only been tested on Windows and Linux platforms. It requires that the openMP C library be installed on the hosts on which the package is intended to run.

2 Measures of Associtation

2.1 Mutual Information Matrix

mRMRe offers a fully parallelized implementation to compute the Mutual Information Matrix (MIM). The object $data_cgps$ should be a dataframe with samples/observations in rows and features/variables in columns. The method supports the following column types: "numeric" ("integer" or "double"), "ordered factor" and "Surv". Mutual information (MI) between two columns is estimated using a linear approximation based on correlation such that MI is estimated as $I(x,y) = -\frac{1}{2} \ln{(1-\rho(x,y)^2)}$, where I and ρ respectively represent the MI and correlation coefficient between features x and y. Correlation between continuous variables can be computed using either Pearson's or Spearman's estimators, while Cramer's V and Somers' Dxy index are used for correlation between discrete variables and between continuous variables and survival data, respectively.

```
> ## Test on a dummy dataset.
>
> # Create a dummy data set
> library(survival)
 df <- data.frame(</pre>
      "surv1" = Surv(runif(100),
                      sample(0:1, 100, replace = TRUE)),
      "cont1" = runif(100),
      "disc1" = factor(sample(1:5, 100, replace = TRUE),
                        ordered = TRUE),
      "surv2" = Surv(runif(100),
                      sample(0:1, 100, replace = TRUE)),
      "cont2" = runif(100),
      "cont3" = runif(100),
      "surv3" = Surv(runif(100),
                      sample(0:1, 100, replace = TRUE)),
      "disc2" = factor(sample(1:5, 100, replace = TRUE),
                        ordered = TRUE))
> dd <- mRMR.data(data = df)</pre>
> # Show a partial mutual information matrix.
> print(mim(subsetData(dd, 1:4, 1:4)))
```

```
surv1
                    cont1
                               disc1
                                          surv2
surv1 0.0000000 0.2231436 0.0204110 0.08717669
cont1 0.2231436
                      Inf 0.1218333
disc1 0.0204110 0.1218333
                                 Inf
                                            Inf
surv2 0.0000000
                      Inf
                                 Inf 0.0000000
> ## Test on the 'cgps' dataset, where the
> ## variables are all of continuous type.
> dd <- mRMR.data(data = data.cgps)</pre>
> dd <- subsetData(dd, 1:10, 1:10)</pre>
> # Uses Spearman as correlation estimator
> spearman_mim <- mim(dd, continuous_estimator = "spearman")</pre>
> print(spearman_mim[1:4, 1:4])
              cgps.ic50 geneid_3310 geneid_2978 geneid_6352
                    Inf 0.025796493 0.000900719 0.108915849
cgps.ic50
geneid_3310 0.025796493
                                 Inf 0.017968244 0.002227175
geneid_2978 0.000900719 0.017968244
                                             Inf 0.050207046
geneid_6352 0.108915849 0.002227175 0.050207046
                                                          Inf
> # Uses Pearson as correlation estimator
> pearson_mim <- mim(dd, continuous_estimator = "pearson")</pre>
> print(pearson_mim[1:4, 1:4])
               cgps.ic50 geneid_3310 geneid_2978 geneid_6352
                     Inf 0.02104964 7.541758e-05 0.09249434
cgps.ic50
                                  Inf 2.450671e-02 0.02740061
geneid_3310 2.104964e-02
geneid_2978 7.541758e-05 0.02450671
                                               Inf
                                                    0.05790450
geneid_6352 9.249434e-02 0.02740061 5.790450e-02
                                                            Inf
```

2.2 Correlations

The mRMRe package offers an efficient, stratified and weighted implementation of the major correlation estimators: Cramer's V, Somers Dxy index (based on the concordance index), Pearson, Spearman correlation coefficients.

```
> # Compute c-index between feature 1 and 2
> correlate(cgps.ge[, 1], cgps.ge[, 2], method = "cindex")
> # Compute Cramer's V
> x <- sample(factor(c("CAT_1", "CAT_2", "CAT_3"),
                      ordered = TRUE), 100, replace = TRUE)
> y <- sample(factor(c("CAT_1", "CAT_2"),</pre>
                      ordered = TRUE), 100, replace = TRUE)
> correlate(x, y, method = "cramersv")
> # Compute Pearson coefficient with random strata and
> # sample weights between features 1 and 2
> strata <- sample(factor(c("STRATUM_1", "STRATUM_2",</pre>
                             "STRATUM_3"),
+
                          ordered = TRUE),
                          nrow(cgps.ge), replace = TRUE)
> weights <- runif(nrow(cgps.ge))</pre>
> correlate(cgps.ge[, 1], cgps.ge[, 2], strata = strata,
            weights = weights, method = "pearson")
```

3 mRMR Feature Selection

mRMRe offers a highly efficient implementation of the mRMR feature selection [2, 4]. The two crucial aspects of our implementation consists first, in parallelizing the key steps of the algorithm and second, in using a lazy procedure to compute only the part of the MIM that is required during the search for the best set of features (instead of estimating the full MIM).

3.1 Classic mRMR

Here is an example of the classic mRMR feature selection [2].

```
> dd <- mRMR.data(data = data.cgps)
> mRMR.classic(data = dd, target_indices = c(1),
+ feature_count = 30)
```

3.2 Ensemble mRMR

```
> dd <- mRMR.data(data = data.cgps)
> # For mRMR.classic-like results
```

4 Fixed Selected Features

The mRMRe package allows to select the features with some features being fixed selected, also supports the return with/without the fixed ones

5 Causality Inference

The mRMRe package allows one to infer causality through the use of the co-information lattice method [1, 3].

6 Session Info

- R Under development (unstable) (2023-04-24 r84317), x86_64-pc-linux-gnu
- Locale: LC_CTYPE=C.UTF-8, LC_NUMERIC=C, LC_TIME=C.UTF-8, LC_COLLATE=C, LC_MONETARY=C.UTF-8, LC_MESSAGES=C.UTF-8, LC_PAPER=C.UTF-8, LC_NAME=C, LC_ADDRESS=C, LC_TELEPHONE=C, LC_MEASUREMENT=C.UTF-8, LC_IDENTIFICATION=C

- Time zone: Europe/Vienna
- TZcode source: system (glibc)
- Running under: Debian GNU/Linux 12 (bookworm)
- Matrix products: default
- BLAS: /home/Hornik/tmp/R-d-gcc-12/lib/libRblas.so
- LAPACK: /usr/lib/x86_64-linux-gnu/lapack/liblapack.so.3.11.0
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: igraph 1.4.2, mRMRe 2.1.2.1, survival 3.5-5
- Loaded via a namespace (and not attached): Matrix 1.5-4, cli 3.6.1, compiler 4.4.0, grid 4.4.0, lattice 0.21-8, magrittr 2.0.3, pkgconfig 2.0.3, rlang 1.1.0, splines 4.4.0, tools 4.4.0

References

- [1] A J Bell. The co-information lattice. In S Amari, A Cichocki, S Makino, and N Murata, editors, *Proceedings of the Fifth International Workshop on Independent Component Analysis and Blind Signal Separation: ICA 2003*, 2003.
- [2] Chris Ding and Hanchuan Peng. Minimum redundancy feature selection from microarray gene expression data. *Journal of bioinformatics and computational biology*, 3(2):185–205, April 2005.
- [3] W McGill. Multivariate information transmission. *IEEE Transactions* on *Information Theory*, 4(4):93–111, September 1954.
- [4] P. E. Meyer, C. Schretter, and Gianluca Bontempi. Information-Theoretic Feature Selection in Microarray Data Using Variable Complementarity. Selected Topics in Signal Processing, IEEE Journal of, 2(3):261–274, 2008.