Processed human microRNA-overexpression data from GEO, and sequence information from TargetScan, and targetScore from TargetScore

Yue Li
yueli@cs.toronto.edu

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1 MicroRNA perturbation datasets

We collected 84 Gene Expression Omnibus (GEO) series corresponding to 6 platforms, 77 human cells or tissues, and 112 distinct miRNAs. To our knowledge, this is by far the largest miRNA-overexpression data compendium. To automate the data download and processing, we developed a pipeline written in R, making use of the function `getGEO` from *GEOquery* R/Bioconductor package (Davis and Meltzer [2007]). For each dataset, the pipeline downloads the raw or processed data (if available) and calculates (when necessary) the log fold-change (logFC) in treatment (miRNA transfected) vs (mock) control, taking into account the unique properties of each data. Next, we combined all of the logFC data columns into a single $N \times M$ matrix for all of the $N = 19177$ RefSeq mRNAs (NM_* obtained from UCSC) and $M = 286$ datasets. Missing data (logFC) for some genes across studies were imputed using `impute.knn` from *impute* R package (Troyanskaya et al. [2001]). For miRNA transfection data having multiple measurements (in different studies), we picked the one whose logFC correlate the most with the validated targets from mirTarBase Hsu et al. [2011] or average them if no validated target available.

```
> library(TargetScoreData)
> transfection_data <- get_miRNA_transfection_data()$transfection_data
> datasummary <-
+ list(  `MicroRNA` = table(names(transfection_data)),
+                 `GEO Series` = table(sapply(transfection_data, function(d
+                 `Platform` = table(sapply(transfection_data, function(df)
+                 `Cell/Tissue` = table(sapply(transfection_data, function(
> print(lapply(datasummary, length))

$MicroRNA
[1] 113

$`GEO Series`
```

```
[1] 84

$Platform
[1] 6

$`Cell/Tissue`
[1] 77
```

2 TargetScan context score and PCT

TargetScan context score and PCT for all of the predicted sites (including conserved and nonconserved sites) downloaded from TargetScan website (`http://www.targetscan.org/cgi-bin/targetscan/data_download.cgi?db=vert_61`)

```
> targetScanCS <- get_TargetScanHuman_contextScore()
> targetScanPCT <- get_TargetScanHuman_PCT()
> head(targetScanCS)
```

```
  Gene Symbol Transcript ID           miRNA 3prime pairing local AU positio
1        A1CF     NM_138932 hsa-miR-4711-3p         -0.018   -0.095   -0.108
2        A1CF     NM_138933 hsa-miR-4711-3p         -0.018   -0.095   -0.108
3        A1CF     NM_014576 hsa-miR-4711-3p         -0.018   -0.095   -0.108
4        A1CF  NM_001198820 hsa-miR-4711-3p         -0.018   -0.095   -0.108
5        A1CF  NM_001198819 hsa-miR-4711-3p         -0.018   -0.095   -0.108
6        A1CF  NM_001198818 hsa-miR-4711-3p         -0.018   -0.095   -0.108
     TA   SPS context+ score context+ score percentile
1 0.003 0.017         -0.448                       99
2 0.003 0.017         -0.448                       99
3 0.003 0.017         -0.448                       99
4 0.003 0.017         -0.448                       99
5 0.003 0.017         -0.448                       99
6 0.003 0.017         -0.448                       99
```

```
> dim(targetScanCS)
```

```
[1] 9569357      10
```

```
> head(targetScanPCT)
```

```
           miR Family Gene Symbol Transcript ID  PCT
1         miR-22/22-3p        A1BG     NM_130786 0.00
2     miR-23abc/23b-3p        A1BG     NM_130786 0.00
7   miR-26ab/1297/4465        A1BG     NM_130786 0.00
8        miR-101/101ab        A1BG     NM_130786 0.00
9   miR-103a/107/107ab        A1BG     NM_130786 0.00
10 miR-103a/107/107ab        A1BG     NM_130786 0.09
```

```
> dim(targetScanPCT)
[1] 2938804       4
```

3 TargetScore

Encouraged by the superior performance of TargetScore (manuscript in peer-review), we applied TargetScore to all of the transfection data above. For further exploring miRNA targetome and their associations, we enclose the targetScores results in this package.

```
> targetScoreMatrix <- get_precomputed_targetScores()
> head(names(targetScoreMatrix))
[1] "hsa-miR-34b"  "hsa-miR-34c"  "hsa-miR-205"  "hsa-miR-124"  "hsa-miR-1"
[6] "hsa-miR-181a"
> head(targetScoreMatrix[[1]])
               logFC targetScanCS targetScanPCT targetScore
SGIP1    0.077526011         0.00             0  0.03489650
AGBL4    0.020639084         0.00             0  0.03388637
NECAP2   0.078650400         0.00             0  0.03492518
CLIC4    0.016043400        -0.03             0  0.24335149
ADC     -0.002303429         0.00             0  0.03417828
SLC45A1 -0.018655797         0.00             0  0.03457975
```

We can reproduce targetScores using the above data as demonstrated in the following example (require *TargetScore* package). As a convenience function, we applied a wrapper function called `getTargetScores` that does the following: (1) given a miRNA ID, obtain fold-change(s) from logFC.imputed matrix or use the user-supplied fold-changes; (2) retrives TargetScan context score (CS) and PCT (if found); (3) obtain validated targets from the local mirTarBase file; (4) compute targetScore. We apply `getTargetScores` function using miRNA hsa-miR-1, which we know has all three types of data, namely logFC, targetScan context score, and PCT.

```
> library(TargetScore)
> library(gplots)
> myTargetScores <- getTargetScores("hsa-miR-1", tol=1e-3, maxiter=200)
> table((myTargetScores$targetScore > 0.1), myTargetScores$validated) # a v
> # obtain all of targetScore for all of the 112 miRNA
>
> logFC.imputed <- get_precomputed_logFC()
> mirIDs <- unique(colnames(logFC.imputed))
>
> # takes time
>
> # targetScoreMatrix <- mclapply(mirIDs, getTargetScores)
>
> # names(targetScoreMatrix) <- mirIDs
```

4 Session Info

```
> sessionInfo()

R version 3.3.0 (2016-05-03)
Platform: x86_64-pc-linux-gnu (64-bit)
Running under: Ubuntu 14.04.4 LTS

locale:
 [1] LC_CTYPE=en_US.UTF-8       LC_NUMERIC=C
 [3] LC_TIME=en_US.UTF-8        LC_COLLATE=C
 [5] LC_MONETARY=en_US.UTF-8    LC_MESSAGES=en_US.UTF-8
 [7] LC_PAPER=en_US.UTF-8       LC_NAME=C
 [9] LC_ADDRESS=C               LC_TELEPHONE=C
[11] LC_MEASUREMENT=en_US.UTF-8 LC_IDENTIFICATION=C

attached base packages:
[1] stats     graphics  grDevices utils     datasets  methods   base

other attached packages:
[1] TargetScoreData_1.8.0

loaded via a namespace (and not attached):
[1] tools_3.3.0
```

References

Sean Davis and Paul S Meltzer. GEOquery: a bridge between the Gene Expression Omnibus (GEO) and BioConductor. *Bioinformatics (Oxford, England)*, 23(14):1846–1847, July 2007.

Sheng-Da Hsu, Feng-Mao Lin, Wei-Yun Wu, Chao Liang, Wei-Chih Huang, Wen-Ling Chan, Wen-Ting Tsai, Goun-Zhou Chen, Chia-Jung Lee, Chih-Min Chiu, Chia-Hung Chien, Ming-Chia Wu, Chi-Ying Huang, Ann-Ping Tsou, and Hsien-Da Huang. miRTarBase: a database curates experimentally validated microRNA-target interactions. *Nucleic acids research*, 39 (Database issue):D163–9, January 2011.

O Troyanskaya, M Cantor, G Sherlock, P Brown, T Hastie, R Tibshirani, D Botstein, and R B Altman. Missing value estimation methods for DNA microarrays. *Bioinformatics (Oxford, England)*, 17(6):520–525, June 2001.