

BISC 577a, Spring 2017

Second Assignment for 3rd section of the course (Rohs)

(1) Application of an open-source and distributed revision control project

(a)

Branch: master ▾	New pull request	Create new file	Upload files	Find file	Clone or download ▾
This branch is 1 commit ahead of rohslab:master. Pull request Compare					
🔑 keith6902 committed on GitHub Update README.md Latest commit a90010c a day ago					
📁 CTF	Add files via upload	12 days ago			
📁 examples	Add files via upload	10 days ago			
📁 gcPBM	Add files via upload	12 days ago			
📄 README.md	Update README.md	a day ago			
📄 your_report.pdf	Add files via upload	12 days ago			
📄 your_script.R	Add files via upload	11 days ago			

(b)

📄 README.md

BISC577

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(c)

(2) High-throughput binding assays

(a) SELEX-seq is an experimental and computational platform used to characterize DNA-binding specificities and determine the relative affinities to any DNA sequence. PBM is a high-throughput technique for characterizing sequence specificity of DNA-binding proteins in vitro.

(b) ChIP-seq is method used to analyze protein interactions with DNA, which combines chromatin immunoprecipitation with massively parallel DNA sequencing to identify the binding sites of DNA-associated proteins.

(c) PBM is good for general characterization of binding specificity for multiple proteins. However, ChIP-seq is good for identifying gene targets bound/regulated under a specific condition. SELEX-seq is more accurate than PBM and ChIP-seq models.

(3) Preparation of high-throughput in vitro data analysis

(a)

```

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/emoise_1.1.0.zip'
Content type 'application/zip' length 29661 bytes (29 KB)
downloaded 29 KB

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/Rcpp_0.12.10.zip'
Content type 'application/zip' length 3316935 bytes (3.2 MB)
downloaded 3.2 MB

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/XML_3.98-1.6.zip'
Content type 'application/zip' length 4305461 bytes (4.1 MB)
downloaded 4.1 MB

package 'XML' successfully unpacked and MD5 sums checked
package 'emoise' successfully unpacked and MD5 sums checked
package 'Rcpp' successfully unpacked and MD5 sums checked
package 'XML' successfully unpacked and MD5 sums checked

The downloaded binary packages are in
C:\Users\xiaoqiang\AppData\Local\Temp\RtmpGuz2H0\downloaded_packages
Warning in install.packages(update[instlib == 1, "Package"], 1, repos = repos, s
  'lib' = "C:/Program Files/R/R-3.3.2/library") is not writable
Error in install.packages(update[instlib == 1, "Package"], 1, repos = repos, :
  unable to install packages
>

```

(b)

```

> ## try http:// if https:// URLs are not supported
> source("https://bioconductor.org/biocLite.R")
Bioconductor version 3.4 (BioInstaller 1.24.0), 'BiocLite' for help
A new version of Bioconductor is available after installing the most recent
version of R: see http://bioconductor.org/install
> biocLite()
Bioc_mirror: https://bioconductor.org
Using Bioconductor 3.4 (BioInstaller 1.24.0), R 3.3.2 (2016-10-31).
Installation path not writeable, unable to update packages: boot, cluster,
foreign, lattice, MASS, Matrix, mgcv, nlme, rpart, survival
Old packages: 'BiocParallel', 'GenomicAlignments', 'GenomicFeatures',
'GenomicRanges', 'IRanges', 'Rsamtools', 'rtracklayer', 'S4Vectors', 'XML',
'XVector'
Update all/some/none? [a/s/n]: a

There is a binary version available but the source version is later:
  binary      source needs compilation
XML 3.98-1.6  3.98-1.7      TRUE

Binaries will be installed
trying URL 'https://bioconductor.org/packages/3.4/bioc/bin/windows/contrib/3.3/
Content type 'application/zip' length 1334913 bytes (1.3 MB)
downloaded 1.3 MB

trying URL 'https://bioconductor.org/packages/3.4/bioc/bin/windows/contrib/3.3/

```

(c)

```

> ## try http:// if https:// URLs are not supported
> source("https://bioconductor.org/biocLite.R")
Bioconductor version 3.4 (BioInstaller 1.24.0), 'BiocLite' for help
A new version of Bioconductor is available after installing the most recent
version of R: see http://bioconductor.org/install
> biocLite("DNAbase")
Bioc_mirror: https://bioconductor.org
Using Bioconductor 3.4 (BioInstaller 1.24.0), R 3.3.2 (2016-10-31).
Installing package(s) 'DNAbase'
also installing the dependencies 'spam', 'maps', 'fields'

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/spam_1.4-0.zip'
Content type 'application/zip' length 1074110 bytes (1.0 MB)
downloaded 1.0 MB

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/maps_3.1.1.zip'
Content type 'application/zip' length 3611720 bytes (3.4 MB)
downloaded 3.4 MB

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/fields_8.10.zip'
Content type 'application/zip' length 360306 bytes (3.4 KB)
downloaded 3.4 KB

trying URL 'https://bioconductor.org/packages/3.4/bioc/bin/windows/contrib/3.3/
Content type 'application/zip' length 7054247 bytes (6.7 MB)

```

(d)

```

> install.packages("colorspace")
Installing package into 'C:/Users/xiaoqiang/Documents/R/win-library/3.3'
(as 'lib' is unspecified)
also installing the dependencies 'colorspace', 'minqa', 'nloptnr', 'RcppEigen', &

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/colorspace_1.3-6
Content type 'application/zip' length 442094 bytes (431 KB)
downloaded 431 KB

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/minqa_1.2.4.zip'
Content type 'application/zip' length 62401 bytes (609 KB)
downloaded 609 KB

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/nloptr_1.6.4.zip'
Content type 'application/zip' length 1172887 bytes (1.1 MB)
downloaded 1.1 MB

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/RcppEigen_0.3.36
Content type 'application/zip' length 2631370 bytes (2.5 MB)
downloaded 2.5 MB

trying URL 'https://cloud.r-project.org/bin/windows/contrib/3.3/RColorBrewer_1.8
Content type 'application/zip' length 26706 bytes (26 KB)
downloaded 26 KB

```

(4) Build prediction models for in vitro data

(a)

Mad 1-mer+shape

```

[1] [2] [3] [4] [5] [6] [7] [8] [9] [10] [11] [12] [13]
seq1 0 0 1 0 0 0 0 1 0 0 0 1 0 0
seq2 0 1 0 0 0 0 0 1 0 0 0 1 0 0
seq3 0 0 1 0 0 0 0 1 0 0 1 0 0 0

[14] [15] [16] [17] [18] [19] [20] [21] [22] [23] [24]
seq1 1 0 0 1 0 0 0 0 0 0 0 0 1
seq2 0 1 0 0 0 0 1 0 1 0 0 0 0
seq3 0 1 0 0 0 0 1 0 0 0 1 0 0

[25] [26] [27] [28] [29] [30] [31] [32] [33] [34] [35]
seq1 0 0 1 0 1 0 0 0 0 1 0 0
seq2 0 0 1 0 0 0 0 1 0 1 0 0
seq3 0 1 0 0 0 0 1 0 0 0 0 1

[36] [37] [38] [39] [40] [41] [42] [43] [44] [45] [46]
seq1 0 1 0 0 0 0 0 0 1 0 0 1
seq2 0 0 0 1 0 0 1 0 0 0 0 1
seq3 0 0 0 1 0 0 0 0 1 0 0 1

[47] [48] [49] [50] [51] [52] [53] [54] [55] [56] [57]
seq1 0 0 0 1 0 0 0 1 0 0 0 0

```

```

seq2  0  0  1  0  0  0  0  1  0  0  0
seq3  0  0  1  0  0  0  0  0  0  1  0
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seq2  1  0  0  0  1  0  0  1  0  0  0
seq3  1  0  0  0  1  0  0  1  0  0  0
      [,69] [,70] [,71] [,72] [,73] [,74] [,75] [,76] [,77] [,78] [,79]
seq1  0  1  0  0  0  0  1  0  0  0  0
seq2  0  1  0  0  0  0  1  0  0  1  0
seq3  0  1  0  0  0  0  1  0  0  0  0
      [,80] [,81] [,82] [,83] [,84] [,85] [,86] [,87] [,88] [,89] [,90]
seq1  1  0  0  1  0  0  0  1  0  0  0
seq2  0  0  0  1  0  0  1  0  0  0  1
seq3  1  0  0  1  0  0  0  1  0  0  0
      [,91] [,92] [,93] [,94] [,95] [,96] [,97] [,98] [,99] [,100] [,101]
seq1  0  1  0  0  0  1  0  0  0  1  0
seq2  0  0  1  0  0  0  0  1  0  0  1
seq3  1  0  0  0  0  1  0  1  0  0  0
      [,102] [,103] [,104] [,105] [,106] [,107] [,108] [,109] [,110] [,111]
seq1  0  0  1  0  0  1  0  0  1  0  0
seq2  0  0  0  0  0  1  0  0  1  0  0
seq3  0  1  0  0  0  1  0  0  0  1  0
      [,112] [,113] [,114] [,115] [,116] [,117] [,118] [,119] [,120] [,121]
seq1  0  1  0  0  0  0  0  1  0  0  0
seq2  0  1  0  0  0  1  0  0  0  0  0
seq3  0  0  1  0  0  0  0  0  0  1  0
      [,122] [,123] [,124] [,125] [,126] [,127] [,128] [,129] [,130] [,131]
seq1  1  0  0  1  0  0  0  1  0  0  0
seq2  0  1  0  0  0  0  0  1  0  1  0
seq3  1  0  0  0  1  0  0  0  0  0  0
      [,132] [,133] [,134] [,135] [,136] [,137] [,138] [,139] [,140] [,141]
seq1  0  0  0  1  0  0  0  0  1  0  0
seq2  0  0  1  0  0  0  0  0  1  0  0
seq3  1  0  0  1  0  0  0  1  0  0  0
      [,142] [,143] [,144] [,145] [,146] [,147] [,148] [,149]
seq1  0  1  0.6477612 0.7402985 0.7910448 0.7223881 0.7910448
seq2  0  1  0.6238806 0.5701493 0.5970149 0.6208955 0.5820896
seq3  0  0  1.07283582 0.7522388 0.6298507 0.5731343 0.6268657
      [,150] [,151] [,152] [,153] [,154] [,155] [,156]
seq1 0.7611940 0.4507463 0.3522388 0.3940299 0.5014925 0.7791045 0.8089552
seq2 0.5313433 0.6567164 0.5432836 0.5014925 0.7791045 0.8089552 0.5731343
seq3 0.6985075 0.6985075 0.6268657 0.6477612 0.7402985 0.7552239 0.5940299
      [,157] [,158] [,159] [,160] [,161] [,162] [,163]
seq1 0.4686567 0.4537313 0.6955224 0.6805970 0.7283582 0.8328358 0.7552239
seq2 0.5402985 0.7641791 0.8328358 0.7164179 0.7014925 0.8029851 0.7641791
seq3 0.6238806 0.8149254 0.8328358 0.5970149 0.5970149 0.8328358 0.7641791
      [,164] [,165] [,166] [,167] [,168] [,169] [,170]
seq1 0.4417910 0.3611940 0.3582090 0.5701493 0.7641791 0.8746269 0.8776119
seq2 0.6597015 0.7791045 0.8805970 0.7373134 0.7343284 0.7223881 0.6656716
seq3 0.5402985 0.4776119 0.5880597 0.8029851 0.7074627 0.6268657 0.5253731
      [,171] [,172] [,173] [,174] [,175] [,176] [,177]
seq1 0.8417910 0.7223881 0.6656716 0.7761194 0.4985075 0.3850746 0.8489078
seq2 0.7761194 0.4985075 0.2656716 0.4955224 0.5850746 0.6179104 0.8834951
seq3 0.5432836 0.6567164 0.5313433 0.6179104 0.7611940 0.6985075 0.8118932
      [,178] [,179] [,180] [,181] [,182] [,183] [,184]
seq1 0.8125000 0.4296117 0.4399272 0.6334951 0.3458738 0.2779126 0.3598301
seq2 0.9144417 0.7226942 0.6529126 0.9751214 0.7099515 0.6334951 0.9696602

```

seq3 0.7754854 0.8367718 0.8847087 0.8361650 0.8040049 0.8040049 0.8361650
[,185] [,186] [,187] [,188] [,189] [,190] [,191]
seq1 0.9077670 0.8343447 0.7572816 0.5703883 0.5989078 0.9484223 0.6183252
seq2 0.8343447 0.7572816 0.5703883 0.6444175 0.7967233 0.8234223 0.5242718
seq3 0.8489078 0.8125000 0.5406553 0.5376214 0.6559466 0.7906553 0.5242718
[,192] [,193] [,194] [,195] [,196] [,197] [,198]
seq1 0.6074029 0.5194175 0.5242718 0.6984223 0.4641990 0.2487864 0.1237864
seq2 0.5175971 0.7148058 0.7457524 0.7961165 0.8209951 0.7572816 0.5570388
seq3 0.4690534 0.4690534 0.5242718 0.8234223 0.7967233 0.6783981 0.5109223
[,199] [,200] [,201] [,202] [,203] [,204] [,205]
seq1 0.1650485 0.3416262 0.7712379 0.7785194 0.5916262 0.8974515 0.7979369
seq2 0.5091019 0.5564320 0.8974515 0.7979369 0.4010922 0.3822816 0.7548544
seq3 0.5928398 0.8246359 0.8361650 0.8513350 0.9696602 0.6334951 0.7099515
[,206] [,207] [,208] [,209] [,210] [,211] [,212]
seq1 0.4010922 0.3822816 0.7299757 0.3945381 0.3893085 0.7576990 0.2562464
seq2 0.5564320 0.6747573 0.9472087 0.3951191 0.3794306 0.4334689 0.3881464
seq3 0.9472087 0.6656553 0.7324029 0.3805927 0.6310285 0.4218478 0.3701336
[,213] [,214] [,215] [,216] [,217] [,218] [,219]
seq1 0.8361418 0.5136549 0.3631610 0.2068565 0.2754213 0.2597327 0.3829169
seq2 0.3201627 0.4195235 0.3759442 0.3381755 0.2969204 0.3829169 0.6589192
seq3 0.3794306 0.4020918 0.6101104 0.4020918 0.3962812 0.3893085 0.7280651
[,220] [,221] [,222] [,223] [,224] [,225] [,226]
seq1 0.6589192 0.3294596 0.3817548 0.3160953 0.4032539 0.7960488 0.3666473
seq2 0.3370134 0.4253341 0.3858222 0.6653109 0.3649041 0.7658338 0.4241720
seq3 0.2382336 0.4369553 0.4677513 0.6717025 0.3393376 0.8256827 0.3393376
[,227] [,228] [,229] [,230] [,231] [,232] [,233]
seq1 0.6891342 0.4665892 0.2667054 0.2492737 0.3126089 0.3271354 0.7466589
seq2 0.6717025 0.3933759 0.4055782 0.6629866 0.3829169 0.7902382 0.3829169
seq3 0.6653109 0.3858222 0.4049971 0.2963393 0.3910517 0.6943637 0.3974433
[,234] [,235] [,236] [,237] [,238] [,239] [,240]
seq1 0.4416037 0.7007554 0.3829169 0.3660662 0.7373620 0.2951772 0.3486345
seq2 0.3660662 0.7373620 0.2951772 0.3131900 0.2277745 0.3625799 0.4398605
seq3 0.3910517 0.3230680 0.3381755 0.3759442 0.4288205 0.3335270 0.6583382
[,241] [,242] [,243] [,244] [,245] [,246]
seq1 0.2359094 0.4050633 0.75105485 0.5344585 0.09845288 0.57383966
seq2 0.3358512 0.3206751 0.37130802 0.3699015 0.65260197 0.07594937
seq3 0.4607786 0.7552743 0.20393812 0.3361463 0.81434599 0.38396624
[,247] [,248] [,249] [,250] [,251] [,252]
seq1 0.5907173 0.69901547 0.75808720 0.2405063 0.9479606 0.32208158
seq2 0.4514768 0.71026723 0.06188467 0.9029536 0.3220816 0.46272855
seq3 0.3375527 0.22362869 0.33755274 0.4022504 0.7510549 0.51758087
[,253] [,254] [,255] [,256] [,257] [,258] [,259]
seq1 0.4627286 0.4472574 0.5836850 0.07735584 0.6343179 0.4078762 0.3811533
seq2 0.4345992 0.5035162 0.3656821 0.45007032 0.3783404 0.3277075 0.6835443
seq3 0.1490858 0.7398031 0.3909986 0.46694796 0.4008439 0.4978903 0.4008439
[,260] [,261] [,262] [,263] [,264] [,265]
seq1 0.4556962 0.5189873 0.6736990 0.80309423 0.8565401 0.6272855
seq2 0.2025316 0.7524613 0.3220816 0.50070323 0.3473980 0.5879044
seq3 0.4500703 0.3656821 0.5007032 0.54008439 0.6526020 0.2672293
[,266] [,267] [,268] [,269] [,270] [,271]
seq1 0.49789030 0.64978903 0.5007032 0.04500703 0.8241913 0.4852321
seq2 0.04922644 0.82419128 0.4852321 0.55836850 0.3094233 0.5991561
seq3 0.36146273 0.37974684 0.8804501 0.06188467 0.7102672 0.4542897
[,272] [,273] [,274]
seq1 0.55836850 0.3066104 0.55836850
seq2 0.69901547 0.4810127 0.03797468
seq3 0.03516174 0.4486639 0.48523207

Mad 1-mer

```
[,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] [,12] [,13]
seq1  0  0  1  0  0  0  1  0  0  0  1  0  0
seq2  0  1  0  0  0  0  1  0  0  0  1  0  0
seq3  0  0  1  0  0  0  1  0  0  1  0  0  0
seq4  0  0  0  1  0  0  1  0  0  1  0  0  0
seq5  0  0  0  1  0  0  1  0  0  1  0  0  0
seq6  0  0  1  0  0  1  0  0  1  0  0  0  0

[,14] [,15] [,16] [,17] [,18] [,19] [,20] [,21] [,22] [,23] [,24]
seq1  1  0  0  1  0  0  0  0  0  0  0  1
seq2  0  1  0  0  0  1  0  1  0  0  0  0
seq3  0  1  0  0  0  1  0  0  1  0  0  0
seq4  0  1  0  0  0  1  0  0  1  0  0  0
seq5  0  0  1  0  1  0  0  0  0  1  0  0
seq6  0  1  0  0  1  0  0  0  0  1  0  0

[,25] [,26] [,27] [,28] [,29] [,30] [,31] [,32] [,33] [,34] [,35]
seq1  0  0  1  0  1  0  0  0  1  0  0  0
seq2  0  0  1  0  0  0  1  0  1  0  0  0
seq3  0  1  0  0  0  1  0  0  0  0  1  0
seq4  0  0  0  1  0  0  0  1  0  1  0  0
seq5  0  1  0  0  0  1  0  0  0  0  0  0
seq6  0  0  1  0  0  1  0  0  0  1  0  0

[,36] [,37] [,38] [,39] [,40] [,41] [,42] [,43] [,44] [,45] [,46]
seq1  0  1  0  0  0  0  0  1  0  0  1  0
seq2  0  0  0  1  0  0  1  0  0  0  1  0
seq3  0  0  0  1  0  0  0  1  0  0  1  0
seq4  0  0  0  1  0  0  0  1  0  0  1  0
seq5  1  0  0  1  0  0  1  0  0  0  1  0
seq6  0  0  1  0  0  0  1  0  0  1  0  0

[,47] [,48] [,49] [,50] [,51] [,52] [,53] [,54] [,55] [,56] [,57]
seq1  0  0  0  1  0  0  1  0  0  0  0  0
seq2  0  0  1  0  0  0  0  1  0  0  0  0
seq3  0  0  1  0  0  0  0  0  0  1  0  0
seq4  0  0  0  0  0  1  0  0  0  1  0  0
seq5  0  0  0  0  0  1  0  0  1  0  0  0
seq6  0  0  0  0  0  1  0  1  0  0  0  0

[,58] [,59] [,60] [,61] [,62] [,63] [,64] [,65] [,66] [,67] [,68]
seq1  1  0  0  0  1  0  0  0  0  0  1
seq2  1  0  0  0  1  0  0  1  0  0  0
seq3  1  0  0  0  1  0  0  1  0  0  0
seq4  1  0  0  0  1  0  0  1  0  0  0
seq5  1  0  0  0  1  0  0  1  0  0  0
seq6  1  0  0  0  1  0  0  1  0  0  0

[,69] [,70] [,71] [,72] [,73] [,74] [,75] [,76] [,77] [,78] [,79]
seq1  0  1  0  0  0  0  1  0  0  0  0
seq2  0  1  0  0  0  0  1  0  0  1  0
seq3  0  1  0  0  0  0  1  0  0  0  0
seq4  0  1  0  0  0  0  1  0  0  1  0
seq5  0  0  0  1  0  0  1  0  0  0  0
seq6  0  1  0  0  0  0  1  0  0  0  0

[,80] [,81] [,82] [,83] [,84] [,85] [,86] [,87] [,88] [,89] [,90]
seq1  1  0  0  1  0  0  0  1  0  0  0
seq2  0  0  0  1  0  0  1  0  0  0  1
seq3  1  0  0  1  0  0  0  1  0  0  0
```

```

seq4  0  0  0  1  0  0  0  1  0  0  1
seq5  1  0  0  1  0  0  1  0  0  1  0
seq6  1  0  0  1  0  0  0  1  0  0  0
    [,91] [,92] [,93] [,94] [,95] [,96] [,97] [,98] [,99] [,100] [,101]
seq1  0  1  0  0  0  1  0  0  0  1  0
seq2  0  0  1  0  0  0  0  1  0  0  1
seq3  1  0  0  0  0  1  0  1  0  0  0
seq4  0  0  1  0  0  0  0  0  0  1  0
seq5  0  0  0  0  1  0  0  1  0  0  0
seq6  0  1  0  0  0  1  1  0  0  0  1
    [,102] [,103] [,104] [,105] [,106] [,107] [,108] [,109] [,110] [,111]
seq1  0  0  1  0  0  1  0  0  1  0
seq2  0  0  0  0  0  1  0  0  1  0
seq3  0  1  0  0  0  1  0  0  0  1
seq4  1  0  0  0  1  0  0  0  0  0
seq5  0  1  0  0  0  1  0  0  1  0
seq6  0  0  0  0  0  1  0  0  0  0
    [,112] [,113] [,114] [,115] [,116] [,117] [,118] [,119] [,120] [,121]
seq1  0  1  0  0  0  0  0  1  0  0
seq2  0  1  0  0  0  1  0  0  0  0
seq3  0  0  1  0  0  0  0  0  1  0
seq4  1  1  0  0  0  0  0  1  0  0
seq5  0  0  1  0  0  0  1  0  0  0
seq6  1  0  0  1  0  0  0  1  0  0
    [,122] [,123] [,124] [,125] [,126] [,127] [,128] [,129] [,130] [,131]
seq1  1  0  0  1  0  0  0  1  0  0
seq2  0  1  0  0  0  0  1  0  1  0
seq3  1  0  0  0  1  0  0  0  0  0
seq4  0  1  0  0  0  0  1  1  0  0
seq5  1  0  0  0  0  0  1  0  0  0
seq6  0  1  0  0  0  0  1  0  0  1
    [,132] [,133] [,134] [,135] [,136] [,137] [,138] [,139] [,140] [,141]
seq1  0  0  0  1  0  0  0  0  1  0
seq2  0  0  1  0  0  0  0  0  1  0
seq3  1  0  0  1  0  0  0  1  0  0
seq4  0  1  0  0  0  0  0  1  0  0
seq5  1  0  0  0  1  0  0  1  0  0
seq6  0  0  0  1  0  0  1  0  0  0
    [,142] [,143] [,144]
seq1  0  1  0
seq2  0  1  0
seq3  0  0  1
seq4  1  0  0
seq5  0  0  1
seq6  1  0  0

```

Max 1-mer+shape

```

    [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] [,12] [,13]
seq1  0  0  1  0  1  0  0  0  1  0  0  0  0
seq2  0  0  0  1  0  1  0  0  0  1  0  0  0
seq3  0  0  1  0  0  0  1  0  0  1  0  0  0
    [,14] [,15] [,16] [,17] [,18] [,19] [,20] [,21] [,22] [,23] [,24]
seq1  0  1  0  0  1  0  0  0  1  0  0
seq2  1  0  0  0  0  1  0  0  0  1  0
seq3  0  1  0  0  1  0  0  0  0  0  1

```

	[,25]	[,26]	[,27]	[,28]	[,29]	[,30]	[,31]	[,32]	[,33]	[,34]	[,35]
seq1	0	1	0	0	0	0	0	1	0	0	1
seq2	0	0	1	0	0	0	1	0	0	1	0
seq3	0	0	1	0	0	1	0	0	0	1	0
	[,36]	[,37]	[,38]	[,39]	[,40]	[,41]	[,42]	[,43]	[,44]	[,45]	[,46]
seq1	0	0	0	1	0	0	1	0	0	0	0
seq2	0	0	0	0	1	1	0	0	0	0	0
seq3	0	0	0	1	0	0	0	1	0	1	0
	[,47]	[,48]	[,49]	[,50]	[,51]	[,52]	[,53]	[,54]	[,55]	[,56]	[,57]
seq1	1	0	0	0	1	0	0	0	1	0	0
seq2	1	0	1	0	0	0	0	0	1	0	0
seq3	0	0	0	1	0	0	0	0	0	1	0
	[,58]	[,59]	[,60]	[,61]	[,62]	[,63]	[,64]	[,65]	[,66]	[,67]	[,68]
seq1	0	1	0	0	1	0	0	0	0	1	0
seq2	0	1	0	0	1	0	0	1	0	0	0
seq3	0	1	0	0	1	0	0	0	0	1	0
	[,69]	[,70]	[,71]	[,72]	[,73]	[,74]	[,75]	[,76]	[,77]	[,78]	[,79]
seq1	0	1	0	0	0	0	1	0	0	0	0
seq2	0	0	0	1	0	0	1	0	0	0	0
seq3	0	1	0	0	0	0	1	0	0	0	0
	[,80]	[,81]	[,82]	[,83]	[,84]	[,85]	[,86]	[,87]	[,88]	[,89]	[,90]
seq1	1	0	0	1	0	0	1	0	0	0	1
seq2	1	0	0	1	0	0	0	1	0	1	0
seq3	1	0	0	1	0	0	0	1	0	1	0
	[,91]	[,92]	[,93]	[,94]	[,95]	[,96]	[,97]	[,98]	[,99]	[,100]	[,101]
seq1	0	0	0	1	0	0	0	0	1	0	0
seq2	0	0	0	1	0	0	0	0	0	1	0
seq3	0	0	0	0	1	0	0	0	0	1	0
	[,102]	[,103]	[,104]	[,105]	[,106]	[,107]	[,108]	[,109]	[,110]	[,111]	
seq1	1	0	0	0	1	0	0	0	0	1	
seq2	1	0	0	1	0	0	0	0	0	1	
seq3	0	1	0	0	0	1	0	0	1	0	
	[,112]	[,113]	[,114]	[,115]	[,116]	[,117]	[,118]	[,119]	[,120]	[,121]	
seq1	0	0	1	0	0	0	1	0	0	0	
seq2	0	0	0	1	0	1	0	0	0	0	
seq3	0	0	0	1	0	0	1	0	0	0	
	[,122]	[,123]	[,124]	[,125]	[,126]	[,127]	[,128]	[,129]	[,130]	[,131]	
seq1	0	1	0	0	1	0	0	0	1	0	
seq2	0	1	0	0	0	1	0	1	0	0	
seq3	0	1	0	0	1	0	0	0	0	0	
	[,132]	[,133]	[,134]	[,135]	[,136]	[,137]	[,138]	[,139]	[,140]	[,141]	
seq1	0	0	0	1	0	0	1	0	0	0	
seq2	0	0	0	0	1	0	0	1	0	1	
seq3	1	0	0	1	0	0	1	0	0	0	
	[,142]	[,143]	[,144]	[,145]	[,146]	[,147]	[,148]	[,149]			
seq1	1	0	0	0.5880597	0.3940299	0.5253731	0.5611940	0.5970149			
seq2	0	0	0	0.6268657	0.6985075	0.6985075	0.6238806	0.5880597			
seq3	0	0	1	0.7641791	0.6955224	0.6805970	0.8417910	0.7641791			
	[,150]	[,151]	[,152]	[,153]	[,154]	[,155]	[,156]				
seq1	0.7611940	0.7701493	0.6597015	0.7283582	0.7313433	0.6238806	0.5880597				
seq2	0.5253731	0.6417910	0.8417910	0.8925373	0.7641791	0.6328358	0.5970149				
seq3	0.6925373	0.7492537	0.7582090	0.6656716	0.4955224	0.6417910	0.7611940				
	[,157]	[,158]	[,159]	[,160]	[,161]	[,162]	[,163]				
seq1	0.6298507	0.7641791	0.8029851	0.7014925	0.7164179	0.8626866	0.8388060				
seq2	0.5880597	0.7402985	0.7910448	0.6388060	0.6865672	0.8805970	0.8149254				
seq3	0.8417910	0.8537313	0.8029851	0.7014925	0.7164179	0.8328358	0.8149254				
	[,164]	[,165]	[,166]	[,167]	[,168]	[,169]	[,170]				

seq1 0.6477612 0.6268657 0.7313433 0.7283582 0.6686567 0.7522388 0.7283582
seq2 0.6985075 0.4955224 0.5014925 0.6089552 0.8089552 0.7820896 0.6179104
seq3 0.6477612 0.5611940 0.5761194 0.7343284 0.7791045 0.6597015 0.7641791
[,171] [,172] [,173] [,174] [,175] [,176] [,177]
seq1 0.6686567 0.7522388 0.7283582 0.6686567 0.7522388 0.7283582 0.5157767
seq2 0.5313433 0.6208955 0.5820896 0.4955224 0.5940299 0.6656716 0.8464806
seq3 0.8029851 0.8029851 0.6955224 0.6805970 0.8417910 0.6895522 0.7961165
[,178] [,179] [,180] [,181] [,182] [,183] [,184]
seq1 0.9077670 0.8513350 0.8877427 0.9933252 0.6656553 0.7991505 0.8209951
seq2 0.8040049 0.8040049 0.8834951 0.8725728 0.8513350 0.9277913 0.6049757
seq3 0.7669903 0.8974515 0.5916262 0.8076456 0.8131068 0.7845874 0.8082524
[,185] [,186] [,187] [,188] [,189] [,190] [,191]
seq1 0.8118932 0.8349515 0.8834951 0.8725728 0.8264563 0.7961165 0.7457524
seq2 0.5782767 0.8064320 0.6146845 0.9593447 0.8574029 0.8125000 0.4296117
seq3 0.6334951 0.5564320 0.7615291 0.5291262 0.7682039 0.7627427 0.7457524
[,192] [,193] [,194] [,195] [,196] [,197] [,198]
seq1 0.7148058 0.5175971 0.4921117 0.7949029 0.8489078 0.8361650 0.8349515
seq2 0.3859223 0.4660194 0.5570388 0.7906553 0.6510922 0.5564320 0.8131068
seq3 0.7148058 0.5175971 0.5242718 0.7906553 0.6711165 0.5922330 0.8009709
[,199] [,200] [,201] [,202] [,203] [,204] [,205]
seq1 0.8118932 0.8094660 0.7754854 0.8118932 0.8094660 0.7754854 0.8118932
seq2 0.5467233 0.6328883 0.6796117 0.9472087 0.7099515 0.6529126 0.9751214
seq3 0.5527913 0.7572816 0.8209951 0.7961165 0.7457524 0.7457524 0.7669903
[,206] [,207] [,208] [,209] [,210] [,211] [,212]
seq1 0.8094660 0.7754854 0.8118932 0.3027310 0.3091226 0.2858803 0.3776874
seq2 0.6808252 0.5376214 0.5546117 0.4450901 0.3957002 0.6101104 0.4003486
seq3 0.8974515 0.5916262 0.7833738 0.3986055 0.6647298 0.3933759 0.3811737
[,213] [,214] [,215] [,216] [,217] [,218] [,219]
seq1 0.3480535 0.3160953 0.6484602 0.4055782 0.3840790 0.6176641 0.3962812
seq2 0.3881464 0.3834980 0.3428239 0.3527019 0.7681580 0.4230099 0.4526438
seq3 0.6990122 0.4189425 0.4230099 0.5967461 0.4654271 0.3765253 0.3137711
[,220] [,221] [,222] [,223] [,224] [,225] [,226]
seq1 0.3881464 0.3939570 0.3997676 0.6717025 0.4241720 0.7658338 0.3672284
seq2 0.3521209 0.3747821 0.3718768 0.7576990 0.2498547 0.8553167 0.3805927
seq3 0.4160372 0.7106334 0.4526438 0.6914585 0.4241720 0.7658338 0.3649041
[,227] [,228] [,229] [,230] [,231] [,232] [,233]
seq1 0.6798373 0.4061592 0.3962812 0.3986055 0.6176641 0.3968623 0.4212667
seq2 0.6531087 0.4729808 0.3660662 0.2701917 0.3463103 0.4212667 0.7274840
seq3 0.6717025 0.4584544 0.3858222 0.3579314 0.3190006 0.6647298 0.4055782
[,234] [,235] [,236] [,237] [,238] [,239] [,240]
seq1 0.6310285 0.3968623 0.4212667 0.6310285 0.3968623 0.4212667 0.6310285
seq2 0.3259733 0.4288205 0.3660662 0.3201627 0.4171993 0.4288205 0.2248693
seq3 0.3933759 0.6717025 0.4311447 0.6722836 0.3933759 0.3811737 0.7100523
[,241] [,242] [,243] [,244] [,245] [,246]
seq1 0.3805927 0.5654008 0.18846695 0.9254571 0.36286920 0.4345992
seq2 0.7315514 0.4472574 0.34599156 0.2236287 0.32208158 0.3727145
seq3 0.3399187 0.7454290 0.17721519 0.8129395 0.04219409 0.4472574
[,247] [,248] [,249] [,250] [,251] [,252]
seq1 0.0281294 0.4528833 0.35302391 0.7580872 0.19127989 0.33333333
seq2 0.3727145 0.8945148 0.05907173 0.5007032 0.07594937 0.62025316
seq3 0.7412096 0.3586498 0.25175809 0.3881857 0.70886076 0.54430380
[,253] [,254] [,255] [,256] [,257] [,258]
seq1 0.37271449 0.39803094 0.7412096 0.2025316 0.6835443 0.3277075
seq2 0.06610408 0.42756681 0.7496484 0.5344585 0.1167370 0.6807314
seq3 0.07594937 0.44303797 0.6526020 0.2348805 0.6835443 0.3277075
[,259] [,260] [,261] [,262] [,263] [,264] [,265]
seq1 0.3952180 0.4978903 0.7524613 0.4022504 0.3488045 0.1912799 0.7510549


```

seq2 0.3319269 0.5091421 0.3980309 0.7046414 0.5597750 0.1462729 0.5794655
seq3 0.3783404 0.4669480 0.4022504 0.6807314 0.1209564 0.4655415 0.4528833
    [,266] [,267] [,268] [,269] [,270] [,271]
seq1 0.3628692 0.20393812 0.7510549 0.362869198 0.20393812 0.75105485
seq2 0.4683544 0.01969058 0.4542897 0.697609001 0.07594937 0.46835443
seq3 0.3220816 0.75246132 0.2025316 0.669479606 0.18565401 0.81293952
    [,272] [,273] [,274]
seq1 0.36286920 0.20393812 0.7552743
seq2 0.73417722 0.15330520 0.5203938
seq3 0.04219409 0.45428973 0.8481013

```

Max 1-mer

```

    [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] [,12] [,13]
seq1  0  0  1  0  1  0  0  0  1  0  0  0  0
seq2  0  0  0  1  0  1  0  0  0  1  0  0  0
seq3  0  0  1  0  0  0  1  0  0  1  0  0  0
seq4  0  0  1  0  0  1  0  0  1  0  0  0  0
seq5  0  0  1  0  0  0  1  0  1  0  0  0  1
seq6  0  0  1  0  0  1  0  0  1  0  0  0  0
    [,14] [,15] [,16] [,17] [,18] [,19] [,20] [,21] [,22] [,23] [,24]
seq1  0  1  0  0  1  0  0  0  1  0  0
seq2  1  0  0  0  0  1  0  0  0  1  0
seq3  0  1  0  0  1  0  0  0  0  0  1
seq4  0  1  0  0  1  0  0  0  0  0  1
seq5  0  0  0  0  0  0  1  0  0  0  1
seq6  0  1  0  0  1  0  0  1  0  0  0
    [,25] [,26] [,27] [,28] [,29] [,30] [,31] [,32] [,33] [,34] [,35]
seq1  0  1  0  0  0  0  0  1  0  0  1
seq2  0  0  1  0  0  0  1  0  0  1  0
seq3  0  0  1  0  0  1  0  0  0  1  0
seq4  0  1  0  0  0  0  1  0  0  1  0
seq5  1  0  0  0  0  1  0  0  0  1  0
seq6  1  0  0  0  0  1  0  0  0  0  1
    [,36] [,37] [,38] [,39] [,40] [,41] [,42] [,43] [,44] [,45] [,46]
seq1  0  0  0  1  0  0  1  0  0  0  0
seq2  0  0  0  0  1  1  0  0  0  0  0
seq3  0  0  0  1  0  0  0  1  0  1  0
seq4  0  0  1  0  0  0  1  0  0  0  0
seq5  0  0  0  0  1  0  0  0  1  0  1
seq6  0  0  0  1  0  0  0  1  0  1  0
    [,47] [,48] [,49] [,50] [,51] [,52] [,53] [,54] [,55] [,56] [,57]
seq1  1  0  0  0  1  0  0  0  1  0  0
seq2  1  0  1  0  0  0  0  0  1  0  0
seq3  0  0  0  1  0  0  0  0  0  1  0
seq4  1  0  0  0  1  0  0  0  1  0  0
seq5  0  0  1  0  0  0  0  0  0  1  0
seq6  0  0  0  0  1  0  1  0  0  0  0
    [,58] [,59] [,60] [,61] [,62] [,63] [,64] [,65] [,66] [,67] [,68]
seq1  0  1  0  0  1  0  0  0  0  1  0
seq2  0  1  0  0  1  0  0  1  0  0  0
seq3  0  1  0  0  1  0  0  0  0  1  0
seq4  1  0  0  0  1  0  0  1  0  0  0
seq5  1  0  0  0  1  0  0  1  0  0  0
seq6  0  1  0  0  1  0  0  0  0  1  0
    [,69] [,70] [,71] [,72] [,73] [,74] [,75] [,76] [,77] [,78] [,79]

```

```

seq1 0 1 0 0 0 0 1 0 0 0 0
seq2 0 0 0 1 0 0 1 0 0 0 0
seq3 0 1 0 0 0 0 1 0 0 0 0
seq4 0 1 0 0 0 0 1 0 0 1 0
seq5 0 1 0 0 1 0 0 0 0 0 0
seq6 0 1 0 0 0 0 1 0 0 0 0
    [,80] [,81] [,82] [,83] [,84] [,85] [,86] [,87] [,88] [,89] [,90]
seq1 1 0 0 1 0 0 1 0 0 0 1
seq2 1 0 0 1 0 0 0 1 0 1 0
seq3 1 0 0 1 0 0 0 1 0 1 0
seq4 0 0 0 1 0 0 0 1 0 0 0
seq5 1 0 0 1 0 0 0 1 0 0 0
seq6 1 0 0 1 0 0 1 0 0 0 0
    [,91] [,92] [,93] [,94] [,95] [,96] [,97] [,98] [,99] [,100] [,101]
seq1 0 0 0 1 0 0 0 0 1 0 0
seq2 0 0 0 1 0 0 0 0 0 1 0
seq3 0 0 0 0 1 0 0 0 0 1 0
seq4 0 1 0 0 1 0 0 1 0 0 0
seq5 0 1 0 0 0 1 0 0 1 0 1
seq6 1 0 0 1 0 0 0 1 0 0 0
    [,102] [,103] [,104] [,105] [,106] [,107] [,108] [,109] [,110] [,111]
seq1 1 0 0 0 1 0 0 0 0 1
seq2 1 0 0 1 0 0 0 0 0 1
seq3 0 1 0 0 0 1 0 0 1 0
seq4 1 0 0 0 0 1 0 0 0 1
seq5 0 0 0 1 0 0 0 0 0 1
seq6 0 1 0 0 1 0 0 0 1 0
    [,112] [,113] [,114] [,115] [,116] [,117] [,118] [,119] [,120] [,121]
seq1 0 0 1 0 0 0 1 0 0 0
seq2 0 0 0 1 0 1 0 0 0 0
seq3 0 0 0 1 0 0 1 0 0 0
seq4 0 0 1 0 0 0 1 0 0 0
seq5 0 0 1 0 0 0 0 0 1 0
seq6 0 0 1 0 0 0 1 0 0 1
    [,122] [,123] [,124] [,125] [,126] [,127] [,128] [,129] [,130] [,131]
seq1 0 1 0 0 1 0 0 0 1 0
seq2 0 1 0 0 0 1 0 1 0 0
seq3 0 1 0 0 1 0 0 0 0 0
seq4 1 0 0 0 0 0 1 0 1 0
seq5 0 1 0 0 0 1 0 0 1 0
seq6 0 0 0 0 0 1 0 1 0 0
    [,132] [,133] [,134] [,135] [,136] [,137] [,138] [,139] [,140] [,141]
seq1 0 0 0 1 0 0 1 0 0 0
seq2 0 0 0 0 1 0 0 1 0 1
seq3 1 0 0 1 0 0 1 0 0 0
seq4 0 0 0 1 0 0 0 1 0 0
seq5 0 0 0 0 1 0 0 1 0 0
seq6 0 0 1 0 0 0 0 1 0 1
    [,142] [,143] [,144]
seq1 1 0 0
seq2 0 0 0
seq3 0 0 1
seq4 1 0 0
seq5 0 1 0
seq6 0 0 0

```

Myc 1-mer+shape

```
[1] [2] [3] [4] [5] [6] [7] [8] [9] [10] [11] [12] [13]
seq1  1  0  0  0  0  1  0  0  0  1  0  0  0
seq2  1  0  0  0  1  0  0  0  0  1  0  0  1
seq3  0  0  1  0  0  1  0  0  0  0  1  0  0
[14] [15] [16] [17] [18] [19] [20] [21] [22] [23] [24]
seq1  0  1  0  1  0  0  0  0  0  1  0  0
seq2  0  0  0  0  0  1  0  0  1  0  0
seq3  0  1  0  0  1  0  0  0  1  0  0
[25] [26] [27] [28] [29] [30] [31] [32] [33] [34] [35]
seq1  0  1  0  0  0  0  1  0  0  0  1
seq2  0  0  1  0  0  1  0  0  0  1  0
seq3  0  0  1  0  0  0  1  0  0  0  0
[36] [37] [38] [39] [40] [41] [42] [43] [44] [45] [46]
seq1  0  0  1  0  0  0  0  1  0  0  1
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(b)

Max 1mer+shape

glmnet

8568 samples
274 predictor

No pre-processing

Resampling: Cross-Validated (10 fold)

Summary of sample sizes: 7712, 7712, 7712, 7712, 7711, 7709, ...

Resampling results across tuning parameters:

lambda	RMSE	Rsquared
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6. 103516e-05	0. 07979423	0. 8642443
1. 220703e-04	0. 07979423	0. 8642443
2. 441406e-04	0. 07979423	0. 8642443
4. 882812e-04	0. 07979423	0. 8642443
9. 765625e-04	0. 07979423	0. 8642443
1. 953125e-03	0. 07979423	0. 8642443
3. 906250e-03	0. 07979423	0. 8642443
7. 812500e-03	0. 07979423	0. 8642443
1. 562500e-02	0. 08290638	0. 8540335
3. 125000e-02	0. 08986680	0. 8312288
6. 250000e-02	0. 09769390	0. 8074125
1. 250000e-01	0. 10777214	0. 7813023
2. 500000e-01	0. 12195072	0. 7481568
5. 000000e-01	0. 14043919	0. 6996691
1. 000000e+00	0. 16036402	0. 6320349
2. 000000e+00	0. 17803561	0. 5563498
4. 000000e+00	0. 19170124	0. 4906228
8. 000000e+00	0. 20111800	0. 4453291
1. 600000e+01	0. 20705524	0. 4180406
3. 200000e+01	0. 21046932	0. 4031887
6. 400000e+01	0. 21232865	0. 3953357
1. 280000e+02	0. 21430041	NaN
2. 560000e+02	0. 21430041	NaN
5. 120000e+02	0. 21430041	NaN
1. 024000e+03	0. 21430041	NaN
2. 048000e+03	0. 21430041	NaN
4. 096000e+03	0. 21430041	NaN
8. 192000e+03	0. 21430041	NaN
1. 638400e+04	0. 21430041	NaN
3. 276800e+04	0. 21430041	NaN

Max 1mer

glmnet

8568 samples

144 predictor

No pre-processing

Resampling: Cross-Validated (10 fold)

Summary of sample sizes: 7711, 7711, 7711, 7712, 7712, 7711, ...

Resampling results across tuning parameters:

lambda	RMSE	Rsquared
3. 051758e-05	0. 09951122	0. 7855663
6. 103516e-05	0. 09951122	0. 7855663
1. 220703e-04	0. 09951122	0. 7855663
2. 441406e-04	0. 09951122	0. 7855663
4. 882812e-04	0. 09951122	0. 7855663
9. 765625e-04	0. 09951122	0. 7855663
1. 953125e-03	0. 09951122	0. 7855663
3. 906250e-03	0. 09951122	0. 7855663
7. 812500e-03	0. 09952114	0. 7855599

1. 562500e-02	0. 10023432	0. 7851275
3. 125000e-02	0. 10262741	0. 7836586
6. 250000e-02	0. 10921830	0. 7790695
1. 250000e-01	0. 12294778	0. 7666436
2. 500000e-01	0. 14326284	0. 7396933
5. 000000e-01	0. 16519530	0. 6946632
1. 000000e+00	0. 18353022	0. 6392797
2. 000000e+00	0. 19646395	0. 5879465
4. 000000e+00	0. 20452072	0. 5507817
8. 000000e+00	0. 20914209	0. 5278996
1. 600000e+01	0. 21164418	0. 5151166
3. 200000e+01	0. 21294796	0. 5083854
6. 400000e+01	0. 21361675	0. 5048975
1. 280000e+02	0. 21429409	NaN
2. 560000e+02	0. 21429409	NaN
5. 120000e+02	0. 21429409	NaN
1. 024000e+03	0. 21429409	NaN
2. 048000e+03	0. 21429409	NaN
4. 096000e+03	0. 21429409	NaN
8. 192000e+03	0. 21429409	NaN
1. 638400e+04	0. 21429409	NaN
3. 276800e+04	0. 21429409	NaN

Mad 1mer+shape

glmnet

7534 samples
274 predictor

No pre-processing

Resampling: Cross-Validated (10 fold)

Summary of sample sizes: 6782, 6779, 6779, 6780, 6781, 6782, ...

Resampling results across tuning parameters:

lambda	RMSE	Rsquared
3. 051758e-05	0. 3018130	0. 8628934
6. 103516e-05	0. 3018130	0. 8628934
1. 220703e-04	0. 3018130	0. 8628934
2. 441406e-04	0. 3018130	0. 8628934
4. 882812e-04	0. 3018130	0. 8628934
9. 765625e-04	0. 3018130	0. 8628934
1. 953125e-03	0. 3018130	0. 8628934
3. 906250e-03	0. 3018130	0. 8628934
7. 812500e-03	0. 3018130	0. 8628934
1. 562500e-02	0. 3018130	0. 8628934
3. 125000e-02	0. 3018130	0. 8628934
6. 250000e-02	0. 3164769	0. 8494464
1. 250000e-01	0. 3511398	0. 8164869
2. 500000e-01	0. 3841694	0. 7864097
5. 000000e-01	0. 4213171	0. 7589079
1. 000000e+00	0. 4717558	0. 7287667
2. 000000e+00	0. 5383830	0. 6878240

4. 000000e+00	0. 6111583	0. 6315115
8. 000000e+00	0. 6760171	0. 5668379
1. 600000e+01	0. 7249502	0. 5098011
3. 200000e+01	0. 7578121	0. 4691378
6. 400000e+01	0. 7776431	0. 4447251
1. 280000e+02	0. 7888355	0. 4311162
2. 560000e+02	0. 7947885	0. 4239883
5. 120000e+02	0. 8010416	NaN
1. 024000e+03	0. 8010416	NaN
2. 048000e+03	0. 8010416	NaN
4. 096000e+03	0. 8010416	NaN
8. 192000e+03	0. 8010416	NaN
1. 638400e+04	0. 8010416	NaN
3. 276800e+04	0. 8010416	NaN

Mad 1mer

glmnet

7534 samples
144 predictor

No pre-processing

Resampling: Cross-Validated (10 fold)

Summary of sample sizes: 6782, 6780, 6780, 6782, 6782, 6779, ...

Resampling results across tuning parameters:

lambda	RMSE	Rsquared
3. 051758e-05	0. 3814439	0. 7746827
6. 103516e-05	0. 3814439	0. 7746827
1. 220703e-04	0. 3814439	0. 7746827
2. 441406e-04	0. 3814439	0. 7746827
4. 882812e-04	0. 3814439	0. 7746827
9. 765625e-04	0. 3814439	0. 7746827
1. 953125e-03	0. 3814439	0. 7746827
3. 906250e-03	0. 3814439	0. 7746827
7. 812500e-03	0. 3814439	0. 7746827
1. 562500e-02	0. 3814439	0. 7746827
3. 125000e-02	0. 3816530	0. 7746503
6. 250000e-02	0. 3847175	0. 7742195
1. 250000e-01	0. 3949555	0. 7727056
2. 500000e-01	0. 4223560	0. 7680281
5. 000000e-01	0. 4770465	0. 7559688
1. 000000e+00	0. 5542697	0. 7320388
2. 000000e+00	0. 6343252	0. 6963678
4. 000000e+00	0. 6991083	0. 6568682
8. 000000e+00	0. 7433124	0. 6228006
1. 600000e+01	0. 7700024	0. 5988878
3. 200000e+01	0. 7848826	0. 5843705
6. 400000e+01	0. 7927978	0. 5762663
1. 280000e+02	0. 7968704	0. 5720114
2. 560000e+02	0. 7990252	0. 5698101
5. 120000e+02	0. 8010430	NaN
1. 024000e+03	0. 8010430	NaN
2. 048000e+03	0. 8010430	NaN

4. 096000e+03	0. 8010430	NaN
8. 192000e+03	0. 8010430	NaN
1. 638400e+04	0. 8010430	NaN
3. 276800e+04	0. 8010430	NaN

Myc 1mer+shape

glmnet

6926 samples
274 predictor

No pre-processing

Resampling: Cross-Validated (10 fold)

Summary of sample sizes: 6234, 6234, 6233, 6233, 6233, 6233, ...

Resampling results across tuning parameters:

lambda	RMSE	Rsquared
3. 051758e-05	0. 3047096	0. 8549888
6. 103516e-05	0. 3047096	0. 8549888
1. 220703e-04	0. 3047096	0. 8549888
2. 441406e-04	0. 3047096	0. 8549888
4. 882812e-04	0. 3047096	0. 8549888
9. 765625e-04	0. 3047096	0. 8549888
1. 953125e-03	0. 3047096	0. 8549888
3. 906250e-03	0. 3047096	0. 8549888
7. 812500e-03	0. 3047096	0. 8549888
1. 562500e-02	0. 3047096	0. 8549888
3. 125000e-02	0. 3047096	0. 8549888
6. 250000e-02	0. 3241223	0. 8370296
1. 250000e-01	0. 3480953	0. 8153897
2. 500000e-01	0. 3757670	0. 7936026
5. 000000e-01	0. 4138085	0. 7695631
1. 000000e+00	0. 4694384	0. 7376329
2. 000000e+00	0. 5405449	0. 6912764
4. 000000e+00	0. 6142656	0. 6296857
8. 000000e+00	0. 6770883	0. 5636472
1. 600000e+01	0. 7232968	0. 5073935
3. 200000e+01	0. 7535666	0. 4679809
6. 400000e+01	0. 7715807	0. 4441754
1. 280000e+02	0. 7816159	0. 4309029
2. 560000e+02	0. 7869178	0. 4239328
5. 120000e+02	0. 7924612	NaN
1. 024000e+03	0. 7924612	NaN
2. 048000e+03	0. 7924612	NaN
4. 096000e+03	0. 7924612	NaN
8. 192000e+03	0. 7924612	NaN
1. 638400e+04	0. 7924612	NaN
3. 276800e+04	0. 7924612	NaN

Myc 1mer

glmnet

6926 samples

144 predictor

No pre-processing

Resampling: Cross-Validated (10 fold)

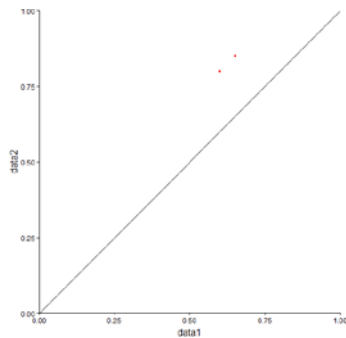
Summary of sample sizes: 6234, 6234, 6234, 6234, 6234, 6234, ...

Resampling results across tuning parameters:

lambda	RMSE	Rsquared
3.051758e-05	0.3739013	0.7781748
6.103516e-05	0.3739013	0.7781748
1.220703e-04	0.3739013	0.7781748
2.441406e-04	0.3739013	0.7781748
4.882812e-04	0.3739013	0.7781748
9.765625e-04	0.3739013	0.7781748
1.953125e-03	0.3739013	0.7781748
3.906250e-03	0.3739013	0.7781748
7.812500e-03	0.3739013	0.7781748
1.562500e-02	0.3739013	0.7781748
3.125000e-02	0.3742715	0.7781077
6.250000e-02	0.3773222	0.7775714
1.250000e-01	0.3874122	0.7757523
2.500000e-01	0.4142908	0.7702824
5.000000e-01	0.4677354	0.7566756
1.000000e+00	0.5435006	0.7308971
2.000000e+00	0.6228532	0.6947852
4.000000e+00	0.6879662	0.6573331
8.000000e+00	0.7330480	0.6264127
1.600000e+01	0.7604246	0.6053231
3.200000e+01	0.7757943	0.5925712
6.400000e+01	0.7839633	0.5855116
1.280000e+02	0.7881827	0.5817870
2.560000e+02	0.7924835	0.5747232
5.120000e+02	0.7925007	NaN
1.024000e+03	0.7925007	NaN
2.048000e+03	0.7925007	NaN
4.096000e+03	0.7925007	NaN
8.192000e+03	0.7925007	NaN
1.638400e+04	0.7925007	NaN
3.276800e+04	0.7925007	NaN

(5) High-throughput in vitro data analysis

(a)



(b) 1mer+shape model shows larger R squared than 1mer model, which means 1mer+shape model is better.

(6) Preparation of high-throughput in vivo data analysis

(a)

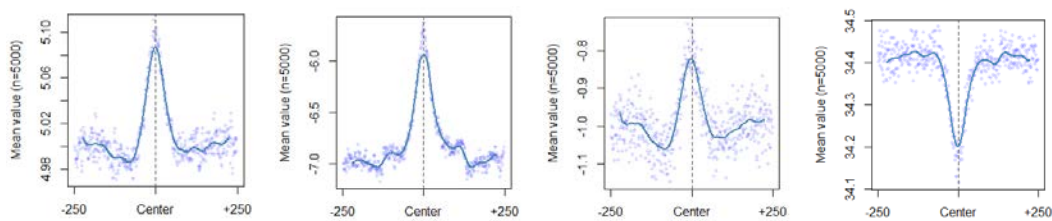
This branch is 1 commit ahead of rohalabmaster.		Pull request	Compare
TsuPeiChu committed on GitHub Add files via upload		Latest commit 45ba223 12 days ago	
..			
README	Create README		12 days ago
bound_30.fa	Add files via upload		12 days ago
bound_500.fa	Add files via upload		12 days ago
unbound_30.fa	Add files via upload		12 days ago
unbound_500.fa	Add files via upload		12 days ago

(b) Installed as shown in question (3).

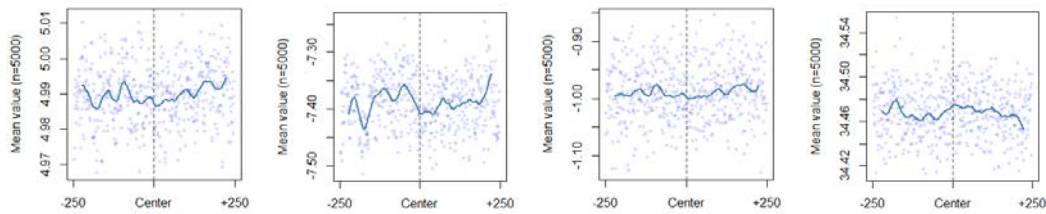
(7) High-throughput in vivo data analysis

(a)

Bound



Unbound

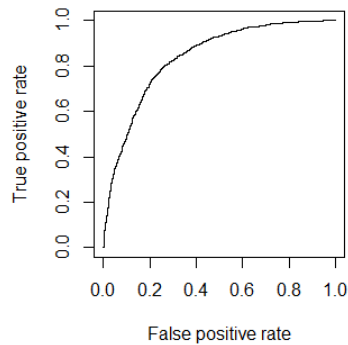


(b) Bound data shows high symmetry, where unbound data does not.

(8) Build prediction models for in vitro data

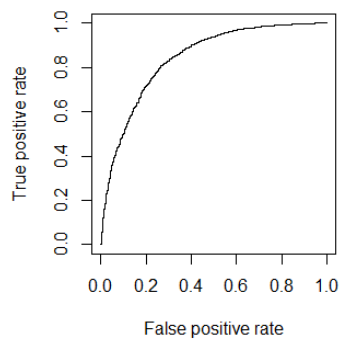
(a)

ROC 1mer+shape



AUC score 0.8386508

ROC 1mer



AUC score 0.8421386

(b) 1mer feature has slightly larger AUC score than 1mer+shape feature, which means 1mer is a better model for the in vitro data bound_30.fa and unbound_30.fa.

