TP –Tests multiples : détection de k-mères exceptionnels

Probabilités et statistique pour la biologie (STAT1)

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Contents

But de ce tutoriel

- Apprendre à manipuler des tableaux de données (objet R data.frame)
- Travailler sur les colonnes de tableaux de données
- Se familiariser par la pratique avec les différentes corrections de tests multples.
- Représentations graphiques associées aux tests multiples (histogramme des P-valeurs, MA plot, Volcano plot)

Jeu de données : contexte

Nous avons utilisé le logiciel *oligo-analysis* de la suite Regulatory Sequence Analysis Tools (RSAT) pour compter les occurrences de chaque octanucléotide dans les pics de liaison du facteur transcriptionnel Sox2 détectés par une expérience de ChIP-seq.

Conditions d'analyse

- Nombre de séquences: $S = 8014$

- Taille totale des séquences: $L = 2776509$

- On dénombre uniquement les occurrences renouvelantes (non-chevauchantes).

- Les octanucléotides ont été regroupés par paires réverse complémentaires (analyse insensible au brin).

- Le programme a également calculé la probabilité a priori de chaque octanucléotide sur base d'un modèle de Markov d'ordre 5. Autrement dit, la probabilité a priori d'un octanucléotide (p) est estimée sur bases des probabilités d'hexanucléotides observées dans l'ensemble des séquences.

Questions à traiter

Durant ce tutoriel, nous allons explorer ce jeu de données, et calculer une série de statistiques pour détecter les octanucléotides (abbréviation: **8nt**) significativement sur-représentés.

Téléchargement du tableau de données

1. A la racine de votre compte, créez un dossier de travail nommé `TP_stat1_multiple_tests_kmers`.

```
## Create work directory
work.dir <- '~/TP_stat1_multiple_tests_kmers'
dir.create(work.dir, recursive = TRUE, showWarnings = FALSE)
setwd(work.dir)
```

2. Téléchargez dans ce dossier le fichier de comptage des k-mères, qui se trouve sur le site Wbe du cours.

https://jvanheld.github.io/stat1/data/Sox2_oligos/Sox2-peaks_8nt_mkv5.tsv.gz

```
kmer.file <- 'Sox2-peaks_8nt_mkv5.tsv.gz'
kmer.url <- file.path("https://jvanheld.github.io/stat1/data/Sox2_oligos/", kmer.file)


## Download the kmer occurrence file in the work directory
download.file(url = kmer.url, destfile = kmer.file)
```

Chargement d'un fichier tabulaire de données

Nous allons charger le tableau de comptage des k-mères dans une variable nomée `kmer.table`, de type `data.frame`.

Les data frames sont des tableaux à deux dimensions (lignes/colonnes) qui permettent d'associer - un nom à chaque ligne, - un nom à chaque colonne - un type de données (nombres, chaînes de caractères, . . .) est défini automatiquement pour chaque colonne sur base de son contenu

```
setwd(work.dir)

## Check the files
list.files()
```

```
[1] "Sox2-peaks_8nt_mkv5.tsv.gz"
```

```
## Load the file
kmer.table <- read.delim(
  file = kmer.file,
  header = 1,
  row.names = 1)

## Check the content of the original data table
names(kmer.table) ## Column content
```

```
[1] "occurrences" "prior"
```

```
head(kmer.table)  ## First rows
```

```
                 occurrences         prior
aaaaaaaa|tttttttt        658 0.000409754
aaaaaaac|gttttttt        285 0.000160186
aaaaaaag|cttttttt        393 0.000194751
aaaaaaat|atttttt         317 0.000143588
aaaaaaca|tgtttttt        317 0.000177584
```

```
aaaaaacc|ggtttttt          166 0.000088000
```

```
tail(kmer.table) ## Last rows
```

```
              occurrences        prior
tttcaaaa|ttttgaaa          223 0.000087900
tttccaaa|tttggaaa          212 0.000074400
tttcgaaa|tttcgaaa           11 0.000003810
tttgaaaa|ttttcaaa          250 0.000103607
tttgcaaa|tttgcaaa          150 0.000065600
ttttaaaa|ttttaaaa          231 0.000074100
```

```
dim(kmer.table)    ## Dimensions of the data frame
```

```
[1] 32860      2
```

Sélection de lines et de colonnes

Il existe plusieurs façons de sélectionner des lignes et colonnes d'un tableau.

```
# Afficher le contenu de la cellule en 10ème ligne, 2ème colonne
kmer.table[10,2]
```

```
[1] 9.95e-05
```

```
## Afficher la 10ème ligne
kmer.table[10,]
```

```
              occurrences      prior
aaaaaagc|gctttttt          148 9.95e-05
```

```
## Afficher la 2ème colonne
kmer.table[,2]
```

```
    [1] 0.000409754 0.000160186 0.000194751 0.000143588 0.000177584
    [6] 0.000088000 0.000019200 0.000072100 0.000145540 0.000099500
   [11] 0.000121909 0.000066500 0.000093000 0.000061100 0.000102422
   [16] 0.000062400 0.000170144 0.000077600 0.000094100 0.000053800
   [21] 0.000067500 0.000056800 0.000012500 0.000059500 0.000009280
   [26] 0.000011400 0.000011900 0.000011200 0.000031900 0.000037500
   [31] 0.000050800 0.000040900 0.000122102 0.000065000 0.000089900
   [36] 0.000047800 0.000080200 0.000069100 0.000014000 0.000059300
   [41] 0.000087000 0.000070200 0.000069800 0.000045200 0.000030700
   [46] 0.000038300 0.000043500 0.000036200 0.000077800 0.000044100
   [51] 0.000047100 0.000038500 0.000044100 0.000038900 0.000007670
   [56] 0.000046200 0.000063000 0.000054000 0.000057400 0.000054300
   [61] 0.000033800 0.000037500 0.000030400 0.000038100 0.000293794
   [66] 0.000078800 0.000100701 0.000183554 0.000121763 0.000074600
   [71] 0.000017200 0.000085500 0.000108664 0.000090300 0.000093200
   [76] 0.000070700 0.000041400 0.000049200 0.000043900 0.000072700
   [81] 0.000071400 0.000059400 0.000080800 0.000048400 0.000076300
   [86] 0.000058800 0.000017100 0.000067000 0.000011000 0.000013500
   [91] 0.000014300 0.000009560 0.000035800 0.000057200 0.000067800
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  [111] 0.000013800 0.000012400 0.000040000 0.000026400 0.000029200
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```

```
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```

```
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```

```
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```

```
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[32106]  0.000003840  0.000001220  0.000004530  0.000007380  0.000001610
[32111]  0.000003090  0.000006360  0.000006600  0.000006840  0.000007340
[32116]  0.000017400  0.000013700  0.000014500  0.000005890  0.000010700
[32121]  0.000011400  0.000011600  0.000016500  0.000009850  0.000007230
[32126]  0.000002400  0.000012500  0.000014000  0.000004540  0.000006270
[32131]  0.000008800  0.000009610  0.000014600  0.000007080  0.000013000
[32136]  0.000002640  0.000002100  0.000003600  0.000005400  0.000014500
[32141]  0.000014400  0.000012100  0.000016100  0.000007860  0.000011300
[32146]  0.000015000  0.000015200  0.000004440  0.000008680  0.000005480
[32151]  0.000004110  0.000005400  0.000005760  0.000008390  0.000007790
[32156]  0.000009510  0.000006690  0.000010600  0.000005470  0.000005960
[32161]  0.000004530  0.000003930  0.000003260  0.000004680  0.000004910
[32166]  0.000002140  0.000002690  0.000004270  0.000007970  0.000006440
[32171]  0.000005190  0.000010500  0.000001280  0.000002010  0.000004430
[32176]  0.000008590  0.000007120  0.000009680  0.000007030  0.000006010
[32181]  0.000008070  0.000007810  0.000009860  0.000004140  0.000006160
[32186]  0.000005590  0.000006580  0.000005670  0.000006360  0.000008040
[32191]  0.000005610  0.000004740  0.000009000  0.000009200  0.000044200
[32196]  0.000053600  0.000054900  0.000055500  0.000032400  0.000053200
[32201]  0.000051100  0.000024400  0.000026800  0.000051600  0.000050500
[32206]  0.000053500  0.000032000  0.000045600  0.000004140  0.000005090
[32211]  0.000021800  0.000034600  0.000053400  0.000040500  0.000051300
[32216]  0.000030600  0.000036200  0.000053800  0.000042300  0.000021000
[32221]  0.000030500  0.000032900  0.000031500  0.000016000  0.000027000
[32226]  0.000027900  0.000036100  0.000041500  0.000025400  0.000062700
[32231]  0.000060400  0.000048700  0.000050100  0.000058200  0.000056100
[32236]  0.000089500  0.000107140  0.000020900  0.000038200  0.000076500
[32241]  0.000091600  0.000099600  0.000068000  0.000115514  0.000009770
[32246]  0.000017700  0.000047600  0.000090200  0.000006650  0.000005980
```

```
[32251]  0.000003850  0.000004280  0.000011400  0.000012900  0.000011500
[32256]  0.000004670  0.000005910  0.000055500  0.000053500  0.000068600
[32261]  0.000131572  0.000095600  0.000118917  0.000052600  0.000083600
[32266]  0.000080000  0.000063300  0.000078500  0.000069600  0.000044800
[32271]  0.000097700  0.000083400  0.000035000  0.000034900  0.000091500
[32276]  0.000082500  0.000065400  0.000051700  0.000075100  0.000007890
[32281]  0.000020900  0.000057200  0.000079259  0.000095300  0.000052400
[32286]  0.000048600  0.000064400  0.000097600  0.000067900  0.000034400
[32291]  0.000040200  0.000074900  0.000044800  0.000051100  0.000059200
[32296]  0.000080300  0.000079300  0.000048700  0.000059100  0.000061200
[32301]  0.000051400  0.000021700  0.000046500  0.000032600  0.000054400
[32306]  0.000057300  0.000028300  0.000033600  0.000067000  0.000062100
[32311]  0.000058600  0.000110817  0.000006980  0.000007460  0.000049600
[32316]  0.000082600  0.000053100  0.000037100  0.000039100  0.000046300
[32321]  0.000063600  0.000044800  0.000048100  0.000044300  0.000106852
[32326]  0.000064500  0.000087100  0.000098100  0.000102082  0.000094100
[32331]  0.000091500  0.000101812  0.000106985  0.000106967  0.000104168
[32336]  0.000050900  0.000109681  0.000082700  0.000051000  0.000042500
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[32481]  0.000038300  0.000037700  0.000031500  0.000036400  0.000047100
[32486]  0.000042200  0.000051600  0.000062500  0.000016900  0.000038300
[32491]  0.000047700  0.000044900  0.000056200  0.000009470  0.000012700
[32496]  0.000029300  0.000006120  0.000005850  0.000005220  0.000012100
[32501]  0.000012400  0.000005260  0.000004490  0.000034800  0.000029600
[32506]  0.000051800  0.000076700  0.000065800  0.000040600  0.000005040
[32511]  0.000005890  0.000006020  0.000005990  0.000005520  0.000008390
[32516]  0.000003360  0.000008600  0.000021400  0.000007570  0.000013700
```

```
[32521] 0.000002900 0.000004090 0.000006730 0.000012000 0.000009920
[32526] 0.000008570 0.000010900 0.000016200 0.000005590 0.000006510
[32531] 0.000006850 0.000004540 0.000009010 0.000010100 0.000004630
[32536] 0.000052900 0.000049200 0.000033300 0.000026600 0.000036700
[32541] 0.000017300 0.000019000 0.000050100 0.000065700 0.000048000
[32546] 0.000067300 0.000005180 0.000040300 0.000074200 0.000061700
[32551] 0.000047600 0.000064600 0.000092100 0.000051800 0.000054900
[32556] 0.000043200 0.000052500 0.000076700 0.000051000 0.000063500
[32561] 0.000072400 0.000098500 0.000102120 0.000039900 0.000089300
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[32576] 0.000083100 0.000105932 0.000029600 0.000035500 0.000024500
[32581] 0.000028400 0.000019300 0.000041800 0.000035000 0.000042300
[32586] 0.000045500 0.000041400 0.000038100 0.000068800 0.000020900
[32591] 0.000043900 0.000076100 0.000036800 0.000061200 0.000007670
[32596] 0.000027600 0.000007770 0.000009180 0.000005050 0.000006770
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[32736] 0.000036800 0.000047700 0.000032100 0.000051100 0.000033600
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[32781] 0.000064100 0.000030600 0.000060700 0.000058500 0.000056700
[32786] 0.000070500 0.000035700 0.000006510 0.000087000 0.000056100
```

```
[32791] 0.000093500 0.000033900 0.000034400 0.000017600 0.000053100
[32796] 0.000049900 0.000088900 0.000070100 0.000064400 0.000010900
[32801] 0.000009830 0.000007730 0.000010900 0.000060800 0.000060800
[32806] 0.000006960 0.000003820 0.000008020 0.000004050 0.000005460
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[32826] 0.000083800 0.000069300 0.000024400 0.000079800 0.000036900
[32831] 0.000040500 0.000012600 0.000064500 0.000039000 0.000032200
[32836] 0.000029300 0.000003870 0.000002480 0.000049000 0.000069900
[32841] 0.000044700 0.000039900 0.000016900 0.000067700 0.000037400
[32846] 0.000070000 0.000018700 0.000051800 0.000058000 0.000088500
[32851] 0.000131653 0.000101473 0.000077700 0.000037400 0.000087900
[32856] 0.000074400 0.000003810 0.000103607 0.000065600 0.000074100
```

```
## Afficher les lignes 10 à 15
kmer.table[10:15,]
```

```
                  occurrences        prior
aaaaaagc|gctttttt         148 0.000099500
aaaaaagg|cctttttt         204 0.000121909
aaaaaagt|actttttt         142 0.000066500
aaaaaata|tatttttt         164 0.000093000
aaaaaatc|gatttttt         136 0.000061100
aaaaaatg|catttttt         156 0.000102422
```

```
## Afficher les colonnes 1 et 2 pour les lignes 10 à 20
kmer.table[10:15, 1:2]
```

```
                  occurrences        prior
aaaaaagc|gctttttt         148 0.000099500
aaaaaagg|cctttttt         204 0.000121909
aaaaaagt|actttttt         142 0.000066500
aaaaaata|tatttttt         164 0.000093000
aaaaaatc|gatttttt         136 0.000061100
aaaaaatg|catttttt         156 0.000102422
```

```
## Sélection d'une ligne par son nom
kmer.table["gattacca|tggtaatc",]
```

```
                  occurrences    prior
gattacca|tggtaatc          53 2.07e-05
```

```
kmer.table[c("gattacca|tggtaatc", "aaaaaaaa|tttttttt"),]
```

```
                  occurrences        prior
gattacca|tggtaatc          53 0.000020700
aaaaaaaa|tttttttt         658 0.000409754
```

```
## Sélection d'une colonne par son nom
## (ici, 50 premières lignes seulement )
head(n = 50, kmer.table[, "occurrences"])
```

```
 [1] 658 285 393 317 317 166  49  92 302 148 204 142 164 136 156  99 556
[18] 182 182 141 183 133  31 149  32  21  21  25  96  75 126  86 481 151
[35] 195 135 206 143  36 139 252 116 162 119  98 113 126  88 249 105
```

```
## Notation rapide
head(n = 50, kmer.table$occurrences)
```

```
 [1] 658 285 393 317 317 166  49  92 302 148 204 142 164 136 156  99 556
[18] 182 182 141 183 133  31 149  32  21  21  25  96  75 126  86 481 151
[35] 195 135 206 143  36 139 252 116 162 119  98 113 126  88 249 105
```

```
## Notation équivalente
kmer.table$occurrences[1:50]
```

```
 [1] 658 285 393 317 317 166  49  92 302 148 204 142 164 136 156  99 556
[18] 182 182 141 183 133  31 149  32  21  21  25  96  75 126  86 481 151
[35] 195 135 206 143  36 139 252 116 162 119  98 113 126  88 249 105
```

Exercice

1. Utilisez la fonction `plot()` pour dessiner un nuage de points indiquant le nombre d'occurrences (Y) en fonction de la probabilité a priori de chaque 8nt (X). Soignez le graphique comme au TP précédent.

2. Dessinez un histogramme des occurrences au moyen de la fonction `hist()`.

Calcul de statistiques sules colonnes

Nous allons calculer le nombre attendu d'occurrences pour chaque oligonucléotide, en tenant compte de sa probabilité a priori.
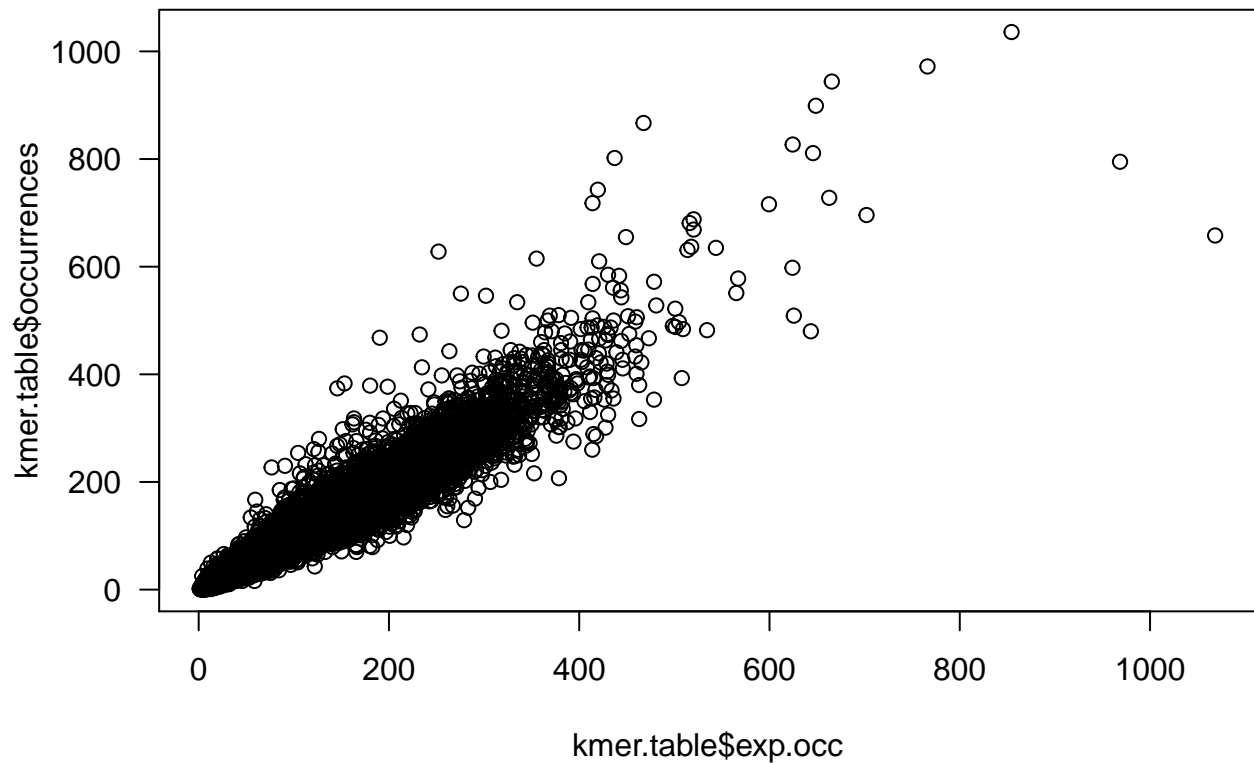
```
kmer.sum <- sum(kmer.table$occurrences)

## Check the sum of prior probabilities
## (~1 but there are some rounding errors)
sum(kmer.table$prior)
```

```
[1] 1.009168
```

```
kmer.table$exp.occ <- kmer.table$prior * kmer.sum

plot(kmer.table$exp.occ, kmer.table$occurrences, las = 1)
```

Exercice

Calculez les statistiques suivantes pour l'ensemble des oligos

1. Rapport entre occurrences observées et attendues (exp/occ)

2. Le logarithme de ce rapport (log-ratio)

3. $P(X = x)$: probabilité binomiale d'observer exactement X occurrences

4. P-valeur de sur-représentation: $P(X \geq x)$ au moyen de la binomiale.

5. P-valeur de sur-représentation: $P(X \geq x)$ au moyen de la Poisson.

6. Dessinez un nuage de points comparant les P-valeurs binomiale et Poisson. Utilisez des axes logarithmiques pour mettre en évidence les faibles p-valeurs.

7. Calculez la E-valeur binomiale.

8. Calculez la significativité de cette E-valeur, définie ici comme $sig_E = -log_{10}(E)$.

9. Dessinez un graphique avec la significativité (Y) en fonction du log-ratio (X).

10. Dessinez un histogramme des p-valeurs.

Contrôle négaitf

1. Générez une colonne de nombre d'occurrences aléatoires tirés selon une loi de Poisson dont l'espérance est prise dans la colonne `prior`.

2. Refaites les calculs et dessins ci-dessus avec ces occurrences aléatoires.

Avant de terminer : conservez la trace de votre session

La traçabilité constitue un enjeu essentiel en sciences. La fonction **R** `sessionInfo()` fournit un résumé des conditions d'une session de travail: version de R, système opérateur, bibliothèques de fonctions utilisées.

```
sessionInfo()
```

R version 3.5.1 (2018-07-02)
Platform: x86_64-apple-darwin15.6.0 (64-bit)
Running under: macOS 10.14.1

Matrix products: default
BLAS: /Library/Frameworks/R.framework/Versions/3.5/Resources/lib/libRblas.0.dylib
LAPACK: /Library/Frameworks/R.framework/Versions/3.5/Resources/lib/libRlapack.dylib

locale:
[1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8

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

other attached packages:
[1] knitr_1.20

loaded via a namespace (and not attached):
 [1] compiler_3.5.1 backports_1.1.2 magrittr_1.5   rprojroot_1.3-2
 [5] tools_3.5.1   htmltools_0.3.6 yaml_2.2.0   Rcpp_1.0.0
 [9] stringi_1.2.4   rmarkdown_1.10 stringr_1.3.1   digest_0.6.18
[13] evaluate_0.12