README

Henrik Christiansen

January 20, 2021

Project: radseq pilot

RADseq optimization pilot experiment with several Antarctic species.

Contact: henrik.christiansen@kuleuven.be

Log:

20/01/2020: added new xml file for run 7, updated bioanalyzer to v0.6.2 and updated 02_empirical_digests.R

20/01/2020: added the project to a github repository

16/12/2020: added a modified read. bioanalyzer function to read in xml file with a missing lower marker in one sample

14/12/2020: small, mostly cosmetic updates in most scripts; updated project and input/output description; finalized $02\,$ empirical digests.R

11/12/2020: added customized plot saving function in recto REs and functions.R

10/12/2020: updated 02_empirical_digests.R, added a customized ggplot plotting function in recto_REs_and_functions.R added in silico functions for comparison in recto_REs_and_functions.R

11-12/2020: updated 02_empirical_digests.R & added a customized plotting function in recto_REs_and_functions.R

11/11/2020: updated to run with R v4.0.3

07-10/2020: added script 02_empirical_digests.R to read results from bioanalyzer and analyze them in R, instead of cumbersome "manual" analysis in spreadsheets

20/07/2019: updated plot ratio scripts

10/07/2019: updated digest scripts

09/07/2019: updated the plots for test library 2

02/07/2019: updated digest scripts

28/06/2019: finalized coverage plot

27/06/2019: re-orderd scripts, included scripts for in silico digestion (previously stored in different R project)

23-27/06/2019: updated parameter plots (now based on correct de novo runs, with PE concatenating); included & updated coverage plot

16-22/06/2019: updated parameter plots; started script to plot targeted and realized coverage

01-14/06/2019: included scripts to plot n_loci and n_snps_per_locus from de novo parameter optimization series

04/12/2018: rerun due to updated input data (Trematomus mainly)

29/11/2018: created script 01_plotting.R and ratio plots

28/11/2018: created R project & input data

Input:

Various reference genomes from target species, or related species in fasta format under:

• /data/refgenomes

Output files from the Agilent Bioanalyzer Software in XML format under:

• data/bioanalyzer results

CSV file with all metadata related to the Bioanalyzer runs, created manually:

• data/bioanalyzer_results/run_overview.csv

 $\mathrm{CSV}/\mathrm{TSV}$ files in data/test_libraries with data from 5 test libraries:

- coverage_stats.csv: coverage for each library under different M values
- various n_snps_per_locus.tsv: files for each library/species and different r/M values with information about the loci and SNPs

R script that contains restriction enzyme information and various functions for analysis and plotting as used in the analyses scripts:

• analyses/recto_REs_and_functions.R

Additional R script to export plots consistently:

• ~/printfig.R

Analyses:

To be run sequentially, all listed under /analyses.

- 01_digests.R: script to perform in silico digestions for different target organisms
- 02_empirical_digests.R: script to read bioanalyzer results and plot output in comparison with in silico results
- $\bullet~03_plot_n_loci.R:$ script based on Rochette & Catchen 2017 to plot the number of (polymorphic) loci for different M parameters
- 04_plot_n_snps_per_locus.R: script based on Rochette & Catchen 2017 to plot the number of SNPs per locus for different M parameters
- 05_plot_coverage.R: script to plot target and realized coverage

Output:

In /data/in_silico_results:

• various tables.csv containing in silico digest results per target taxa

In /figures:

- genome digestion curves, empirical and in silico, created with 02_empirical_digests.R
- various n_loci_Mn plots per library, created with 03_plot_n_loci.R
- various n_snps per library/species, created with 04_n_snps_per_locus.R
- coverage plots, created by 05_plot_coverage.R

Session info:

Package citations:

```
## Warning in FUN(X[[i]], ...): no date field in DESCRIPTION file of package
## 'bioanalyzeR'
## [[1]]
##
## To cite package 'here' in publications use:
##
     Kirill Müller (2020). here: A Simpler Way to Find Your Files. R
##
##
     package version 1.0.0. https://CRAN.R-project.org/package=here
##
## A BibTeX entry for LaTeX users is
##
##
     @Manual{,
##
       title = {here: A Simpler Way to Find Your Files},
##
       author = {Kirill Müller},
##
       year = \{2020\},\
##
       note = {R package version 1.0.0},
       url = {https://CRAN.R-project.org/package=here},
##
##
##
##
## [[2]]
##
## To cite package 'SimRAD' in publications use:
##
##
     Olivier Lepais and Jason Weir (2016). SimRAD: Simulations to Predict
     the Number of RAD and GBS Loci. R package version 0.96.
##
     https://CRAN.R-project.org/package=SimRAD
##
##
## A BibTeX entry for LaTeX users is
##
##
     @Manual{,
##
       title = {SimRAD: Simulations to Predict the Number of RAD and GBS Loci},
```

```
##
       author = {Olivier Lepais and Jason Weir},
##
       year = \{2016\},\
##
       note = {R package version 0.96},
       url = {https://CRAN.R-project.org/package=SimRAD},
##
##
##
##
## [[3]]
##
## To cite seqinr in publications use:
     Charif, D. and Lobry, J.R. (2007)
##
##
## A BibTeX entry for LaTeX users is
##
##
     @InCollection{,
##
       author = {D. Charif and J.R. Lobry},
##
       title = {Seqin{R} 1.0-2: a contributed package to the {R} project for statistical computing devo
##
       booktitle = {Structural approaches to sequence evolution: Molecules, networks, populations},
##
       year = \{2007\},\
##
       editor = {U. Bastolla and M. Porto and H.E. Roman and M. Vendruscolo},
##
       series = {Biological and Medical Physics, Biomedical Engineering},
##
       pages = \{207-232\},
       address = {New York},
##
       publisher = {Springer Verlag},
##
##
       note = \{\{ISBN :\} 978-3-540-35305-8\},
##
##
##
## [[4]]
##
## To cite package 'bioanalyzeR' in publications use:
##
##
     Joseph Foley (2021). bioanalyzeR: Analysis of Agilent electrophoresis
##
     data. R package version 0.6.2.
##
## A BibTeX entry for LaTeX users is
##
##
     @Manual{,
       title = {bioanalyzeR: Analysis of Agilent electrophoresis data},
##
       author = {Joseph Foley},
##
##
       year = \{2021\},\
##
       note = {R package version 0.6.2},
##
##
##
## [[5]]
##
##
     Wickham et al., (2019). Welcome to the tidyverse. Journal of Open
##
     Source Software, 4(43), 1686, https://doi.org/10.21105/joss.01686
##
## A BibTeX entry for LaTeX users is
##
##
     @Article{,
```

```
##
       title = {Welcome to the {tidyverse}},
       author = {Hadley Wickham and Mara Averick and Jennifer Bryan and Winston Chang and Lucy D'Agosti
##
##
       year = \{2019\},\
       journal = {Journal of Open Source Software},
##
##
       volume = \{4\},
       number = \{43\},
##
       pages = \{1686\},
##
       doi = {10.21105/joss.01686},
##
##
##
##
## [[6]]
##
## To cite package 'ggsci' in publications use:
##
##
     Nan Xiao (2018). ggsci: Scientific Journal and Sci-Fi Themed Color
##
     Palettes for 'ggplot2'. R package version 2.9.
##
     https://CRAN.R-project.org/package=ggsci
##
## A BibTeX entry for LaTeX users is
##
##
     @Manual{,
       title = {ggsci: Scientific Journal and Sci-Fi Themed Color Palettes for
##
## 'ggplot2'},
       author = {Nan Xiao},
##
##
       year = \{2018\},\
##
       note = {R package version 2.9},
       url = {https://CRAN.R-project.org/package=ggsci},
##
##
     }
##
##
## [[7]]
##
## To cite package 'gridExtra' in publications use:
##
##
     Baptiste Auguie (2017). gridExtra: Miscellaneous Functions for "Grid"
##
     Graphics. R package version 2.3.
##
     https://CRAN.R-project.org/package=gridExtra
## A BibTeX entry for LaTeX users is
##
##
     @Manual{,
       title = {gridExtra: Miscellaneous Functions for "Grid" Graphics},
##
       author = {Baptiste Auguie},
##
       year = {2017},
       note = {R package version 2.3},
##
       url = {https://CRAN.R-project.org/package=gridExtra},
##
##
     }
R Session:
## R version 4.0.3 (2020-10-10)
## Platform: x86_64-pc-linux-gnu (64-bit)
## Running under: Ubuntu 18.04.5 LTS
```

```
##
## Matrix products: default
          /usr/lib/x86 64-linux-gnu/blas/libblas.so.3.7.1
## LAPACK: /usr/lib/x86_64-linux-gnu/lapack/liblapack.so.3.7.1
## locale:
## [1] LC CTYPE=en US.UTF-8
                                   LC NUMERIC=C
## [3] LC TIME=en US.UTF-8
                                   LC COLLATE=en US.UTF-8
   [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] stats4
                 parallel stats
                                     graphics grDevices utils
                                                                    datasets
## [8] methods
                 base
##
## other attached packages:
## [1] gridExtra_2.3
                                    ggsci_2.9
## [3] forcats_0.5.0
                                    stringr 1.4.0
## [5] dplyr_1.0.2
                                    purrr_0.3.4
## [7] readr 1.4.0
                                    tidyr_1.1.2
## [9] tibble_3.0.4
                                    ggplot2_3.3.2
## [11] tidyverse 1.3.0
                                    bioanalyzeR 0.6.2
## [13] seqinr_4.2-4
                                    SimRAD 0.96
## [15] zlibbioc_1.36.0
                                    ShortRead_1.48.0
## [17] GenomicAlignments_1.26.0
                                    SummarizedExperiment_1.20.0
## [19] Biobase_2.50.0
                                    MatrixGenerics_1.2.0
## [21] matrixStats_0.57.0
                                    Rsamtools_2.6.0
## [23] GenomicRanges_1.42.0
                                    GenomeInfoDb_1.26.1
## [25] BiocParallel_1.24.1
                                    Biostrings_2.58.0
## [27] XVector_0.30.0
                                    IRanges_2.24.0
## [29] S4Vectors_0.28.0
                                    BiocGenerics_0.36.0
## [31] here_1.0.0
## loaded via a namespace (and not attached):
## [1] bitops 1.0-6
                               fs 1.5.0
                                                       lubridate 1.7.9.2
## [4] RColorBrewer_1.1-2
                               progress_1.2.2
                                                       httr_1.4.2
## [7] rprojroot_2.0.2
                               tools_4.0.3
                                                       backports_1.2.0
## [10] R6_2.5.0
                                                       colorspace_2.0-0
                               DBI_1.1.0
                                                       tidyselect_1.1.0
## [13] ade4 1.7-16
                               withr 2.3.0
## [16] prettyunits_1.1.1
                               compiler 4.0.3
                                                       cli_2.2.0
                               xml2 1.3.2
## [19] rvest 0.3.6
                                                       DelayedArray_0.16.0
## [22] scales_1.1.1
                               digest_0.6.27
                                                       rmarkdown_2.5
## [25] base64enc_0.1-3
                               jpeg_0.1-8.1
                                                       pkgconfig_2.0.3
## [28] htmltools_0.5.0
                               dbplyr_2.0.0
                                                       rlang_0.4.8
## [31] readxl_1.3.1
                               rstudioapi_0.13
                                                       generics_0.1.0
## [34] hwriter_1.3.2
                               jsonlite_1.7.1
                                                       RCurl_1.98-1.2
## [37] magrittr_2.0.1
                               GenomeInfoDbData_1.2.4 Matrix_1.3-2
## [40] fansi_0.4.1
                               Rcpp_1.0.5
                                                       munsell_0.5.0
## [43] lifecycle_0.2.0
                               stringi_1.5.3
                                                       yaml_2.2.1
## [46] MASS_7.3-53
                               grid_4.0.3
                                                       crayon_1.3.4
## [49] lattice_0.20-41
                               haven_2.3.1
                                                      hms_0.5.3
## [52] knitr 1.30
                               pillar_1.4.7
                                                       reprex_0.3.0
```

## [55] XML_3.99-0.5	glue_1.4.2	evaluate_0.14
## [58] latticeExtra_0.6-29	modelr_0.1.8	png_0.1-7
## [61] vctrs_0.3.5	cellranger_1.1.0	gtable_0.3.0
## [64] assertthat_0.2.1	xfun_0.19	broom_0.7.2
## [67] ellipsis_0.3.1		