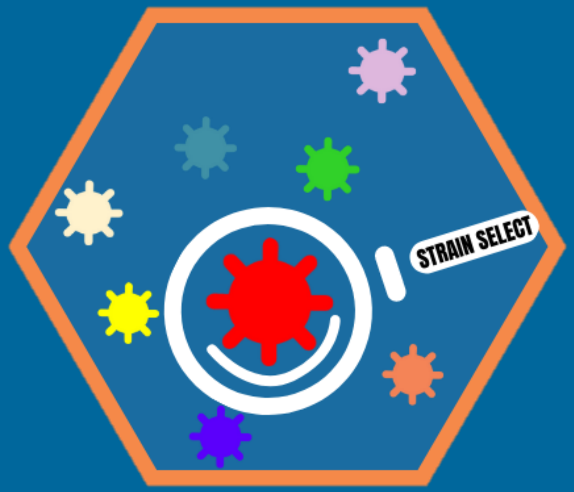
Strain select Package: a R-tool for strain selection



L. Guillier

Laurent.guillier@anses.fr

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The Strain select R package

Impact

Aim: Propose a formal and reproducible method to select strains in a collection based on their metadata

Areas on applications:

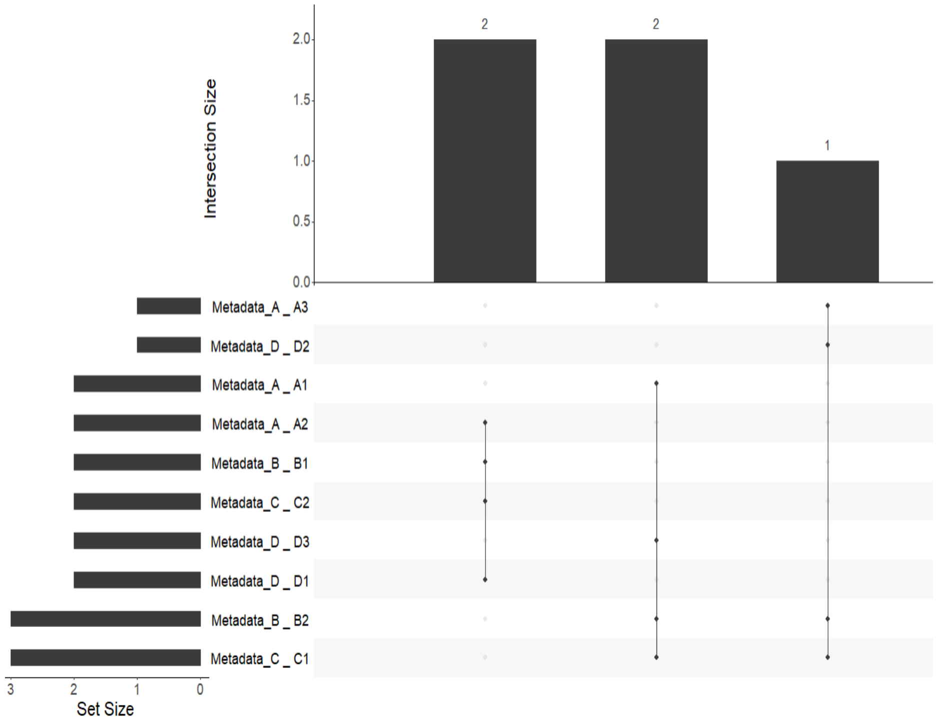
- Any pathogens
- Many contexts in One Health studies
  - Choosing strains to be sequenced for epi. investigations
  - Establishing a set of strains for phenotyping
  - Selecting strains representative of consumer exposure or risk
  - Selecting strains based on their virulence/antimicrobial profiles
  - …

Added values

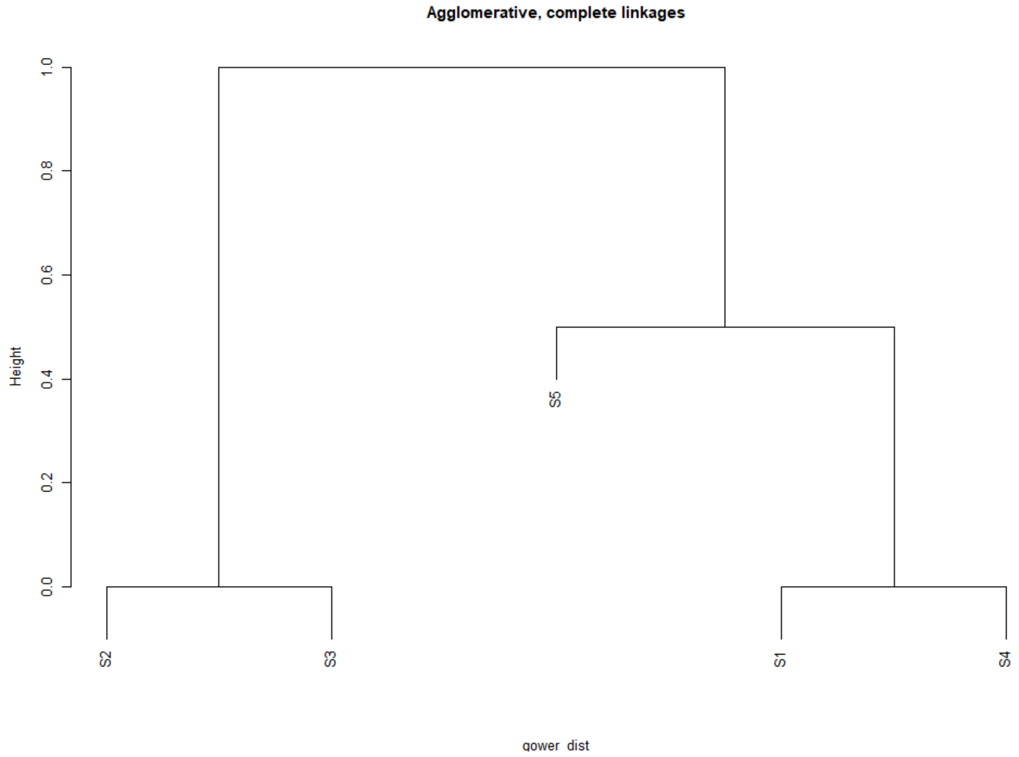
- Reference laboratories (NL- EU-)
- Research teams working on population structure, source attribution

Strain select R package: Two methods for selecting strains

❶ Intersection-based method



❷ Clustering method (Gower)



Strain select R package: Two methods for selecting strains

Same structure of data frame for the two methods

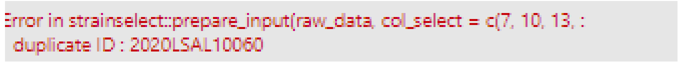
prepare_input(filename, metadata)

Mystrains.xlsx

Selection of metadata (column numbers)

Outputs:

- quality checks (e.g. duplicate strain names)
- data input for selection methods



```
Error in strainselect::prepare_input(raw_data, col_select = c(7, 10, 13, :
  duplicate ID : 2020LSAL10060
```

Strain ID	Metadata_A	Metadata_B	Metadata_C	Metadata_D
S1	A1	B2	C1	D2
S2	A2	B1	C2	D1
S3	A2	B1	C2	D1
S4	A1	B2	C1	D2
S5	A2	B2	C2	D2

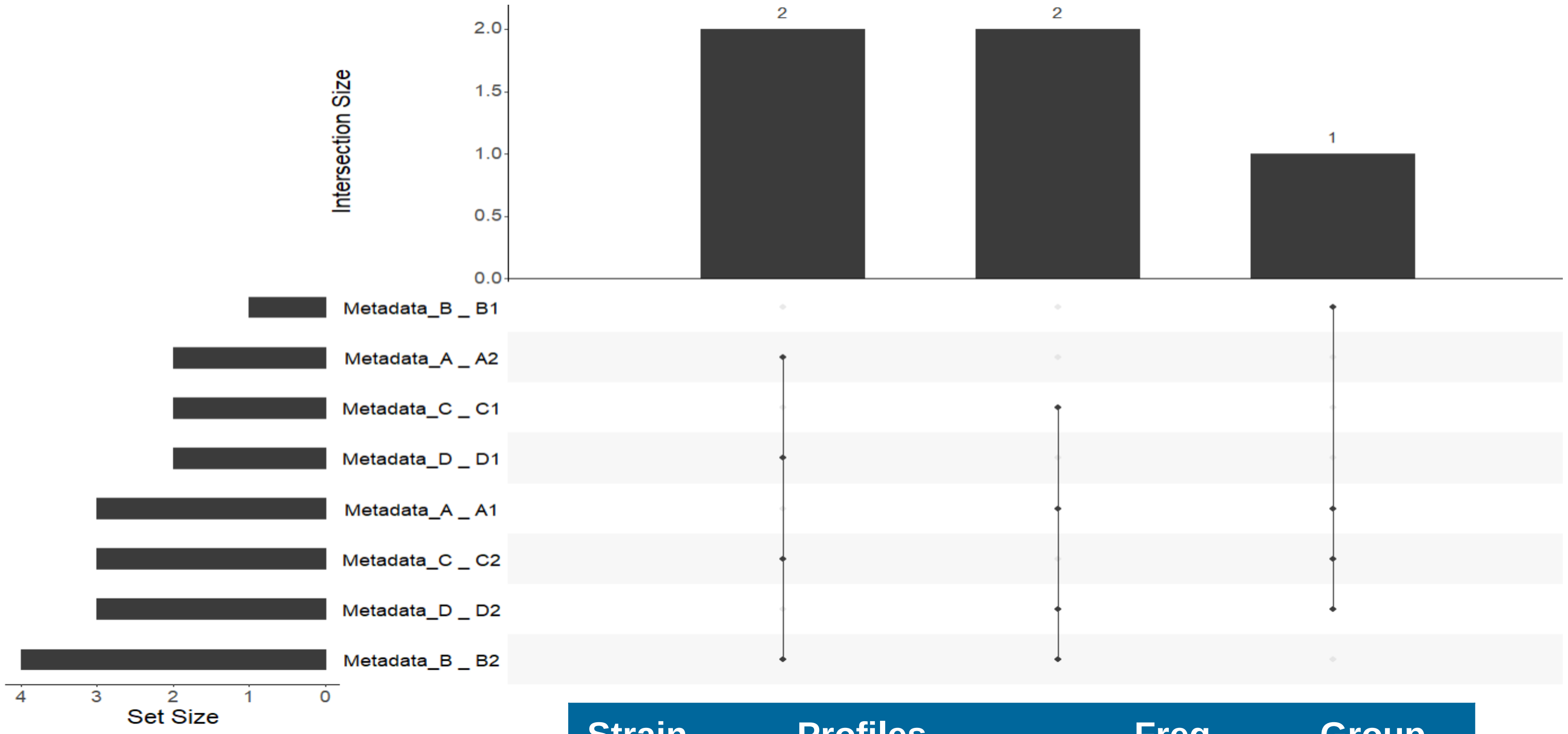
Strain select R package: ❶ Intersection-based method

Strain ID	Metadata_A	Metadata_B	Metadata_C	Metadata_D
S1	A1	B2	C1	D2
S2	A2	B1	C2	D1
S3	A2	B1	C2	D1
S4	A1	B2	C1	D2
S5	A2	B2	C2	D2

prepare_upset()

Strain ID	Metadata_A_A1	Metadata_A_A2	Metadata_B_B1	...	Metadata_D_D2
S1	1	0	0	...	1
S2	0	1	1	...	0
S3	0	1	1	...	0
S4	1	0	0	...	1
S5	0	1	0	...	1

Strain select R package: ❶ Intersection-based method



Strain	Profiles	Freq	Group
S1	10011001	2	1
S2	01100110	2	2
S3	01100110	2	2
S4	10011001	2	1
S5	01010101	1	3

define_profiles() and select_profiles()

→ Random selection in groups

Group	Selected strain
1	S4
2	S3
3	S5

Strain select R package: ❷ Clustering method (Gower)

Strain	Metadata_A	Metadata_B	Metadata_C	Metadata_D
S1	A1	B2	C1	D2
S2	A2	B1	C2	D1
S3	A2	B1	C2	D1
S4	A1	B2	C1	D2
S5	A2	B2	C2	D2

assess_gower()

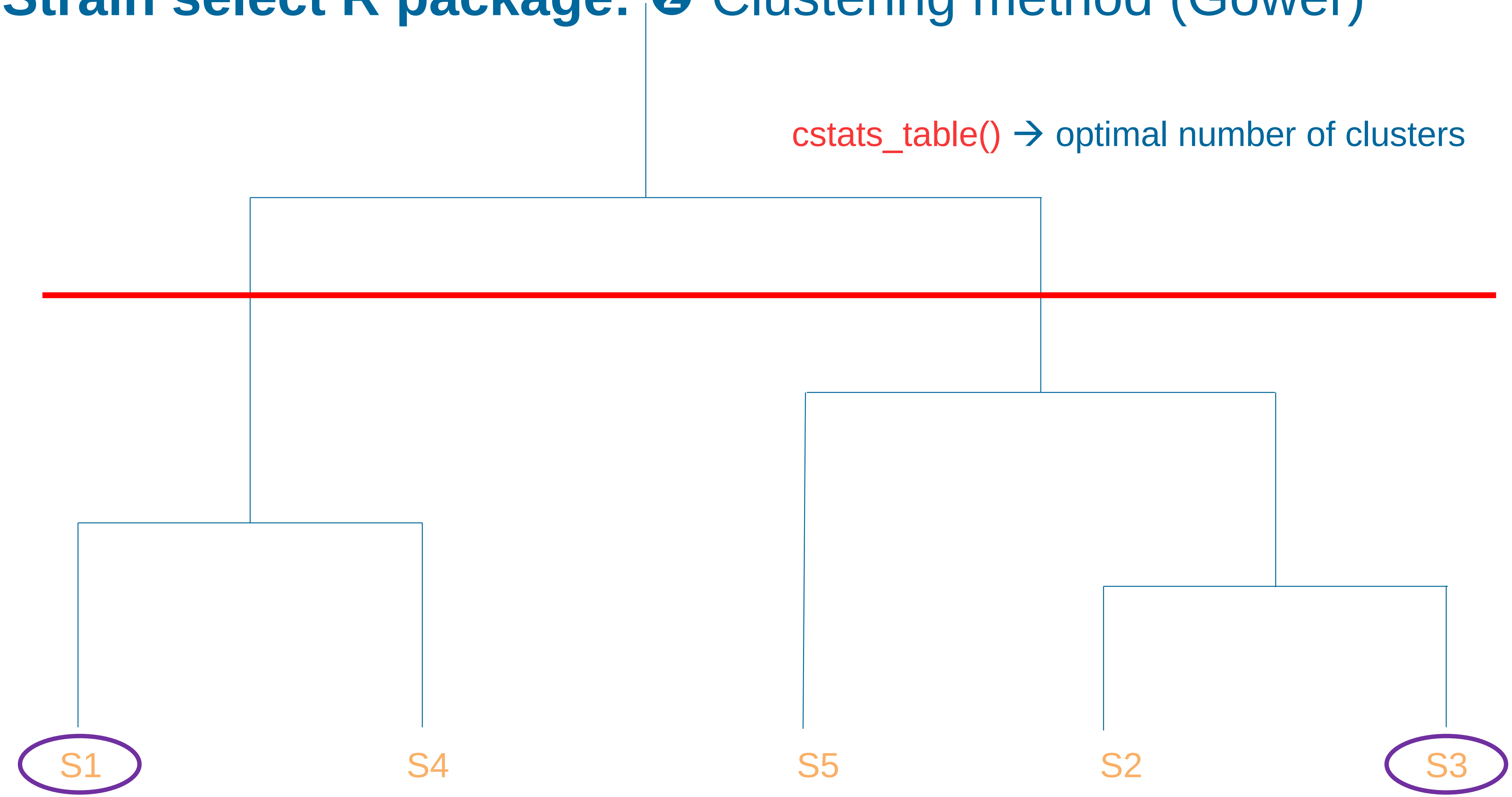
$$D_{Gower}(x_i, x_j) = 1 - S_{Gower}(x_i, x_j)$$

$$S_{Gower}(x_i, x_j) = \frac{\sum_{k=1}^{p} s_{ijk}}{p}$$

	S1	S2	S3	S4	S5
S1	0	4	4	0	2
S2		0	0	4	2
S3			0	4	3
S4				0	2
S5					0

Strain select R package: ❷ Clustering method (Gower)

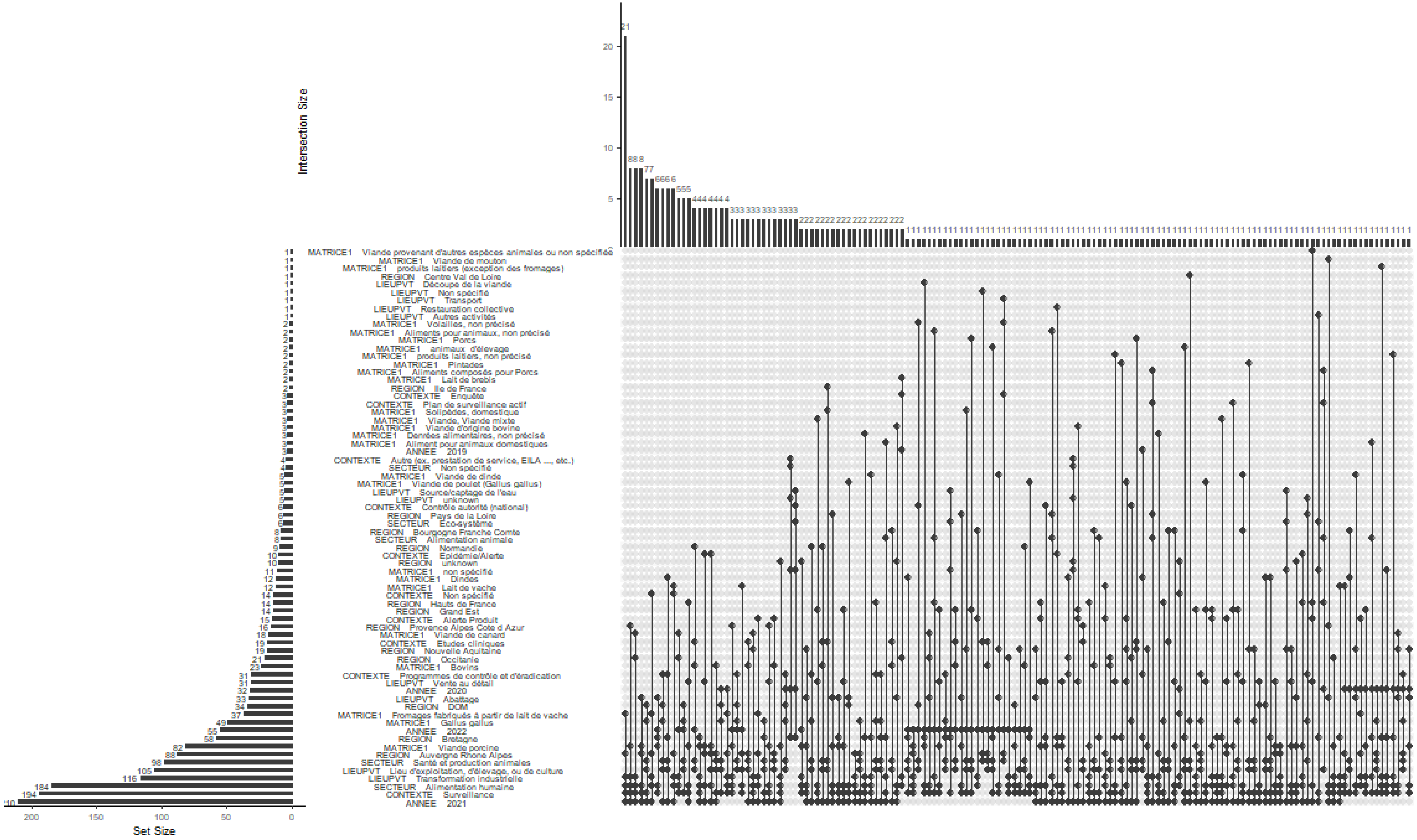
cstats_table() → optimal number of clusters



select_silhouette() → Random selection of strains in clusters

Strain select R package: Example of application

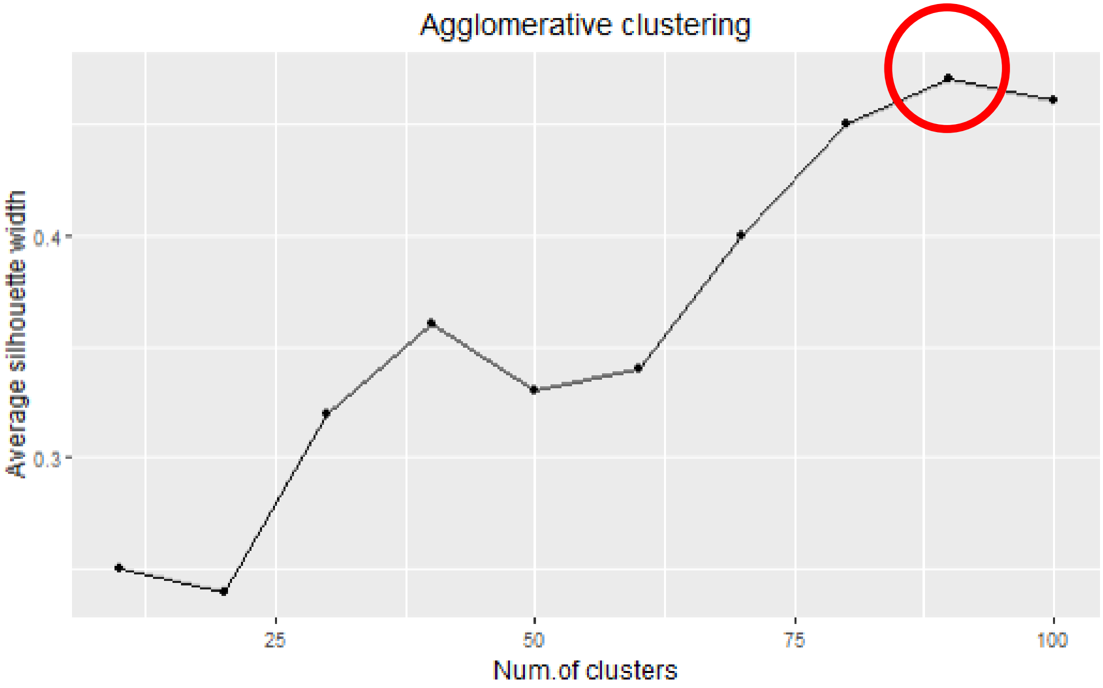
Dataset of 300 *Salmonella* Typhimurium strains – Metadata: 24 variables
→ 6 variables selected with prepare_input() + ❶ Intersection-based method



→ 149 different profiles are identified

Strain select R package: Example of application

Dataset of 300 *Salmonella* Typhimurium strains – Metadata: 24 variables
→ 6 variables selected with prepare_input() + ❷ Clustering method (Gower)



User constraints = no more than 100

→ Optimal number of clusters = 90

90 strains selected tagged in the output

- Metadata (reminder of input)
- Group (n° 1:90)
- Selection (Y/N)

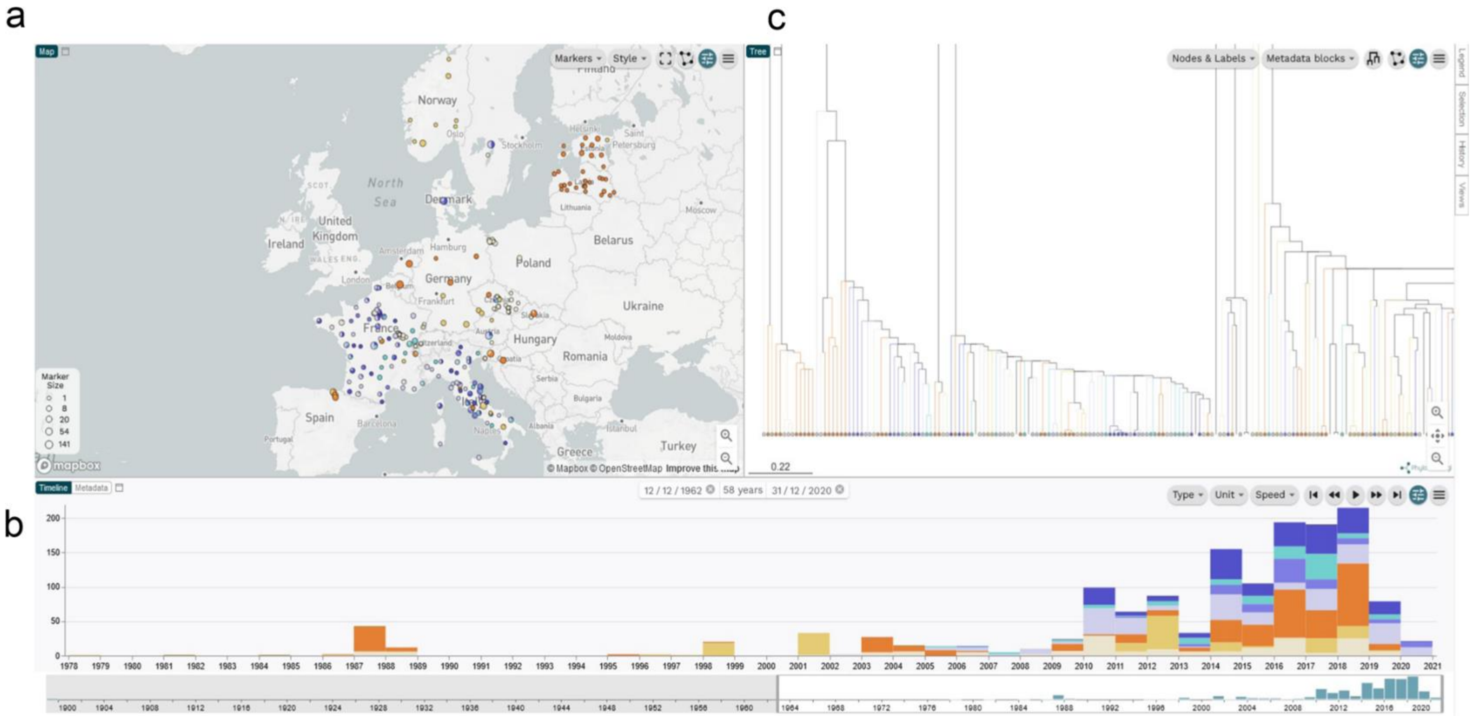
Mystrains_selection.xlsx

Projects that have used Strain select method

Selection of environmental *L. monocytogenes* strains

Felix et al. (2022)

https://doi.org/10.1038/s41597-022-01278-6

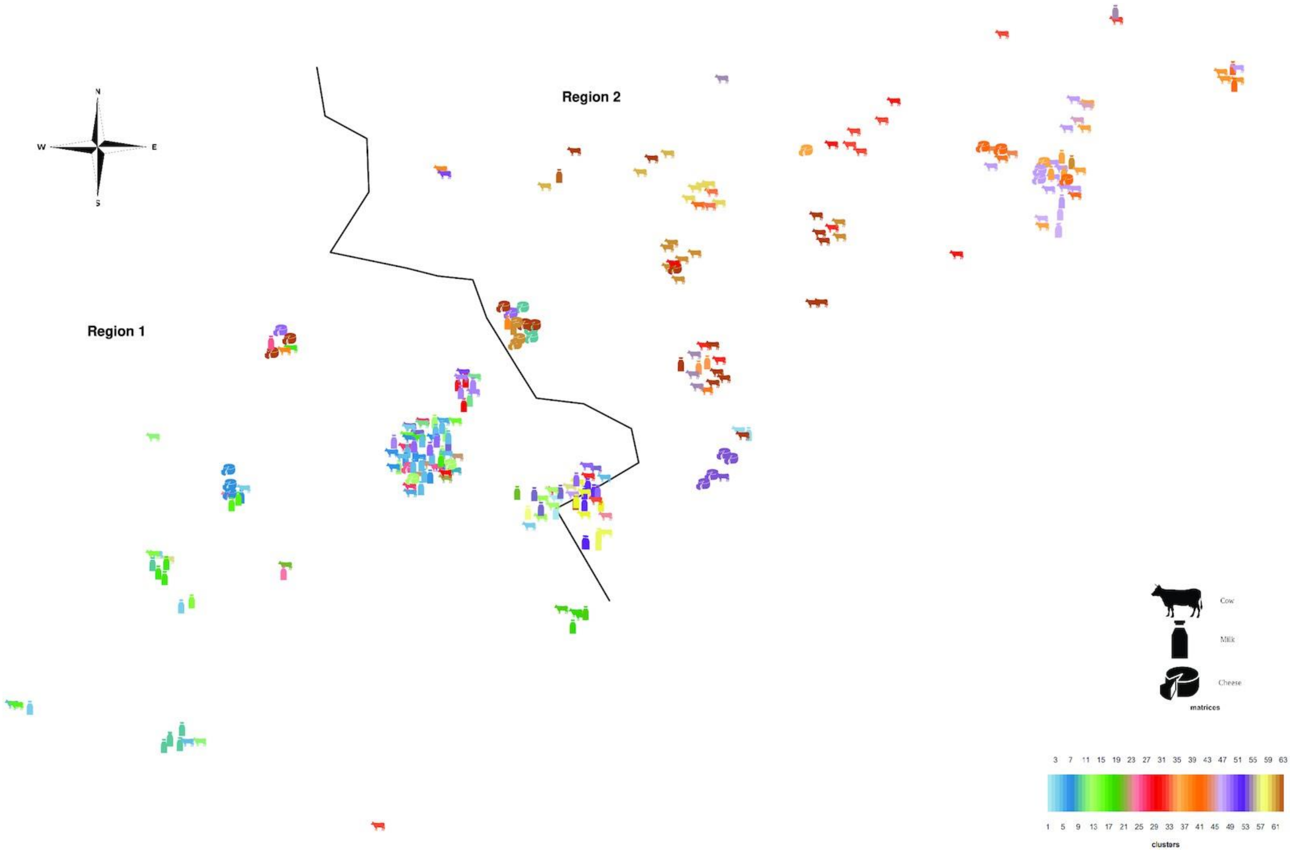


Projects that have used Strain select method

Selection on *Salmonella* Dublin strains: population structure and epidemiological investigations (France)

De Sousa Violante et al. (2022)

https://doi.org/10.1093/nargab/lqac047



Additional informations on Strain select

Availability: https://github.com/valleemarie/strainselect_package

Publication (2023) submission to https://open-research-europe.ec.europa.eu/browse/articles

Follow on activities

- Continuation of the work of the CARE project:
  - Method to select strains within CARE collection
  - Method to integrate potential new strains
- Support to EU-RLs: feel free to contact laurent.guillier@anses.fr

Marie Vallée

Thank you for your attention!

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