

RuReady?

Rolling out a blueprint for software design: discussion on Epiverse's *linelist* package

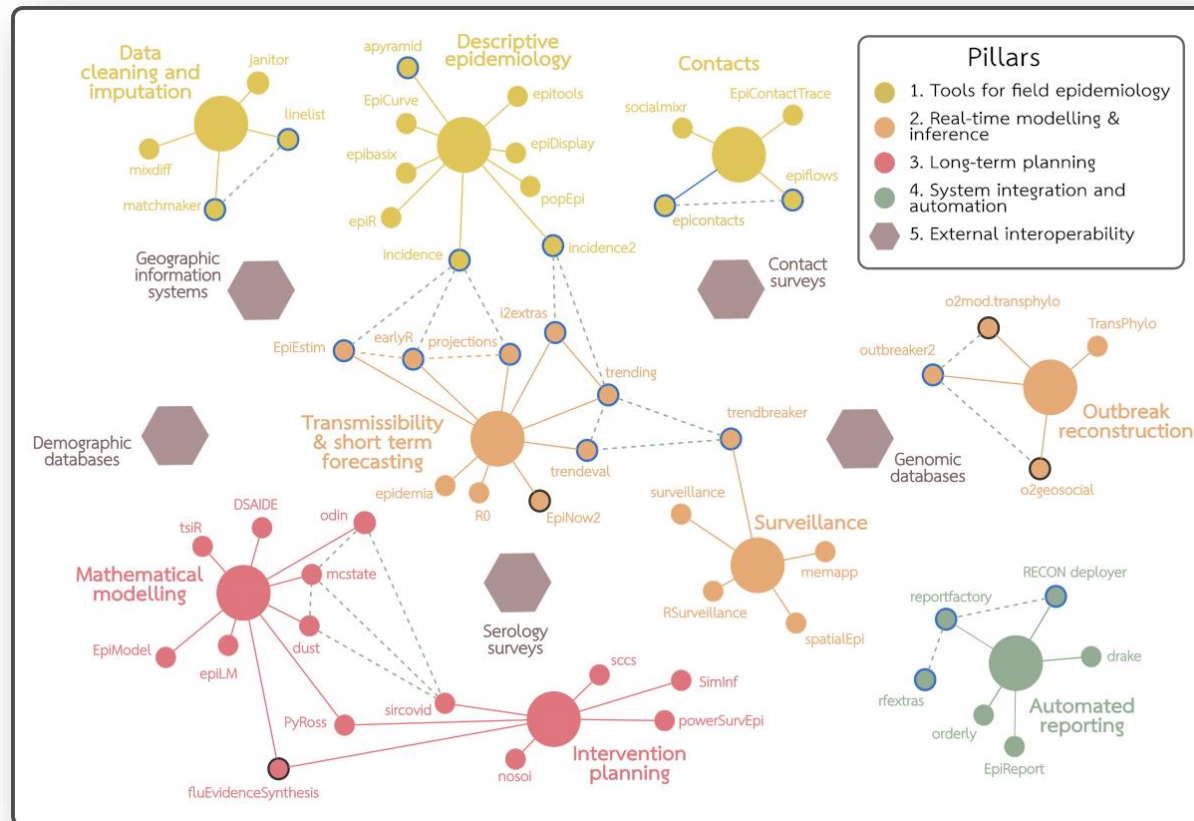
London - 7 June 2022

Thibaut Jombart

Software Design and Implementation Lead, Data.org

Current ecosystem of R package for outbreak analytics

CURRENT LANDSCAPE

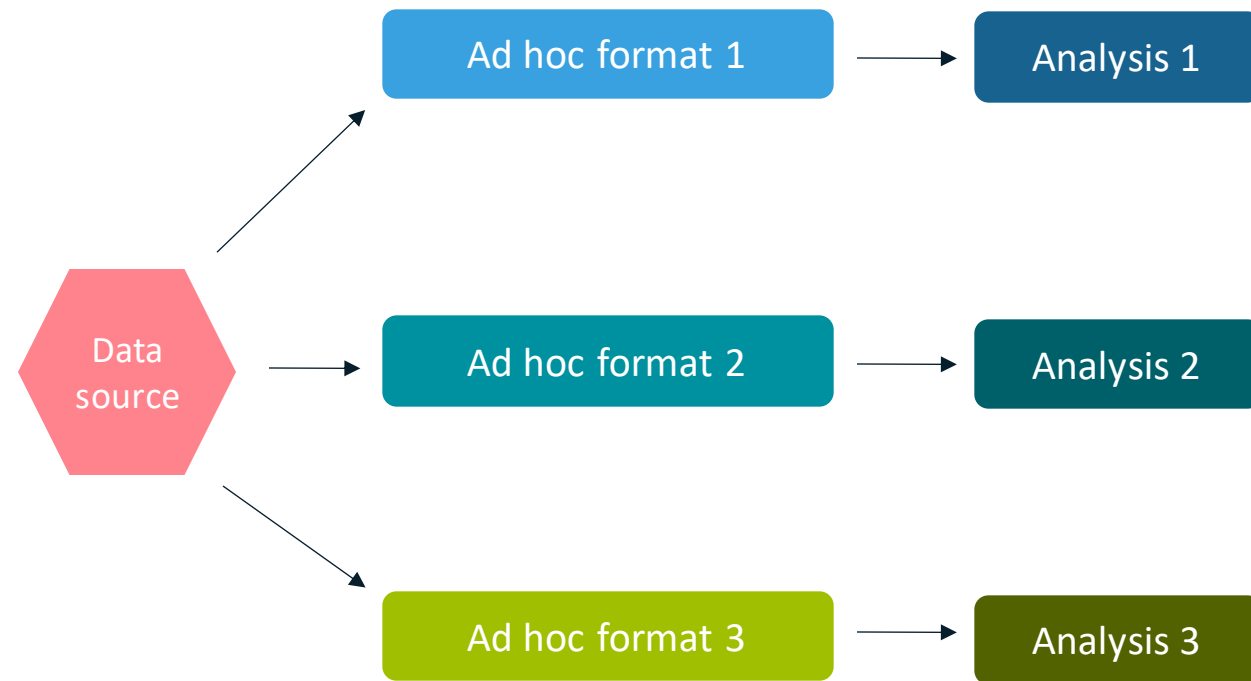


CHALLENGES

- Limited interoperability
- Lack of common data structures
- Data pipelines harder to build

Ad hoc versus canonical data representations

CURRENTLY COMMON MODEL



ISSUES

- Pre-processing overhead
 - Requires **ad-hoc scripts**
 - Sometimes **more complex** than analysis itself
 - May require **dedicated import functions**
 - Discourages multiple analyses and methods **comparisons**
- Prone to data discrepancies
 - **Mistakes** can be introduced during pre-processing
 - **Hinders comparison** of methods and results

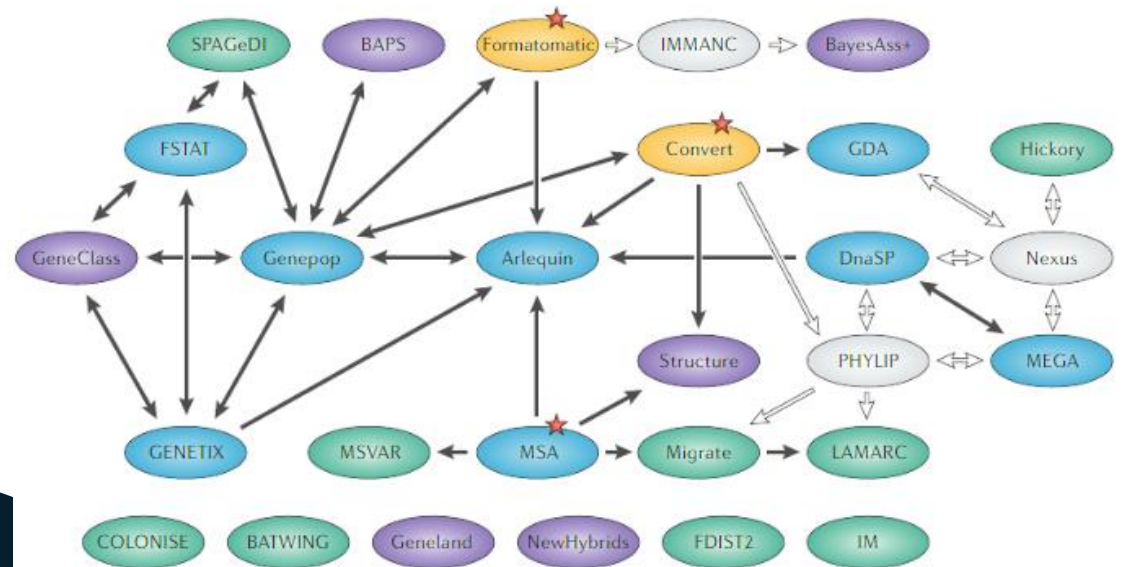
Why *ad hoc* formats are a problem: lessons from population genetics

Computer programs for population genetics data analysis: a survival guide

Laurent Excoffier and Gerald Heckel

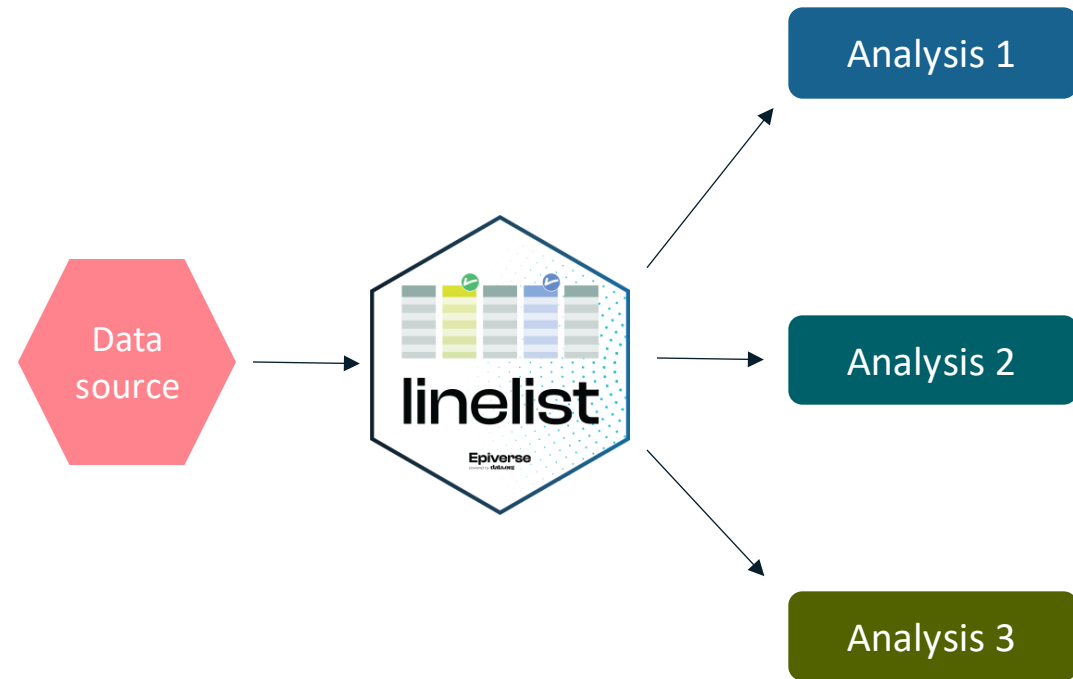
Abstract | The analysis of genetic diversity within species is vital for understanding evolutionary processes at the population level and at the genomic level. A large quantity of data can now be produced at an unprecedented rate, requiring the use of dedicated computer programs to extract all embedded information. Several statistical packages have been recently developed, which offer a panel of standard and more sophisticated analyses. We describe here the functionalities, special features and assumptions of more than 20 such programs, indicate how they can interoperate, and discuss new directions that could lead to improved software and analyses.

- Interoperability but...
 - Requires many conversion steps
 - Complicated data pathways
 - Prone to mistakes/errors
- No coding, testing, or documentation standards



Excoffier & Heckel 2006 *Nature Reviews Genetics*

linelist: a package to handle case line list data



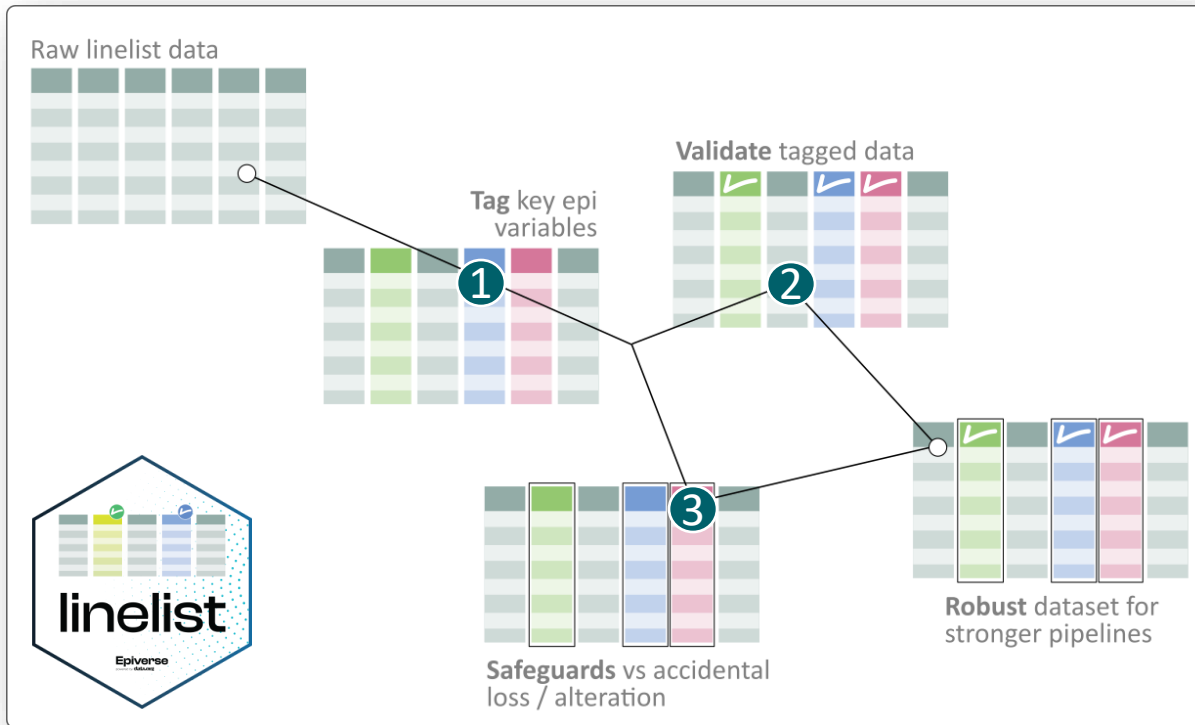
■ Case line list data

- Spreadsheet-like dataset
- Rows = different patients
- Columns = variables, including:
 - Dates of events: symptom onset, case reporting, ...
 - Case data: epi case definition, disease outcome, symptoms
 - Patient info: age, gender, occupation, location, ...

■ Common issues

- No standardized names for key epi variables
- Data have the wrong type / class e.g.:
 - dates stored as factors rather than Date,
 - Epi case definition coded as integer rather explicit character strings
- Key data may be altered or lost accidentally

linelist in a nutshell



<https://github.com/epiverse-trace/linelist>

1 Tagging system

- **linelist**: S3 class extending `data.frame` or `tibble`
- **Tags** identify columns storing **key epi variables** in a dataset
- Tags are stored as named **list** in `attr(., "tags")`

2 Data validation

- Validate tagged variables against their **expected types**
- Easy to extend to more advanced validations (e.g. consistency in timing of events)

3 Safeguards

- Protections against alteration / loss of tagged variables
- Done through **S3 dispatching** with dedicated methods for 'dangerous' operations
- Implementation for non-generic more cumbersome

Documentation

The screenshot shows the GitHub repository page for `linelist` by `epiverse-trace`. The page title is `linelist: Tagging and Validating Epidemiological Data`. It includes sections for **Installation** (Stable and Development versions), **Usage** (with a diagram showing the workflow from raw data to a robust dataset), and a **Links** sidebar. The diagram illustrates the process: Raw linelist data is processed by tagging key epidemiological variables, which then leads to validating the tagged data. This results in safeguards against accidental loss or alteration, ultimately creating a robust dataset for stronger pipelines.

linelist: Tagging and Validating Epidemiological Data

linelist provides a safe entry point to the *Epiverse* software ecosystem, adding a foundational layer through *tagging*, *validation*, and *safeguarding* epidemiological data, to help make data pipelines more straightforward and robust.

Installation

Stable version

Our stable versions are released on CRAN, and can be installed using:

```
install.packages("linelist", build_vignettes = TRUE)
```

Development version

The development version of *linelist* can be installed from [GitHub](#) with:

```
if (!require(remotes)) {  
  install.packages("remotes")  
}  
remotes::install_github("epiverse-trace/linelist", build_vignettes = TRUE)
```

Usage

Raw linelist data

Tag key epi variables

Validate tagged data

Safeguards vs accidental loss / alteration

Robust dataset for stronger pipelines

linelist works by tagging key epidemiological data in a `data.frame` or a `tibble` to facilitate and strengthen data pipelines. The resulting object is a `linelist` object, which extends `data.frame` (or `tibble`) by providing three types of features:

1. a **tagging system** to identify key data, enabling access to these data using their tags rather than actual names, which may change over time and across datasets
2. **validation** of the tagged variables (making sure they are present and of the right type/class)
3. **safeguards** against accidental losses of tagged variables in common data handling operations

Links

- [View on CRAN](#)
- [Browse source code](#)
- [Report a bug](#)
- License**
- [Full license](#)
- [MIT + file LICENSE](#)
- Community**
- [Code of conduct](#)
- Citation**
- [Citing linelist](#)
- Developers**
- Thibaut Jombart
Author, maintainer
- Dev status**
- License: [MIT](#)
- CRAN: [OK](#)
- R-CMD-check: [passing](#)
- codecov: [100%](#)
- RECON: [experimental](#)
- downloads: [362/month](#)
- downloads: [362](#)
- DOI: [10.5281/zenodo.6556047](#)

- All functions documented using **roxygen2**
- All exported functions have examples
- README.Rmd
- Vignette
- Website (**pkgdown**)
- Infographics
- Hex sticker!!
- Cheat-sheet underway

Testing and continuous integration



```
1 test_that("tests for make_linelist", {
2
3   # test errors
4   msg <- "Assertion on 'x' failed: Must be of type 'data.frame', not 'NULL'."
5   expect_error(make_linelist(NULL), msg)
6
7   msg <- "Assertion on 'x' failed: Must have at least 1 cols, but has 0 cols."
8   expect_error(make_linelist(data.frame()), msg)
9
10  msg <- "Assertion on 'var_name' failed: Must be element of set \\{'speed','dist'\\}, but is 'bar'."
11  expect_error(make_linelist(cars, outcome = "bar"), msg)
12
13  msg <- "Unknown variable types: foo\n Use only tags listed in `tags_names()`, or set `allow_extra = TRUE`"
14  expect_error(make_linelist(cars, foo = "speed", allow_extra = FALSE), msg, fixed = TRUE)
15
16  # test functionalities
17  expect_identical(tags_defaults(), tags(make_linelist(cars), TRUE))
18
19  x <- make_linelist(cars, date_onset = "dist", date_outcome = "speed")
20  expect_identical(tags(x)$date_onset, "dist")
21  expect_identical(tags(x)$date_outcome, "speed")
22  expect_null(tags(x)$outcome)
23  expect_null(tags(x)$date_reporting)
24
25  x <- make_linelist(cars, foo = "speed", bar = "dist", allow_extra = TRUE)
26  expect_identical(tags(x, TRUE), c(tags_defaults(), foo = "speed", bar = "dist"))
27
28  x <- make_linelist(cars, date_onset = "dist", date_outcome = "speed")
29  y <- make_linelist(cars, list(date_onset = "dist", date_outcome = "speed"))
30  expect_identical(x, y)
31
32 })
```

- Full test coverage for all functions
- Each function has its own test file
- Testing guides coding
- ~ 50% tests on errors and warnings ;
~50% tests on functionalities
- Github actions for CI (usethis)

Code reviews, collaboration workflows, communities

Solo project is a bad example but...

```
`[.linelist` <- function(x, i, j, drop = FALSE) {  
  # Strategy for subsetting  
  #  
  # Subsetting is done using the next method in line, for which we drop the  
  # linelist class (we cannot use NextMethod because of the extra argument  
  # `lost_action`). Then we need to check two things:  
  #  
  # 1. that the subsetting object is still a `data.frame` or a `tibble`; if not,  
  # we automatically drop the `linelist` class and tags  
  # 2. if the output is going to be a `linelist` we need to restore previous  
  # tags with the appropriate behaviour in case of missing tagged variables  
  
  lost_action <- get_lost_tags_action()  
  
  # Case 1  
  out <- drop_linelist(x)[i, j, drop = drop]  
  if (is.null(ncol(out))) {  
    return(out)  
  }  
}
```

```
`[<-.linelist` <- function(x, i, j, value) {  
  lost_action <- get_lost_tags_action()  
  out <- NextMethod()  
  old_tags <- tags(x, TRUE)  
  out <- restore_tags(out, old_tags, lost_action)  
  out  
}
```

- Code reviews
 - Useful, but non-trivial
 - Pair-programming better?
 - Part of Pull Requests, or separate exercise?
- Lean / Agile development
 - Important to incorporate user feedback early and often
 - Short cycles with regular production of MVPs better for user engagement?
- Dev and user community
 - How to engage end-users?
 - Metrics of community health or performance?

Blueprints: how many boxes to ticks?



- ❑ Coding standards
- ❑ Documentation standards
- ❑ Testing and continuous integration
- ❑ Collaboration framework
 - ❑ Code reviews
 - ❑ Pair programming
 - ❑ Agile/Lean methodologies
- ❑ Community engagement and monitoring
- ❑ ...

THANK YOU

Senior RSE position for *Epiverse* open until Friday at data.org!

Contact:



Thibaut Jombart



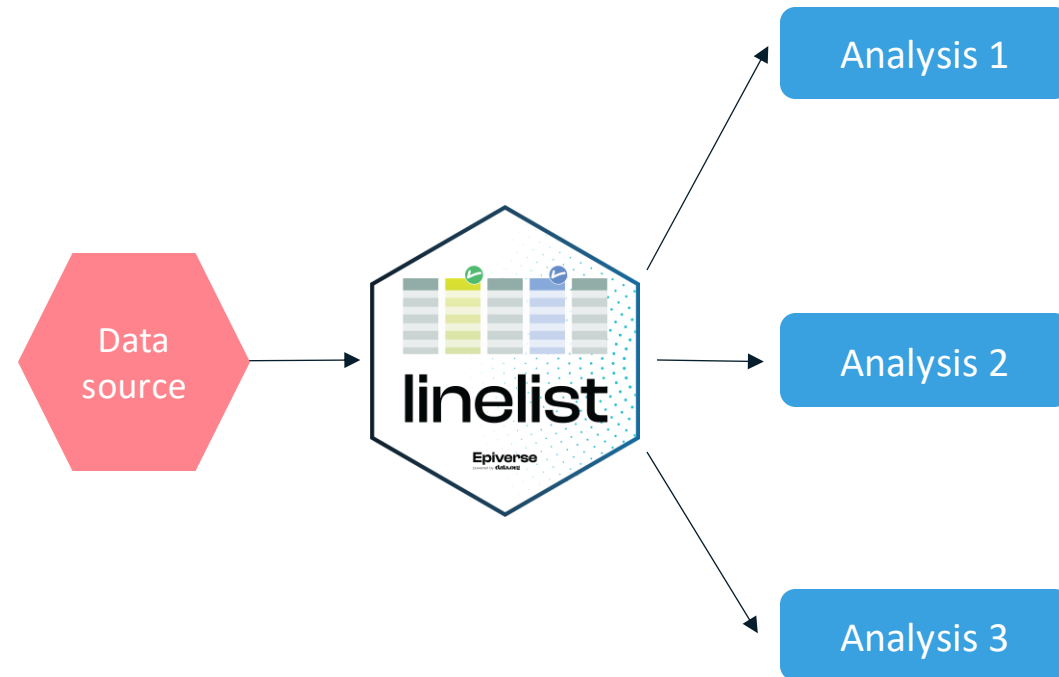
thibaut@data.org



linelist: tagging, validating, and safeguarding key epi data

Linelist = S3 class extending `data.frame`

- Tagging system: identify key epi data
 - `set_tags()`: identify columns storing key epi variables (e.g. date of onset, disease outcome, age)
 - `select()`, `select_tags()`, `tags_df()`: access tagged variables
 - Tags are stored in the attributes of the object
- Data validation
 - Key epi variables have pre-defined acceptable types
 - `validate_linelist()`: check tags consistency and types
- Safeguards
 - Protections against alteration / loss of tagged variables
 - `lost_tags_action()`: defines behaviour to adopt
 - `rename()`, `names() <-`: update tags as needed
 - `select()`, `[`, `[[`, `...`: issues warnings/errors if variable lost



Context

Epiverse-TRACE: building a coherent ecosystem for outbreak analytics in R

- Simplest workflows rely on:

```
import_data() %>%
```

```
  preprocess_data() %>%
```

```
  use_analysis() %>%
```

```
  summarise_or_plot()
```

- Complications:
 - Lack of **canonical representations**
 - Multiple inputs (e.g. case counts + serial interval)
 - Multiple layers of analysis (e.g. estimate R -> make projections)

