universität innsbruck

The R System: From Open Source to Open Science

An Insider’s View

Achim Zeileis

https://eeecon.uibk.ac.at/~zeileis/

Overview

R:

- System for statistical computing.
- Open-source software under General Public License (GPL).
- `https://www.R-project.org/`

Insider: Achim Zeileis.

- Statistician.
- Co-editor: Journal of Statistical Software.
- Ordinary member: R Foundation.
- Co-creator: useR! conference, R-Forge, . . .

What is R?

Based on: ACM award-winning S language (core of commercial S-PLUS).

Early 1990s: **R**oss Ihaka and **R**obert Gentleman start reimplementation, with underlying semantics derived from Scheme, eventually called **R**.

Since 1997:

- Base system developed by R Core Team.
- Highly extensible through packages.
- Openly shared through Comprehensive R Archive Network.

Since 2000s: Lingua franca in statistics. Around $\sim$100 CRAN packages in 2000, more than 15,000 today ($\sim$ 25% nominal growth rate per year).

Since 2010s: Popular programming language (#5, IEEE Spectrum 2019), esp. for data science (KDnuggets 2015–2019, Top 3: Python, R, RapidMiner).

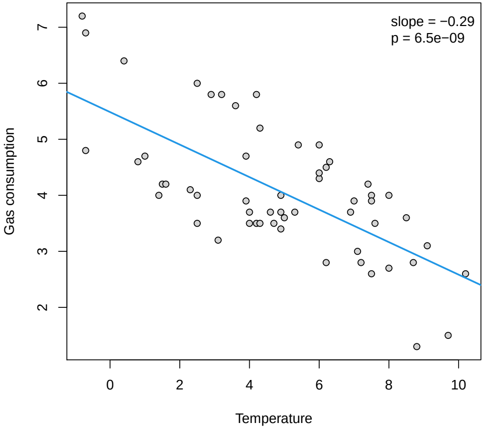
What is R?

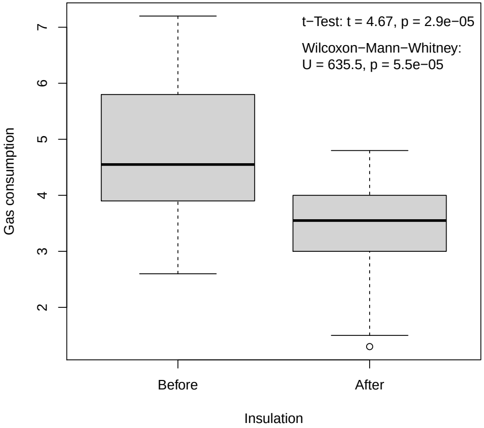
Vantage points:

- Data analysis vs. programming.
- Statistics vs. data science.
- Community vs. app.
- Science vs. commerce.

What is R used for?

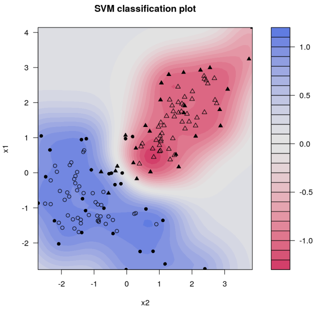
Classically: Statistics and graphics.
Linear regression, two-sample tests, scatter plots, bar charts, . . .



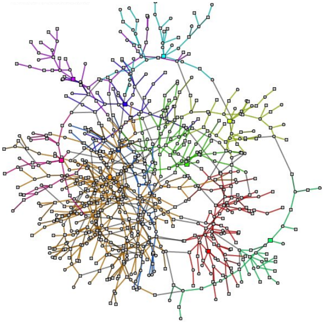


What is R used for?

Diversified methods: Machine learning, social network analysis, econometrics, environmetrics, psychometrics, ...



doi:10.18637/jss.v015.i09



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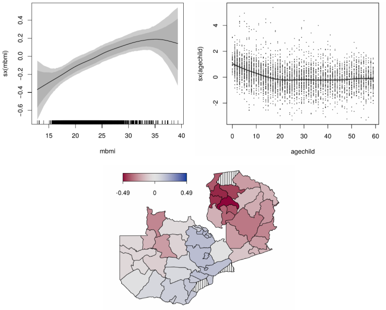
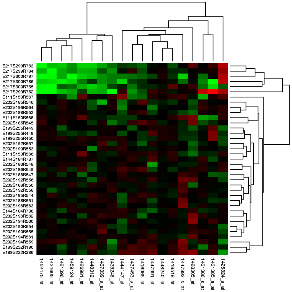


doi:10.18637/jss.v063.i21

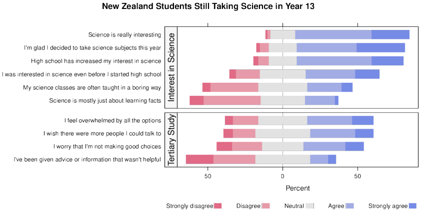
What is R used for?

Data structures: Genomic data, spatial and space-time data, surveys, text corpora, connections to databases, ...



https://en.wikipedia.org/wiki/Heat_map

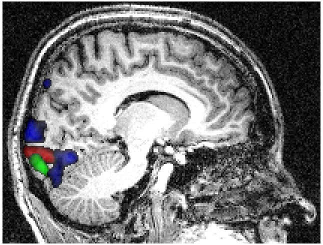
doi:10.18637/jss.v082.i07



doi:10.18637/jss.v057.i05

What is R used for?

Specific applications: Bioinformatics, business analytics, atmospheric sciences, finance, natural language processing, . . .



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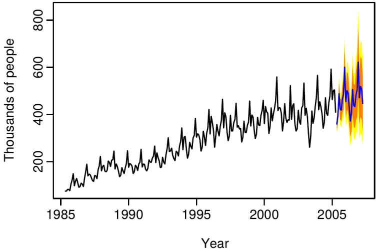

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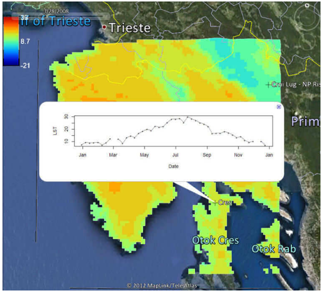

doi:10.18637/jss.v063.i05

Why is R so successful?

- Open source.
- By statisticians for statisticians (in a very broad sense).
- Highly modular and extensible.
- Many subcommunities.
- Spillovers through joint journals, conferences, . . .
- “Big Data Science.”

How does the R community work?

R Core/Foundation

Base system

CRAN

Mailing lists

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Why do you contribute to the R community?

In 1999: Undergraduate.

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Since 2004: Postdoc onwards.

- *“Why do you volunteer to edit a free journal and organize conferences?
  You should make some money.”*
- Open and reproducible science!

From open source to open science in R

R package system:

- Inspired by the Debian package system.
- Standard way of sharing R code with easy installation.
- Packages can contain: R code, source code (e.g., C, C++, Fortran, . . .), data, manual pages, other documentation, examples, tests, demos, . . .
- Package can *depend* on other packages.
- CRAN (Comprehensive R Archive Network) is the main repository for sharing R packages (sources plus binary versions). Daily checks of the entire network on different platforms.
- Other repositories include Bioconductor, R-Forge but also platforms such as GitHub or Bitbucket.

From open source to open science in R

Dynamic documents:

- **2002:** `Sweave` introduced in R 1.5.0 by Friedrich Leisch.
  Ideas: From literate programming to literate data analysis.
  Basis for: R package vignettes.
  First (?) contributed example: *strucchange* based on previous JSS paper.
- **2006:** *weaver* in Bioconductor by Seth Falcon.
  Ideas: Caching code chunks.
- **2012:** *knitr* by Yihui Xie.
  Initial ideas: Extended/improved `Sweave` alternative.
  Later: R/Markdown support.
- **2014:** *rmarkdown* by J.J. Allaire, Yihui Xie, *et al.*
  Ideas: Wide range of output formats via pandoc. Flexibility/extensibility.

From open source to open science in R

Research compendium: Robert Gentleman & Duncan Temple Lang (2004).

- Integrate computations, code, and data used in empirical analyses, simulations, etc.
- In R based on package infrastructure, leveraging dynamic documents (`Sweave`, *knitr*, ...) and automatic checking.

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In 2010s:

- Support R package development: *devtools* (Wickham), *roxygen(2)* (Danenberg, Eugster, Wickham), ...
- Package reproducibility: *checkpoint* (Microsoft), *packrat* (RStudio), ...
- Pipelines and workflows: *drake* (Landau), ...

Scientific review of R packages

Journal of Statistical Software

- Founded in 1996 by Jan de Leeuw for publishing statistical software (any language).
- Publication: Software – along with paper plus replication materials.
- Papers: Explains statistical technique, code, and provides examples.
- Trick: Fit publication of software into classical journal publications.
- Review: Classical single-blind review.
- Audience: Broad community of practitioners, teachers, and researchers in the field of statistics
- Emphasis: Careful review of existing implementations and discussion of relative (dis)advantages. Interesting case study highlighting the typical workflow.

Scientific review of R packages

The R Journal

- Founded in 2001 as *R News*.
- Papers: Reasonably short, clearly written, not too technical, focused on R.
- Content: Not just packages – also reviews, comparisons, or applications.
- Review: Classical single-blind review.
- Audience: Users and developers of R.
- Emphasis: Contribution in context of related functions/packages. Reproducible code.

Scientific review of R packages

rOpenSci

- Founded in 2011 as non-profit initiative for reproducible data retrieval.
- Peer review process for R packages.
- Focus: Data processing and infrastructure.
- Submission: Open in GitHub repository.
- Review: Open conversation using GitHub issues.
- Recommendations for good practices: Naming conventions, code style, documentation, testing.
- Journal publication: Subsequently in *Journal of Open Source Software*.

Implementation strategies

Task: Turn conceptual statistical tools into computational tools

Goals: Desirable features.

- Easy to use.
- Numerically reliable.
- Computationally efficient.
- Flexible and extensible.
- Reusable components.
- Object-oriented.
- Reflect features of the conceptual method.

Problem: Often antagonistic, e.g., computational efficiency vs. extensibility.

Implementation strategies

Guiding principle: The implementation should be guided by the properties of the underlying statistical methods while trying to ensure as much efficiency and accuracy as possible.

The resulting functions should do what we think a method does conceptually.

In practice: Many implementations are instead guided by the limitations that programming languages used to have where everything had to be represented by numeric vectors and matrices.

Question: What language features are helpful for improving this?

Implementation strategies

Object orientation: Create objects of a certain class with methods performing typical tasks. Particularly easy: S3 paradigm, based on generic functions.

Functions as first-class objects: Functions are a basic data type that can be passed to and returned by another function.

Lexical scope: Returned *nested lexically scoped functions* can have free variables stored in function closure.

Compiled code: Combine convenience of interpreted code and efficiency of (byte) compilation or dynamic linking.

Reusable components: Build on standard and widely-used tools. Likewise, provide tools that other implementations can build on.

Illustration: Heteroscedastic censored regression

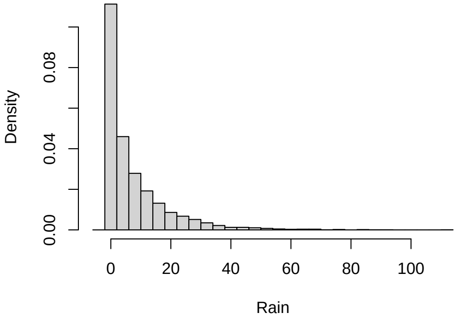
Examples:

- Linear regression in base R.
- Heteroscedastic censored and truncated regression models in package *crch* (Messner, Mayr, Zeileis 2016, *The R Journal*, `doi:10.32614/RJ-2016-012`).

Illustration:

- Precipitation forecasts for Innsbruck, Austria (`RainIbk`).
- Observed 3 day-accumulated precipitation amounts (`rain`) from SYNOP station Innsbruck Airport from 2000-01-01 to 2013-09-17.
- Corresponding GEFS 11-member ensemble reforecasts of total accumulated precipitation between 5 and 8 days in advance with mean `ensmean` and standard deviation `enssd`.

Illustration: Heteroscedastic censored regression



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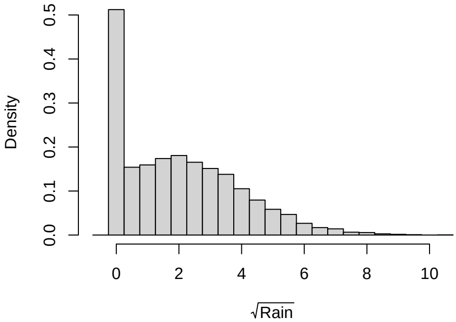

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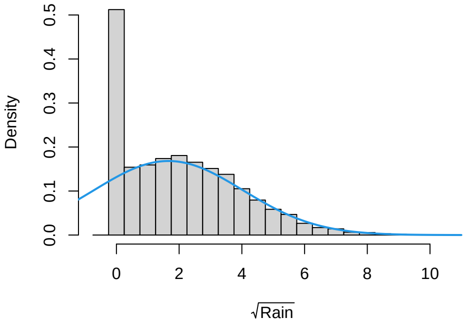

Hence:

- Gaussian model on square root scale.
- Account for zeros by “censoring”.

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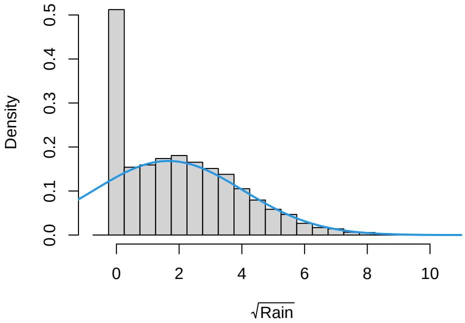

Hence:

- Gaussian model on square root scale.
- Account for zeros by “censoring”.
- Mean precipitation explained by GEFS ensemble mean.
- Standard deviation explained by GEFS standard deviation (using a log link).

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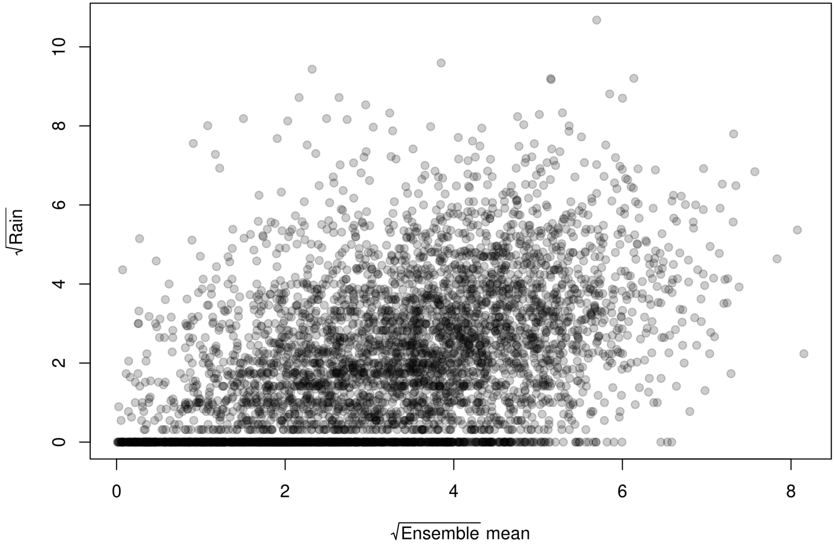

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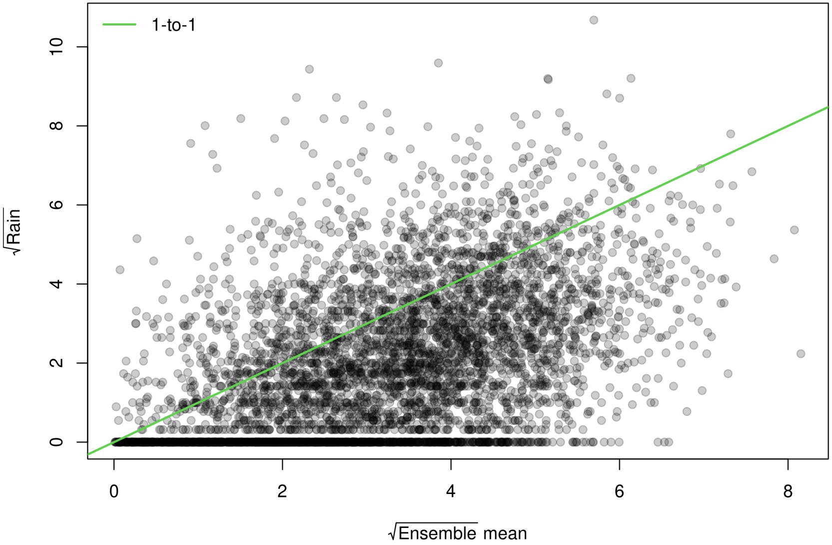

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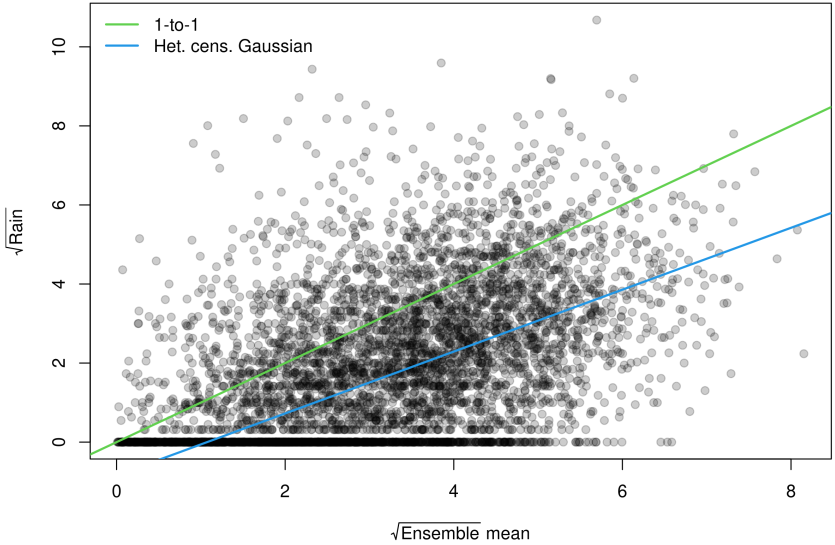

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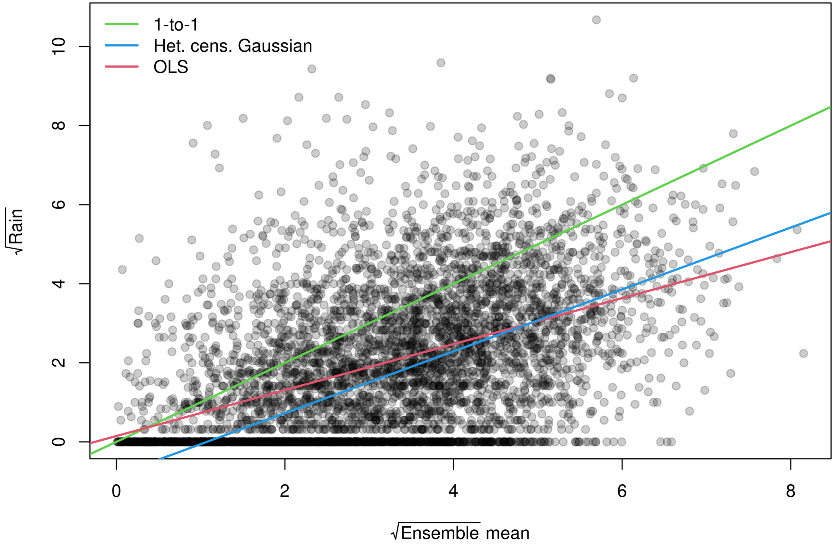

Implementation strategies in practice

Example: Linear regression in R.

- **Object orientation:** `lm()` returns an "`lm`" object with suitable methods and extractor functions.
- **Reusable components:** Underlying workhorse `lm.fit()` without pre- and postprocessing is also provided.
- **Compiled code:** At its core `lm.fit()` has a `.Fortran("dqrls", ...)` call.

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Application:

```
R> m1 <- lm(rain ~ ensmean, data = RainIbk)
R> coef(m1)
(Intercept)     ensmean
      0.147       0.582
R> vcov(m1)
            (Intercept)   ensmean
(Intercept)    0.003026 -0.000772
ensmean       -0.000772  0.000240
```

Implementation strategies in practice

Note: S3 uses naming convention for methods (plus registration).

Here: `coef.lm()` and `vcov.lm()`.

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Also: Smart default methods like `confint.default()` that reuse other methods.

```
R> confint(m1)
              2.5 % 97.5 %
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ensmean     0.5512  0.612
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Furthermore: Methods for inference, prediction, data handling, etc.

Implementation strategies in practice

Package: *crch* for censored regression with conditional heteroscedasticity.

- **Object orientation**: Object structure and methods mimic `lm()`/`glm()`.
- **Functions as first-class objects**: Model components can be supplied as functions, e.g., the log-likelihood (and its gradient and Hessian) or the link function (and its inverse and derivative).
- **Lexical scope**: Log-likelihood (and its gradient and Hessian) may access data through lexical scoping.
- **Compiled code:** Density/score/Hessian functions for censored distributions are implemented in C.
- **Reusable components**:
  - Uses `lm.fit()` for starting values.
  - Provide: `crch.fit()` and `dcnorm()` for other applications.
  - Optional: CRPS estimation from *scoringRules*.

Implementation strategies in practice

```
R> library("crch")
R> m2 <- crch(rain ~ ensmean | log(enssd), data = RainIbk, left = 0)
R> coef(m2)
        (Intercept)                 ensmean (scale)_(Intercept)
             -0.840                   0.783               0.687
 (scale)_log(enssd)
              0.220
```

```
R> confint(m2)
                     2.5 % 97.5 %
(Intercept)         -0.983 -0.697
ensmean              0.743  0.822
(scale)_(Intercept)  0.662  0.712
(scale)_log(enssd)   0.161  0.279
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```

Reproducibility: Paper from the *The R Journal* is provided in the package as a dynamic `Sweave` vignette.

Where are we going from here?

Quite certainly: More growth and more diversity.

High potential: Exciting and innovative collaborations across disciplines.

Unclear: Whether “one” R community will persist.

Crucial: Communication and exchange within and beyond the community.

Strength: Rooting in academia, tools for reproducibility and open science.