Good Practices in R Programming

Martin Mächler

maechler@R-project.org
The R Core Team

maechler@stat.math.ethz.ch
Seminar für Statistik
ETH Zurich, Switzerland

useR! – July 1, 2014

Outline

Introduction

Seven Guidelines for Good Practices in R Programming

FAQ 7.31 — generalized: Loss of Accuracy

Specific Hints — to give your friends

Prehistoric – 10 years ago

- May 2004: First UseR! conference in Vienna
- 8 (eight!) keynote talks by R Core members (about exciting new features, such as namespaces)
- R version 1.9.1 a month later in June

This talk is . . .

- *not* systematic and comprehensive like a *book* such as
  John Chambers "Programming with Data" (1998),
  Venables + Ripley "S Programming" (2000),
  Uwe Ligges "R Programmierung" (2004) [in German]
  Norm Mattloff's "The Art of R Programming" (2011)
- *not* for complete newbies
- *not* really for experts either
- *not* about C++ (or C or Fortran or . . .) programming
- *not* always entirely serious ☺

This talk **is** . . .

- on R language programming
- my own view, and hence *biased*
- hopefully helping userR s to improve
- . . . . . . somewhat entertaining ?

“Good Practices in R Programming”

- “Good”, not “best practice”
- “Programming” using R : useR!
- “Practice”: What I’ve learned over the years, with examples

What is Programming ?

Is Programming

- like driving a car, a skill you learn and then know to do?
- a scientific process to be undertaken with care?
- a creative art?

$\longrightarrow$ all of them, but not the least an $\boxed{\text{art}}$.
$\longrightarrow$ Your R 'programs' should become *works of art* ... ☺

In spite of this,
$\longrightarrow$ *Guidelines* (or *Rules) for Good Practices in R Programming*:

Rule 1: Work with Source files!

R Source files aka 'R Scripts' (but more).

- obvious to some,
  not intuitive for useRs used to GUIs.
- *Paradigm* (shift):
  Do not `edit` *objects* or `fix()` them, but modify (and re-evaluate) their source!

  In other words (from the ESS manual):

  The source code is real.
  The objects are realizations of the source code.

(*Rule 1*: Work with Source files!)

- Use a *smart* editor or IDE (Interactive Development Environment)
  - syntax-aware: parentheses matching "(..))"
    highlighting (differing *fonts* & colors syntax dependently)
  - able to *evaluate* R code, by line, whole selection (region), `function`, and the whole file
  - command completion on R objects

such as (available on all platforms):

- Emacs + ESS (**E**macs **S**peaks **S**tatistics)
- RStudio
- StatET (R + Eclipse)
- ......and more

Good source code

1. is well readable by humans
2. is as much self-explaining as possible

Rule 2: Keep R source well readable & maintainable

Good, well readable R source code $\rightarrow$ is also well <u>maintainable</u>

1. Do indent lines!   (i.e. initial spaces)
2. Do use spaces!

   e.g., around $<-$, $=$, $<=$,..., $+$, $-$, ...;

   after ',' ; before '{'
3. Do wrap long lines!

   (at column 70–80; $\longrightarrow$ do not put the editor in fullscreen mode)

well maintainable (*Rule 2* cont.)

4. Do use comments copiously! (about every 10 lines)
   We recommend
   '##' for the usually indented comments,
   '#' for end-of-line comments, and
   '###' for the (major) "sectioning" or beginning-of-line ones.
5. Sometimes even better (but more laborious): Use <u>Sweave</u> or <u>knitr</u> (or `org-mode` or another "weave & tangle" system (`noweb`))
6. E.g., R source in R Markdown (`*.Rmd`) format.

… well readable code and the assignment operator

Beware: this is very controversial, and I am severely biased!

Some (including me, but by far not all!) believe that

using $<-$ instead of $=$ leads to *far* easier readable code:

- ' $=$ ' is also used much in function *calls* (incl. `list(a=.., b=..)` and definitions (argument defaults)

$<-$ stands out visually

- $<-$ can be marked up (by font/color) quite easily
- something hard to achieve correctly with $=$ (distinguishing *assignment* from function arguments (both calls *and* formals)

Keyboard shortcut for $<-$: `Alt`+`-` in both Rstudio and ESS (configurable)

\end{really-controversial}

. . . . . . well maintainable (*Rule 2* (end))

2 x. Do follow *naming conventions* for function **argument names**, and if available also for new functions and/or classes.

But do *not* impose rigid rules here, since

1. programming is *art* (☺)
2. The S language has a long history with many contributers:
   Live with some historical misnomers . . .

2 . . . Modularity, Clarity: *"refine and polish your code"* (V&R): More on "well maintainable" in the following rules

Rule 3: Do read the documentation

and read it again and again ......
(and—only then—submit bug reports ☺)

1. Books (see above), ...
2. The manuals "An Introduction to R" (early),
   "Writing R Extensions" (when you're mutating from
   useR to programmeR)
3. R package vignettes
4. The help pages! and try their **examples**
5. Use `help.search()` (and read its help page to find out about fuzzy matching and the `agrep` argument!)
6. Websearch ('G..gl.') Blogs, etc — *are* dated. Compare with *"official"* docs: help pages, vignettes: The package authors' reference.

Rule 4: Do learn from the masters

An art is learned from the master artists:
Picasso, Van Gogh, Gauguin, Manet, Klimt . . .
John Chambers, Bill Venables, Bill Dunlap, Luke Tierney, Brian Ripley, R-core in general :-), Dirk Eddelbuettel, Hadley Wickham
. . .

Read others' source — Learning by examples

. . . learn from the masters – Read the Source:

Obi-Wan Kenobi . . . :

"Use the source, Luke!"

```
> install.packages("fortunes")
> fortune(250)
As Obi-Wan Kenobi may have said in Star Wars: "Use the sour
Luke!"
   -- Barry Rowlingson (answering a question on the
      documentation of some implementation details)
      R-devel (January 2010)
```

Reading Source for '?' ... → Find Easter egg

```
> Anybody ? there ???
  ?
  ,,
```

(Demo)

```
Contacting Delphi...the oracle is unavailable.
We apologize for any inconvenience.
```

Read the source – of packages

- Note: The R source of an R package (in *source* state) is inside ⟨pkg⟩/R/*.R, and *not* what you get when you display the function in R(by typing its name).
- R FAQ 7.40 *How do I access the source code for a function?* ⟶ Uwe Ligges (2006), "Help Desk: Accessing the sources", *R News*, **6/4**, 43–45 (http://CRAN.R-project.org/doc/Rnews/Rnews_2006-4.pdf)
- Download the *source* package, ⟨pkg⟩_⟨n.m⟩.tar.gz typically from CRAN, unpack it and
  - read it,
  - experiment with it, and
  - learn from it,
- Or browse the package source code on R-forge or github, or …

Rule 5: Do not Copy & Paste !

because the result is *not* well maintainable:
Changes in one part do not propagate to the copy!

1. write functions instead
2. break a long function into *several* smaller ones, if possible
3. Inside functions : still *Rule 5*: "Do not Copy & Paste !!"
   $\longrightarrow$ write local or (package) global helper functions
   $\longrightarrow$ use many small helper functions (nicely hidden in `NAMESPACE`).

"Use functions", e.g., use

```
mat[complicated, compcomp] <-
   if(A) A.expr   else   B.expr
```

instead of

```
if(A)   mat[complicated, compcomp] <- A.expr
else    mat[complicated, compcomp] <- B.expr
```

Use Functions

Everything you do in R is calling functions anyway: In R,

Everything that exists is an object;
Everything that happens is a function call.

(John Chambers — **this** morning, first two of three principles)

Quiz:

When `if(*)` ... *is regarded as function with three arguments, the last being optional with a default,*
What is the default?

```
if(C) A
if(C) A else B
```

Answer: `NULL`: **if** (FALSE) A returns `NULL` invisibly

Rule 6: Strive for clarity and simplicity

first! . . . and second . . . and again, e.g.,
think about naming of intermediate results with “self-explainable” variable names
but use short names (plus comments) for formulae

> *Venables & Ripley:*
> *“Refine and polish your code in the same way you would polish your English prose”*

(prose: using as “dictionary” your reference material)

$\longrightarrow$ modularity (“granularity”)

Optimization: much much later, see below

Rule 7: Test your code!

1. Carefully write (small) testing examples, for each function
   ("modularity", "unit testing")
2. Next step: Start a 'package' via `package.skeleton()`. This allows (via `R CMD check`)
   - auto-testing (all the help pages examples).
     use `example(`*your_function*`)`
   - specific testing (in a `./tests/` subdirectory, with or without strict comparison to previous results)
   - documenting your functions (and data, classes, methods): takes time, but almost always leads you to improve your code !

Test your code! (*Rule 7* cont.)

3. Use software tools for testing:
   - Those of `R CMD check` are in the standard R package `tools`, and
     codetools (by Luke Tierney)
   - Unit testing by packages, `RUnit`, `testthat`, etc.

After Testing, maybe Optimizing

Citing from V&R's "S Programming" (p.172):

> *Jackson "Principles of Program Design" (on 'code optimization'):*
>
> - *Rule 1 Don't do it.*
> - *Rule 2 (for experts only) Don't do it yet—not until you have a perfectly clear and unoptimized solution.*
>
> *'to the right problem by an efficient method'.*

Premature optimization is the root of all evil – Donald Knuth

Optimizing code - 2

1. Really do clean up and *test* your code and think twice before you even start contemplating optimizing the code . . .
2. do **measure**, not guess:

> *In 2001, when R was at version 1.1.x,*
>
> ```
> From: Thomas Lumley (tlumley@u.washington.edu)
> To  : R-help
> ```
>
> *There are two fundamental principles of optimisation*
> *1) Don't do it unless you need it*
> *2) Measure, don't guess, about speed.*
>
> *The simple way to answer questions about which way is slower/more memory intensive is to try it and see. Between Rprof(), unix.time() and gc(), you have all the information you need. . . . .*

In 2014: Have packages `rbenchmark`, `microbenchmark`, `pbdPROF`, and more.

Seven Guidelines ("Rules") – still relevant

1. Work with Source files
2. Keep R source code well readable and maintainable
3. Do read the documentation
4. Do learn from the masters — Read R (package) sources
5. Do not Copy & Paste! — Modularize into (small) Functions
6. Strive for clarity and simplicity
7. Test your code — and test, and test!

New Guidelines:

8. Maintain R code in Packages (extension of “Test!”)
9. → Source code management, e.g., subversion(svn) or github(git)
10. `Rscript` or `R CMD BATCH` ⟨`mysource`⟩`.R` should “always” work!

    ⟶ *Reproducible* Data Analysis and Research

    - → Do not use `.RData` no, really, not ever! ...
    - Rather, use `save()` explicitly only for *expensive* parts.
    - Consider `attach("myStuff.rda")` instead of `load("myStuff.rda")`
    - Use the following outline:

```
savefile <- "<myThings>.rda"
if(file.exists(savefile)) attach(savefile) else
    ........
    ........
    save(o1, o2,..., o.n, file = savefile)
}
```

FAQ 7.31 — Floating Point Numbers are Limited

R FAQ 7.31

Why doesn't R think these numbers are equal?

> *The only numbers that can be represented exactly in R's numeric type are integers and fractions whose denominator is a power of 2. Other numbers have to be rounded to (typically) 53 binary digits accuracy. As a result, two floating point numbers will not reliably be equal unless they have been computed by the same algorithm, and not always even then. For example*

```
> a <- sqrt(2)
> a * a == 2  # mathematically, yes,  ...
[1] FALSE
> a * a - 2
[1] 4.440892e-16
```

For more, ... David Goldberg (1991), "*What Every Computer Scientist Should Know About Floating-Point Arithmetic*", *ACM Computing Surveys*, **23/1**, 5–48. . .

FAQ 7.31 — Floating Point – 2 –

R FAQ 7.31

Why doesn't R think these numbers are equal?

To quote from "*The Elements of Programming Style*" by Kernighan and Plauger:

> *10.0 times 0.1 is hardly ever 1.0.*

Actually, it is in R, (always / typically (?)), nowadays.

FAQ 7.31 ++ : The "log" in the dpq-functions

All "dpq" distribution functions in R, i.e. **d**ensity cumulative **p**robability and **q**uantile functions, have a `log` or `log.p` argument (FALSE / TRUE).

Why ?

$\longrightarrow$ Compute Likelihoods via `d<foo>(*, log = TRUE)`
$\longrightarrow$ Probalistic Networks, MC(MC): $P = P_1 \cdot P_2 \cdot \cdots \cdot P_n$ quickly underflows to zero.

Solution: Work in "log space": $\log P = \sum_j \log P_j$, where $\log P_j$ are computed via R's `d⟨foo⟩(*, log=TRUE)` or `p⟨foo⟩(*, log.p=TRUE)`, rather than taking logs

FAQ 7.31 . . . Why R needs even more functions

1. `log1p()` (since R 1.0.0), `expm1()` (since R 1.5.0)

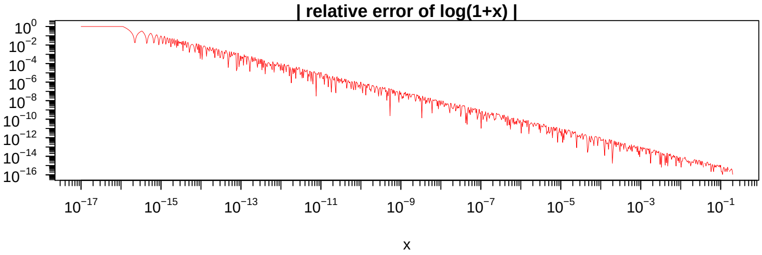
Why $\log(1+x)$ is not good enough, but $\text{log1p}(x)$ is

$1 + x$ cannot be numerically accurate when $|x| \ll 1$. In double precision (53 bits ≈ 16 digits) accuracy, $1 + x$ "sees" only 2–3 digits of x when $x = 10^{-14}$,

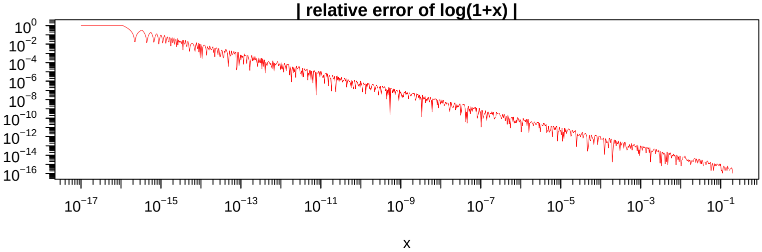
```
> u <- 1 + (e <- 4e-13/9)  ## then   u - 1 == e  mathematically:
> rbind(‘u-1‘ = u - 1, e)
            [,1]
u-1 4.440892e-14
e   4.444444e-14
```

And the consequence for $\log(1+x)$,

```
> curve(abs(1 - log(1+x) / log1p(x)), 1e-17, .2,  log = 'xy', ma
> sfsmisc :: eaxis(1); eaxis(2)
```



Why $\log1p(x)$ beats $\log(1+x)$



Solution: Expand $\log(1+x)$ around $x = 0$. Well known

$$\log(1+x) = x - x^2/2 + x^3/3 \pm \ldots = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{x^n}{n},$$

for $|x| < 1$.

Fast version of this expansion: typically used in `log1p()`.

FAQ 7.31 ... Why R needs even more functions –2–

2. `cospi()`, `sinpi()`, `tanpi()` (from R 3.2.0), e.g., `cospi(x)`$:= \cos(\pi \cdot x)$, accurately, e.g., for $x = \frac{1}{2}$:

```
> cos(pi/2) ## mathematically == 0
[1] 6.123234e-17
> cospi(1/2)
[1] 0
```

3. `log1mexp()` ... (my research; in R's Rmathlib C code, named differ.)

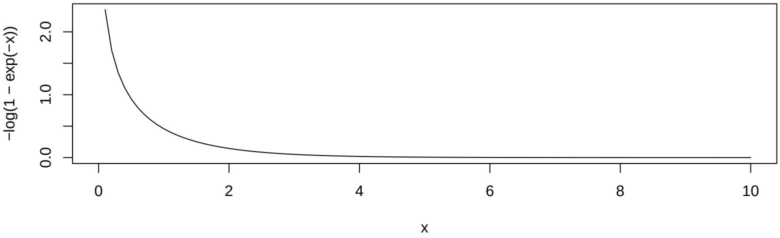
Simple (semi-artificial!) Example: logit(exp(-L))

Logistic regression: Computing "logit()"s, $\log \frac{p}{1-p}$ accurately for very small p, i.e., $p = \exp(-L)$, or

$$\log \frac{p}{1-p} = \log p - \log(1-p) = -L - \log(1 - \exp(-L)),$$

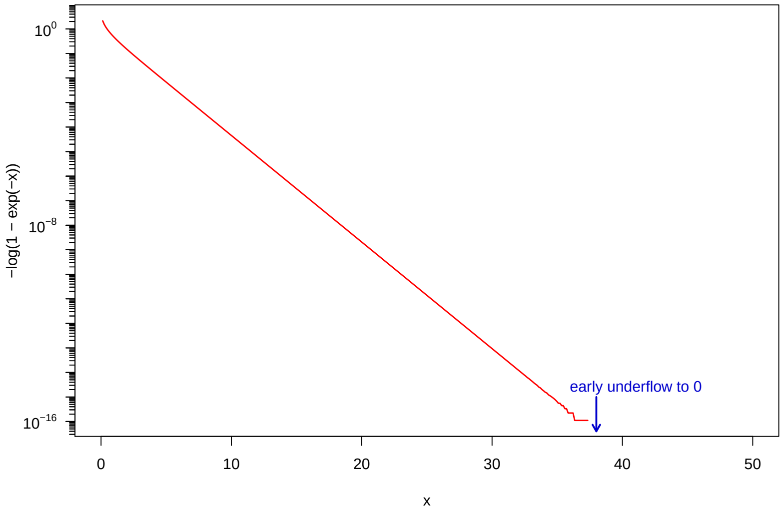
and hence $-\log(1 - \exp(-L))$ is needed, e.g., when p is really really close to 0, say $p = 10^{-1000}$, as then we can only compute $\mathrm{logit}(p)$, if we specify $L := -\log(p) \leftrightarrow p = \exp(-L)$.

```
> curve(-log(1 - exp(-x)), 0, 10)
```



seems fine. — — However, . . .

However, further out to 50 (and on a log scale), we observe



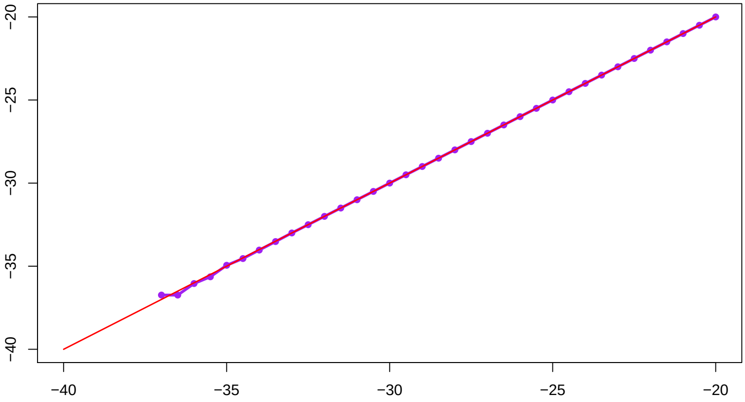
which shows early underflow.

What did happen? Look at

```
> x <- -40:-35
>     -log(1 - exp(x))
[1] 0.000000e+00 0.000000e+00 0.000000e+00 1.110223e-16 2.220446
[6] 6.661338e-16
> log(-log(1 - exp(x)))# --> -Inf values
[1]      -Inf      -Inf      -Inf -36.73680 -36.04365 -34.94504
> ## ok, how about more accuracy
> x. <- mpfr(x, 120)
> log(-log(1 - exp(x.)))# aha... looks perfect now
6 'mpfr' numbers of precision  120   bits
[1] -39.999999999999999979329048775382417334
[2]  -38.99999999999999994233721967569358070
[3]  -37.99999999999999984304517159810296111
[4] -36.999999999999999957331848579613165434
[5] -35.999999999999999884024061830552087239
[6] -34.999999999999999684744214015307532692
```

Visually, and with "high accuracy" `mpfr`-numbers:

```
> x <- seq(-40, -20, by = .5)
> plot(x,x, type="n", ylab="", ann=FALSE)
> lines(x, log(-log(1 - exp(x))), type = "o", col = "purple", lw
> x. <- mpfr(x, 120)
> lines(x, log(-log(1 - exp(x.))), col=2, lwd=1.5)
```



The "real" solution uses a <u>piecewise</u> implementation of

Specific Hints, Tips:

1. Subsetting ("[..]"):
   1.1 Matrices, arrays (& data.frames):
   Instead of `x[ind ,]`, use `x[ind, , drop = FALSE]` !
   1.2 tricky because of NAs
   Inside "[..]", often use `%in%` (wrapper of `match()`) or `which()`.
2. Not x == NA but **is**.**na**(x)
3. Use '1:n' only when you *know* that n is positive:
   Instead of `1:length(obj)`, use **seq**_along(obj)

Specific Hints – 2:

4. Do not *grow* objects:
   If you cannot avoid a `for` loop, replace

```
rmat <- NULL
for(i in 1:n) {
  rmat <- rbind(rmat, long.computation(i, .....))
}
```

   by

```
rmat <- matrix(0., n, k)
for(i in 1:n) {
  rmat[i, ] <- long.computation(i, .....)
}
```

   and almost always, column by column instead of row by row (creating the *transpose*):

```
tmat <- matrix(0., k, n)
for(i in 1:n) {
  tmat[, i ] <- long.computation(i, .....)
}
```

Specific Hints, Tips (cont.)

5. Use `lapply()`, `sapply()`, sometimes preferably `vapply()` `mapply()` (Apply to **m**ultiple arguments), or sometimes the `replicate()` wrapper:

```r
sample <- replicate(1000, median(rt(100, df=3)))
hist(sample)
```

6. Use `with(<d.frame>, ......)` and do *not* attach data frames
7. Use `TRUE` and `FALSE`, not 'T' and 'F' !
8. know the difference between '|' vs '||' and '&' vs '&&' and inside **if**(....) almost always use '||' and '&&'!
9. use `which.max()`, `...`, `findInterval()`
10. Learn about 'Regular Expressions': `?regexp` etc

What Style is your R programming?
Perform the art, enjoy and be productive!

Martin.Maechler@R-project.org