

Good Practices in R Programming

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useR! – July 1, 2014

Outline

- 1 Introduction
- 2 Seven Guidelines for Good Practices in R Programming
- 3 FAQ 7.31 — generalized: Loss of Accuracy
- 4 Specific Hints — to give your friends



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Prehistoric – 10 years ago

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- 2 Seven Guidelines for Good Practices in R Programming
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- May 2004: First UseR! conference in Vienna
- 8 (eight!) keynote talks by R Core members (about exciting new features, such as namespaces)
- Discussion on the mailing lists in June



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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 ?


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“Good Practices in R Programming”

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

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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?

→ all of them, but not the least an art.

→ Your R 'programs' should become *works of art* ... ☺

In spite of this,

→ Guidelines (or Rules) for Good Practices in R Programming:

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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.*

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(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

Good source code

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- 2 is as much self-explaining as possible

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Rule 2: Keep R source well readable & maintainable

Good, well readable R source code → is also well maintainable

- 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; → do not put the editor in fullscreen mode)

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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 Sweave or knitr (or `org-mode` or another “weave & tangle” system (`noweb`))
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... 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)

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.....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 contributors:
Live with some historical misnomers ...

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

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

- 1 Books (see above), . . .
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An art is learned from the master artists:
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... 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 source, 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 ???
?
,,
```

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

(Demo)

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- 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)
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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 !!"
 → write local or (package) global helper functions
 → use many small helper functions

"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
```

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

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 → write local or (package) global helper functions
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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?

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1 if(C) A
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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)

→ modularity ("granularity")

Optimization: much much later, see below

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Test your code! (Rule 7 cont.)

- ④ 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

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- Rule 1 Don't do it.
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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.

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Outline

- 1 Introduction
- 2 Seven Guidelines for Good Practices in R Programming
- 3 FAQ 7.31 — generalized: Loss of Accuracy
- 4 Specific Hints — to give your friends

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 –

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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.



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

Why ?

- Compute Likelihoods via `d<foo>(*, log = TRUE)`
- Probabilistic Networks, MC(MC): $P = P_1 \cdot P_2 \cdot \dots \cdot P_n$ 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



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FAQ 7.31 ... Why R needs even more functions

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

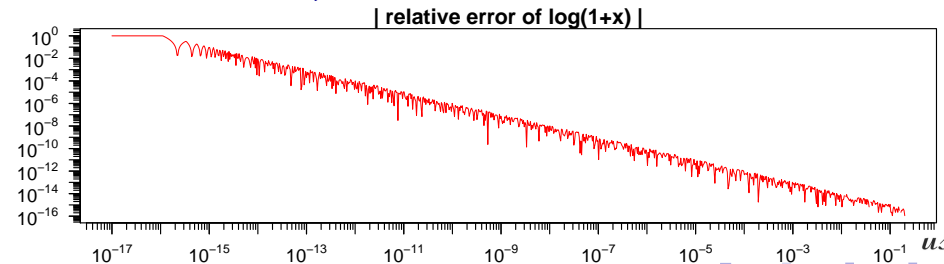
Why $\log(1 + x)$ is not good enough, but $\log1p(x)$ is

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

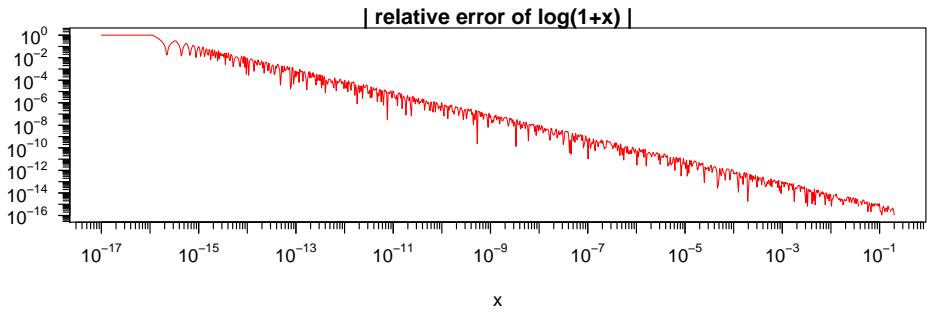
```
> u <- 1 + (e <- 4e-13/9) ## then u - 1 == e mathematically:
> rbind('u-1' = u - 1, e)
```

```
      [,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', main =
> sfsmisc :: eaxis(1); eaxis(2)
```



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



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

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

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(π · x), accurately, e.g., for x = 1/2:

```
> cos(pi/2) ## mathematically == 0
```

```
[1] 6.123234e-17
```

```
> cospi(1/2)
```

```
[1] 0
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- 3 log1mexp() ... (my research; in R's Rmathlib C code, named differ.)

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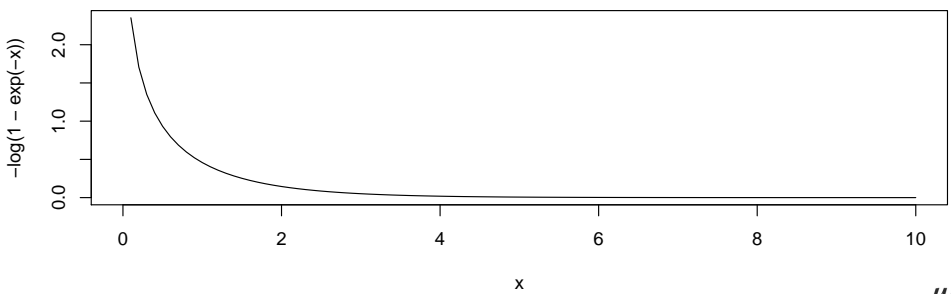
Simple (semi-artificial!) Example: logit(exp(-L))

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

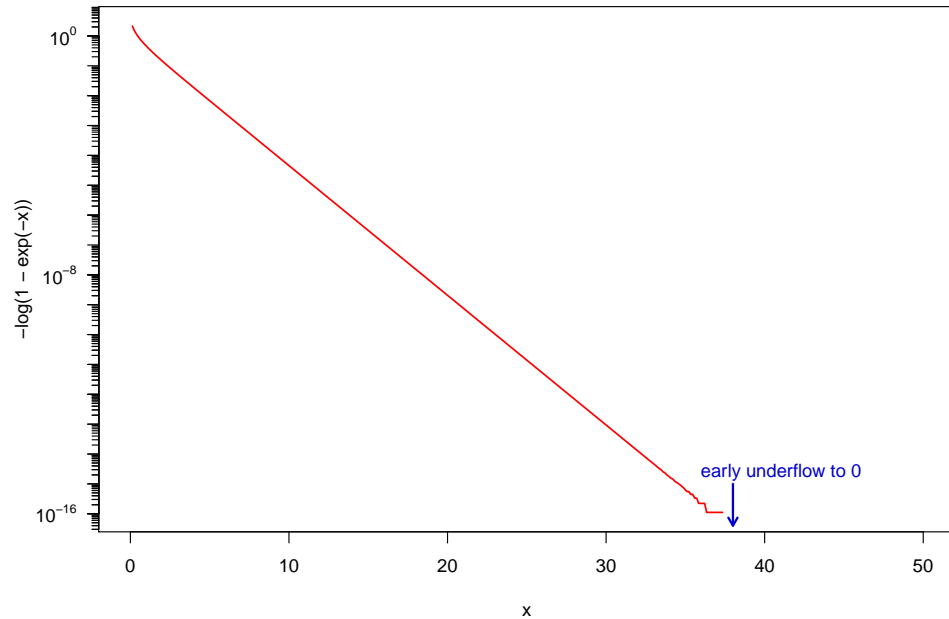
$$\log \frac{p}{1-p} = \log p - \log(1-p) = -L - \log(1 - \exp(-L)),$$

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 logit(p), if we specify $L := -\log(p) \leftrightarrow p = \exp(-L)$.

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



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



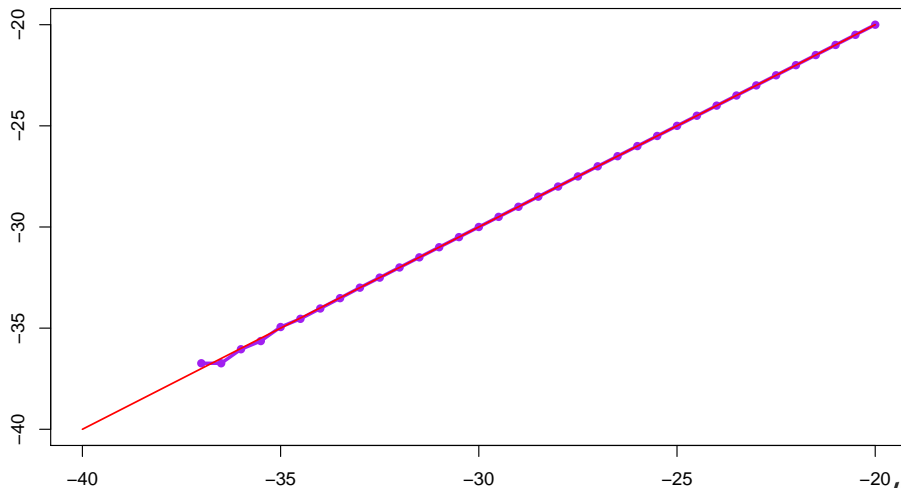
What did happen? Look at

```
> x <- -40:-35
> -log(1 - exp(x))
[1] 0.000000e+00 0.000000e+00 0.000000e+00 1.110223e-16 2.220446e-16
[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] -39.9999999999999997932904877538241734
[2] -38.999999999999999423372196756935807
[3] -37.9999999999999998430451715981029611
[4] -36.99999999999999957331848579613165434
[5] -35.999999999999999884024061830552087239
[6] -34.999999999999999684744214015307532692
```

which shows early underflow.

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", lwd=3)
> x. <- mpfr(x, 120)
> lines(x, log(-log(1 - exp(x.))), col=2, lwd=1.5)
```



Outline

- 1 Introduction
- 2 Seven Guidelines for Good Practices in R Programming
- 3 FAQ 7.31 — generalized: Loss of Accuracy
- 4 Specific Hints — to give your friends

Specific Hints, Tips:

- 1 Subsetting (“[..]”):
 - 1 Matrices, arrays (& data.frames):
Instead of `x[ind ,]`, use `x[ind, , drop = FALSE]` !
 - 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)`

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Specific Hints – 2:

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

```

1 rmat <- NULL
2 for(i in 1:n) {
3   rmat <- rbind(rmat, long.computation(i, .....))
4 }

```

 by


```

1 rmat <- matrix(0., n, k)
2 for(i in 1:n) {
3   rmat[i, ] <- long.computation(i, ..... )
4 }

```

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


```

1 tmat <- matrix(0., k, n)
2 for(i in 1:n) {
3   tmat[, i] <- long.computation(i, ..... )
4 }

```

Specific Hints, Tips (cont.)

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

```
1 sample <- replicate(1000, median(rt(100, df=3)))
2 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 '&&'!
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