

## Assignment 3

- Two numerical approximations to the derivative of a function  $f$  at a point  $x$  are the forward difference quotient

$$\delta_F(f, x, h) = \frac{f(x+h) - f(x)}{h}$$

and the central, or symmetric, difference quotient

$$\delta_S(f, x, h) = \frac{f(x+h) - f(x-h)}{2h}$$

for a step size  $h$ . A third option that is available when the function  $f$  is analytic near  $x$  is

$$\delta_C(f, x, h) = \frac{\Im(f(x+hi))}{h}$$

where  $i = \sqrt{-1}$  is the imaginary unit and  $\Im(z)$  is the imaginary part of the complex number  $z$ .

Choose a few functions and argument values and examine these approximations graphically by plotting the approximations against  $-\log_2 h$  for  $h$  values in the range  $2^{-1}, \dots, 2^{-64}$ . Some functions and argument values you might consider:

$$\begin{array}{ll} f_1(x) = \sin(x) & \text{at } x = 1 \\ f_2(x) = 10000 \sin(x) & \text{at } x = 1 \\ f_3(x) = \tan(x) & \text{at } x = 1.59 \\ f_4(x) = \phi(x) & \text{at } x = 0.5 \end{array}$$

where  $\phi$  is the standard normal density. Comment on the behavior you see. Can you suggest a guideline for choosing the step size  $h$ ?

- Create an R package `pareto` that contains a function `dpareto` to compute the density of the Pareto distribution. Include an example in the help page and some test code in a `tests` directory. Your package should pass R CMD `check` without errors or warnings. Your writeup should contain a simple example of using your package, and you should include your package as a source package file created by R CMD `build` in your submission archive file.

The *Writing R Extensions* manual provides documentation on creating R packages. The function `package.skeleton` may help you get started. There is also a small sample package available called `AddOne` that you can start with. You can unpack the package sources with the command

```
tar xzf AddOne_1.0-1.tar.gz
```

You can find further documentation, tutorials, and tools by searching the web, e.g. for “create R package.”

Commit your package source code to your UI GitLab repository in a directory named `pareto`. After your commit your repository should look like

```
<your repo>/
  README.md
  pareto/
    DESCRIPTION
    NAMESPACE
    README
    man/
      ...
    R/
      ...
    tests/
      ...
```

You should submit your assignment electronically using Icon. Your submission should include

- your writeup as a PDF file
- a source code package as created by `R CMD build`.

Submit your work as a single compressed tar file. If your work is in a directory `mywork` then you can create a compressed tar file with the command

```
tar czf mywork.tar.gz mywork
```

## Solutions and Comments

General comments:

1.
  - If you use separate plots for symmetric and forward differences then you should use common axes.
  - Numerical derivatives are often used in optimization.
  - It is important to choose a step size that is not too large or too small. This balances the *truncation error* ( $h$  too large) against the *round-off error* ( $h$  too small).
  - Central differences can use larger step sizes but require more function evaluations.
  - Simple calculus can help understand why central differences will be more accurate than forward differences for a given small  $h$  value.
  - Complex differences avoid the round-off error, but require the algorithm computing the function to be able to handle complex arguments.
  - Dennis and Schnabel (1983) recommend for forward difference quotients

$$h = \sqrt{\eta} \max\{x, t_x\}$$

where  $\eta$  is the relative error in computing  $f(x)$  and  $t_x$  is the typical size of  $x$ .

- Using this rule, if  $\eta = 10^D$  with  $D$  the number of accurate base 10 digits in  $f(x)$  then the number of accurate digits in  $\delta_F(f, x, h)$  is about  $D/2$ .
- Their recommendation for central difference quotients is

$$h = \sqrt[3]{\eta} \max\{x, t_x\}$$

For  $\eta = 10^D$  the number of accurate digits in the approximate derivative should be about  $2D/3$ .

- Extrapolation methods can be useful.
2.
    - Your submission should include a package tarball as created by `R CMD build`.
    - Your package should pass `R CMD check` without errors, warnings or notes.
    - Package tests:
      - You should include test code in a `tests` directory.
      - Your tests should try to test all important cases.
      - Be careful about floating point equality tests.
      - It is best to not put tests in examples in the help pages.

- If you include a `README` file then its contents should be appropriate for a user of your package. You can also use a `README.md` file; GitLab will render these nicely.
- Make sure your help file includes useful information.
- Make sure examples in your help file are useful as examples.
- Please follow the coding standards on use of spaces, avoiding long lines, and proper indentation.
- Use vectorized arithmetic, not `for` loops or `apply` functions in your R code.
- Vectorization should work for `x`, `a`, and `b`.
- You do not need to check for missing arguments without a default as R will do that.
- Make sure your package is in your GitLab repo and at the right place as specified in the assignment. If you have not done this please fix before the next assignment.
- The tests I used:

```

stopifnot(is.na(dpareto(3,-2, 1)))
stopifnot(is.na(dpareto(3,2, -1)))
stopifnot(all.equal(dpareto(3,2,1), 0.222222222))
stopifnot(all.equal(dpareto(1,2,3), 0.0))
stopifnot(all.equal(dpareto(3:5,2, 1),
                    c(0.222222222, 0.1250000, 0.0800000)))
stopifnot(all.equal(dpareto(1:5,2, 1),
                    c(0.0, 0.0, 0.222222222, 0.1250000, 0.0800000)))
stopifnot(all.equal(dpareto(6,2:4, 1),
                    c(0.05555555556, 0.08333333333, 0.11111111111)))
stopifnot(all.equal(log(dpareto(1:5,2, 1)),
                    dpareto(1:5,2, 1, log = TRUE)))
stopifnot(all.equal(dpareto(6,1,2:4),
                    c(0.0092592593, 0.0023148148, 0.0005144033)))
stopifnot(all.equal(dpareto(1:6,1:2, 1),
                    c(0.0, 0.0, 0.11111111111, 0.125, 0.04, 0.05555555556)))
stopifnot(all.equal(dpareto(1, 2, 1:2), c(0, 0)))

```