Enhancing Target Functions

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Why and How: Enhancing a Target Function

There are many methods for sensitivity analysis and optimisation (calibration) that take a target function, generate parameters and run the function with these parameters.

When performing sensitivity and optimisation tasks,

- we may impose some constraints on the parameters
- we might be interested not only in the final result, but also on all generated parameters to track how the method came to the result

Depending on the implementation of the sensitivity or optimisation method, this options might or might not be available. If the optimisation method does not offer a possibility to limit parameters or to track intermediate runs, then we have to add this functionality to our target function:

- checking parameters and return a high penalty value instead of real function value for parameters outside the boundaries
- recording parameters and results of each function run

Instead of doing this manually by writing the corresponding code inside the target function, we can use R to enhance our target function automatically.

Respecting boundaries

The function `enhanceWithBoundaries` takes as arguments

- our target function
- lower and upper bounds as vectors which have as many elements as our parameterset has

and returns a new function which checks first, if the parameters are within the boundaries. In this case, it calls our original target function. If the parameters are outside the boundaries, it returns Infitiy, i.e. the maximum possible error.

There are some additional optional arguments

- `penalty_value` we may change the penalty value to another value (e.g. -Inf)
- `boundary_fun` maybe we want to supply a more sophisticated function for checking if parameters are within boundaries
- `param_pos` can be used, if our target function takes the parameter set not as the first argument, but as the second or third etc.

```
enhanceWithBoundaries <- function(fun, l_bound, u_bound,
                                  penalty_value=Inf,
                                  boundary_fun=NULL,
                                  param_pos=1,
                                  ...) {
```

```
  function(...) {
    invalid <- FALSE
    if(!is.null(boundary_fun)) {
      invalid <- boundary_fun(...elt(param_pos))
    }
    else {
      invalid <- !all(l_bound <= ...elt(param_pos) & ...elt(param_pos) <= u_bound)
    }
    if(invalid) {
      penalty_value
    }
    else {
      fun(...)
    }
  }
}
```

Example

The function $f(x, y) = (x^2 + y^2 - 1)^2 + (x + y - 1)^2$ has two minima, at (0,1) and at (1,0). Let's assume that for some reasons a value for x smaller than 0.6 would not be acceptable.

```
target_fun <- function(p) (p[1]^2 + p[2]^2 -1)^2 + (p[1] + p[2] -1)^2
o1 <- optim(c(.7,.7), target_fun, control=list(reltol=1e-20))

round(o1$par,10)
```

```
## [1] 0 1
```

```
round(o1$value,10)
```

```
## [1] 0
```

When running an optimisation of our function, we get the minimum at (0,1), which we could not accept.

```
target_fun_bd <- enhanceWithBoundaries(target_fun,c(.6,-100),c(100,100))

o2 <- optim(c(.7,.7), target_fun_bd,  control=list(reltol=1e-20))
round(o2$par,10)
```

```
## [1] 1 0
```

```
round(o2$value,10)
```

```
## [1] 0
```

By imposing a boundary on our function, the optimisation process would give us only values with x bigger than 0.6

Recording all runs

When we want to record all parameters and function calls used by the sensitivity or optimisation method, we need some object to store this data.

For this we create a so called *Reference Class* in R. We name this class "FunctionRecorder". The class has a slot `runInfo` that holds the information for each run and some methods:

- `add` to add the information of a run to the `runInfo` list

- `get` and `get_as_df` to get the `runInfo` either as list or dataframe
- `reset` to clear the `runInfo`

And there is the method `enhanceWithRecorder` that takes our target function and returns a new function that takes the parameter set, runs our target function and stores parameters as well as the result in the function recorder.

The `enhanceWithRecorder` takes an optional argument `info_fun`. We can create a function that takes a parameter set and a result value and restructure them before being stored in the recorder. By default parameters and result are added as a vector. With an own function, we can put them e.g. in a named vector so that the recorded dataframes has our prefered column names.

```
FunctionRecorder <- setRefClass(
  "FunctionRecorder",

  fields=list(runInfo="list",temporaryInfo="list", count="numeric",temporarycount="numeric"),

  methods = list(
    add = function(x) {
      count <<- count + 1
      temporarycount <<- temporarycount + 1
      if(length(temporaryInfo)<temporarycount) {
        ls <- list()
        v <- rep(0.0,length(x))
        for(i in 1:1000) {
          ls[[length(ls)+1]]<-v
        }
        runInfo <<-c(runInfo,temporaryInfo)
        temporarycount <<- 1
        temporaryInfo <<- ls
      }
      temporaryInfo[[temporarycount]]<<-x
    },
    get = function() {
      c(runInfo, temporaryInfo)[1:count]
    } ,
    get_as_df = function() tryCatch({
      df <- data.frame(do.call(rbind, get()),row.names = NULL)
      if(length(get())>0 && is.null(names(get()[[1]]))){
        names(df)<-c(paste0("P",1:(ncol(df)-1)),"Value")
      }
      df
    }),
    reset = function() {
      runInfo <<-list()
      temporaryInfo <<- list()
      temporarycount <<- 0
      count <<- 0
    },
    enhanceWithRecorder = function(fun,info_fun=\(p,r)c(p,r), ...) {
      reset()
      function(...) {
        r <- fun(...)
        add(info_fun(...,r))
        r
      }
    },
    initialize = function() {
      runInfo <<-list()
      temporaryInfo <<- list()
      temporarycount <<- 0
      count <<- 0
    }
  )
)
```

Notice: As the time to add elements to a list seems to increase with the lenght of the list, we add the information to a shorter temporary list, which we then add to the full list. This will speed up the adding process, if we have a large amount of runs recorded (>100000).

Example

We create a function recorder and enhance our initial target function before supplying it to the optimisation function.

```
FR <- FunctionRecorder$new()

target_fun_rec <- FR$enhanceWithRecorder(target_fun)

o3 <- optim(c(.7,.7), target_fun_rec,  control=list(reltol=1e-20))
round(o3$par,10)
```

```
## [1] 0 1
```

```
round(o3$value,10)
```

```
## [1] 0
```

After the optimisation, we can get the dataframe of all runs

```
runs3 <- FR$get_as_df()
head(runs3)
```

```
##     P1    P2     Value
## 1 0.70 0.700 0.1604000
## 2 0.77 0.700 0.2277724
## 3 0.70 0.770 0.2277724
## 4 0.63 0.770 0.1601040
## 5 0.56 0.805 0.1346976
## 6 0.56 0.735 0.1083921
```

Same procedure with the function that respects boundaries

```
target_fun_bd_rec <- FR$enhanceWithRecorder(target_fun_bd)

o4 <- optim(c(.7,.7), target_fun_bd_rec,  control=list(reltol=1e-20))
round(o2$par,10)
```

```
## [1] 1 0
```

```
round(o2$value,10)
```

```
## [1] 0
```

```
runs4 <- FR$get_as_df()

head(runs4)
```

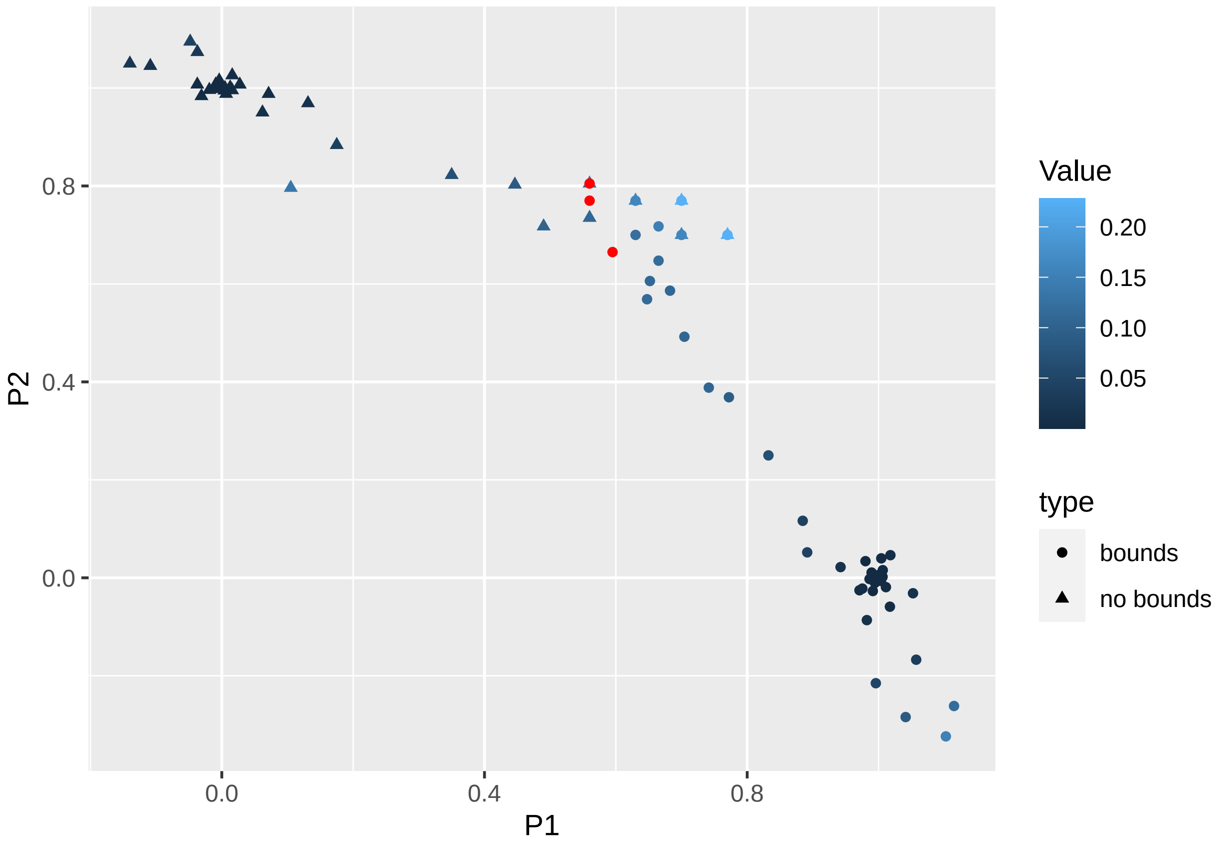
```
##      P1    P2     Value
## 1 0.70 0.700 0.1604000
## 2 0.77 0.700 0.2277724
## 3 0.70 0.770 0.2277724
## 4 0.63 0.770 0.1601040
## 5 0.56 0.805       Inf
## 6 0.63 0.700 0.1216916
```

Notice the value `Inf` where P1 (i.e x) is smaller than 0.6:

Plotting the runs

```
runs3$type<-"no bounds"
runs4$type<-"bounds"
runs <- rbind(runs3,runs4)

library(ggplot2)
ggplot(runs) + geom_point(aes(x=P1,y=P2,colour=Value,shape=type)) +
  scale_colour_continuous(na.value="red")
```



The parameters for the non-bounded function move during optimisation towards (0,1), whereas those for bounded function are "punished" (red dots) if they move towards 0 on x-Axis. So the optimisation method will move the parameters towards the allowed area and then taking the road towards the other minimum at (1,0)

Performance test

Running pure function 1 million times

```
system.time(
  for(i in 1:1000000)
    target_fun(c(runif(1,.55,1),runif(1,0,1)))
)
```

```
##        User      System verstrichen
##        5.93        0.83        6.94
```

Running boundary check function 1 million times

```
system.time(
  for(i in 1:1000000)
    target_fun_bd(c(runif(1,.55,1),runif(1,0,1)))
)
```

```
##        User      System verstrichen
##       11.64        0.69       13.36
```

Running recording function 1 million times

```
FR$reset()
tm <- system.time(
  for(i in 1:1000000)
    target_fun_bd_rec(c(runif(1,.55,1),runif(1,0,1)))
)
tm
```

```
##        User      System verstrichen
##      185.23        1.55      205.21
```

Recording the result of 1 million runs adds an overhead of around 3.4 minutes. Considering the fact, that running usual models 1 million times will take rather hours than minutes, then the overhead of the recording will be neglectable for most cases.

Extending FunctionRecorder to write to disk

Optimisation process may not finish always properly. Common failures can be

- crashing of the task (e.g. when running out of memory)
- aborting the task (e.g. when assigned computation time on clusters expires)

Recorded run data will vanish from memory in these cases. Therefore it's recommended for long running tasks to write the logged data to disk from time to time.

We extend the FunctionRecorder to accomplish the intermediate storage of data to disk.

The new recorder has a method `write()` that writes the data to disk. Actually it does not write the complete data at once, but it appends the new data to the file. The write method is called every time a new entry is added, but it will write to disk only if the time after the last write exceeds a given time interval.

When creating a new instance of the `FunctionRecorderToDisk`, the user has to supply a filename where to write and optionally the time interval (in minutes) between automatic writes. The minimum time interval is 1 minute, the default one is 5 minutes.

```
FunctionRecorderToDisk <- setRefClass(
  "FunctionRecorderToDisk",
  fields = list(
    filename = "character",
    writeinterval = "numeric",
    lastwrittentime = "numeric",
    lastwrittencount = "numeric"
  ),

  contains = "FunctionRecorder",

  methods = list(

    write = function(force=TRUE) {
      if(count > lastwrittencount &
         (force || as.numeric(Sys.time()) > lastwrittentime + writeinterval*60)) {
        append <- lastwrittencount!=0
        write.table(
          get_as_df()[(lastwrittencount +1):count,],
          filename,
          col.names = !append,
          append = append,
          row.names = FALSE,
          sep=","
        )
        lastwrittencount <<- count
        lastwrittentime <<- as.numeric(Sys.time())
      }
    },

    add = function(...) {
      callSuper(...)
      write(force=FALSE)
    },

    reset = function(newfile = NULL) {
      if(count > lastwrittencount) {
        write()
      }
      if(!is.null(newfile) && newfile!="")
      {
        filename <<- newfile
      }
      callSuper()
      lastwrittentime <<- 0
      lastwrittencount <<- 0

    },

    initialize = function(file, interval=5) {
      callSuper()
      lastwrittentime <<- 0
      lastwrittencount <<- 0
      filename <<- file
      writeinterval <<- min(1,interval)
    },
    finalize = function() {
      write()
    }
  )

)
```

Example of writing recorded data to disk

We create a function that needs at least two seconds to execute (by letting it sleep for 2 seconds).

```
longcomputation <- function (p) {
  Sys.sleep(1)
  p^2
}
```

We create a function recorder that will log the data to the file `longrun_recorded.csv` every minute. and enhance our function.

```
FRD <- FunctionRecorderToDisk$new("longrun_recorded.csv",1)



longcomputation_recorded <- FRD$enhanceWithRecorder(longcomputation)
```

Now we run the enhanced function 100 times, which will take appx. 100 seconds. We expect that after appx. 60 seconds the intermediate data will be written to disk.

```
for(i in 1:100) {
  longcomputation_recorded(i)
}
```

Let's check the written file:

```
recdata <- read.table("longrun_recorded.csv", sep=",", header=TRUE)
tail(recdata)
```

```
##    P1 Value
## 55 55  3025
## 56 56  3136
## 57 57  3249
## 58 58  3364
## 59 59  3481
## 60 60  3600
```

```
writtenrows <- nrow(recdata)
writtenrows
```

```
## [1] 60
```

The file contains 60 rows - which where written after 1 minute. After finishing the calculation, we call the `write()` function one more time explicitely to write the remaining data since the automatic write.

```
FRD$write()

recdata <- read.table("longrun_recorded.csv", sep=",", header=TRUE)
tail(recdata)
```

```
##      P1 Value
## 95   95  9025
## 96   96  9216
## 97   97  9409
## 98   98  9604
## 99   99  9801
## 100 100 10000
```

```
writtenrows <- nrow(recdata)
writtenrows
```

```
## [1] 100
```

Wrap up

If you want to use the enhancing functions, you can download the files

- `boundaries.R`
- `FunctionRecorder.R`

and include (`source`) them into your scripts.

Pure functional recorder

We don't really need references classes, we can also use R's standard mechanisms for closures. The benefits of reference classes are,

- their definition is more explicit
- we can use inheritance to extend functionality

Anyway, here the code for a recorder that does not use reference classes.

```
create_function_recorder <- function() {

  runInfo <- list()
  temporaryInfo <- list()
  count <- 0
  temporarycount <- 0


    add <- function(x) {
      count <<- count + 1
      temporarycount <<- temporarycount + 1
      if(length(temporaryInfo)<temporarycount) {
        ls <- list()
        v <- rep(0.0,length(x))
        for(i in 1:1000) {
          ls[[length(ls)+1]]<-v
        }
        runInfo <<-c(runInfo,temporaryInfo)
        temporarycount <<- 1
        temporaryInfo <<- ls
      }
      temporaryInfo[[temporarycount]]<<-x
    }
    get <- function() {
      c(runInfo, temporaryInfo)[1:count]
    }
    get_as_df = function() tryCatch({
```

```r
      df <- data.frame(do.call(rbind, get()),row.names = NULL)
      if(length(get())>0 && is.null(names(get()[[1]]))){
        names(df)<-c(paste0("P",1:(ncol(df)-1)),"Value")
      }
      df
    })
    reset <- function() {
      runInfo <<-list()
      temporaryInfo <<- list()
      temporarycount <<- 0
      count <<- 0
    }
    enhanceWithRecorder <- function(fun,info_fun=\(p,r)c(p,r), ...) {
      reset()
      function(...) {
        r <- fun(...)
        add(info_fun(...,r))
        r
      }
    }
    list(
      add=add,
      get=get,
      get_as_df=get_as_df,
      reset=reset,
      enhanceWithRecorder = enhanceWithRecorder
    )
}

FR <- create_function_recorder()
```