Quantessentials
R advice – optimising in R

Equities

Global
Quantitative

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Introducing Quantessentials

Following the client feedback for our recent note offering useful tips for the R programming language (see R advice, 29 June 2016), we decided to formally introduce a new product line, called Quantessentials. The purpose of this product will be to present hints and tips covering the broad toolkit of a quant analyst. The R programming language is again our focus for this issue.

Optimising in R

We first highlight the nloptr package, which offers a general approach to non-linear optimisation. We provide an overview of the functionality and we present a hands-on example by constructing (solving for) a Maximum Diversification portfolio.

Reproducible research

There is more and more demand for reproducible research. Two answers to this have been the knitr/R-markdown and Jupyter Notebook projects – both produce an output that includes both code and the results in an easy-to-read format. Adding to this, the Jupyter Notebook offers this in a web-based format.

Optimising in R using `nloptr`

nloptr is a package to help with non-linear optimisations. It is a one-stop shop for a large variety of different optimisation algorithms, each with their own strengths and weaknesses. It is an R wrapper around the NLopt library.[1]

`nloptr` provides access to lots of different optimisation algorithms

Quant analysts use optimisation across a wide variety of fields, but perhaps the most common is in portfolio construction. Many of the classic quantitative approaches to portfolio construction, including mean-variance and risk-parity, require optimisation, and the **nloptr** package is extremely helpful for this.

Useful for portfolio construction

As an example, suppose you wanted to build a maximum diversification portfolio with a few constraints:

Maximise the diversification ratio: $\frac{\sum_i w_i \sigma_i}{\sqrt{w^T \Sigma w}}$

Subject to: $\sum_i w_i = 100\%$ and $0\% \leq w_i \leq 50\%, \forall i$

The **nloptr** package is well suited to these kinds of problem.

Before we run the optimisation, we have to define a series of functions that get our problem into the right form for the **nloptr(.)** function:

Define functions

- **Objective function** – what we want the optimiser to minimise. If you want to maximise something (as we do in this example) then we express this as minimising minus one times our objective.
- **Equality constraint function** – in our example, the weights sum to 100%. These functions have to be written in the form $f(w) = 0$, so in this case it would be $f(w) = \sum_i w_i - 1$. Notice that you can have multiple equality constraints.
- **Inequality constraint function** – we can also include inequality constraints here, which are of the form $f(w) \leq 0$. Again, you can have multiple inequality constraints.
- **Gradient functions** – Optionally, we can also give the optimiser gradient functions, ∇f, which explicitly define the gradients of the objective and constraint functions. This nearly always makes it easier for the optimiser to find the minimum accurately, so provided your gradient is well defined, this is usually a good idea.

  However, it can be difficult to code up gradient functions without introducing bugs or mathematical errors like dropping a minus sign, particularly for complicated functions. Fortunately, there is a useful function called **check.derivatives(.)** in the **nloptr** package which can help you. It will compare the gradient computed numerically (using finite differences) with the result of your gradient function at a particular point. This can help to de-bug your gradient function.

These functions let us specify the problem in a way that can be interpreted by the **nloptr(.)** function. As a reference, we have included the code for these functions for the maximum diversification problem in the Appendix.

[1] See http://ab-initio.mit.edu/wiki/index.php/NLopt_Introduction

Starting vector

Next, you need to specify a vector for the search algorithm to start from. It has to satisfy all of your constraints so, in our example, you would need to give it a vector of weights which sum to 100%. For portfolio construction optimisations, we often start from an equal weighted portfolio.

It is sometimes useful to run the optimisation multiple times from different starting points. This helps you to see if the optimiser is finding the global minima or has "got stuck" in a local minima. In addition, one could create a loop within the code which updates the starting point with the new optimal weights and continues running the algorithm until the difference between old and new weights is below a certain threshold. This is not required if a deterministic solution exists but can be useful for certain objective functions and algorithms used.

Choose an optimisation algorithm

The final step is to choose our optimisation algorithm. There are more than 30 different algorithms to choose from, including a broad array of different approaches.[2] You can narrow it down to just a few by answering a few questions:

- Do you want a local or global minima?
- Do you have explicit gradient functions for your objective and constraint functions?
- What kind of constraints do you have? For example, not all of the algorithms accept equality constraints.

These questions will reduce the list of possible algorithms down to a much shorter list. Then you can experiment with those algorithms and different stopping criteria and see what is most successful with your problem. In our example, we found the SLSQP algorithm worked.

It can sometimes be effective to run the optimisation with a global optimisation algorithm and then further refine the solution by running the optimisation again with a local optimisation, but this time using the global solution as the starting vector.

We include Figure 6 in the appendix which identifies the algorithms available and which criteria they satisfy.

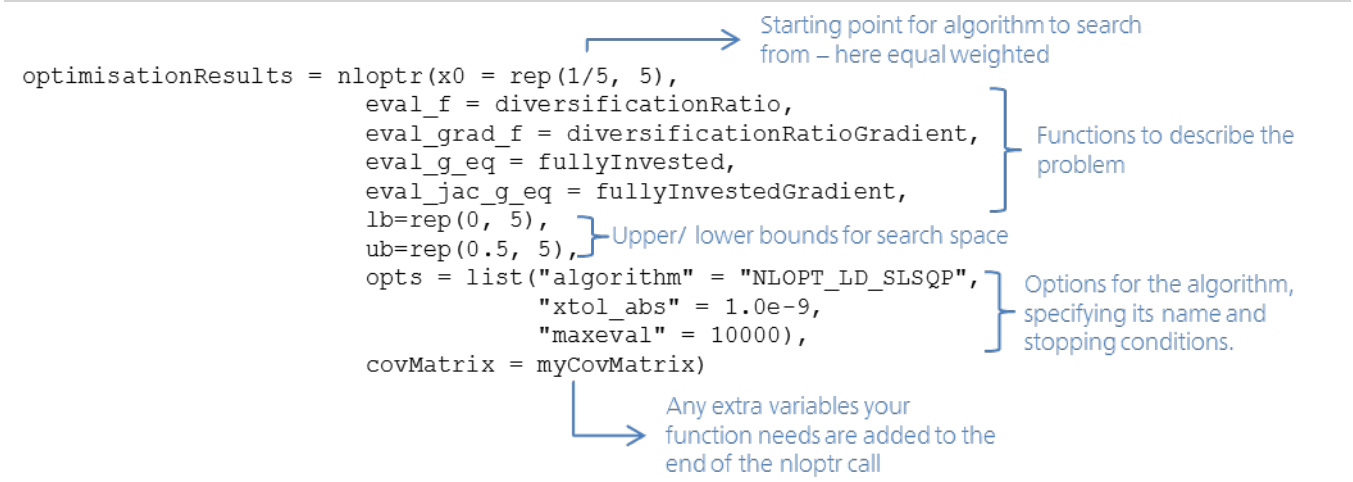
The algorithm names have a fixed pattern, which is `NLOPT_{G,L}{N,D}_xxxx`, where G/L denotes global/local optimisation and N/D denotes derivative-free/gradient-based algorithms, respectively. The "xxxx" is the name of the algorithm. For example the algorithm we use for our example is `NLOPT_LD_SLSQP` so it finds a local minimum and needs gradients.

[2] The NLopt website: http://ab-initio.mit.edu/wiki/index.php/NLopt_Algorithms, can provide much more detail about the methods for each optimisation algorithm and is a very helpful reference.

Ultimately, here is what a call to the **nloptr(.)** function looks like:

Run optimisation

Figure 1: Example of code to run an optimisation using the nloptr(.) function



Source: UBS Quantitative Research.

Output

The output of the optimisation is a list showing the solution (in this case the vector of asset weights which maximise the diversification ratio), the value of the objective function at that solution, a status code showing why the optimiser stopped and various other pieces of information.

nloptr is an extremely convenient package and makes a wide variety of algorithms accessible to practitioners, but it is not as simple as "point and click". Expressing your problem in terms the optimiser can understand is not trivial and requires writing functions in a specific format – and sometimes manually differentiating the objective function in order to find the gradient. Also, as ever in optimisation, there is "no free lunch" – you will have to experiment with different algorithms and their parameters to find the best approach to your problem.

Reproducible research using knitr/R-markdown and Jupyter Notebooks

There is a growing awareness of the difficulty people can have in reproducing published research. We have (occasionally) found this when writing our Academic Research Monitor[3] – we attempt to reproduce the results from a paper and we struggle with either the algorithm or reproducing the data set used by the authors.

Another example of this problem was highlighted in a recent paper in Science where the authors attempted to reproduce 100 published results in psychology – whereas in the original papers 97% had significant results, only 36% of the replications managed to achieve significance.

This has led to calls for "reproducible research". As an example of this call, the IEEE Transactions on Signal Processing "*encourages authors to make their publications reproducible by making all information needed to reproduce the presented results available online. This typically requires publishing the code and data used to produce the publication`s figures and tables on a website*".

This concept is based on the idea of "literate programming" (Knuth, 1992), which is explained as "*Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to human beings what we want a computer to do*". This involves interweaving text explaining what is happening with pieces of code which do the calculations.

knitr and R Markdown

The R environment has a number of tools to help with this interweaving of text, analysis and results.[4] The original function to encourage this was **Sweave**. The **knitr** package is an easier way to achieve the same thing, and together with the **R Markdown** language allows the generation of analysis and reports on the fly.[5] As an example, the code in Figure 2 would be complied into the file in Figure 3.

Figure 2: R Markdown example - input

````
Analysis of S&P 500 vs Oil price
================================

We analyse the relationship between the oil price and the S&P
500.  We start by simply plotting the
chart of weekly returns.  The data goes from 1994 to today.

```{r, echo=FALSE}
data = read.csv ("SPX and Oil.csv", row.names = 1)
rets = data.frame (apply (log (data), 2, diff))
colnames (rets) = c ("SPX", "OIL")

ggplot (rets, aes (x = OIL, y = SPX)) + geom_point ()
```

This shows that the relationship is fairly weak.  We then
regress the S&P return on the oil price.

```{r, echo=FALSE}
model = lm (SPX~OIL, rets)
summary (model)
```
````

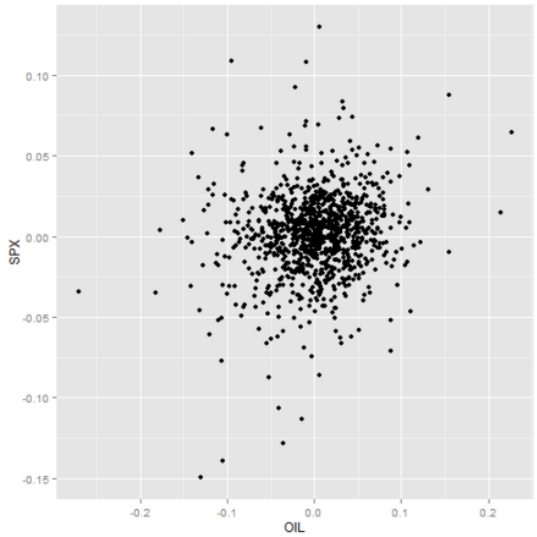
Source: UBS

[3] See our latest ARM on Portfolio Construction and Overfitting (18 July 2016)
[4] See https://cran.r-project.org/web/views/ReproducibleResearch.html for a discussion of this.
[5] knitr / R Markdown are well supported within R Studio.

Figure 3: R Markdown example - output

Analysis of S&P 500 vs Oil price

We analyse the relationship between the oil price and the S&P 500. We start by simply plotting the chart of weekly returns. The data goes from 1994 to today.



This shows that the relationship is fairly weak. We then regress the S&P return on the oil price.

```
##
## Call:
## lm(formula = SPX ~ OIL, data = rets)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.13923 -0.01282  0.00134  0.01367  0.12773
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 0.001279   0.000791    1.62     0.11
## OIL         0.085922   0.016399    5.24  1.9e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0255 on 1042 degrees of freedom
## Multiple R-squared:  0.0257, Adjusted R-squared:  0.0247
## F-statistic: 27.5 on 1 and 1042 DF,  p-value: 1.95e-07
```

Source: UBS

The obvious advantage of this is that one can update the data and then reproduce a whole analysis with commentary.

Another approach - Jupyter

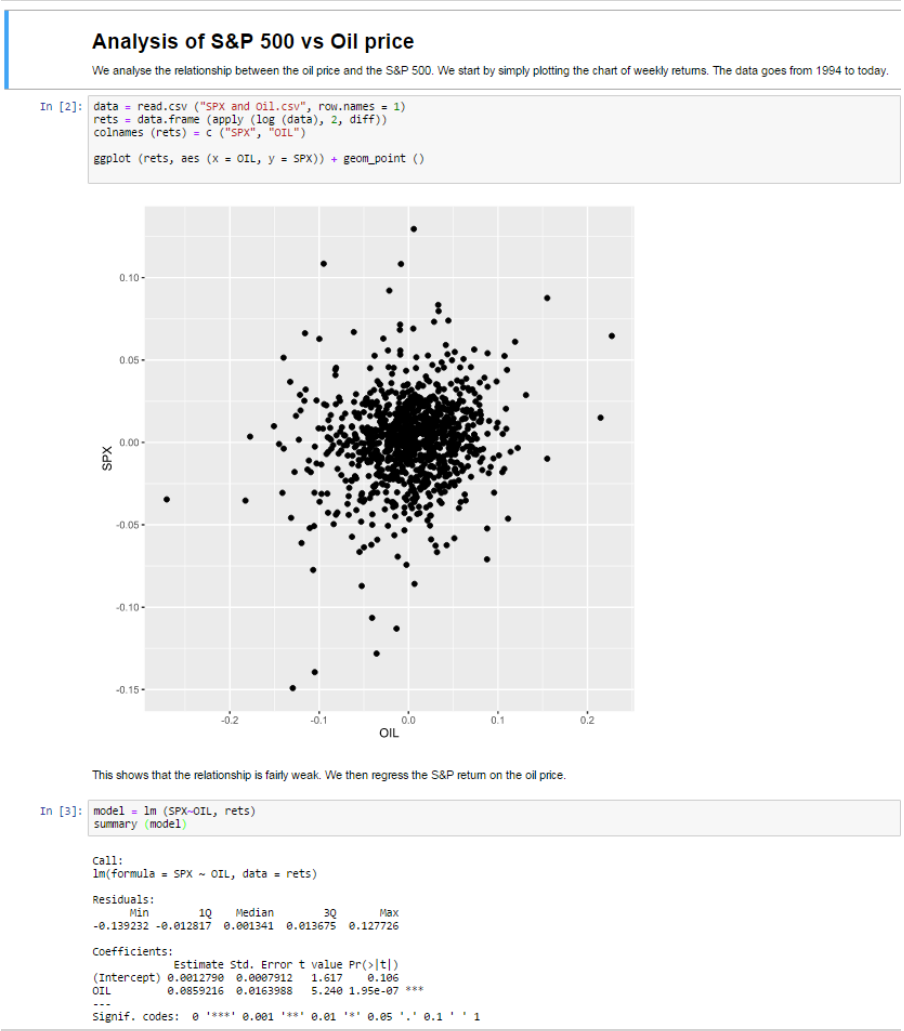
There is a new kid on the block which has migrated from the Python world, and this is the **Jupyter Notebook** project[6]. The Notebooks are described as "a web application for interactive data science and scientific computing". They embed code, text and results in a browser environment. This is very similar to R Markdown / knitr but the difference is everything in the notebook is executed within the browser itself.

Jupyter is written in python, so in order to install it one has to first install python, and then install the R kernel. The Anaconda project (https://www.continuum.io) can be used to do all of this.

[6] Jupyter notebooks (which comes from an elision of JUlia, PYThon and R) used to be called IPython notebooks. See https://jupyter.org/ to get started.

Once this is installed one can create a notebook which is made up of a number of cells which can either show Markdown (as in the first cell below) or code and the output from the code. An example of the same analysis as above is shown below in Figure 4.

Figure 4: Example of Jupyter Notebook



Source: UBS

The advantage of the Notebook format is that everything is in one place – you don't have to compile it. One disadvantage is that, behind the scenes, the notebook is stored as JSON and so both code and output are in the same place, which makes tracking changes in the code, say via version control, difficult.

However both approaches have lots of benefits in terms of both one being able to revisit analysis later and understand what you did, as well as passing analysis onto other people in an easy-to-read format.

Appendix

Figure 5: Case study – optimising for maximum diversification ratio

```
#Define functions for the optimisation
diversificationRatio = function(w, covMatrix)
{
  weightedAvgVol = sum(w * sqrt(diag(covMatrix)))
  portfolioVariance = (w %*% covMatrix %*% w)[1,1]

  -1 * weightedAvgVol / sqrt(portfolioVariance)
}

fullyInvested = function(w, covMatrix)
{
  sum(w)-1
}

diversificationRatioGradient = function(w, covMatrix)
{
  weightedAvgVol = sum(w * sqrt(diag(covMatrix)))
  portfolioVariance = (w %*% covMatrix %*% w)[1,1]

  -1 * sqrt(diag(covMatrix)) / sqrt(portfolioVariance) +
              weightedAvgVol * portfolioVariance^-(3/2) * (w %*% covMatrix)[1,]
}

fullyInvestedGradient = function(w, covMatrix)
{
  rep(1,length(w))
}

#-------------------------------------------------------------------------------------
#Generate some random data for this example
set.seed(3142)
myRet = matrix(runif(100*5, -0.1, 0.1), ncol=5)
myCovMatrix = cov(myRet)

#-------------------------------------------------------------------------------------
#Check the gradient functions at the point w = (0.2, 0.2, 0.2, 0.2, 0.2)
check.derivatives(rep(1/5,5), diversificationRatio, diversificationRatioGradient,
covMatrix=myCovMatrix)
check.derivatives(rep(1/5,5), fullyInvested, fullyInvestedGradient, covMatrix=myCovMatrix)

#-------------------------------------------------------------------------------------
#Run the optimisation
library(nloptr)
optimisationResults = nloptr(x0 = rep(1/5, 5),
                         eval_f = diversificationRatio,
                         eval_grad_f = diversificationRatioGradient,
                         eval_g_eq = fullyInvested,
                         eval_jac_g_eq = fullyInvestedGradient,
                         lb=rep(0, 5),
                         ub=rep(0.5, 5),
                         opts = list("algorithm" = "NLOPT_LD_SLSQP",
                                     "xtol_abs" = 1.0e-9,
                                     "maxeval" = 10000),
                         covMatrix = myCovMatrix)
```

Source: UBS Quantitative Research

Figure 6: NLoptr Algorithms

Algorithm	Global	Local	Requires/Supports Bound Constraints	Supports NL Inequality Constraints	Supports NL Equality Constraints	Requires a Gradient/Derivative
NLOPT_GN_DIRECT	√		√			
NLOPT_GN_DIRECT_L	√		√			
NLOPT_GN_DIRECT_L_RAND	√		√			
NLOPT_GN_DIRECT_NOSCAL	√		√			
NLOPT_GN_DIRECT_L_NOSCAL	√		√			
NLOPT_GN_DIRECT_L_RAND_NOSCAL	√		√			
NLOPT_GN_ORIG_DIRECT	√		√			
NLOPT_GN_ORIG_DIRECT_L	√		√			
NLOPT_GD_STOGO	√		√			√
NLOPT_GD_STOGO_RAND	√		√			√
NLOPT_LD_SLSQP		√		√	√	√
NLOPT_LD_LBFGS		√				√
NLOPT_LN_PRAXIS		√				
NLOPT_LD_VAR1		√				√
NLOPT_LD_VAR2		√				√
NLOPT_LD_TNEWTON		√				√
NLOPT_LD_TNEWTON_RESTART		√				√
NLOPT_LD_TNEWTON_PRECOND		√				√
NLOPT_LD_TNEWTON_PRECOND_RESTART		√				√
NLOPT_GN_CRS2_LM	√		√			
NLOPT_GN_MLSL	√					
NLOPT_GD_MLSL	√					√
NLOPT_GN_MLSL_LDS	√					
NLOPT_GD_MLSL_LDS	√					√
NLOPT_LD_MMA		√		√		√
NLOPT_LN_COBYLA		√	√	√	√	
NLOPT_LN_NEWUOA		√				
NLOPT_LN_NEWUOA_BOUND		√	√			
NLOPT_LN_NELDERMEAD		√				
NLOPT_LN_SBPLX		√	√			
NLOPT_LN_AUGLAG		√	√	√	√	
NLOPT_LD_AUGLAG		√	√	√	√	√
NLOPT_LN_AUGLAG_EQ		√	√	√	√	
NLOPT_LD_AUGLAG_EQ		√	√	√	√	√
NLOPT_LN_BOBYQA		√	√	√	√	
NLOPT_GN_ISRES	√		√	√	√	

Source: UBS Quantitative Research

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