mages' blog (http://www.magesblog.com/)

How to use optim in R

② 12 Mar 2013 07:49 (2013-03-12T07:49:00Z) ❖ optim (http://www.magesblog.com/search/label/optim), R (http://www.magesblog.com/search/label/R), Tutorials (http://www.magesblog.com/search/label/Tutorials)

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A friend of mine asked me the other day how she could use the function <code>optim</code> in R to fit data. Of course there are built in functions for fitting data in R and I wrote about this earlier (http://www.magesblog.com/2011/12/fitting-distributions-with-r.html). However, she wanted to understand how to do this from scratch using <code>optim</code>.

The function optim provides algorithms for general purpose optimisations and the documentation is perfectly reasonable, but I remember that it took me a little while to get my head around how to pass data and parameters to optim. Thus, here are two simple examples.

I start with a linear regression by minimising the residual sum of square and discuss how to carry out a maximum likelihood estimation in the second example.

Minimise residual sum of squares

I start with an x-y data set, which I believe has a linear relationship and therefore I'd like to fit y against x by minimising the residual sum of squares.

```
dat=data.frame(x=c(1,2,3,4,5,6),
y=c(1,3,5,6,8,12))
```

Next, I create a function that calculates the residual sum of square of my data against a linear model with two parameter. Think of y = par[1] + par[2] * x.

```
min.RSS <- function(data, par) {
      with(data, sum((par[1] + par[2] * x - y)^2))
}</pre>
```

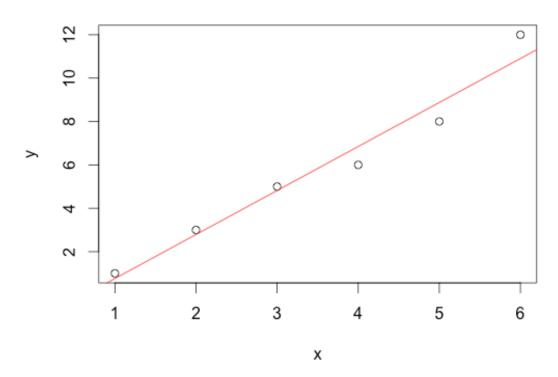
Optim minimises a function by varying its parameters. The first argument of <code>optim</code> are the parameters I'd like to vary, <code>par</code> in this case; the second argument is the function to be minimised, <code>min.RSS</code>. The tricky bit is to understand how to apply <code>optim</code> to your data. The solution is the ... argument in <code>optim</code>, which allows me to pass other arguments through to <code>min.RSS</code>, here my data. Therefore I can use the following statement:

```
result <- optim(par = c(0, 1), min.RSS, data = dat)
# I find the optimised parameters in result$par
# the minimised RSS is stored in result$value
result
## $par
## [1] -1.267 2.029
##
## $value
## [1] 2.819
##
## $counts
## function gradient
         89
##
##
## $convergence
## [1] 0
##
## $message
## NULL
```

Let me plot the result:

```
plot(y ~ x, data = dat, main="Least square regression")
abline(a = result$par[1], b = result$par[2], col = "red")
```

Least square regression



(http://3.bp.blogspot.com/-oeg1_8ypw6Y/VbP5VqJcHcI/AAAAAAAACKI/LzsWAfUfUFQ/s1600/LeastSquare.png)

Great, this looks reasonable. How does it compare against the built in linear regression in R?

Spot on! I get the same answer.

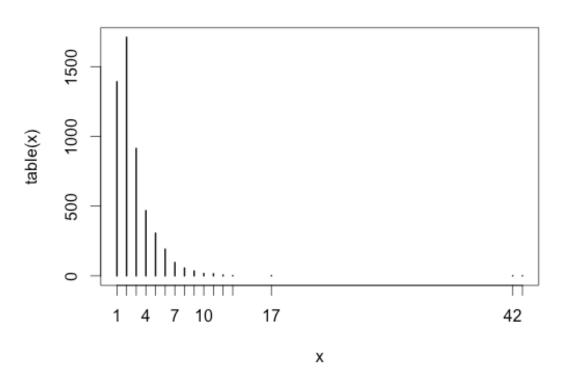
Maximum likelihood

In my second example I look at count data and I would like to fit a Poisson distribution to this data.

Here is my data:

```
obs = c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 17, 42, 43)
freq = c(1392, 1711, 914, 468, 306, 192, 96, 56, 35, 17, 15, 6, 2, 2, 1, 1)
x <- rep(obs, freq)
plot(table(x), main="Count data")
```

Count data



(http://2.bp.blogspot.com/-8ReSaQIaBw4/VbP5Vn31RpI/AAAAAAAACKE/r0M079FRkM4/s1600/CountData.png) To fit a Poisson distribution to x I don't minimise the residual sum of squares, instead I maximise the likelihood for the chosen parameter lambda.

The likelihood function is given by:

```
lklh.poisson <- function(x, lambda) lambda^x/factorial(x) * exp(-lambda)</pre>
```

and the sum of the log-liklihood function is:

```
log.lklh.poisson <- function(x, lambda){
        -sum(x * log(lambda) - log(factorial(x)) - lambda)
    }</pre>
```

By default optim searches for parameters, which minimise the function fn. In order to find a maximium, all I have to do is change the sign of the function, hence -sum(...).

```
optim(par = 2, log.lklh.poisson, x = x)
## Warning: one-diml optimization by Nelder-Mead is unreliable: use "Brent"
## or optimize() directly
## $par
## [1] 2.704
##
## $value
## [1] 9966
##
## $counts
## function gradient
         24
##
                  NA
##
## $convergence
## [1] 0
##
## $message
## NULL
```

Ok, the warning message tells me that I shoud use another optimisation algorithm, as I have a one dimensional problem - a single parameter. Thus, I follow the advise and get:

```
optim(par = 2, log.poisson, x = x, method = "Brent", lower = 2, upper = 3)
## $par
## [1] 2.704
##
## $value
## [1] 9966
##
## $counts
## function gradient
##
         NA
                  NA
##
## $convergence
## [1] 0
##
## $message
## NULL
```

It's actually the same result. Let's compare the result to fitdistr, which uses maximum liklihood as well.

```
library(MASS)
fitdistr(x, "Poisson")
## lambda
## 2.70368
## (0.02277)
```

No surprise here, it gives back the mean, which is the maximum likelihood parameter.

```
mean(x)
## [1] 2.704
```

For more information on optimisation and mathematical programming with R see the CRAN Task View on this subject (http://cran.r-project.org/web/views/Optimization.html).

Session Info

```
sessionInfo()
## R version 2.15.2 (2012-10-26)
## Platform: x86_64-apple-darwin9.8.0/x86_64 (64-bit)
##
## locale:
## [1] en_GB.UTF-8/en_GB.UTF-8/C/en_GB.UTF-8/en_GB.UTF-8
##
## attached base packages:
## [1] stats graphics grDevices utils datasets methods base
##
## other attached packages:
## [1] MASS_7.3-22
```

Newer Post (http://www.magesblog.com/2013/03/googlevis-042-with-support-for-shiny.html)
Older Post (http://www.magesblog.com/2013/03/create-r-package-from-single-r-file.html)





Tahir • 2 months ago

Hello Markus

I'm trying to run this code using optim(), but I got an error (Error in optim(c(0, 0), f): objective function in optim evaluates to length 0 not 1), pleas, can you guide me to know where is the

the code is:

error.

```
M<-10
N<-10
L<-0.8
Mu<-0.1
y<-matrix(rnorm(M*N),M,N)
AB<-function(L,Mu){
A11.<-NULL
A11<-function(M,N){cos(m*L+n*Mu)^2}
for(m in 1:M){
for(n in 1:N){
A11.<-cbind(A11.,A11(m,n))
}
```

see more

```
Reply • Share >
```



Anand • a year ago

Hi Sir,

Could you please tell me how to use optim for finding the maximum of a function? Thanks

Anand



Jenny · 2 years ago

Hello Markus,

I'm trying to find the optimum values (a and b) for a function's minumum value or a constant minimum level. I used the optim and optimize function but I can't find the optimal pairs of the parameters of a and b. My function is some more complicated and I create this function as $\min.RSS(a)(b)$ (two functions are nested) when I used the optim function and I received the following error from this code: error in optim(c(1,1), min.RSS): cannot coerce type 'closure' to vector of type 'double' Could you please help me on finding the optimal pairs of parameters.

Thanks in advance

```
Reply • Share >
```



Markus Gesmann Mod → Jenny • 2 years ago

Hi Jenny,

You will have to provide a minimal reproducible example for anyone to help you. Those questions are best asked by email, or at stackoverflow or R-help.

```
Reply • Share >
```



Arjun Kavallur • 2 years ago

Hello Markus

The blog you have posted has been very informative and helpful! I have been trying to calculate the maximum likelihood estimate of an ARMA process using optim.

In the process I have to recursively find the error terms (white noise) using a for loop which involves the use of parameters. I want to optimize the sum of the square of the error terms and hence estimate the parameters. I believe that both the processes cannot be done under the same function(fn). If I calculate the for loop under a different function the error message of "parameters" are missing crops up.

Moreover I have found that if we optimized a function using two different parameters an error message of "second parameter" missing with no default comes up.

Could you please advice me on these two issues.

Thanks

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Markus Gesmann Mod → Arjun Kavallur • 2 years ago

I think your question is best asked on stackoverflow: http://stackoverflow.com/quest... Please ensure that you provide a small reproducible example in R.



Ashish Verma · 3 years ago

Hi Markus,

I am grad student and I have written a custom function for piece wise continuous fit with constraints on boundaries. I have used optim() and I am getting decent results but in order to improve these results I am trying to program in the gradient as well, but when I put the gradient in optim returns the exact same parameters which I give it to initialize. If you have any suggestions please share. Also, I faced same problem with optimx() and lab.optim(). Thanks in advance.

```
Reply • Share >
```



Markus Gesmann Mod → Ashish Verma • 3 years ago

I suggest you post your question with a small reproducible example to R-help: http://www.r-project.org/mail.....



ayush ⋅ 3 years ago

Hi,

I tried the same thing as yours. But I am getting different answers from optim and Im(). Please look into it.

Following is the data.

Int Ext y

1 89 21 2625

2 93 24 2700

3 91 21 3100

4 122 23 3150

5 115 27 3175

6 100 18 3100

7 98 19 2700

8 105 16 2475

9 112 23 3625

10 109 28 3525

11 130 20 3225

see more

Reply • Share >



Markus Gesmann Mod → ayush · 3 years ago

Change you initial parameters from c(0,1,2) to c(100, 1, 2) and see if this has an impact.



Ayush Raj Singh → Markus Gesmann • 3 years ago

Hi Markus,

It worked. Awesome. But could you please explain why it worked? I just followed your code. I really do not understand how par =c(0,1,2) or par =c(100,1,2) are related to par[1], par[2] and par[3] ?

Thank you for the help.

ayush



Markus Gesmann Mod → Ayush Raj Singh • 3 years ago

The parameters par[1], par[2], par[3] are initialised via the vector par=c(0,1,2). I believe, you should have used a different optimisation method for your problem, as optim(par=c(0,1,2), min.function, data=dat, method="BFGS") would give you the answer you are looking for. I don't know which fitting method 'lm' is using in the background, but I am sure the answer is in the documentation or online.



ayush → Markus Gesmann • 3 years ago



-

Ok. But, how does initialization of parameters affects the answer. Acc. to me answer should come out to be the same from both initial values (100 or 0).

Also, what other optimization method would you suggest for my problem.

Thank you.



Markus Gesmann Mod → ayush · 3 years ago

Well, optim is looking for minima and what do you do if your function has serval minima and your start close a local one? I think you have to take a text book and look into this in more detail and read the documentation.

ALSO ON MAGES' BLOG WHAT'S THIS?

Extended Kalman filter example in R

4 comments • a year ago



Adrian Lisko — Hi, I think that there are mistakes in your code, because you are first doing the filtering step (update) and then ...

Adding mathematical notations to R plots

2 comments • 7 months ago



Mick Cooney — I think latex2exp may prove to be a hugely useful package. Getting mathematical symbols onto plots has ...

googleVis version 0.5.8 released

5 comments • a year ago



Markus Gesmann — The following works for me: plot(gvisLineChart(Andrew, "Date/Time UTC", "Speed_kt"))

Reading Arduino data directly into R

2 comments • a year ago



Markus Gesmann — Or use a Raspberry Pi and WebIOPi to do something similar: http://www.magesblog.com/2014/.... Oh ...





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A friend of mine asked me the other day how

she could use the function optim in R to fit data. Of course there are built in functions for f...



First steps of using googleVis

(http://www.magesblog.com/2013/02/first-steps-of-using-googlevis-on-shiny.html) on shiny

(http://www.magesblog.com/2013/02/first-steps-of-using-googlevis-on-shiny.html)

The guys at RStudio have done a fantastic job with shiny. It is really easy to build web apps with R using shiny. With the help of Joe Ch...

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Formatting table output in R

(http://www.magesblog.com/2016/01/formatting-table-output-in-r.html)

(http://www.magesblog.com/2016/01/formatting-table-output-in-r.html)

Formatting data for output in a table can be a bit of a pain in R. The package formattable by Kun Ren and Kenton Russell provides some intu...



Interactive pivot tables with R

(http://www.magesblog.com/2015/03/pivot-tables-with-r.html) (http://www.magesblog.com/2015/03/pivot-tables-with-r.html)

I love interactive pivot tables . That is the number

one reason why I keep using spreadsheet software. The ability to look at data quickly ...

Say it in R with "by", "apply" and friends (http://www.magesblog.com/2012/01/say-it-in-r-with-by-apply-and-friends.html)

Iris versicolor By Danielle Langlois License: CC-BY-SA R is a language, as Luis Apiolaza pointed out in his recent post. This is ab...



Changing colours and

(http://www.magesblog.com/2012/12/changing-colours-and-legends-in-lattice.html) legends in lattice plots

(http://www.magesblog.com/2012/12/changing-colours-and-legends-in-lattice.html)

Lattice plots are a great way of displaying multivariate data in R. Deepayan Sarkar, the author of lattice, has written a fantastic book ab...



Data.table rocks! Data

(http://www.magesblog.com/2012/11/datatable-rocks-data-manipulation-fast.html) manipulation the fast way in

(http://www.magesblog.com/2012/11/datatable-rocks-data-manipulation-fast.html)

I really should make it a habit of using data.table. The speed and simplicity of this R package are astonishing. Here is a simple exampl...



Transforming subsets of data

(http://www.magesblog.com/2012/06/transforming-subsets-of-data-in-r-with.html) in R with by, ddply and

(http://www.magesblog.com/2012/06/transforming-subsets-of-data-in-r-with.html)

Transforming data sets with R is usually the starting point of my data analysis work. Here is a scenario which comes up from time to time: t...



Plotting tables alsongside

(http://www.magesblog.com/2015/04/plotting-tables-alsongside-charts-in-r.html) charts in R

(http://www.magesblog.com/2015/04/plotting-tables-alsongside-charts-in-r.html)

Occasionally I'd like to plot a table alongside a chart in R, e.g. to present summary statistics of the graph itself. Thanks to the grid...



Fitting distributions with R

(http://www.magesblog.com/2011/12/fitting-distributions-with-r.html)

(http://www.magesblog.com/2011/12/fitting-distributions-with-r.html)

Fitting distribution with R is something I have to do once in a while, but where do I start? A good starting point to learn more about dis...

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Package xgboost updated to version 0.4-3 with previous version 0.4-2 dated 2015-08-02 (http://dirk.eddelbuettel.com/cranberries/2016/02/15#xgboost_0.4-3)

R bloggers (http://www.r-bloggers.com)

Using Microsoft R Server to Address Scalability Issues in R (http://feedproxy.google.com/~r/RBloggers/~3/3908R4EDEB4/)

Freakonometrics (http://freakonometrics.hypotheses.org)

Central Limit Theorem (http://freakonometrics.hypotheses.org/48061)

Seth's Blog (http://sethgodin.typepad.com/seths_blog/)

"I've got this" (http://feeds.feedblitz.com/~/138055095/0/sethsblog~Ive-got-this.html)

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