

Introduction to `ipoptr`: an R interface to Ipopt *

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Abstract

This document describes how to use `ipoptr`, which is an R interface to Ipopt (Interior Point Optimizer). Ipopt is an open source software package for large-scale nonlinear optimization (Wächter & Biegler, 2006). It can be used to solve general nonlinear programming problems with nonlinear constraints and lower and upper bounds for the controls. Ipopt is written in C++ and is released as open source code under the Eclipse Public License (EPL). It is available from the COIN-OR initiative. The code has been written by Carl Laird and Andreas Wächter, who is the COIN project leader for Ipopt.

1 Introduction

Ipopt is designed to find (local) solutions of mathematical optimization problems of the form

$$\begin{aligned} \min_{x \in R^n} & f(x) \\ \text{s.t.} & g_L \leq g(x) \leq g_U \\ & x_L \leq x \leq x_U \end{aligned}$$

where $f(x) : R^n \rightarrow R$ is the objective function, and $g(x) : R^n \rightarrow R^m$ are the constraint functions. The vectors g_L and g_U denote the lower and upper bounds on the constraints, and the vectors x_L and x_U are the bounds on the variables x . The functions $f(x)$ and $g(x)$ can be nonlinear and nonconvex, but should be twice continuously differentiable. Note that equality constraints can be formulated in the above formulation by setting the corresponding components of g_L and g_U to the same value.

This vignette describes how to formulate minimization problems to be solved with the R interface to Ipopt. If you want to use the C++ interface directly or are interested in the Matlab interface, there are other sources of documentation available. Some of the information here is heavily based on the Ipopt Wiki¹ and generally that is a good source to find additional information, for instance

*This package should be considered in beta and comments about any aspect of the package are welcome. Thanks to Alexios Ghalanos for comments. This document is an R vignette prepared with the aid of `Sweave`, Leisch(2002). Financial support of the UK Economic and Social Research Council through a grant (RES-589-28-0001) to the ESRC Centre for Microdata Methods and Practice (CeMMAP) is gratefully acknowledged.

¹<https://projects.coin-or.org/Ipopt>

on which options to use. All credit for implementing the C++ code for `Ipoptr` should go to Andreas Wächter and Carl Laird. Please show your appreciation by citing their paper.

2 Installation

Installing the `ipoptr` package is not as straightforward as most other R packages, because it depends on `Ipoptr`. To install (and compile) `Ipoptr` and the R interface a C/C++ compiler has to be available. On Windows I was succesful using `MSYS` to compile `Ipoptr` and then use `Rtools`² to compile the R interface from source. On Ubuntu no additional tools were needed.

The code for the R interface to `Ipoptr` is available from R-Forge and from the `Ipoptr` website. Additional information is also available on <http://www.ucl.ac.uk/~uctpjyy/ipoptr.html>. The R interface to `Ipoptr` comes with the most recent version of `Ipoptr`, so there is no need to download it separately.

Detailed installation instructions for `Ipoptr` are available on <http://www.coin-or.org/Ipoptr/documentation>. You should follow these first, before trying to install the R interface. `Ipoptr` needs to be configured using the `-fPIC` flag for all GNU compilers. For 64bit Linux one needs to specify

```
ADD_CXXFLAGS='-fPIC' ADD_FFLAGS='-fPIC' ADD_CFLAGS='-fPIC'
```

For the installation of the R interface, I will assume that you have a working installation of `Ipoptr` (i.e. `configure`, `make` and `make install` executed without problems).

During the installation of `Ipoptr` a file `Makevars` has been created in the source directory of the R interface, e.g. `$IPOPTDIR/build/Ipoptr/contrib/RInterface/src` if you used the same build directory as in the `Ipoptr` installation notes, `$IPOPTDIR/build`. The file `Makevars` in this directory has been configured for your system.

To install the R interface, this file has to be copied to the `Ipoptr` directory containing the source code, `$IPOPTDIR/Ipoptr/contrib/RInterface/src`. Notice that the path of this directory is different from the directory where you built `Ipoptr` (`build` is not there).

The source directory `$IPOPTDIR/Ipoptr/contrib/RInterface/src` contains four files, `ipoptr.cpp`, `IpoptrNLP.cpp`, `IpoptrNLP.hpp` and `Makevars.in`. Copy `Makevars` in this directory and, if you're on Windows, rename it to `Makevars.win`.

You can then install the package from R with the command

```
> install.packages('$IPOPTDIR/Ipoptr/contrib/RInterface', repos=NULL, type='source')
```

where the first argument specifies the directory where the source code for the R interface to `Ipoptr` is located. You should now be able to load the R interface to `Ipoptr` and read the help.

```
> library('ipoptr')
> ?ipoptr
```

²<http://www.murdoch-sutherland.com/Rtools/>

3 Minimizing the Rosenbrock Banana function

As a first example we will solve an unconstrained minimization problem. The function we look at is the Rosenbrock Banana function

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2,$$

which is also used as an example in the documentation for the standard R optimizer `optim`. The gradient of the objective function is given by

$$\nabla f(x) = \begin{pmatrix} -400 \cdot x_1 \cdot (x_2 - x_1^2) - 2 \cdot (1 - x_1) \\ 200 \cdot (x_2 - x_1^2) \end{pmatrix}.$$

`Ipopt` always needs gradients to be supplied by the user. After loading the library

```
> library(ipoptr)
```

we start by specifying the objective function and its gradient

```
> eval_f <- function(x) {
  return( 100 * (x[2] - x[1] * x[1])^2 + (1 - x[1])^2 )
}
> ## Gradient of Rosenbrock Banana function
> eval_grad_f <- function(x) {
  return( c( -400 * x[1] * (x[2] - x[1] * x[1]) - 2 * (1 - x[1]),
            200 * (x[2] - x[1] * x[1]) ) )
}
```

We define initial values

```
> x0 <- c( -1.2, 1 )
```

and then minimize the function using the `ipoptr` command. This command runs some checks on the supplied inputs and returns an object with the exit code of the solver, the optimal value of the objective function and the solution. The checks do not always return very informative messages, but usually there is something wrong with dimensions (e.g. `eval_grad_f` returns a vector that doesn't have the same size as `x0`).

```
> res <- ipoptr( x0=x0,
                eval_f=eval_f,
                eval_grad_f=eval_grad_f )
*****
This program contains Ipopt, a library for large-scale nonlinear optimization.
Ipopt is released as open source code under the Eclipse Public License (EPL).
For more information visit http://projects.coin-or.org/Ipopt
*****
```

```
NOTE: You are using Ipopt by default with the MUMPS linear solver.
      Other linear solvers might be more efficient (see Ipopt documentation).
```

This is Ipopt version 3.9stable, running with linear solver mumps.

Number of nonzeros in equality constraint Jacobian...: 0
 Number of nonzeros in inequality constraint Jacobian.: 0
 Number of nonzeros in Lagrangian Hessian.....: 0

Total number of variables.....: 2
 variables with only lower bounds: 0
 variables with lower and upper bounds: 0
 variables with only upper bounds: 0
 Total number of equality constraints.....: 0
 Total number of inequality constraints.....: 0
 inequality constraints with only lower bounds: 0
 inequality constraints with lower and upper bounds: 0
 inequality constraints with only upper bounds: 0

| iter | objective | inf_pr | inf_du | lg(mu) | d | lg(rg) | alpha_du | alpha_pr | ls |
|------|---------------|----------|----------|--------|----------|--------|----------|-----------|----|
| 0 | 2.4200000e+01 | 0.00e+00 | 1.00e+02 | 0.0 | 0.00e+00 | - | 0.00e+00 | 0.00e+00 | 0 |
| 1 | 4.5132962e+00 | 0.00e+00 | 1.12e+01 | -11.0 | 1.00e+02 | - | 1.00e+00 | 1.95e-03f | 10 |
| 2 | 4.1352907e+00 | 0.00e+00 | 1.79e+00 | -11.0 | 1.97e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 3 | 4.1190197e+00 | 0.00e+00 | 6.93e-01 | -11.0 | 4.07e-03 | - | 1.00e+00 | 1.00e+00f | 1 |
| 4 | 4.1150551e+00 | 0.00e+00 | 6.49e-01 | -11.0 | 2.30e-03 | - | 1.00e+00 | 1.00e+00f | 1 |
| 5 | 3.9227578e+00 | 0.00e+00 | 4.69e+00 | -11.0 | 1.29e-01 | - | 1.00e+00 | 1.00e+00f | 1 |
| 6 | 3.6726950e+00 | 0.00e+00 | 8.55e+00 | -11.0 | 4.40e-01 | - | 1.00e+00 | 5.00e-01f | 2 |
| 7 | 3.4018752e+00 | 0.00e+00 | 8.83e+00 | -11.0 | 1.61e-01 | - | 1.00e+00 | 1.00e+00f | 1 |
| 8 | 2.7843438e+00 | 0.00e+00 | 4.79e+00 | -11.0 | 1.61e-01 | - | 1.00e+00 | 1.00e+00f | 1 |
| 9 | 2.4059304e+00 | 0.00e+00 | 5.07e+00 | -11.0 | 1.81e-01 | - | 1.00e+00 | 1.00e+00f | 1 |
| iter | objective | inf_pr | inf_du | lg(mu) | d | lg(rg) | alpha_du | alpha_pr | ls |
| 10 | 1.7000439e+00 | 0.00e+00 | 1.07e+00 | -11.0 | 1.96e-01 | - | 1.00e+00 | 1.00e+00f | 1 |
| 11 | 1.6771291e+00 | 0.00e+00 | 5.14e+00 | -11.0 | 5.32e-01 | - | 1.00e+00 | 2.50e-01f | 3 |
| 12 | 1.4393650e+00 | 0.00e+00 | 1.50e+00 | -11.0 | 5.34e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 13 | 1.2550640e+00 | 0.00e+00 | 1.20e+00 | -11.0 | 7.71e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 14 | 1.1507383e+00 | 0.00e+00 | 4.95e+00 | -11.0 | 3.74e-01 | - | 1.00e+00 | 5.00e-01f | 2 |
| 15 | 9.6590056e-01 | 0.00e+00 | 8.93e-01 | -11.0 | 5.09e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 16 | 8.2734120e-01 | 0.00e+00 | 7.20e-01 | -11.0 | 7.46e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 17 | 8.2045779e-01 | 0.00e+00 | 5.18e+00 | -11.0 | 3.87e-01 | - | 1.00e+00 | 5.00e-01f | 2 |
| 18 | 6.4544893e-01 | 0.00e+00 | 6.70e-01 | -11.0 | 8.97e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 19 | 5.5855730e-01 | 0.00e+00 | 4.95e-01 | -11.0 | 5.77e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| iter | objective | inf_pr | inf_du | lg(mu) | d | lg(rg) | alpha_du | alpha_pr | ls |
| 20 | 4.5925683e-01 | 0.00e+00 | 1.91e+00 | -11.0 | 3.99e-01 | - | 1.00e+00 | 2.50e-01f | 3 |
| 21 | 3.9287824e-01 | 0.00e+00 | 2.25e+00 | -11.0 | 6.74e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 22 | 2.4068628e-01 | 0.00e+00 | 3.34e-01 | -11.0 | 1.05e-01 | - | 1.00e+00 | 1.00e+00f | 1 |
| 23 | 1.9757043e-01 | 0.00e+00 | 1.75e+00 | -11.0 | 1.76e-01 | - | 1.00e+00 | 5.00e-01f | 2 |
| 24 | 1.5237414e-01 | 0.00e+00 | 1.01e+00 | -11.0 | 4.17e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 25 | 1.0985011e-01 | 0.00e+00 | 2.61e+00 | -11.0 | 1.49e-01 | - | 1.00e+00 | 1.00e+00f | 1 |
| 26 | 5.9419120e-02 | 0.00e+00 | 9.25e-01 | -11.0 | 5.60e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 27 | 3.1250980e-02 | 0.00e+00 | 8.92e-01 | -11.0 | 1.08e-01 | - | 1.00e+00 | 1.00e+00f | 1 |
| 28 | 2.3414933e-02 | 0.00e+00 | 1.28e+00 | -11.0 | 6.13e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| 29 | 7.4967612e-03 | 0.00e+00 | 1.55e-01 | -11.0 | 8.07e-02 | - | 1.00e+00 | 1.00e+00f | 1 |
| iter | objective | inf_pr | inf_du | lg(mu) | d | lg(rg) | alpha_du | alpha_pr | ls |

```

30 4.0777005e-03 0.00e+00 8.87e-01 -11.0 8.61e-02 - 1.00e+00 1.00e+00f 1
31 1.1222234e-03 0.00e+00 1.19e-01 -11.0 1.42e-02 - 1.00e+00 1.00e+00f 1
32 1.5923668e-04 0.00e+00 9.72e-02 -11.0 4.19e-02 - 1.00e+00 1.00e+00f 1
33 1.0924731e-05 0.00e+00 3.72e-02 -11.0 1.76e-02 - 1.00e+00 1.00e+00f 1
34 3.3816594e-06 0.00e+00 2.92e-02 -11.0 3.35e-03 - 1.00e+00 1.00e+00f 1
35 2.9021805e-06 0.00e+00 1.50e-02 -11.0 4.91e-03 - 1.00e+00 1.00e+00f 1
36 3.1189724e-07 0.00e+00 6.99e-03 -11.0 3.83e-03 - 1.00e+00 1.00e+00f 1
37 5.7345880e-08 0.00e+00 4.33e-03 -11.0 9.35e-04 - 1.00e+00 1.00e+00f 1
38 4.6169682e-08 0.00e+00 4.98e-04 -11.0 6.37e-04 - 1.00e+00 5.00e-01f 2
39 5.1943636e-09 0.00e+00 6.97e-04 -11.0 5.50e-04 - 1.00e+00 1.00e+00f 1
iter objective inf_pr inf_du lg(mu) ||d|| lg(rg) alpha_du alpha_pr ls
40 2.6580142e-11 0.00e+00 9.57e-05 -11.0 1.23e-04 - 1.00e+00 1.00e+00f 1
41 1.1074711e-11 0.00e+00 3.08e-05 -11.0 1.20e-05 - 1.00e+00 5.00e-01f 2
42 1.2243668e-14 0.00e+00 8.26e-07 -11.0 5.98e-06 - 1.00e+00 1.00e+00f 1
43 9.0765507e-16 0.00e+00 4.92e-07 -11.0 2.32e-07 - 1.00e+00 1.00e+00f 1
44 5.4495359e-17 0.00e+00 1.17e-07 -11.0 2.10e-08 - 1.00e+00 1.00e+00f 1
45 7.9765903e-18 0.00e+00 1.60e-08 -11.0 1.31e-08 - 1.00e+00 1.00e+00f 1
46 7.8031102e-19 0.00e+00 1.11e-08 -11.0 6.69e-09 - 1.00e+00 1.00e+00f 1
47 3.0972849e-19 0.00e+00 6.67e-09 -11.0 1.81e-09 - 1.00e+00 2.50e-01f 3

```

Number of Iterations.....: 47

| | (scaled) | (unscaled) |
|---------------------------|------------------------|------------------------|
| Objective.....: | 1.4365885378475596e-19 | 3.0972848875993381e-19 |
| Dual infeasibility.....: | 6.6696582319005021e-09 | 1.4379783147977480e-08 |
| Constraint violation....: | 0.0000000000000000e+00 | 0.0000000000000000e+00 |
| Complementarity.....: | 0.0000000000000000e+00 | 0.0000000000000000e+00 |
| Overall NLP error.....: | 6.6696582319005021e-09 | 1.4379783147977480e-08 |

```

Number of objective function evaluations = 109
Number of objective gradient evaluations = 48
Number of equality constraint evaluations = 0
Number of inequality constraint evaluations = 0
Number of equality constraint Jacobian evaluations = 0
Number of inequality constraint Jacobian evaluations = 0
Number of Lagrangian Hessian evaluations = 0
Total CPU secs in IPOPT (w/o function evaluations) = 0.065
Total CPU secs in NLP function evaluations = 0.003

```

EXIT: Optimal Solution Found.

These are the minimal arguments that have to be supplied. If, like above, no Hessian is defined, Ipopt uses an approximation. The Ipopt website has a detailed explanation of the output. We can see a summary of the results by printing the resulting object.

```

> print( res )
Call:

```

```
ipoptr(x0 = x0, eval_f = eval_f, eval_grad_f = eval_grad_f)
```

```
Ipopt solver status: 0 ( SUCCESS: Algorithm terminated
successfully at a locally optimal point, satisfying the
convergence tolerances (can be specified by options). )
```

```
Number of Iterations....: 47
Optimal value of objective function: 3.09728488759934e-19
Optimal value of controls: 1 1
```

It's advised to always check the exit code for convergence of the problem and in this case we can see that the algorithm terminated successfully. Ipopt used 47 iterations to find the solution and the optimal value of the objective function and the controls are given as well.

If you do not want to, or cannot calculate the gradient analytically, you can supply a function `eval_grad_f` that approximates the gradient. However, this is not advisable and might result in convergence problems, for instance by not finding the minimum, or by finding the wrong minimum. We can see this from the following example where we approximate `eval_grad_f` using finite differences

```
> finite.diff <- function( func,
                           x,
                           minAbsValue=0,
                           stepSize=sqrt( .Machine$double.eps ), ... ) {

  stepSizeVec <- pmax( abs(x), 1 ) * stepSize

  fx <- func( x, ... )
  approx.gradf.index <- function(i, x, func, fx, stepSizeVec, ...) {
    x_prime <- x
    x_prime[i] <- x[i] + stepSizeVec[i]
    stepSizeVec[i] <- x_prime[i] - x[i]
    fx_prime <- func( x_prime, ... )
    return( ( fx_prime - fx )/stepSizeVec[i] )
  }
  grad_fx <- sapply( 1:length(x),
                    approx.gradf.index,
                    x=x,
                    func=func,
                    fx=fx,
                    stepSizeVec=stepSizeVec,
                    ... )

  return( grad_fx )
}
> # Approximate eval_f using finite differences
> approx_grad_f <- function( x ) {
```

```

    return( finite.diff( eval_f, x ) )
}

```

and using this approximation to minimize the same Rosenbrock Banana function. We suppress the output by the `printe_level` option.

```

> opts <- list("tol"=1.0e-8, "max_iter"=5000, "print_level"=0)
> # solve Rosenbrock Banana function with approximated gradient
> print( ipoptr( x0=x0,
                eval_f=eval_f,
                eval_grad_f=approx_grad_f,
                opts=opts) )

```

Call:

```

ipoptr(x0 = x0, eval_f = eval_f, eval_grad_f = approx_grad_f,
       opts = opts)

```

```

Ipoptr solver status: 1 ( MAXITER_EXCEEDED:Maximum number
of iterations exceeded (can be specified by an option). )

```

```

Number of Iterations....: 5000
Current value of objective function: 1.9797812650522e-11
Current value of controls: 0.9999956 0.999991

```

In this case 5000 iterations are not enough to solve the minimization problem to the required tolerance. This has to do with the step size we choose to approximate the gradient

```

> sqrt( .Machine$double.eps )
[1] 1.490116e-08

```

which is of the same order of magnitude. If we decrease the tolerance, the algorithm converges, but the solution is less precise than if we supply gradients and it takes more iterations to get there.

```

> opts <- list("tol"=1.0e-7, "print_level"=0)
> # solve Rosenbrock Banana function with approximated gradient
> print( ipoptr( x0=x0,
                eval_f=eval_f,
                eval_grad_f=approx_grad_f,
                opts=opts) )

```

Call:

```

ipoptr(x0 = x0, eval_f = eval_f, eval_grad_f = approx_grad_f,
       opts = opts)

```

```

Ipoptr solver status: 0 ( SUCCESS: Algorithm terminated
successfully at a locally optimal point, satisfying the
convergence tolerances (can be specified by options). )

```

```

Number of Iterations....: 49
Optimal value of objective function: 1.97994053116301e-11
Optimal value of controls: 0.9999956 0.999991

```

4 Sparse matrix structure

Ipopt can handle sparseness in the Jacobian of the constraints and the Hessian. The sparseness structure should be defined in advance and stay the same throughout the minimization procedure. A sparseness structure can be defined as a list of vectors, where each vector contains the indices of the non-zero elements of one row. E.g. the matrix

$$\begin{pmatrix} . & . & . & 1 \\ 1 & 1 & . & . \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

has a non-zero element in position 4 in the first row. In the second row it has non-zero elements in position 1 and 2, and the third row contains non-zero elements at every position. Its structure can be defined as

```
> sparse_structure <- list( c( 4 ), c( 1, 2 ), c( 1, 2, 3, 4 ) )
```

The function `make.sparse` can simplify this procedure

```

> make.sparse( rbind( c(0, 0, 0, 1), c( 1, 1, 0, 0 ), c( 1, 1, 1, 1 ) ) )
[[1]]
[1] 4

[[2]]
[1] 1 2

[[3]]
[1] 1 2 3 4

```

This function takes a matrix as argument. All non-zero elements in this matrix will be defined as non-zero in the sparseness structure, `NA` or `NaN` are not allowed. The function `print.sparseness` shows the non-zero elements

```

> print.sparseness( sparse_structure )
 1 2 3 4
1 . . . 1
2 2 3 . .
3 4 5 6 7

```

By default `print.sparseness` shows the indices of the non-zero elements in the sparse matrix. Values for the non-zero elements of a sparse matrix have to be supplied in one vector, in the same order as the the non-zero elements occur in the structure. I.e. the order of the indices matters and the values of the following two matrices should be supplied in a different order


```

> print.sparseness( list( c(1,3,6,8), c(2,5), c(3,7,9) ) )
  1 2 3 4 5 6 7 8 9
1 1 . 2 . . 3 . 4 .
2 . 5 . . 6 . . . .
3 . . 7 . . . 8 . 9
> print.sparseness( list( c(3,1,6,8), c(2,5), c(3,9,7) ) )
  1 2 3 4 5 6 7 8 9
1 2 . 1 . . 3 . 4 .
2 . 5 . . 6 . . . .
3 . . 7 . . . 9 . 8

```

Since the sparseness structure defines the indices of non-zero elements by row, the order of the rows cannot be changed in the R implementation. In principle a more general order of the non-zero elements (independent of row or column) could be specified, which can be added as a feature on request. Below are two final examples on sparseness structure (see `?print.sparseness` for more options and examples)

```

> A_lower <- make.sparse( lower.tri( matrix(1, nrow=5, ncol=5), diag=TRUE ) )
> print.sparseness( A_lower )
  1 2 3 4 5
1 1 . . . .
2 2 3 . . .
3 4 5 6 . .
4 7 8 9 10 .
5 11 12 13 14 15
> # print a diagonal 5x5 matrix without indices counts
> A_diag <- make.sparse( diag(5) > 0 )
> print.sparseness( A_diag, indices=FALSE )
  1 2 3 4 5
1 x . . . .
2 . x . . .
3 . . x . .
4 . . . x .
5 . . . . x

```

For larger matrices it is easier to plot them using the `plot.sparseness` command

```

> s <- do.call( "cbind", lapply( 1:5, function(i) {
                                     diag(5) %x% matrix(1, nrow=5, ncol=20)
                                 } ) )
> s <- do.call( "rbind", lapply( 1:5, function(i) { s } ) )
> s <- cbind( matrix( 1, nrow=nrow(s), ncol=40 ), s )
> plot.sparseness( make.sparse( s ) )

```

The resulting sparse matrix structure from this code can be seen in figure 1. All non-zero elements are shown as black dots by default.

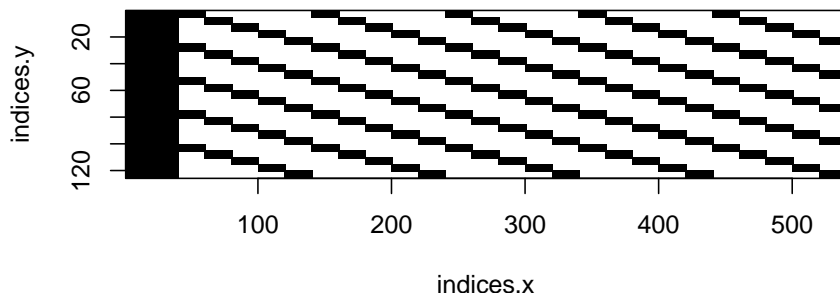


Figure 1: Plot of large sparseness structure

5 Supplying the Hessian

Now that we know how to define a sparseness structure we can supply the Hessian to the Rosenbrock Banana function from above. Its Hessian is given by

$$\nabla^2 f(x) = \begin{pmatrix} 2 - 400 \cdot (x_2 - x_1^2) + 800x_1^2 & -400x_1 \\ -400x_1 & 200 \end{pmatrix}$$

Ipoptr needs the Hessian of the Lagrangian in the following form

$$\sigma_f \nabla^2 f(x) + \sum_{i=1}^m \lambda_i \nabla^2 g_i(x),$$

where $g_i(x)$ represents the i th of m constraints, λ_i are the multipliers of the constraints and σ_f is introduced so that Ipoptr can ask for the Hessian of the objective or the constraints independently if required.

In this case we don't have any constraints. The user-defined function `eval_h` to define the Hessian takes three arguments. The first argument contains the value of the control variables, x , the second argument contains the multiplication factor of the Hessian of the objective function, σ_f , and the third argument contains a vector with the multipliers of the constraints, λ . We can define the structure of the Hessian and the function to evaluate the Hessian as follows

```
> eval_h_structure <- list( c(1), c(1,2) )
> eval_h <- function( x, obj_factor, hessian_lambda ) {
  return( obj_factor*c( 2 - 400*(x[2] - x[1]^2) + 800*x[1]^2,      # 1,1
                      -400*x[1],                                  # 2,1
                      200 ) )                                     # 2,2
}
```

Note that we only specify the lower half of the Hessian, since it is a symmetric matrix. Also, `eval_h` returns a vector with all the non-zero elements of the Hessian in the same order as the non-zero indices in the sparseness structure. Then we minimize the function using the `ipoptr` command

```

> opts <- list("print_level"=0,
              "file_print_level"=12,
              "output_file"="banana.out",
              "tol"=1.0e-8)
> # solve Rosenbrock Banana function with analytic Hessian
> print( ipoptr( x0=x0,
                eval_f=eval_f,
                eval_grad_f=eval_grad_f,
                eval_h=eval_h,
                eval_h_structure=eval_h_structure,
                opts=opts) )

```

Call:

```

ipoptr(x0 = x0, eval_f = eval_f, eval_grad_f = eval_grad_f, eval_h = eval_h,
       eval_h_structure = eval_h_structure, opts = opts)

```

```

Ipoptr solver status: 0 ( SUCCESS: Algorithm terminated
successfully at a locally optimal point, satisfying the
convergence tolerances (can be specified by options). )

```

```

Number of Iterations....: 21
Optimal value of objective function:  3.74397564313947e-21
Optimal value of controls: 1 1

```

Here we also supplied options to not print any intermediate information to the R screen (`print_level=0`). Printing output to the screen directly from `Ipoptr` does not work in all R terminals correctly, so it might be that even though you specify a positive number here, there will still be no output visible on the screen. If you want to print things to the screen, a workaround is to do this directly in the R functions you defined, such as `eval_f`.

Also, to inspect more details about the minimization we can write all the output to a file, which will be created in the current working directory. For larger problems, having a large number for `file_print_level` can easily generate very large files, which is probably not desirable. Many more options are available, and a full list of all the options can be found at the `Ipoptr` website, http://www.coin-or.org/Ipoptr/documentation/node59.html#app.options_ref. Options can also be supplied from an option file, which can be specified in `option_file_name`.

6 Adding constraints

To look at how we can add constraints to a problem, we take example problem number 71 from the Hock-Schittkowsky test suite, which is also used in the `Ipoptr` C++ tutorial. The problem is

$$\begin{aligned}
 & \min_x x_1 \cdot x_4 \cdot (x_1 + x_2 + x_3) + x_3 \\
 & s.t. \\
 & x_1 \cdot x_2 \cdot x_3 \cdot x_4 \geq 25
 \end{aligned}$$

$$x_1^2 + x_2^2 + x_3^2 + x_4^2 = 40$$

$$1 \leq x_1, x_2, x_3, x_4 \leq 5,$$

and we use $x = (1, 5, 5, 1)$ as initial values. In this problem we have one inequality constraint, one equality constraint and upper and lower bounds for all the variables. The optimal solution is $(1.00000000, 4.74299963, 3.82114998, 1.37940829)$. First we define the objective function and its gradient

```
> eval_f <- function( x ) {
  return( x[1]*x[4]*(x[1] + x[2] + x[3]) + x[3] )
}
> eval_grad_f <- function( x ) {
  return( c( x[1] * x[4] + x[4] * (x[1] + x[2] + x[3]),
            x[1] * x[4],
            x[1] * x[4] + 1.0,
            x[1] * (x[1] + x[2] + x[3]) ) )
}
```

Then we define a function that returns the value of the two constraints. We define the bounds of the constraints (in this case the g_L and g_U are 25 and 40) later.

```
> eval_g <- function( x ) {
  return( c( x[1] * x[2] * x[3] * x[4],
            x[1]^2 + x[2]^2 + x[3]^2 + x[4]^2 ) )
}
```

Then we define the structure of the Jacobian, which is a dense matrix in this case, and function to evaluate it

```
> eval_jac_g_structure <- list( c(1,2,3,4), c(1,2,3,4) )
> eval_jac_g <- function( x ) {
  return( c( x[2]*x[3]*x[4],
            x[1]*x[3]*x[4],
            x[1]*x[2]*x[4],
            x[1]*x[2]*x[3],
            2.0*x[1],
            2.0*x[2],
            2.0*x[3],
            2.0*x[4] ) )
}
```

The Hessian is also dense, but it looks slightly more complicated because we have to take into account the Hessian of the objective function and of the constraints at the same time, although you could write a function to calculate them both separately and then return the combined result in `eval_h`.

```
> eval_h_structure <- list( c(1), c(1,2), c(1,2,3), c(1,2,3,4) )
> eval_h <- function( x, obj_factor, hessian_lambda ) {

  values <- numeric(10)
  values[1] = obj_factor * (2*x[4]) # 1,1
```

```

values[2] = obj_factor * (x[4]) # 2,1
values[3] = 0 # 2,2

values[4] = obj_factor * (x[4]) # 3,1
values[5] = 0 # 4,2
values[6] = 0 # 3,3

values[7] = obj_factor * (2*x[1] + x[2] + x[3]) # 4,1
values[8] = obj_factor * (x[1]) # 4,2
values[9] = obj_factor * (x[1]) # 4,3
values[10] = 0 # 4,4

# add the portion for the first constraint
values[2] = values[2] + hessian_lambda[1] * (x[3] * x[4]) # 2,1

values[4] = values[4] + hessian_lambda[1] * (x[2] * x[4]) # 3,1
values[5] = values[5] + hessian_lambda[1] * (x[1] * x[4]) # 3,2

values[7] = values[7] + hessian_lambda[1] * (x[2] * x[3]) # 4,1
values[8] = values[8] + hessian_lambda[1] * (x[1] * x[3]) # 4,2
values[9] = values[9] + hessian_lambda[1] * (x[1] * x[2]) # 4,3

# add the portion for the second constraint
values[1] = values[1] + hessian_lambda[2] * 2 # 1,1
values[3] = values[3] + hessian_lambda[2] * 2 # 2,2
values[6] = values[6] + hessian_lambda[2] * 2 # 3,3
values[10] = values[10] + hessian_lambda[2] * 2 # 4,4

return ( values )
}

```

After the hard part is done, we only have to define the initial values, the lower and upper bounds of the control variables, and the lower and upper bounds of the constraints. If a variable or a constraint does not have lower or upper bounds, the values `-Inf` or `Inf` can be used. If the upper and lower bounds of a constraint are equal, Ipopt recognizes this as an equality constraint and acts accordingly.

```

> x0 <- c( 1, 5, 5, 1 )
> # lower and upper bounds of control
> lb <- c( 1, 1, 1, 1 )
> ub <- c( 5, 5, 5, 5 )
> # lower and upper bounds of constraints
> constraint_lb <- c( 25, 40 )
> constraint_ub <- c( Inf, 40 )
> opts <- list("print_level"=0,
               "file_print_level"=12,
               "output_file"="hs071_nlp.out")
> print( ipoptr( x0=x0,

```

```

eval_f=eval_f,
eval_grad_f=eval_grad_f,
lb=lb,
ub=ub,
eval_g=eval_g,
eval_jac_g=eval_jac_g,
constraint_lb=constraint_lb,
constraint_ub=constraint_ub,
eval_jac_g_structure=eval_jac_g_structure,
eval_h=eval_h,
eval_h_structure=eval_h_structure,
opts=opts) )

```

Call:

```

ipoptr(x0 = x0, eval_f = eval_f, eval_grad_f = eval_grad_f, lb = lb,
       ub = ub, eval_g = eval_g, eval_jac_g = eval_jac_g, eval_jac_g_structure = eval_jac.
       constraint_lb = constraint_lb, constraint_ub = constraint_ub,
       eval_h = eval_h, eval_h_structure = eval_h_structure, opts = opts)

```

Ipoptr solver status: 0 (SUCCESS: Algorithm terminated successfully at a locally optimal point, satisfying the convergence tolerances (can be specified by options).)

Number of Iterations....: 8
Optimal value of objective function: 17.0140171451792
Optimal value of controls: 1 4.743 3.82115 1.379408

7 Using data

The final subject we have to cover, is how to pass data to an objective function or the constraints. There are two ways to do this. The first is to supply additional arguments to the user defined functions and `ipoptr`. The second way is to define an environment that holds the data and pass this environment to `ipoptr`. Both methods are shown in `tests/parameters.R`.

As a very simple example³ suppose we want to find the minimum of

$$f(x) = a_1x^2 + a_2x + a_3$$

for different values of the parameters a_1 , a_2 and a_3 .

First we define the objective function and its gradient using, assuming that there is some variable `params` that contains the values of the parameters.

```

> eval_f_ex1 <- function(x, params) {
  return( params[1]*x^2 + params[2]*x + params[3] )
}
> eval_grad_f_ex1 <- function(x, params) {

```

³A more interesting example is given in `tests/lasso.R`

```

    return( 2*params[1]*x + params[2] )
}

```

Note that the first parameter should always be the control variable. All of the user-defined functions should contain the same set of additional parameters. You have to supply them as input argument to all functions, even if you're not using them in some of the functions.

Then we can solve the problem for a specific set of parameters, in this case $a_1 = 1$, $a_2 = 2$ and $a_3 = 3$, from initial value $x_0 = 0$, with the following command

```

> ipoptr( x0          = 0,
          eval_f      = eval_f_ex1,
          eval_grad_f = eval_grad_f_ex1,
          opts        = list("print_level"=0),
          params      = c(1,2,3) )

```

Call:

```

ipoptr(x0 = 0, eval_f = eval_f_ex1, eval_grad_f = eval_grad_f_ex1,
       opts = list(print_level = 0), params = c(1, 2, 3))

```

```

Ipoptr solver status: 0 ( SUCCESS: Algorithm terminated
successfully at a locally optimal point, satisfying the
convergence tolerances (can be specified by options). )

```

```

Number of Iterations....: 1
Optimal value of objective function:  2
Optimal value of controls: -1

```

For the second method, we don't have to supply the parameters as additional arguments to the function.

```

> eval_f_ex2 <- function(x) {
  return( params[1]*x^2 + params[2]*x + params[3] )
}
> eval_grad_f_ex2 <- function(x) {
  return( 2*params[1]*x + params[2] )
}

```

Instead, we define an environment that contains specific values of `params`

```

> auxdata      <- new.env()
> auxdata$params <- c(1,2,3)

```

To solve this we supply `auxdata` as an argument to `ipoptr`, which will take care of evaluating the functions in the correct environment, so that auxiliary data is available.

```

> ipoptr( x0          = 0,
          eval_f      = eval_f_ex2,
          eval_grad_f = eval_grad_f_ex2,
          ipoptr_environment = auxdata,
          opts        = list("print_level"=0) )

```

Call:

```
ipoptr(x0 = 0, eval_f = eval_f_ex2, eval_grad_f = eval_grad_f_ex2,  
      opts = list(print_level = 0), ipoptr_environment = auxdata)
```

```
Ipoptr solver status: 0 ( SUCCESS: Algorithm terminated  
successfully at a locally optimal point, satisfying the  
convergence tolerances (can be specified by options). )
```

```
Number of Iterations....: 1  
Optimal value of objective function: 2  
Optimal value of controls: -1
```

8 Options

There are many options available, all of which are described on the Ipoptr website. One of the options can test whether your derivatives are correct. This option is activated by setting `derivative_test` to `first-order` or `second-order` if you want to test second derivatives as well. This process can take quite some time. To see all the output from this process you can set `derivative_test_print_all` to `yes`, preferably when writing to a file, because of the problems with displaying on some terminals mentioned above. Without this option the derivative checker only shows those lines where an error occurs if a high enough `print_level` is supplied.

9 Remarks

If you run many large optimization problems in a row on Windows, at some point you'll get errors that Mumps is running out of memory and you won't get any solutions. On Linux this same problem hasn't occurred yet.

From version 0.8.2 output is shown in the R terminal under Windows as well.

References

- Leisch, F. (2002). Sweave: Dynamic generation of statistical reports using literate data analysis. In W. Härdle & B. Rönz (Eds.), *Compstat 2002 — proceedings in computational statistics* (pp. 575–580). Physica Verlag, Heidelberg. Available from <http://www.stat.uni-muenchen.de/~leisch/Sweave> (ISBN 3-7908-1517-9)
- Wächter, A., & Biegler, L. T. (2006). On the implementation of a primal-dual interior point filter line search algorithm for large-scale nonlinear programming. *Mathematical Programming*, 106(1), 25–57.