

Mathematics 2, Part 4, Homework 1

I. NELDER-MEAD IMPLEMENTATION

2-D implementation

Firstly we implemented the two dimensional version of the Nelder-Mead method and tested it on a simple function:

$$f(x, y) = x^2 + y^2$$

On Figure 1 we can see the convergence of the best points using the 2-d implementation of the method.

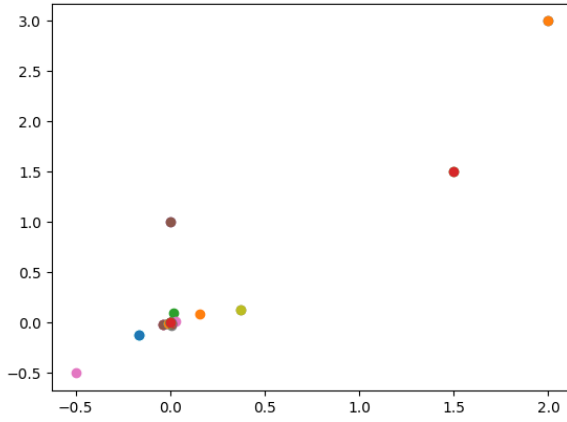


Figure 1. Convergence of the best points on a simple function for a 2-d implementation of the Nelder-Mead method

Implementation for arbitrary dimension

Next, we implemented Nelder-Mead for arbitrary dimensions and tested it on the same function. On Figure 2 We can see that, when using the same starting points, we achieve the same convergence as for the previous implementation. Note that, we require the user to specify one starting point for this implementation. The other starting points are determined by taking the first starting point and adding a constant r (which is another parameter for the method) to a different dimension each time.

II. COMPARISON OF NELDER-MEAD WITH DESCENT METHODS

We compared the implemented method with the previously implemented descent methods on 3 different functions. To compare the implemented method with the descent methods, we used the results from the second homework, where we looked at the number of steps needed to reach convergence, where our convergence condition was where the difference in our positions (of consecutive steps) is small enough. We add our results for the Nelder-Mead method to our results from the second homework. For each function we used both starting points given in the second homework and we evaluate the Nelder-Mead method with three different r -s, those being 1, 2 and 5.

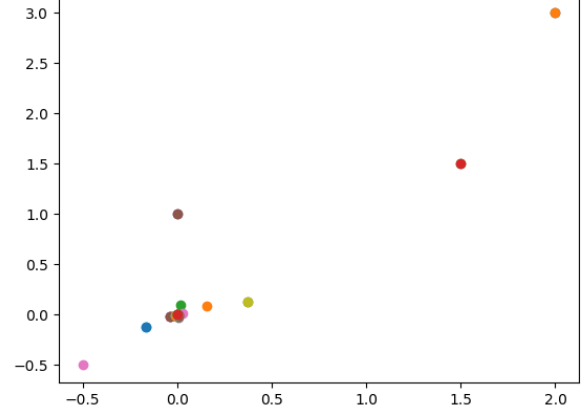


Figure 2. Convergence of the best points on a simple function for the arbitrary dimensional implementation of the Nelder-Mead method

Function 1

The first function is given as:

$$f_1(x) = (x_0 - x_2)^2 + (2x_1 + x_2)^2 + (4x_0 - 2x_1 + x_2)^2 + x_0 + x_1$$

For this function we used the starting points of $(0, 0, 0)$ and $(1, 1, 0)$. We can see the results in Table I. Note that here and the other tables S1 and S2 denote the first and second starting points and f denotes the value of the function in the final point. We can see that Nelder-Mead was outperformed by second degree methods (of their approximations) and Adagrad, however it outperformed the basic gradient descent and its Polyak and Nesterov modifications. Changing r did not influence the result much for this function.

Method	S1: f	S1: Steps	S2: f	S2: Steps
GD	-0.1979	3142	-0.1979	3611
Polyak	-0.1979	1561	-0.1979	1794
Nesterov	-0.1979	1565	-0.1979	1798
AdaGrad	-0.1979	101	-0.1979	79
Newton	-0.1979	1	-0.1979	1
Bfgs	-0.1979	20	-0.1979	22
L-Bfgs	-0.1979	8	-0.1979	11
NM, $r=1$	-0.1979	126	-0.1979	141
NM, $r=2$	-0.1979	136	-0.1979	131
NM, $r=5$	-0.1979	138	-0.1979	132

Table I
COMPARISON OF THE NELDER-MEAD METHOD WITH DESCENT METHODS ON THE FIRST FUNCTION

Function 2

Next, we used the function:

$$f_2(x) = (x_1 - 1)^2 + (x_2 - 1)^2 + 100(x_2 - x_1^2)^2 + 100(x_3 - x_2^2)^2$$

Here, the starting points were $(1.2, 1.2, 1.2)$ and $(-1, 1.2, 1.2)$. We can see the comparison in Table II. Note that here the

descent methods were only allowed 2 second of runtime, since that was the task in the second homework. We can quickly see that with an appropriate choice of r the Nelder-Mead method performs really nicely even in comparison to second degree methods, however when choosing an r that is too large, the method does not converge properly.

Method	S1: f	S1: Steps	S2: f	S2: Steps
GD	3.271×10^{-8}	24966	3.268×10^{-8}	30730
Polyak	3.268×10^{-8}	12430	3.268×10^{-8}	15350
Nesterov	3.266×10^{-8}	14134	3.267×10^{-8}	13784
AdaGrad	3.601×10^{-9}	13498	4.622×10^{-9}	15915
Newton	1.840×10^{-1}	67541	3.831×10^{-1}	66239
Bfgs	1.939×10^{-15}	319	4.709×10^{-16}	188
L-Bfgs	5.161×10^{-11}	369	2.255×10^{-8}	509
NM, r=1	6.330×10^{-15}	178	3.460×10^{-14}	1294
NM, r=2	1.091×10^{-13}	169	0.246	113
NM, r=5	7.339	123	2.325	102

Table II

COMPARISON OF THE NELDER-MEAD METHOD WITH DESCENT METHODS ON THE SECOND FUNCTION

Function 3

The last function was given as:

$$f_3(x) = (1.5 - x_1 + x_1 x_2)^2 + (2.25 - x_1 + x_1 x_2^2)^2 + (2.625 - x_1 + x_1 x_2^3)^2$$

The starting points were (1, 1) and (4.5, 4.5). We can see the comparison on Table III. Here, we can see that for the second starting point, all the other methods fail to reach the optimum, while the Nelder-Mead method finds it really quickly, if we choose the correct r .

Method	S1: f	S1: Steps	S2: f	S2: Steps
GD	1.656×10^{-8}	23234	nan	100000
Polyak	1.655×10^{-8}	11607	nan	100000
Nesterov	1.657×10^{-8}	11617	nan	100000
AdaGrad	1.08×10^{-12}	318	0.227	27017
Newton	14.203	1	14.203	12
BFGS	4.661×10^{-18}	31	nan	71794
L-BFGS	1.189×10^{-14}	29	1.748×10^5	3
NM, r=1	6.587×10^{-15}	65	0.125	48
NM, r=2	4.879×10^{-15}	61	1.373×10^{-14}	91
NM, r=5	1.761×10^{-15}	73	5.441×10^{-14}	81

Table III

COMPARISON OF THE NELDER-MEAD METHOD WITH DESCENT METHODS ON THE THIRD FUNCTION