# Selective Reflections for the Nelder-Mead Algorithm

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## Abstract

The Nelder-Mead Algorithm is an established algorithm to search for a minimum to a function. Since its first description, the algorithm has had various improvements made to it. With this project, I searched for improvements to the algorithm through changes to its reflective direction and geometric structure. I found in testing that directions that maintain the shape of the algorithm’s search structure perform better than those that do not. The algorithm’s speed can also be increased in higher test dimensions by increasing the number of points in the simplex by one. With these alterations, the Nelder-Mead algorithm can find solutions to problems it previously could not and do so with fewer function evaluations.

## Methods

In a single iteration, the basic algorithm does not directly use all the information that is stored within the simplex. The algorithm overlooks the fullest extent of rank and value of the n-best points during an iteration. To use this information, I calculated new direction vectors to use as a basis for the reflection. To gather more information, I added an extra point to the simplex as a second point of reflection and used another mirror reflection to allow more movement of the simplex.

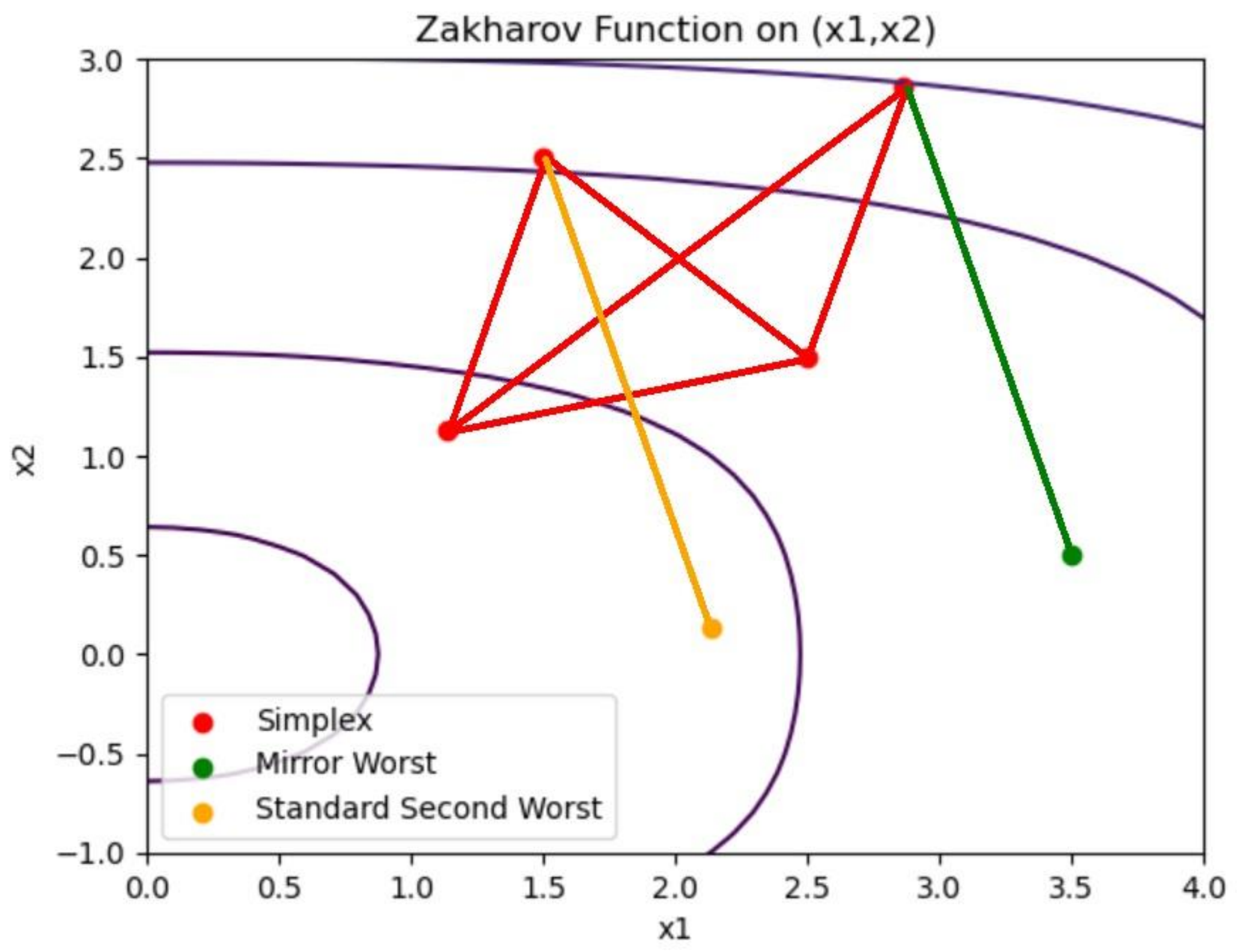

Figure 1. An example of the reflection and mirror steps on an n+2 point simplex evaluated on the Zhakarov function.

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## Introduction

The Nelder-Mead method optimizes a function of n variables by creating a simplex with n+1 points in an n-dimensional space. It then uses a combination of five steps to transform the simplex by moving the point with the worst evaluation to a hopefully better location. The direction in which it moves this point is what this project focused on studying. The standard algorithm moves the point in the direction of the center of the rest of the points, called the centroid. The centroid is calculated by taking the mean of the n-best points. Once the last ranked point has been moved, the algorithm starts again with the new set of points and iterates until a stopping condition is met. In a single iteration, the basic algorithm does not directly use a lot of information that is stored within the simplex.

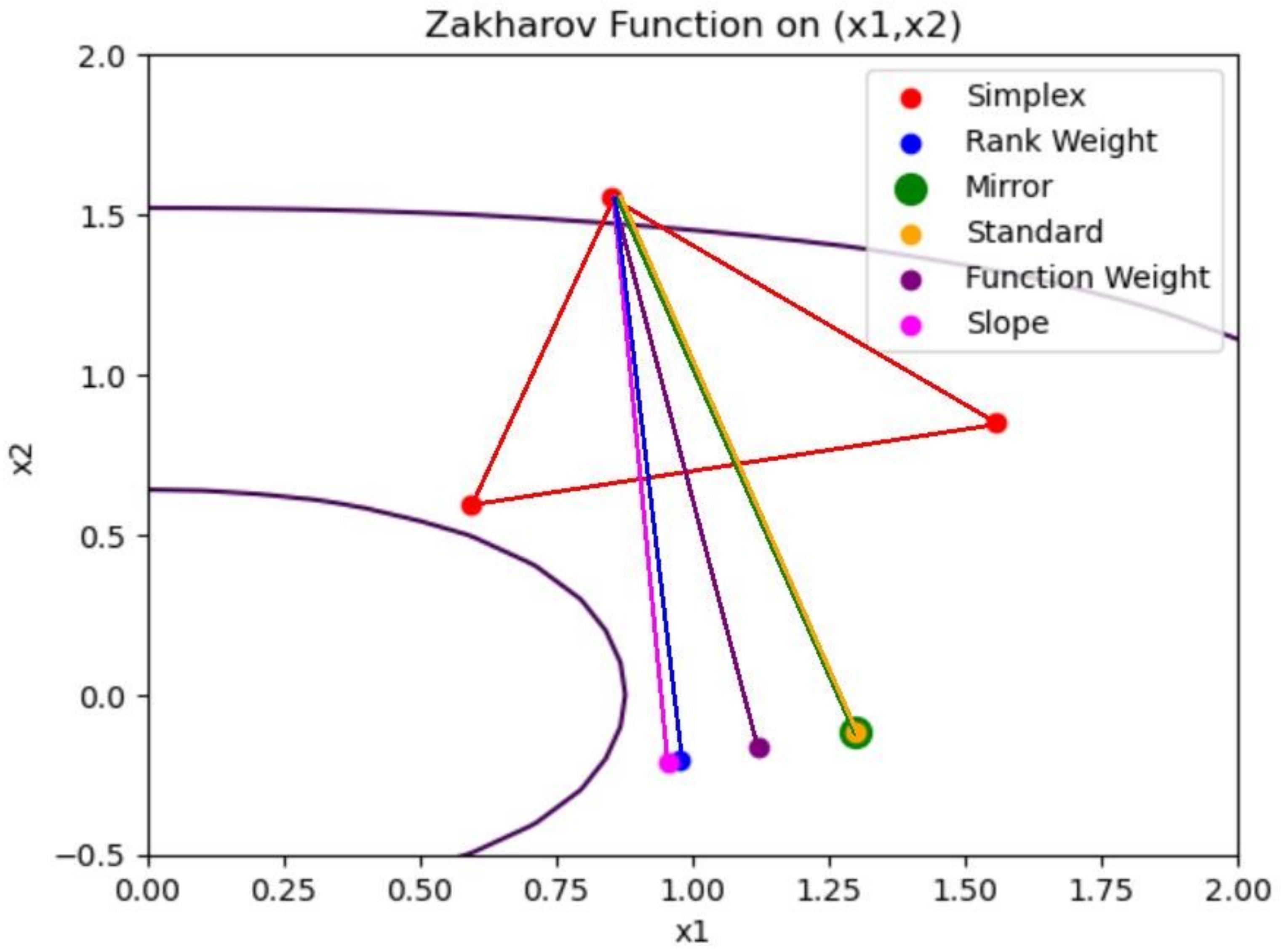


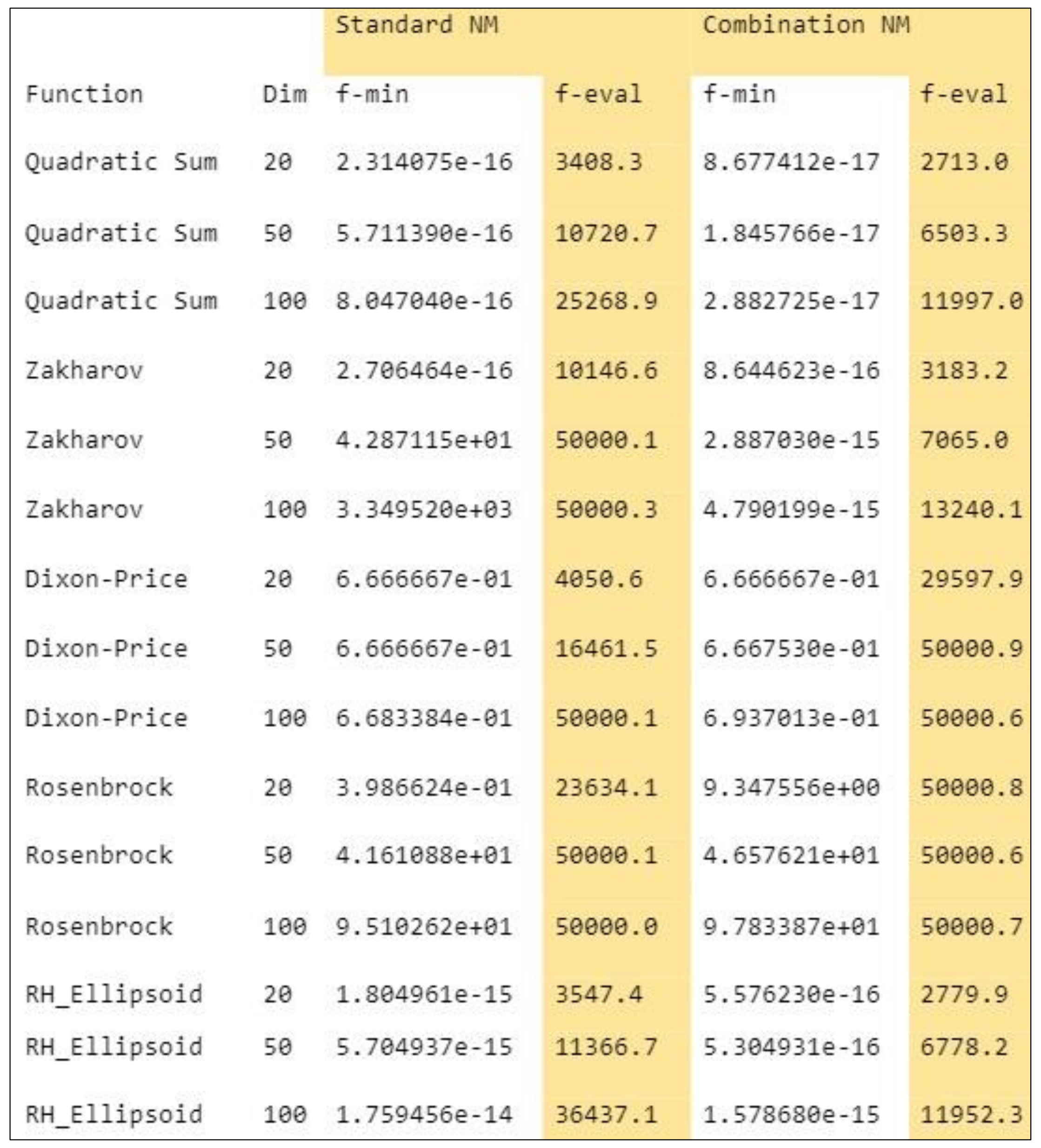
Figure 2. An example of each of the five tested reflections given a simplex evaluated on the Zhakarov function.

## References

Nelder, J. A., & Mead, R. (1965). A simplex method for function minimization. *The Computer Journal*, *7*(4), 308–313. https://doi.org/10.1093/comjnl/7.4.308

## Results

This project found that the additional point to the simplex improved the performance of the base algorithm without any changes to the reflective direction as the dimension of the function increased. The mirror transformation used with the extra point also helped the algorithm perform faster on multiple test functions and find more accurate minimums. However, more aggressive reflections that did not uphold the shape of the simplex as closely as the standard reflection or mirror reflection would often cause the algorithm to fail to find an acceptable minimum or perform within an acceptable speed.



| | | Standard NM | | Combination NM | |
|---|---|---|---|---|---|
| Function | Dim | f-min | f-eval | f-min | f-eval |
| Quadratic Sum | 20 | 2.314075e-16 | 3408.3 | 8.677412e-17 | 2713.0 |
| Quadratic Sum | 50 | 5.711390e-16 | 10720.7 | 1.845766e-17 | 6503.3 |
| Quadratic Sum | 100 | 8.047040e-16 | 25268.9 | 2.882725e-17 | 11997.0 |
| Zakharov | 20 | 2.706464e-16 | 10146.6 | 8.644623e-16 | 3183.2 |
| Zakharov | 50 | 4.287115e+01 | 50000.1 | 2.887030e-15 | 7065.0 |
| Zakharov | 100 | 3.349520e+03 | 50000.3 | 4.790199e-15 | 13240.1 |
| Dixon-Price | 20 | 6.666667e-01 | 4050.6 | 6.666667e-01 | 29597.9 |
| Dixon-Price | 50 | 6.666667e-01 | 16461.5 | 6.667530e-01 | 50000.9 |
| Dixon-Price | 100 | 6.683384e-01 | 50000.1 | 6.937013e-01 | 50000.6 |
| Rosenbrock | 20 | 3.986624e-01 | 23634.1 | 9.347556e+00 | 50000.8 |
| Rosenbrock | 50 | 4.161088e+01 | 50000.1 | 4.657621e+01 | 50000.6 |
| Rosenbrock | 100 | 9.510262e+01 | 50000.0 | 9.783387e+01 | 50000.7 |
| RH_Ellipsoid | 20 | 1.804961e-15 | 3547.4 | 5.576230e-16 | 2779.9 |
| RH_Ellipsoid | 50 | 5.704937e-15 | 11366.7 | 5.304931e-16 | 6778.2 |
| RH_Ellipsoid | 100 | 1.759456e-14 | 36437.1 | 1.578680e-15 | 11952.3 |

Figure 3. Data collected comparing the standard Nelder-Mead algorithm to the one found in the project. Note that "Dim" stands for dimension of the test function. "RH_Ellipsoid" stands for the Rotated Hyper-Ellipsoid function.

## Conclusions

These results open avenues to understanding the functioning of the Nelder-Mead algorithm and improving its design. Future research can be done to explore the effect of using even more points in the simplex, new transformations that continue to maintain the shape of the simplex and fine-tune the selection of multiple types of reflections in a single algorithm run.