

MANE 6710 - Numerical Design Optimization Lab 5

Human 6966

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Executive Summery

Unconstrained optimization algorithms are powerful tools for engineers, as they form a basic method of solving complex multivariable optimization problems found across engineering disciplines. The purpose of this lab was for us to implement an unconstrained optimization problem from scratch to learn more about how they work. The algorithm I implemented was the Broyden–Fletcher–Goldfarb–Shanno algorithm, which is a nonlinear multivariable Quasi-Newton algorithm, that is relatively efficient for medium to large smooth optimization problems. I was successfully able to implement this algorithm in Python, which runs with reasonable efficiency and accuracy.

1 Introduction

Optimization algorithms are an important tool for engineers as they enable us to numerically determine a viable solution to a complex problem that balances various design criteria (such as weight, cost, or strength). Optimization algorithms solve these problems by numerically solving a given input equation set (called the objective function) for a local minimum. These algorithms use various methods to solve for these local minimums, which have different strengths and weaknesses.

For example, genetic algorithms can solve nonlinear equations that have a discontinuous first derivative as it relies solely on the objective function. However, the downside of this particular method is its computational cost as sampling the objective function several times each iteration to determine the best movement direction takes more time and power than other methods like the Broyden–Fletcher–Goldfarb–Shanno algorithm (BFGS).

The BFGS algorithm is a non-linear Quasi-Newton optimization algorithm that is significantly more efficient than the genetic algorithm. This is because it uses derivative and approximated second derivative information to reduce the number of function calls and iterations used to determine a local minimum. However, the downside to using this and other Quasi-Newton methods is they rely on the function having a continuous, easily computed first derivative. This means that there are problems the genetic algorithm is capable of solving that the BFGS algorithm cannot.

2 Methodology

The BFGS algorithm I implemented in this project is from algorithms 6.1, 3.5, and 3.6 [1] shown in Figures 1, 2, and 3 respectively.

My implementation of this algorithm works by using the complex step method to calculate the gradient (∇f_k) at the current position (x_k) using a step size of 10^{-30} . Then my code calculates the step direction (p_k) from the gradient and the current approximation of the hessian (H_k) using the equation $p_k = -H_k \nabla f_k$. From this and the given objective function ($f(x)$), an anonymous scalar function is defined as $\phi(\alpha) = f(x_k + \alpha p_k)$ and an anonymous function for the derivative is defined as $\phi'(\alpha) = \nabla \phi(\alpha)$, which are given to the line search algorithm to solve for a minimum in the search direction.

The Line Search algorithm iterates through values of α until it either finds values on both sides of the directional minimum, finds an increasingly positive first derivative, or runs out of allowed iterations. In the first case, the line search method calls the Zoom algorithm, passing it the two endpoints and the scalar functions, and returns its output. In the second case, the function returns the current value of α and in the third case the algorithm throws a runtime error.

The Zoom algorithm performs a bisection search on the given interval of the scalar function, checking if the current α satisfies the strong Wolfe conditions for each iteration. When the strong Wolfe conditions are satisfied, the algorithm returns the current step length ($\alpha_{\text{current step}} = 0.5(\alpha_{\text{high bound}} + \alpha_{\text{low bound}})$). In iterations where the strong Wolfe conditions aren't met, the algorithm sets the high bound of the interval to the current step if the sufficient decrease condition ($\phi(\alpha_{\text{current step}}) < \phi(0) +$

Algorithm 6.1 (BFGS Method).

Given starting point x_0 , convergence tolerance $\epsilon > 0$,
 inverse Hessian approximation H_0 ;
 $k \leftarrow 0$;
while $\|\nabla f_k\| > \epsilon$;
 Compute search direction

$$p_k = -H_k \nabla f_k; \quad (6.18)$$

 Set $x_{k+1} = x_k + \alpha_k p_k$ where α_k is computed from a line search
 procedure to satisfy the Wolfe conditions (3.6);
 Define $s_k = x_{k+1} - x_k$ and $y_k = \nabla f_{k+1} - \nabla f_k$;
 Compute H_{k+1} by means of (6.17);
 $k \leftarrow k + 1$;
end (while)

Figure 1: Algorithm 6.1: BFGS Method

Algorithm 3.5 (Line Search Algorithm).

Set $\alpha_0 \leftarrow 0$, choose $\alpha_{\max} > 0$ and $\alpha_1 \in (0, \alpha_{\max})$;
 $i \leftarrow 1$;
repeat
 Evaluate $\phi(\alpha_i)$;
 if $\phi(\alpha_i) > \phi(0) + c_1 \alpha_i \phi'(0)$ or $[\phi(\alpha_i) \geq \phi(\alpha_{i-1}) \text{ and } i > 1]$
 $\alpha_* \leftarrow \text{zoom}(\alpha_{i-1}, \alpha_i)$ and **stop**;
 Evaluate $\phi'(\alpha_i)$;
 if $|\phi'(\alpha_i)| \leq -c_2 \phi'(0)$
 set $\alpha_* \leftarrow \alpha_i$ and **stop**;
 if $\phi'(\alpha_i) \geq 0$
 set $\alpha_* \leftarrow \text{zoom}(\alpha_i, \alpha_{i-1})$ and **stop**;
 Choose $\alpha_{i+1} \in (\alpha_i, \alpha_{\max})$;
 $i \leftarrow i + 1$;
end (repeat)

Figure 2: Algorithm 3.5: BFGS Line Search Method

$c_1 \alpha_{\text{current step}} \phi'(0)$) isn't satisfied and the low bound of the interval to the current step if the sufficient decrease condition is met but the flatness condition ($|\phi'(\alpha_{\text{current step}})| \leq -c_2 \phi'(0)$). Note: c_1 and c_2 were chosen to be 0.0001 and 0.9 respectively based on the advice from the textbook [1].

Once the Zoom and Line Search algorithms return the current step length (α), the BFGS algorithm updates the current position, gradient, and Hessian estimate. The Hessian estimate update equation is given in Equation 1 [1] (y_k , and s_k , and ρ_k are given in Equations 2, 3, and 4 respectively). Then the current step statistics are printed to the terminal and the ending condition ($\|\nabla f(x_k)\| < \text{Error Tolerance}$) is checked to determine if the algorithm needs another iteration and, if not, returns the final position.

$$H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T \quad (1)$$

$$y_k = \nabla f(x_{k+1}) - \nabla f(x_k) \quad (2)$$

Algorithm 3.6 (zoom).

```

repeat
    Interpolate (using quadratic, cubic, or bisection) to find
        a trial step length  $\alpha_j$  between  $\alpha_{lo}$  and  $\alpha_{hi}$ ;
    Evaluate  $\phi(\alpha_j)$ ;
    if  $\phi(\alpha_j) > \phi(0) + c_1\alpha_j\phi'(0)$  or  $\phi(\alpha_j) \geq \phi(\alpha_{lo})$ 
         $\alpha_{hi} \leftarrow \alpha_j$ ;
    else
        Evaluate  $\phi'(\alpha_j)$ ;
        if  $|\phi'(\alpha_j)| \leq -c_2\phi'(0)$ 
            Set  $\alpha_* \leftarrow \alpha_j$  and stop;
        if  $\phi'(\alpha_j)(\alpha_{hi} - \alpha_{lo}) \geq 0$ 
             $\alpha_{hi} \leftarrow \alpha_{lo}$ ;
         $\alpha_{lo} \leftarrow \alpha_j$ ;
end (repeat)

```

Figure 3: Algorithm 3.6: BFGS Zoom Method

$$s_k = \alpha p_k \tag{3}$$

$$\rho_k = \frac{1}{y_k^T s_k} \tag{4}$$

3 Testing and Results

Once I implemented the algorithm in Python, the algorithm needed to be tested to ensure it worked. The test cases and the algorithm's results are summarized in Table 1. I chose a scalar function for the first test case, as it is a special case that isn't affected by matrix algebra errors while still testing the different algorithms and their integration. Once I ensured the algorithm was running as intended with the scalar case, I chose to implement two simple two-dimensional polynomial cases to test the matrix algebra implementation and how the code handles vectors. There were several matrix algebra errors due to how the Numpy library handles arrays that were fixed using these test cases. The final set of test cases I chose to test the algorithm's ability to handle more complex problems. The Two-dimensional Rosenbrock function was suggested by the instructor as a good single-objective optimization test case used in research. The fifth test case tested how the algorithms reacted to multimodal cases and the sixth tested the algorithm's ability to handle higher dimensional problems. See Table 2 for the initial conditions used in each test case.

As is shown in Table 1, the algorithm I implemented was able to consistently find a minimum within a reasonable time frame (the largest number of iterations used being 34 in the used test cases). While there is some error between the calculated and actual minima locations, particularly in cases with unequal scaling. As shown in the Appendix section for each test case, the First-order Optimality (magnitude of the gradient) decreased by at least nine orders of magnitude demonstrating a properly functioning optimization algorithm converging on a viable solution. Between the low error in the results and the convergence history, my implementation of the BFGS algorithm is shown to work in all of the test cases.

Table 1: Test Cases and Algorithm Results

| Test Case | Actual Minima Location | Calculated Minima Location | Appendix |
|--|------------------------|---------------------------------------|----------|
| x^2 | 0 | 0,0 | 5.1.1 |
| $x_1^4 + x_2^2$ | (0,0) | (1.28e-3,-2.10e-8),(1.28e-3,-2.10e-8) | 5.1.2 |
| $(x_1 - 1)^4 + (x_2 + 2)^2$ | (1,-2) | (0.999,-1.9999), (1.001,-1.99999) | 5.1.3 |
| two dimensional Rosenbrock | (1,1) | (1,1) | 5.1.4 |
| $x_1^4 + x_2^4 - 17x_2^3 + 45x_2^2$ | (1,3), (1,13.6342) | (1.0002,3),(0.9972,13.6342) | 5.1.5 |
| $(x_1 - 1)^4 + (x_2 + 2)^2 + 1 + 5(x_3 - 3)^4$ | (1,-2,3) | (0.9996,-2,3), (1.0015,-2,3) | 5.1.6 |

Table 2: Initial Conditions for Test Cases

| Test Case | x_0 | H_0 |
|--|--------------------|-------|
| x^2 | 10,-10 | 0.1I |
| $x_1^4 + x_2^2$ | (10,10),(-10,-10) | 0.1I |
| $(x_1 - 1)^4 + (x_2 + 2)^2$ | (4,4),(-7,-7) | 0.05I |
| two dimensional Rosenbrock | (1,1) | 0.1I |
| $x_1^4 + x_2^4 - 17x_2^3 + 45x_2^2$ | (4,4),(-7,-7) | 0.1I |
| $(x_1 - 1)^4 + (x_2 + 2)^2 + 1 + 5(x_3 - 3)^4$ | (4,4,4),(-7,-7,-7) | 0.1I |

4 Conclusions

I was able to successfully implement the nonlinear unconstrained optimization algorithm BFGS. As shown in the results, the implemented algorithm was able to handle simple and complex smooth nonlinear multivariable optimization problems efficiently. However, my implementation of the BFGS algorithm has significant limitations. Firstly, it only handles unconstrained optimization algorithms. This limits the potential applications for this algorithm as most problems in engineering have constraints. This can be somewhat mitigated by adding barrier functions to the objective function, however, it will likely be less efficient and accurate than an algorithm designed for handling constraints. Secondly, the algorithm only works with deterministic functions that are 'smooth' and have a continuous first derivative. Thirdly, this implementation is less efficient for linear optimization problems than purpose-made algorithms. Finally, this algorithm doesn't handle functions that go to negative infinity well (it usually throws an error), so it should only be used on functions with real minima.

References

- [1] S. W. Jorge Nocedal, *Numerical optimization second edition*, Book, 2006.

5 Appendix

5.1 Optimization Algorithm Test Case Output

5.1.1 One Dimentional Polynomial

```
Iterations:      |grad|
1              16.0
2              0.0
bfgs[0.]
Iterations:      |grad|
1              16.0
2              0.0
bfgs[0.]
```

Figure 4: Function output for one dimensional polynomial from two starting points

5.1.2 Two Dimentional Polynomial

| Iterations: | grad | Iterations: | grad |
|---------------------------------------|------------------------|-------------------------------------|------------------------|
| 1 | 65.58403483318178 | 1 | 65.58403483318178 |
| 2 | 51.680716658179655 | 2 | 51.680716658179655 |
| 3 | 15.290466011992974 | 3 | 15.290466011992974 |
| 4 | 12.394032704204294 | 4 | 12.394032704204294 |
| 5 | 9.477798608410072 | 5 | 9.477798608410072 |
| 6 | 5.178661875102632 | 6 | 5.178661875102632 |
| 7 | 2.1773968474436325 | 7 | 2.1773968474436325 |
| 8 | 0.8221514143987172 | 8 | 0.8221514143987172 |
| 9 | 0.454889195063089 | 9 | 0.454889195063089 |
| 10 | 0.2857348166513772 | 10 | 0.2857348166513772 |
| 11 | 0.13584582547710278 | 11 | 0.13584582547710278 |
| 12 | 0.0464531951190135 | 12 | 0.0464531951190135 |
| 13 | 0.023335755179815895 | 13 | 0.023335755179815895 |
| 14 | 0.01747223023161133 | 14 | 0.01747223023161133 |
| 15 | 0.008776985597580767 | 15 | 0.008776985597580767 |
| 16 | 0.002147450337541808 | 16 | 0.002147450337541808 |
| 17 | 0.0015736080969060552 | 17 | 0.0015736080969060552 |
| 18 | 0.0014467020121639686 | 18 | 0.0014467020121639686 |
| 19 | 0.0006259883329915933 | 19 | 0.0006259883329915933 |
| 20 | 7.49960770268807e-05 | 20 | 7.49960770268807e-05 |
| 21 | 0.00016772994998276555 | 21 | 0.00016772994998276555 |
| 22 | 0.00013212992776993662 | 22 | 0.00013212992776993662 |
| 23 | 4.261952044649142e-05 | 23 | 4.261952044649142e-05 |
| 24 | 8.982231749875275e-06 | 24 | 8.982231749875275e-06 |
| 25 | 1.9101024019070267e-05 | 25 | 1.9101024019070267e-05 |
| 26 | 1.156345652089891e-05 | 26 | 1.156345652089891e-05 |
| 27 | 2.318783372309847e-06 | 27 | 2.318783372309847e-06 |
| 28 | 1.7494845845582582e-06 | 28 | 1.7494845845582582e-06 |
| 29 | 2.0258010729966285e-06 | 29 | 2.0258010729966285e-06 |
| 30 | 9.257729385853145e-07 | 30 | 9.257729385853145e-07 |
| 31 | 4.274642526164209e-08 | 31 | 4.274642526164209e-08 |
| bfgs[-1.28237509e-03 -2.09529297e-08] | | bfgs[1.28237509e-03 2.09529297e-08] | |

Figure 5: Function output for two dimensional polynomial from two starting points

5.1.3 Shifted Two Dimentional Polynomial

| Iterations: | grad | Iterations: | grad |
|------------------------------|------------------------|-------------------------------|------------------------|
| 1 | 56.340816607500486 | 1 | 442.47820629834433 |
| 2 | 8.975456017530629 | 2 | 64.99383329095672 |
| 3 | 6.806647524875654 | 3 | 38.73384423230395 |
| 4 | 0.14184863330781683 | 4 | 12.508293226775423 |
| 5 | 0.0009714744472591841 | 5 | 5.621957850248754 |
| 6 | 0.00013065326931259422 | 6 | 3.3311886758200204 |
| 7 | 0.00015399075436447785 | 7 | 2.5168181853149805 |
| 8 | 0.0005565454995007706 | 8 | 1.5894162989075442 |
| 9 | 0.0005638851609230319 | 9 | 0.7803443511994075 |
| 10 | 0.00024382693631504204 | 10 | 0.24323989043595762 |
| 11 | 1.3841268955275838e-05 | 11 | 0.0955112574814264 |
| 12 | 5.1579251356273843e-05 | 12 | 0.0810742678993822 |
| 13 | 4.828845594752732e-05 | 13 | 0.0635624062272388 |
| 14 | 1.8009211663722587e-05 | 14 | 0.033153143446662 |
| 15 | 1.1317081371780335e-06 | 15 | 0.007823257469121702 |
| 16 | 5.779569120065623e-06 | 16 | 0.0048387151658952085 |
| 17 | 4.1401531711586605e-06 | 17 | 0.005123317104651325 |
| 18 | 1.0917889818202174e-06 | 18 | 0.0028512099436148177 |
| 19 | 3.9756649753852955e-07 | 19 | 0.0005466242011692326 |
| 20 | 6.212506800217101e-07 | 20 | 0.00042434541697837887 |
| 21 | 3.2924237491447375e-07 | 21 | 0.0004814519071360643 |
| 22 | 4.199133178057899e-08 | 22 | 0.00023268283105266655 |
| bfgs[0.9993471 -1.99999998] | | 23 | 2.3110256159098433e-05 |
| Iterations: | grad | 24 | 5.053119100994786e-05 |
| 1 | 442.47820629834433 | 25 | 4.621663701041531e-05 |
| 2 | 64.99383329095672 | 26 | 1.7414490196882007e-05 |
| 3 | 38.73384423230395 | 27 | 1.3515939120023806e-06 |
| 4 | 12.508293226775423 | 28 | 6.051021320554987e-06 |
| 5 | 5.621957850248754 | 29 | 4.216913487507347e-06 |
| 6 | 3.3311886758200204 | 30 | 1.1102194694811617e-06 |
| 7 | 2.5168181853149805 | 31 | 4.4165021324450455e-07 |
| 8 | 1.5894162989075442 | 32 | 6.709111904820717e-07 |
| 9 | 0.7803443511994075 | 33 | 3.55566553371198e-07 |
| 10 | 0.24323989043595762 | 34 | 4.674735595228893e-08 |
| 11 | 0.0955112574814264 | bfgs[1.00072178 -1.99999998] | |

Figure 6: Function output for two dimensional polynomial from two starting points

5.1.4 Two Dimentional Rosenbrock Function

| Iterations: | grad | Iterations: | grad |
|---------------------------------------|------------------------|-------------------------------------|------------------------|
| 1 | 65.58403483318178 | 1 | 65.58403483318178 |
| 2 | 51.680716658179655 | 2 | 51.680716658179655 |
| 3 | 15.290466011992974 | 3 | 15.290466011992974 |
| 4 | 12.394032704204294 | 4 | 12.394032704204294 |
| 5 | 9.477798608410072 | 5 | 9.477798608410072 |
| 6 | 5.178661875102632 | 6 | 5.178661875102632 |
| 7 | 2.1773968474436325 | 7 | 2.1773968474436325 |
| 8 | 0.8221514143987172 | 8 | 0.8221514143987172 |
| 9 | 0.454889195063089 | 9 | 0.454889195063089 |
| 10 | 0.2857348166513772 | 10 | 0.2857348166513772 |
| 11 | 0.13584582547710278 | 11 | 0.13584582547710278 |
| 12 | 0.0464531951190135 | 12 | 0.0464531951190135 |
| 13 | 0.023335755179815895 | 13 | 0.023335755179815895 |
| 14 | 0.01747223023161133 | 14 | 0.01747223023161133 |
| 15 | 0.008776985597580767 | 15 | 0.008776985597580767 |
| 16 | 0.002147450337541808 | 16 | 0.002147450337541808 |
| 17 | 0.0015736080969060552 | 17 | 0.0015736080969060552 |
| 18 | 0.0014467020121639686 | 18 | 0.0014467020121639686 |
| 19 | 0.0006259883329915933 | 19 | 0.0006259883329915933 |
| 20 | 7.49960770268807e-05 | 20 | 7.49960770268807e-05 |
| 21 | 0.00016772994998276555 | 21 | 0.00016772994998276555 |
| 22 | 0.00013212992776993662 | 22 | 0.00013212992776993662 |
| 23 | 4.261952044649142e-05 | 23 | 4.261952044649142e-05 |
| 24 | 8.982231749875275e-06 | 24 | 8.982231749875275e-06 |
| 25 | 1.9101024019070267e-05 | 25 | 1.9101024019070267e-05 |
| 26 | 1.156345652089891e-05 | 26 | 1.156345652089891e-05 |
| 27 | 2.318783372309847e-06 | 27 | 2.318783372309847e-06 |
| 28 | 1.7494845845582582e-06 | 28 | 1.7494845845582582e-06 |
| 29 | 2.0258010729966285e-06 | 29 | 2.0258010729966285e-06 |
| 30 | 9.257729385853145e-07 | 30 | 9.257729385853145e-07 |
| 31 | 4.274642526164209e-08 | 31 | 4.274642526164209e-08 |
| bfgs[-1.28237509e-03 -2.09529297e-08] | | bfgs[1.28237509e-03 2.09529297e-08] | |

Figure 7: Function output for two dimensional Rosenbrock Function from one starting point

5.1.5 Two Dimentional Polynomial with Multiple Minima

| Iterations: | grad | Iterations: | grad |
|--------------------|------------------------|-------------------------------|------------------------|
| 1 | 7.039391029514307 | 1 | 593.3935263992481 |
| 2 | 0.12004658381253484 | 2 | 319.545937420049 |
| 3 | 0.08533043356255114 | 3 | 473.8574794033544 |
| 4 | 0.2120188355121932 | 4 | 418.86976790550654 |
| 5 | 0.3061268958883217 | 5 | 139.28932091766006 |
| 6 | 0.24986420826773392 | 6 | 66.1096109011661 |
| 7 | 0.084396360063551 | 7 | 30.966000339939256 |
| 8 | 0.008266180032129837 | 8 | 13.742972535708395 |
| 9 | 0.027488657118786147 | 9 | 4.511687908107179 |
| 10 | 0.022357723969299387 | 10 | 1.967816628197473 |
| 11 | 0.007168978343351536 | 11 | 0.8339069908811855 |
| 12 | 0.0011358951261645814 | 12 | 0.3584670399901734 |
| 13 | 0.0029053581940634977 | 13 | 0.15417390831930014 |
| 14 | 0.0019573841005107746 | 14 | 0.06631074550623645 |
| 15 | 0.000468341081580844 | 15 | 0.028524865867473246 |
| 16 | 0.0002137114339111993 | 16 | 0.01227008769633971 |
| 17 | 0.0003069119577110067 | 17 | 0.005278116286219785 |
| 18 | 0.00016073866662605544 | 18 | 0.0022704296340439224 |
| 19 | 1.972859591231157e-05 | 19 | 0.000976647846380209 |
| 20 | 3.1915001661787985e-05 | 20 | 0.0004201144698644053 |
| 21 | 3.0503928730416796e-05 | 21 | 0.00018071633162249212 |
| 22 | 1.1924910273030958e-05 | 22 | 7.773688236734789e-05 |
| 23 | 6.577248836736022e-07 | 23 | 3.34392750698766e-05 |
| 24 | 4.02999940591284e-06 | 24 | 1.4384228771538615e-05 |
| 25 | 2.800042786074979e-06 | 25 | 6.187515672800093e-06 |
| 26 | 7.406320693787607e-07 | 26 | 2.661619939565364e-06 |
| 27 | 3.02775543023223e-07 | 27 | 1.1449216589576383e-06 |
| 28 | 4.508901751938955e-07 | 28 | 4.92499167601005e-07 |
| 29 | 2.3417408605071746e-07 | 29 | 2.118532986312597e-07 |
| 30 | 2.8304108422669455e-08 | 30 | 9.113075333215174e-08 |
| bfgs[1.00025018 3. |] | bfgs[0.99716512 13.63418126] | |

Figure 8: Function output for two dimensional polynomial from two starting points

5.1.6 Three Dimentional Polynomial

| Iterations: | grad | Iterations: | grad |
|---------------------------------------|------------------------|-------------------------------------|------------------------|
| 1 | 65.58403483318178 | 1 | 65.58403483318178 |
| 2 | 51.680716658179655 | 2 | 51.680716658179655 |
| 3 | 15.290466011992974 | 3 | 15.290466011992974 |
| 4 | 12.394032704204294 | 4 | 12.394032704204294 |
| 5 | 9.477798608410072 | 5 | 9.477798608410072 |
| 6 | 5.178661875102632 | 6 | 5.178661875102632 |
| 7 | 2.1773968474436325 | 7 | 2.1773968474436325 |
| 8 | 0.8221514143987172 | 8 | 0.8221514143987172 |
| 9 | 0.454889195063089 | 9 | 0.454889195063089 |
| 10 | 0.2857348166513772 | 10 | 0.2857348166513772 |
| 11 | 0.13584582547710278 | 11 | 0.13584582547710278 |
| 12 | 0.0464531951190135 | 12 | 0.0464531951190135 |
| 13 | 0.023335755179815895 | 13 | 0.023335755179815895 |
| 14 | 0.01747223023161133 | 14 | 0.01747223023161133 |
| 15 | 0.008776985597580767 | 15 | 0.008776985597580767 |
| 16 | 0.002147450337541808 | 16 | 0.002147450337541808 |
| 17 | 0.0015736080969060552 | 17 | 0.0015736080969060552 |
| 18 | 0.0014467020121639686 | 18 | 0.0014467020121639686 |
| 19 | 0.0006259883329915933 | 19 | 0.0006259883329915933 |
| 20 | 7.49960770268807e-05 | 20 | 7.49960770268807e-05 |
| 21 | 0.00016772994998276555 | 21 | 0.00016772994998276555 |
| 22 | 0.00013212992776993662 | 22 | 0.00013212992776993662 |
| 23 | 4.261952044649142e-05 | 23 | 4.261952044649142e-05 |
| 24 | 8.982231749875275e-06 | 24 | 8.982231749875275e-06 |
| 25 | 1.9101024019070267e-05 | 25 | 1.9101024019070267e-05 |
| 26 | 1.156345652089891e-05 | 26 | 1.156345652089891e-05 |
| 27 | 2.318783372309847e-06 | 27 | 2.318783372309847e-06 |
| 28 | 1.7494845845582582e-06 | 28 | 1.7494845845582582e-06 |
| 29 | 2.0258010729966285e-06 | 29 | 2.0258010729966285e-06 |
| 30 | 9.257729385853145e-07 | 30 | 9.257729385853145e-07 |
| 31 | 4.274642526164209e-08 | 31 | 4.274642526164209e-08 |
| bfgs[-1.28237509e-03 -2.09529297e-08] | | bfgs[1.28237509e-03 2.09529297e-08] | |

Figure 9: Function output for three dimensional polynomial from two starting points

5.2 Code

5.2.1 BFGS Algorithm

[illegible]

```

45     #calc yk
46     yk=grad( func , xk1)-grad( func , xk);
47     #calc rho k
48     rhok=1/((yk)@cols(sk))[0]
49
50     #calc Hk+1
51     #eqn 6.17
52     if dim==1:
53         h=((np.eye(dim)-rhok*(sk*np.transpose(yk)))*h*(np
54             .eye(dim)-rhok*(yk*np.transpose(sk)))+rhok*(sk
55             *np.transpose(sk)));
56     else:
57         a1=rhok*mult( cols( sk) , sk)
58         # print(a1)
59         a21=np.eye(dim)-rhok*mult( cols( sk) , yk)
60         a22=np.eye(dim)-rhok*mult( cols( yk) ,( sk))
61         a2=a21@(h@a22)
62         h=a2+a1;
63
64     # iterate count
65     count +=1;
66
67     # update gradient
68     fk=grad( func , xk1 , isfk=1);
69
70     # update position
71     xk=xk1;
72
73     # print step info
74     print( str( count)+'\t\t'+str( np.linalg.norm( fk)))
75
76     # print warning if maximum number of iterations are reached
77     if count>=maxIterations:
78         print("warning max maxIterations reached");
79
80     # return final position
81     return xk
82
83 def grad( func , x , step=0.00000000000000000000000000000001 , isfk=0):
84     """use complex step to calculate function gradient
85
86     Inputs:
87         func - the function to calculate gradient of
88         x - the point to evaluate at
89         step - (optional) the imaginary step size to use
90
91     Output:
92         the complex step approximation of the gradient"""

```

```

93     # initialize complex inputs
94     y=np.zeros(np.shape(x), dtype=complex)
95     for i in range(np.size(y)):
96         y[i]=x[i];
97
98     #         initialize outputs
99     z=np.zeros(np.shape(y))
100
101 # iterate through the input directions and get derivative in each
    direction using complex step
102     for i in range(np.size(z)):
103         # keep indices in correct bounds
104         if i==np.size(x):
105             break;
106         # add complex step to correct input direction
107         y[i] =complex(x[i],step)
108         # calculate derivative in that direction
109         z[i]=func(y)[0].imag/step;
110         # remove the complex step from the variable
111         y[i] =x[i]
112     # convert to column vector if needed
113     if isfk:
114         z=cols(z)
115 # return output
116     return z
117
118 def cols(x):
119     """define a row numpy array as a column matrix. Note this was
        implamented due to native python methods/python libraries
        acting oddly
120
121     Inputs:
122         x – the array to transpose
123     Output:
124         z – the transposed array"""
125     y=np.zeros((np.size(x),1));
126     cont=0;
127     for i in x:
128         y[cont,0]=i;
129         cont+=1;
130     return y;
131 def mult(x,y):
132     """define a row numpy array as a column matrix. Note this was
        implamented due to native python methods/python libraries
        acting oddly
133
134     Inputs:
135         x – the first array to multiply
136         y – the second array to multiply
137     Output:

```

```

138         z – the matrix resulting from the multiplication"""
139     z=np.zeros((np.shape(x)[0],np.shape(x)[0]))
140     for i in range(np.size(x)):
141         for j in range(np.size(x)):
142             z[i,j]=x[i][0]*y[j]
143         # print(z)
144     return z
145
146 #————— test casses —————
147
148 # one dimentional quadratic
149 func=lambda x: np.array(x*x);
150 h0=np.array(np.eye(1))*1
151 x0=10*np.ones(1);
152 print("bfgs"+str(bfgs(func,x0,h0,.000001)))
153 x0=-10*np.ones(1);
154 print("bfgs"+str(bfgs(func,x0,h0,.000001)))
155
156 # two dimensional polynomial
157 func = lambda x: np.array([x[0]*x[0]*x[0]*x[0]+ x[1]*x[1]])
158 h0=np.array(np.eye(2))*1;
159 x0=10*np.ones(2);
160 print("bfgs"+str(bfgs(func,x0,h0,.0000001)))
161 x0=-10*np.ones(2);
162 print("bfgs"+str(bfgs(func,x0,h0,.0000001)))
163
164 #two dimensional polynomial non-zeros minimum/position
165 func = lambda x: np.array([(x[0]-1)*(x[0]-1)*(x[0]-1)*(x[0]-1)+ (x[1]+2)*(
    x[1]+2)+1])
166 h0=np.array(np.eye(2))*1;
167 x0=4*np.ones(2);
168 print("bfgs"+str(bfgs(func,x0,h0,.0000001)))
169 x0=-7*np.ones(2);
170 print("bfgs"+str(bfgs(func,x0,h0,.0000001)))
171
172 # two dimensional rosenbrock function
173 func = lambda x: np.array((((1-x[0])*(1-x[0]))+ 100*((x[1]-(x[0]*x[0]))*(
    x[1]-(x[0]*x[0])))))
174 h0=np.array(np.eye(2))*0.05;
175 x0=0*np.ones(2);
176 print("bfgs"+str(bfgs(func,x0,h0,.0000001)))
177
178 # two dimensional polynomial, multiple minima
179 func = lambda x: np.array([(x[0]-1)*(x[0]-1)*(x[0]-1)*(x[0]-1)+ 45*(x
    [1]-3)*(x[1]-3)+(x[1]-3)*(x[1]-3)*(x[1]-3)*(x[1]-3)-17*(x[1]-3)*(x
    [1]-3)*(x[1]-3)])
180 h0=np.array(np.eye(2))*1;
181 x0=4*np.ones(2);
182 print("bfgs"+str(bfgs(func,x0,h0,.0000001)))
183 x0=-7*np.ones(2);

```



```

184 print("bfgs"+str(bfgs(func,x0,h0,.0000001)))
185
186 #three dimensional polynomial
187
188 func = lambda x: np.array([(x[0]-1)*(x[0]-1)*(x[0]-1)*(x[0]-1)+ (x[1]+2)*(
      x[1]+2)+1+5*(x[2]-3)*(x[2]-3)+(x[2]-3)*(x[2]-3)*(x[2]-3)*(x[2]-3)])
189 h0=np.array(np.eye(3))*1;
190 x0=4*np.ones(3);
191 print("bfgs"+str(bfgs(func,x0,h0,.0000001)))
192 x0=-7*np.ones(3);
193 print("bfgs"+str(bfgs(func,x0,h0,.0000001)))

```

5.2.2 Line Search Algorithm

```
1 from zoom import zoom;
2 import numpy as np;
3
4 def lineSearch(amax, phi, phiprime, c1=0.0001, c2=.9, maxIterations=100000):
5
6     ai=1.0
7     # print(amax)
8     # initialize variables
9     ai2= 0.0;
10    count=0;
11    # print("eval0: "+str(phi(0)))
12    # print("deval0: "+str(hiprime(0)))
13    # print("eval1: "+str(phi(ai)))
14    # print("deval1: "+str(hiprime(ai)))
15    while count<maxIterations:
16
17        # print(str(c1*hiprime(0)));
18        # check sufficient decrease
19        if (phi(ai)>(phi(0)+c1*ai*hiprime(0))) or ((phi(ai)>=phi(
20            ai2)) and (count>0)):
21            # print("zooomingg"+str(count))
22            # call zoom and return value
23            return zoom(ai2, ai, phi, hiprime, c1, c2);
24            #check curavture condition
25            # print(abs(hiprime(ai)))
26            # print(-1*c2*hiprime(0))
27            # break
28            if (abs(hiprime(ai))<=(-1*c2*hiprime(0))):
29                # print("succsssss")
30                #return current value
31                return ai;
32                #if phi increasing
33            if hiprime(ai)>=0:
34                #call zoom and return
35                return zoom(ai, ai2, phi, hiprime, c1, c2);
36            #reset ai2
37            ai2=ai;
38            count +=1;
39
40            # interpolate ai
41            ai*=1.1;
42
43            # if viable point not found print warning and return Null
44            print("Warning: max number of itterations reached"+ai);
45            return None;
```

5.2.3 Zoom algorithm

```
1 import numpy as np;
2
3
4 def zoom(a0,ahi,phi, phiPrime, c1, c2, maxIterations=100000):
5
6     # print(a0)
7     # print(ahi)
8     alo=a0;
9     count=0;
10    aj=0;
11    # print("eval0: "+str(phi(0)))
12    # print("deval0: "+str(phiPrime(0)))
13    # print("eval1: "+str(phi(ahi)))
14    # print("deval1: "+str(phiPrime(ahi)))
15    # while number of itterations < some max number (to prevent
        infinite loops)
16    while count<maxIterations:
17        count+=1;
18        # interpolate aj
19        aj=(ahi+alo)/2
20        # print(ahi)
21        # print(aj)
22        # print(alo)
23        # print("evalj: "+str(phi(aj)))
24        # print("devalj: "+str(phiPrime(aj)))
25        # check sufficient decrease condition
26        if(( phi(aj)>phi(0)+c1*(aj)*phiPrime(0) )or (phi(aj)>= phi
            (alo))):
27            # if not viable move upper bound
28            ahi=aj;
29
30        else:
31            # evaluate flatness condition
32            if abs(phiPrime(aj))<=-c2*phiPrime(0):
33                # if flat enough return aj
34                return aj;
35            if phiPrime(aj)*(ahi-alo)>=0:
36                # enforce phi(ahi)>phi(alo)
37                ahi=alo;
38                # print(ahi)
39            # if sufficient decrease satisfied but not
                flatness, update alo
40            alo=aj;
41            # print(alo)
42            # if count>10:
43            #     return
44    # if viable point not found print warning and return Null
45    print("Warning: max number of itterations reached -z"+str(aj));
```

```
return a0;
```