Comparative Study of Unconstrained Mechanical Optimization Methods Based on Two-variable Rosenbrock Function

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Abstract. The unconstrained optimization method (UOM) plays an important role in the field of physics, mathematics, statistics, etc. Rosenbrock function is a 4-degree function with a curved canyon. It is most suitable for testing UOM. However, the test hasn't done. We have written 14 UOM computer programs, 12 of which contain our new algorithm. From the optimal result, the 2-order approximation direction is the best, followed by the conjugate direction, followed by the negative gradient direction. For quadratic fitting function method, linear fitting gradient method and unbounded polyhedron deformation method, a new algorithm for moving points was proposed. When the new point is better than all of the other points, the other points should close up to it. And when the new point is worse than all of the other points, it should close up to the best point or center point. The improvement of moving points makes these optimization directions be effective for complex objective functions.

Introduction

Any algorithm for finding global extreme point or optimal parameters can be called optimization methods. It belongs to the field of applied mathematics and computational mathematics. The optimization problem exists in other fields too, such as classical continuum physics, theoretical, mathematical & computational physics, particle and nuclear physics, physical chemistry, pure mathematics, mathematical physics, fluid dynamics, actuarial science, applied information economics, astrostatistics, biostatistics, business statistics, mechanical, etc. The research on optimization method not only needs the algorithm innovation, but also needs the computer program verification. Instead of relying on computational software, we write computer programs and validate algorithms in time. Among the research of related projects, we haven't found any reference on UOM comparative study.

According to the basic idea of the algorithm, there are mainly 14 kinds of unconstrained optimization methods, 1 negative gradient direction method; 2 zigzag line negative gradient direction method based on the blind pathfinding idea; 3 higher-degree multidimensional two-order approximate direction method and the fixed point method(Newton method); 4 quasi-uniform coordinate transformation method (the coordinate transformation method); 5 geometric constructing conjugate direction method; 6 conjugate direction group method based on gradient(conjugate gradient method); 7 conjugate direction group method based on the linear independent vector group (conjugate direction method); 8 adjacent conjugate direction method based on auxiliary direction and the three-search method; 9 multidimensional quadratic fitting function method and the linear fitting gradient method; 10 alternating coordinate direction method and its improved algorithm; 11 basic and improved algorithm of classic Powell method; 12 constructing conjugate-direction method without partial derivative; 13 unbounded polyhedron deformation method (simplex substitution method); 14 adaptive coordinate descent method, etc.
Rosenbrock function is a 4-degree non-convex function, introduced by Howard H. Rosenbrock in 1960\(^1\), which is known as Rosenbrock Canyon or Banana function. It can test algorithms.

In this paper, a computer program is compiled to test all optimization methods with the same objective function. On the basis of classical optimization methods, we have made the following improvements and innovations:

1. One-dimensional blindwalking optimization method\(^2\).
2. The obtaining conjugate directions method based on geometric relations\(^3\).
3. The obtaining conjugate direction method based on auxiliary direction\(^4\).
4. Three-search method to obtain conjugate direction based on negative gradient direction\(^5\).
5. Multidimensional quadratic fitting function method\(^6\).
6. Linear fitting gradient method\(^6\).
7. Constructing conjugate direction method. Powell method is the most classical optimization method. Three improvements are based on it\(^7\).
8. Improved unbounded polyhedron deformation method (simplex and complex method)\(^8\).
9. Second-order approximate direction method (Newton direction method)\(^2\).
10. The improved second-order approximate fixed-point method based on the idea of blind path finding\(^9\).
11. An improved negative gradient direction method based on the idea of blind path finding\(^10\).
12. The algorithm of moving new points (for the first time in this paper).

**Rosenbrock Function**

Two-dimensional Rosenbrock function is following.

\[
\begin{align*}
\min f(x) &= 100(x_2 - x_1^2)^2 + (1 - x_1)^2 \\
\nabla f(x) &= \begin{bmatrix} 400x_1^3 - 400x_1x_2 + 2x_1 - 2 \\
200x_2 - 200x_1^2 \end{bmatrix} \\
H_{f(x)} &= \begin{bmatrix} 1200x_1^2 - 400x_2 + 2 & -400x_1 \\
-400x_1 & 200 \end{bmatrix}
\end{align*}
\]

(1)

The global minimum point is \([-1, 1]^T\). It is difficult to find the descent direction pointing to the extremum point in Rosenbrock Canyon. It can only be approached by small step ceaselessly and circuitously. When a certain section bottom of Canyon is meted, even if a better descent direction is found, it can only go forward by micro step. If the termination condition value is too large, or the scope of the search direction is limited, it is difficult to approach the extremum point.

**The Adaptive Coordinate Descent Method**

The optimal point whose objective function value is less than \(10^{-10}\) can be found after 325 times of objective function calculation\(^11\). This process is not reproduced by writing computer program.

**The Negative Gradient Direction Method and Three Newton Methods**

The optimal point \(x^{(k+1)}\) at the direction \(s^{(k)}\) is obtained by 1D optimization method\(^2\). The sawtooth phenomenon occurs in the algorithm. If the current point is closer to the extremum point, the worse the optimization effect is.

The two-order approximation of the objective function at the current point is regarded as the fitting function. The direction points to the extremum point (Eq. 2). If the objective function power is less
than 1, the fixed-point method (Eq. 3) is not suitable. The inverse matrix can be insted by its adjugate matrix.

\[ s^{(k)} = -H^{-1} f'(x^{(k)}) \]  \hspace{2cm} (2)

\[ x^{(k+1)} = x^{(k)} + \left[-H^{-1} f'(x^{(k)}) \right] \]  \hspace{2cm} (3)

The initial point is \([-0.4 \ 0.6]^T\). The termination condition value is \(1.0 \times 10^{-6}\). The initial step size of one-dimensional blind pathfinding optimization is 0.1. For the negative gradient direction method, the process is the solid line 1 in Fig.1. The computation of blind pathfinding negative gradient direction method\[^{[10]}\] will be smaller. For higher-degree multi-dimensional 2-order approximate fixed-point method based on the blind pathfinding idea\[^{[9]}\], the process is the dash-dot line 2 in Fig.1. For the classical fixed-point method which is also called as Newton iteration method, the process is the dashed line 3 in Fig.1. For higher-degree multidimensional two-order approximate direction method, the process is the dotted line 4 in Fig.1.

![Figure 1. The negative gradient direction method and three Newton methods.](image)

**The Quasi-uniform Coordinate Transformation Method**

In order to avoid the zigzag phenomenon, the eccentricity of the objective function is online can be reduced by coordinate transformation. Then a better optimal result can be obtained along the negative gradient direction. For DFP (Davidon, Fletcher, Powell) algorithm, and BFGS (Broyden, Fletcher, Goldfarb, Shanno) algorithm formula, the similar search process is obtained, which is shown in fig.2.

![Figure 2. The quasi-uniform coordinate transformation method.](image)
The Gradient Related Conjugate Direction Methods

For a general objective function, if it is replaced by its second-order approximation at a certain point, then it is the formula (4).

\[ f(x) = \frac{1}{2} x^T G x + b^T x + c \]  

(4)

Where, a real symmetric positive definite matrix \( G \) is the two-order partial derivative matrix at the point \( x \). According to the optimization characteristics and the condition of new direction pointing to the extremum point, after the optimizing along \( s^{(0)} \), the direction \( s^{(i)} \) should satisfies Eq.(5).

\[ (s^{(0)})^T G (s^{(i)}) = 0 \]  

(5)

After the optimal point \( x^{(k+1)} \) is obtained by 1-dimensional optimization along \( s^{(k)} \) starting from \( x^{(k)} \), the conjugate direction \( s^{(k+1)} \) of \( s^{(k)} \) can be obtained from the gradients \( g^{(k)} \) and \( g^{(k+1)} \).

If \( s^{(k+1)} \) is in the plane determined by \( s^{(k)} \), \( g^{(k+1)} \), it can be obtained by undetermined coefficient method (UCM). For 2-dimensional Rosenbrock function, an optimization round is carried out along the negative gradient direction and its conjugate direction in turn.

The conjugate direction group method is based on the linear independent vector group (CDM). Figure 3 is the optimization process. The reference [3] and UCM coincides with dashed line 1 and 2. The optimization efficiency of CDM is poor. If the orthogonal vector group changes at each round, the process is shown as solid line 3. If the orthogonal vector group doesn't change, the process is shown as solid line 4.

![Figure 3. Three conjugate direction methods.](image)

Two Contiguous Conjugate-direction Methods Based on Auxiliary Direction

For the optimization problem with the objective function (4), the \( x^{(k)} \) and \( x^{(k+1)} \) are optimal points (the numerical approximate point of the extreme point on this direction) along the direction \( s^{(j)} \) by 1-dimensional optimization starting from different points. The direction \( s^{(k)} = x^{(k+1)} - x^{(k)} \) and \( s^{(j)} \) are conjugative relating to \( G \). After an optimal point is obtained along a direction, another optimal point is obtained along the same direction starting from an auxiliary point outside the above optimization route. The link of two optimal points is regarded as the next optimization direction. The auxiliary point can be gotten at the negative gradient direction of the first optimal point. Along the negative gradient direction, three-search method is obtained[5].

In figure 4, the solid line is the optimization process of the first method, and the dashed line is the optimization process of three-search method.
The Multidimensional Quadratic Fitting Function and Linear Fitting Gradient Method

In accordance with the 1-dimensional quadratic fitting function method, according to the objective function value of some points, the quadratic fitting function of the objective function is constructed by the undetermined coefficient method. The extremum point of the fitting function is regarded as the new point. The worst point or the most edge point is removed. Then the new fitting function can be constructed. So an iterative is completed\(^6\). In order to avoid multimodal influence, several nearest points construct the fitting function.

The optimization process is shown as dotted line in Fig. 5. When the parameter reaches the software limit, the error is larger, but the optimal point is still good. It shows that the algorithm has good robustness.

The Alternate Coordinate Direction Method and the Improved Powell Method

The improved and basic algorithm of classic Powell method is well-known. Reference \(^7\) has improved it. In figure 6, the dashed line 1 in Fig.6 shows the process of the alternate coordinate direction method, and the solid line 2 in Fig. 6 shows the improved Powell method. For the unbounded polyhedron deformation method, the vertex number is \(N+1\). If the new point is by mapping coefficient, the optimization is failure.
Conclusion

1) the quasi-uniform coordinate transformation method and the conjugate direction are the best.

2) all classic optimization methods with deterministic direction are proposed based on the unimodal assumption in which the objective function is regarded as quadratic function. The change of initial point will not affect the optimization result.

3) since the computer programs have written, the theoretical system can be developed.

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Figure 6. The alternate coordinate direction method and Powell method.
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