SEMARAK ILMU PUBLISHING
202103268166(003316878-P)

Journal of Advanced Research in Applied Mechanics

Journal homepage:
https://semarakilmu.com.my/journals/index.php/appl_mech/index
ISSN: 2289-7895

The Application of Conjugate Gradient Methods to Optimize 3D Printed Parameters

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ARTICLE INFO

Article history:
Received 4 April 2024
Received in revised form 29 May 2024
Accepted 12 June 2024
Available online 30 June 2024

Keywords:
Conjugate gradients method; optimization; exact line search; regression

ABSTRACT

The Conjugate Gradient (CG) method stands as an evolved computational technique designed for addressing unconstrained optimization problems. Its attractiveness stems from its simplicity, making it straightforward to implement, and its proven track record in effectively addressing real-world applications. Despite the recent surge in interest in this field, certain newer versions of the CG algorithm have failed to outperform the efficiency of their predecessors. Consequently, this paper introduces a fresh CG variant that upholds essential properties of the original CG methods, including sufficient descent and global convergence. In this paper, three types of new CG coefficients are presented with applications in optimizing data. Numerical experiments show that the proposed methods have succeeded in solving problems under exact line search conditions.

1. Introduction

Mathematical optimization is a field of study focused on finding the best possible solution from a set of feasible solutions to a particular problem. Optimization methods play a crucial role in various disciplines, including engineering, economics, finance, machine learning, and operations research. These methods are employed to minimize or maximize an objective function, subject to a set of constraints, and they are instrumental in addressing complex decision-making problems across diverse domains. The unconstrained optimization function is stated as follows:

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https://doi.org/10.37934/aram.120.1.136141

$$\min_{x \in R^n} f(x)$$

where $f: \mathbb{R}^n \to \mathbb{R}$ is a continuously differentiable function and $x = [x_1, x_2, ..., x_n]^T$ is the vector of decision variables. The goal is to find the values of x that minimize the objective function $f(x)$. This equation represents a broad class of optimization problems, and the specific form of $f(x)$ and any additional constraints would depend on the context particular optimization problem.

The conjugate gradient method is an iterative optimization technique that refines the current approximation x_k to the solution through a series of updates. At each iteration, the algorithm employs the gradient g_k, a line search stepsize α_k, and a search direction d_k, along with a conjugate gradient coefficient β_k:

$$x_{k+1} = x_k + \alpha_k d_k$$

This update is based on the current approximation and the chosen search direction. In the context of the conjugate gradient method, the search direction is a pivotal element in guiding the iterative updates toward an optimal solution. The selection of this direction involves a strategic consideration of both the gradient information and the conjugate gradient coefficient, ensuring an effective exploration of the optimization landscape:

$$d_k = \begin{cases} -g_k, & \text{for} \quad k = 0 \\ -g_k + \beta_k d_{k-1}, & \text{for} \quad k \geq 1 \end{cases},$$

The exact line search is employed according to the following formula:

$$\alpha_k = \arg \min_{\alpha > 0} f(x_k + \alpha d_k)$$

In this equation, α_k represents the optimal step size, x_k is the current approximation, d_k is the search direction, and f is the objective function. This approach ensures that the step size is precisely chosen to minimize the objective function along the search direction. The integration of this exact line search enhances the precision and efficiency of our novel conjugate gradient method.

Subsequently, the gradient g_{k+1} is computed for the updated point x_{k+1} using the gradient of the objective function $\nabla f(x_{k+1})$:

$$g_{k+1} = \nabla f(x_{k+1})$$

These iterative steps play a crucial role in navigating the search space and converging towards an optimal solution. The choice of the conjugate gradient coefficient β_k influences the efficiency of the algorithm. Various methods, such as Fletcher-Reeves (FR) [1], Hestenes-Steifel (HS) [2], and NPRP [3], employ specific strategies for determining β_k to enhance convergence performance.

$$\beta_k^{FR} = \frac{g_k^T g_k}{\|g_{k-1}\|^2},\ \beta_k^{HS} = \frac{g_k^T (g_k - g_{k-1})}{d_{k-1}^T (g_k - g_{k-1})},\ \beta_k^{NPRP} = \frac{\|g_k\|^2 - \frac{\|g_k\|}{\|g_{k-1}\|}\left|g_k^T g_{k-1}\right|}{\|g_{k-1}\|^2},$$

In this study, we investigated well-established conjugate gradient methods, including Fletcher-Reeves (FR) [1], Wei *et al.,* (HS) [2], and NPRP [13]. For further insights and exploration of innovative methods, readers are encouraged to refer to [4-11].

Nowadays, the CG method finds extensive applications across diverse fields, providing efficient solutions to a variety of real-life problems. In the domain of medical imaging, CG is employed for image reconstruction from incomplete or noisy data. Linear systems of equations, a common outcome of image reconstruction processes, can be effectively solved using the CG method, leading to clearer and more accurate medical images [19].

In machine learning, the CG method is often applied to optimize quadratic objective functions or to solve linear systems that arise during the training of certain models [20]. The CG method stands as a versatile and powerful tool with applications spanning machine learning, medical imaging, finite element analysis, quantum chemistry, computer graphics, and numerous other disciplines [14-18]. Its iterative nature, efficiency in solving large-scale problems, and adaptability make it a cornerstone in the toolkit of scientists, engineers, and researchers addressing complex real-life challenges. Hence, in this paper the CG method is applied in 3D printing process to determine the best solution for its parameters.

This paper is organized as follows: In Section 2, we introduce a conjugate gradient method. Section 3 data analysis of compared methods. The implementation details are discussed in Section 4, followed by concluding remarks in Section 5.

2. New CG method

These modifications are proposed based on the WYL method [3], where its coefficient is defined as

$$\beta_k^{WYL} = \frac{g_k^T\left(g_k - \frac{\|g_k\|}{\|g_{k-1}\|} g_{k-1}\right)}{g_{k-1}^T g_{k-1}}.$$

This new β_k known as NHMR (Nurul Hajar, Mustafa and Rivaie) and the numerator of β_k^{NHMR} is retained from β_k^{WYL} but their new denominators are designed as follows:

$$\beta_k^{NHMR} = \frac{g_k^T\left(g_k - \frac{\|g_k\|}{\|g_{k-1}\|} g_{k-1}\right)}{g_{k-1}^T (g_k - d_{k-1})}.$$

The following algorithm will implement the β_k^{NHMR} method.

Step 1: Initialization.
Given x_0, set $k = 0$.
Step 2: Compute the CG coefficient.

Step 3: Compute the search direction.
Step 4: Determine the stepsize.
Step 5: Update the new point.
$x_{k+1} = x_k + \alpha_k d_k$.
Step 6: Convergence test and stopping criteria.
If $f(x_{k+1}) < f(x_k)$ and $\|g_k\| \le \varepsilon$ then stop
Otherwise go to Step 1 with $k = k+1$.

In order to support of our method, the convergence properties of β_k^{NHMR} will be studied. An algorithm must satisfy the sufficient descent condition and the global convergence properties. In this case, the global convergence properties are already established in the previous paper [11].

The relation between two or more variables can be found using regression, and this relationship can then be used for optimization or estimation. The multiple linear regression model is defined by the following algorithm,

$$y = a + b_1x_1 + b_2x_2 + b_3x_3$$

where y is the dependent variable, x_1, x_2 and x_3 represent the three different independent variables, a is the intercept value and b_1, b_2 and b_3 are three regression coefficients.

3. Data analysis

Table 1 below shows the actual data obtained from Lim *et al.,* [12]. This study aims to obtain the optimum tensile strength and printing time using the conjugate gradient method.

Table 1
Tensile strength and printing time of each experiment

Experiment no	Nozzle Diameter (mm)	Layer Thickness (mm)	Printing velocity (mm/s)	Tensile Strength	Printing time (minutes)
1	0.6	0.3	30	65.786	65.47
2	0.6	0.39	40	57.417	40.53
3	0.6	0.48	50	57.811	31.47
4	0.8	0.3	40	56.501	41.17
5	0.8	0.39	50	50.857	27.48
6	0.8	0.48	30	65.636	35.05
7	1.0	0.3	50	56.518	29.47
8	1.0	0.39	30	60.597	31.98
9	1.0	0.48	40	64.347	23.45

The function utilized in this experiment to resolve the above problem is regarded as a linear case and is resolved using the FR, WYL, and NHMR methods. In addition, the problem is also solved using the sum squares method for comparison. Then, the results are analyzed by finding the relative error of the CG and sum squares methods using the formula shown below,

$$Relative\ error = \left|\frac{exact\ value - approximate\ value}{exact\ value}\right|$$

The "exact value" and "approximate value" refer to the optimized results obtained from the optimization methods. Calculation of relative error is important to determine the best method to optimize tensile strength and printing time for 3D printer parameters.

4. Results and Discussion

The data is implemented in FR, WYL, NHMR and sum squares methods. All calculations involve the use of Microsoft Excel and Matlab 12 subroutine programs. The results of the multiple linear regression model are shown below in Table 2.

Table 2
The multiple linear regression model

Method	Result	
	Tensile strength	Printing time
FR	70.5946+0.3733x_1+16.6463x_2-0.4472x_3	133.9867-43.8083x_1-85.4445x_2-0.7347x_3
WYL	70.5946+0.3734x_1+16.6463x_2-0.4472x_3	133.9867-43.8084x_1-85.4446x_2-0.7347x_3
NHMR	70.5944+0.3734x_1+16.6467x_2-0.4472x_3	133.9867-43.8083x_1-85.4444x_2-0.7347x_3
Sum squares	77.3853-0.4472x_3	133.9867-43.8083x_1 -85.4444x_2-0.7347x_3

The relative error for each data is defined by comparing the actual data and the approximation data (see Table 3). The model that gives the smallest sum of relative error is considered the best approximation function.

Table 3
The relative error

Method	Relative error	
	Tensile strength	Printing time
FR	0.0515235764	0.0831316633
WYL	0.0515235764	0.0831325798
NHMR	0.0515208403	0.0831312051
Sum squares	0.0276152980	0.0831312051

Based on the above results, we can see the NHMR and sum squares method is comparable which gives the smallest relative error value in terms of printing time compared to FR and WYL methods. But for tensile strength, the sum squares method is superior to NHMR, FR, and WYL methods. Thus, the NHMR and sum squares method are the best methods to optimize tensile strength and printing time for 3D printer parameters.

5. Conclusions

The data is applied to the CG methods which are FR, WYL, NHMR method and sum squares methods. Then, it is found that all methods can solve the problem for a linear case. In conclusion, the CG method presents a valuable approach for optimizing tensile strength in materials. By formulating the optimization problem to maximize tensile strength while considering relevant constraints, the CG method efficiently navigates the solution space, iteratively updating design parameters. In conclusion, the optimization of parameters will give the best result for 3D printers in future.

Acknowledgement
We would like to thank Universiti Teknikal Malaysia Melaka (UTeM) and the Forecasting and Engineering Technology Analysis (FETA) research group.

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