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PERFORMANCE ASSESSMENT OF STEEPEST DESCENT METHOD CONSIDERING GRADIENT BASED LINE SEARCH CONDITIONS IN GEOMETRY FITTING OF 2D MEASURED PROFILES

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ABSTRACT

This paper focuses on exploring effect of the step length, used in the line search, computation techniques on the performance of steepest descent (SD) method in the geometry fitting of the 2D measured profiles. To this end, the three step length computation techniques or line search conditions accommodating Weak Wolfe (WWC), Strong Wolfe (SWC) and the exact minimizer finder have been implemented during the fitting process. To test the line search conditions performances, the 2D primitive geometry test set consisting of five different geometries such as circle, square, triangle, ellipse and rectangle have been employed. The 2D profiles of those geometries have been extracted using coordinate measuring machine (CMM) with high precision. For performance assessments, the total number of function evaluations when the SD method-line search condition combination satisfies the required converge tolerance have been used. By means of those data, the performance profiles have been created to conduct reliable and efficient assessments on the line search conditions. The results have shown that the step length computation technique plays a crucial role for the SD method performance. Based on the performance profiles, it has been determined that the fastest line search condition is the WWC. Besides that, it has been revealed that the optimum technique is the exact minimizer finder for the geometry fitting process in the study.

Keywords: *Steepest descent method, Performance profiles, Line search, Geometry fitting, Optimization*

ÖLÇÜLEN 2B PROFİLLERE GEOMETRİ UYDURULMASINDA GRADYAN TEMELLİ DOĞRU BOYUNCA ARAMA ŞARTLARI DİKKATE ALINARAK EN DİK İNİŞ YÖNTEMİNİN PERFORMANS DEĞERLENDİRMESİ

ÖZET

Bu çalışmada ölçülen 2B profillere geometri uydurulmasında doğru boyunca aramada kullanılan adım uzunluğu hesaplama yöntemlerinin en dik iniş yönteminin performansına etkisi incelenmiştir. Bu amaçla, zayıf Wolfe, güçlü Wolfe ve tam olarak minimize eden adım uzunluğunu bulan olmak üzere üç adım uzunluğu hesaplama yöntemi ya da doğru boyunca arama şartları geometri uydurma sürecinde kullanılmıştır. Doğru boyunca arama şartlarının performansını test etmek amacıyla, daire, kare, üçgen, elips ve dikdörtgen geometrilerini içeren bir 2B temel geometri seti kullanılmıştır. Bu geometrilerin profilleri yüksek hassasiyet ile koordinat ölçme cihazı ile elde edilmiştir. Performans değerlendirmeleri için ilgili en dik iniş yöntemi-doğru boyunca arama şartı kombinasyonu istenen tolerans değerini sağladığında ortaya çıkan toplam fonksiyon kullanım sayısından yararlanılmıştır. Doğru boyunca arama şartlarının güvenilir ve verimli bir şekilde performans değerlendirilmesini yapmak için bu veriler vasıtasıyla performans profilleri oluşturulmuştur. Sonuçlar adım uzunluğu hesaplama tekniklerinin en dik iniş yöntemi performansında önemli bir rol oynadığını göstermektedir. Performans profillerine dayanarak, en hızlı doğru boyunca arama şartı zayıf Wolfe olarak saptanmıştır. Bunun yanı sıra, çalışmada geometri uydurma süreci için optimum yöntemin tam olarak minimize eden adım uzunluğunu bulan yöntem olduğu ortaya çıkarılmıştır.

Anahtar kelimeler: *En dik iniş yöntemi, Performans profilleri, Doğru boyunca arama, Geometri uydurma, Optimizasyon*

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1. Introduction

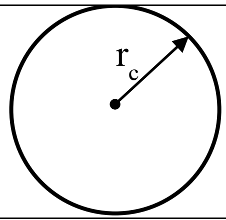
The steepest descent [1] is a basic optimization method that has been frequently used in many areas such as engineering, science, business etc. It has been implemented in many studies along with the various line search conditions. For instance, Bento et al. [2] provided an inexact SD method including Armijo's rule for multicriteria optimization. A general application of the SD method on the mechanical systems was completed by Haug et al. [3]. Liu and Reynolds [4] derived a multi-objective SD method. They performed applications for optimal well control and it was shown that the proposed method is quite efficient. In [5], the circularity value of a mechanical part was found using a novel SD algorithm. The data measured with CMM was used for the input to the proposed algorithm. Much more applications of the SD method can be found in the literature such those in [6-10]. On the other hand, the SD method performance or any other optimization algorithm performance may differ from problem-to-problem. Thus, researchers have been performing benchmarking studies to make assessments on the particular problem set. Those studies can be seen in many areas. Khan and Lobiyal [11], for instance, carried out performance analysis on the three different algorithms (i.e., Newton-Raphson, conjugate gradient and SD) in application of backbone based wireless networks. Different optimization algorithms were compared to each other for the finite element based structural topology optimization by Rojas-Labanda and Stolpe [12]. The other significant efforts on the benchmarking of optimization algorithms can be found in [13-16].

From the point of view given above, this paper focuses on the performance evaluation of the SD method considering line search conditions in the nonlinear least squares geometry fitting of 2D measured profiles. The primitive geometry set containing circle, square, triangle, ellipse and rectangle have manufactured using 3D printer with PLA material. And then, 2D profiles of these geometries are extracted using the CMM with high precision. All the scanned profiles are subjected to nonlinear least squares fitting process through the SD method along with three different step length computation techniques (i.e., WWC, SWC and exact minimizer finder). During the fitting process, the total number of function evaluations, when the algorithm converges, are recorded and they are used for performance evaluations. Henceforth, the paper is organized as follows: Section 2 provides the primitive test geometry set including their mathematical models and their parameters. The nonlinear least squares fitting procedure is given in Section 3. In Section 4 a brief mathematical background on the step length computation techniques is included. Section 5 shows the experimental setup. Section 6 reports the results with discussions. Finally, the conclusions are made in Section 7.

2. Test Geometries

The five 2D primitive geometries (i.e., circle, square, triangle, ellipse and rectangle) are chosen for the nonlinear least squares geometry fitting process. They are listed in Table 1. that accommodates corresponding mathematical models [17] and parameter vectors.

Table 1. Test geometries and their mathematical models

Geometry number	Mathematical model	Parameter vector	Geometry
1	$x = r_c \cos(u) + x_c$ $y = r_c \sin(u) + y_c$	$p = [r_c\ x_c\ y_c\ u]$	

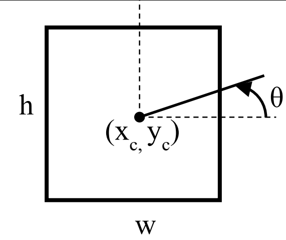
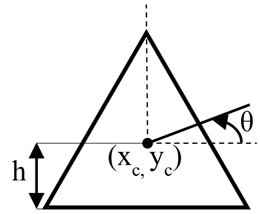
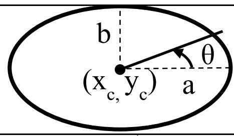
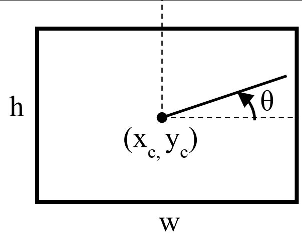
2	$x_u = \frac{w}{2}(\lvert\cos(u)\rvert\cos(u) + \lvert\sin(u)\rvert\sin(u))$ $y_u = \frac{h}{2}(\lvert\cos(u)\rvert\cos(u) - \lvert\sin(u)\rvert\sin(u))$ $x = x_u\cos(\theta) - y_u\sin(\theta) + x_c$ $y = x_u\sin(\theta) + y_u\cos(\theta) + y_c$	$p = [w\ h\ x_c\ y_c\ \theta\ u]$	
3	$r = \frac{h}{\cos\left(\frac{2}{n_s}arcsin\left(sin\left(\frac{n_s}{2}u\right)\right)\right)}$ $x_u = r\cos(u)$ $y_u = r\sin(u)$ $x = x_u\cos(\theta) - y_u\sin(\theta) + x_c$ $y = x_u\sin(\theta) + y_u\cos(\theta) + y_c$	$p = [h\ x_c\ y_c\ \theta\ u]$	
4	$x_u = a\cos(u)$ $y_u = b\sin(u)$ $x = x_u\cos(\theta) - y_u\sin(\theta) + x_c$ $y = x_u\sin(\theta) + y_u\cos(\theta) + y_c$	$p = [a\ b\ x_c\ y_c\ \theta\ u]$	
5	$x_u = \frac{w}{2}(\lvert\cos(u)\rvert\cos(u) + \lvert\sin(u)\rvert\sin(u))$ $y_u = \frac{h}{2}(\lvert\cos(u)\rvert\cos(u) - \lvert\sin(u)\rvert\sin(u))$ $x = x_u\cos(\theta) - y_u\sin(\theta) + x_c$ $y = x_u\sin(\theta) + y_u\cos(\theta) + y_c$	$p = [w\ h\ x_c\ y_c\ \theta\ u]$	

Table 1- Continue

3. Nonlinear Least Squares Geometry Fitting Procedure

As well-known, in least squares fitting method, the sum of squared error between the measured and modeled data is minimized to find the best parameters that belong to function or the mathematical model. The measured data dimensions may vary by depending on the application or problem. In this study we deal with 2D profiles acquired via the CMM. Therefore, the measured data is described to be (x_i, y_i) that consist of n data points. The sum of squared errors [18] is:

$$\epsilon^2(p) = \sum_{i=1}^{n}\left[x_i - x_i^{model}(p)\right]^2 + \sum_{i=1}^{n}\left[y_i - y_i^{model}(p)\right]^2 \tag{1}$$

where the $x_i^{model}(p)$ and $y_i^{model}(p)$, which depend upon parameter vector (i.e., p), are the data computed using the mathematical model of the geometry. To minimize those errors, there are many methods in the literature. In this study we use a general one called steepest descent. This method progresses with gradient information of the objective function. In other words, the method updates the model parameters along with the opposite direction of the objective function gradient. This can be mathematically defined as:

$$h = J^T D \tag{2}$$

where J is the Jacobian matrix of the objective function, which is calculated using finite difference approach, $D = \begin{bmatrix} D_x \\ D_y \end{bmatrix}$, $D_x = x_i - x_i^{model}(p)$ and $D_y = y_i - y_i^{model}(p)$. The next parameter vector is then:

$$p_{i+1} = p_i + \alpha h \tag{3}$$

In this equation $\alpha > 0$ is the step length, which is computed by the line search conditions or other algorithms. This line search process keeps searching the best model parameters until the inequality is satisfied as follows:

$$maximum|J^T D| \leq \partial \tag{4}$$

where the $\partial = 10^{-3}$ is the converge tolerance used in this work.

4. Step Length Computation Techniques

The step length computation is actually a one-dimensional minimization problem as described in Equation 5. For a remarkable progress along the given direction (e.g., opposite direction of the objective function gradient in this study), the one of the exact minimizers of the $F(\alpha)$ is required. However, in general, it brings high computational cost. Therefore, the approximation methods, called line search conditions, are employed to overcome this problem in the literature. In this study, to compute step length during the fitting process, the two well-known line search conditions (i.e., WC and SWC) are used. Besides, an algorithm is proposed to find one of the exact minimizers because it is only option for the fitting of some geometries.

$$minimize_{\alpha>0} F(\alpha) \equiv \epsilon(p_i + \alpha h) \tag{5}$$

4.1. Wolfe conditions

The Wolfe conditions are basically a combination of sufficient decrease and curvature conditions [19]. Those conditions are respectively:

$$\epsilon(p_i + \alpha h) \leq \epsilon(p_i) + c_1 \alpha G^T h \tag{6}$$

$$G(p_i + \alpha h)^T h \geq c_2 G(p_i)^T h \tag{7}$$

where $G = -J^T D$ is the gradient of the objective function, c_1 and c_2 are the scalars satisfying $0 < c_1 < c_2 < 1$. $c_1 = 10^{-4}$ and $c_2 = 10^{-1}$ are used in the fitting process. The condition in this form is referred to as weak Wolfe. To obtain the strong Wolfe condition, we only need to modify the curvature condition as follows:

$$|G(p_i + \alpha h)^T h| \leq c_2 |G(p_i)^T h| \tag{8}$$

These two similar conditions provide step length α that is close to one of the exact minimizers of the $F(\alpha)$. In general, Wolfe conditions work very well. However, in some cases, it is inevitable to use exact local minimizer for the minimization algorithm success.

4.2. Exact minimizer finder

To find the one of the exact minimizers of the $F(\alpha)$, an algorithm is proposed. It proceeds as follows:

- apply sufficient decrease condition, Equation 6, for finding initial α.
- check the slope of the $F(\alpha)$ if it is negative. In case of positive slope, reduce the α until the slope is negative and set the α as α_{low}.
- increase α_{low} to where the slope of the $F(\alpha)$ is being positive and set it as α_{up}.
- employ Golden section method between α_{low} and α_{up} to find local minimizer of the $F(\alpha)$.

5. Experimental Setup

The test geometries were built with 3D printer using PLA material. The 2D profiles of the geometries were collected via Renishaw Cyclone 2 coordinate measuring machine, as seen in Figure 1.

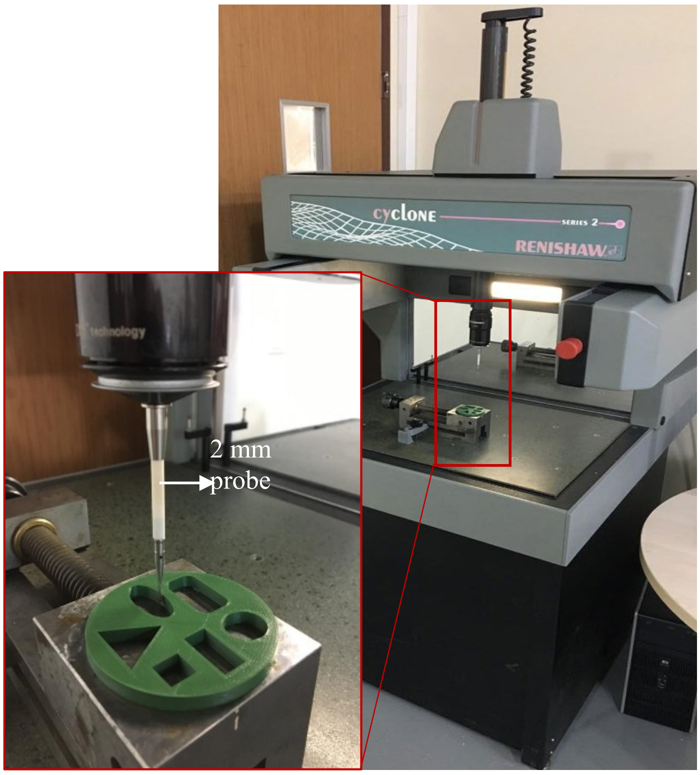


Figure 1. Scanning process with CMM

In the 2D scanning process, 2 mm touch probe was used and the scanning speed was set to 100 mm/min. All the collected data for CMM were processed with MATLAB.

6. Results and Discussion

All the scanned geometries have been subjected to fitting process with all the SD method-line search conditions. As an example, a circle fitting is compared with actual and measured geometries in Figure 2. This example belongs to the fitting process completed with exact minimizer algorithm. In addition to that, the circle fitting parameters (i.e., $p = [r_c\ x_c\ y_c]$), the sum of squared error, the norm of the gradient of objective function and step length are kept track for each iteration, as seen in Figure 3.

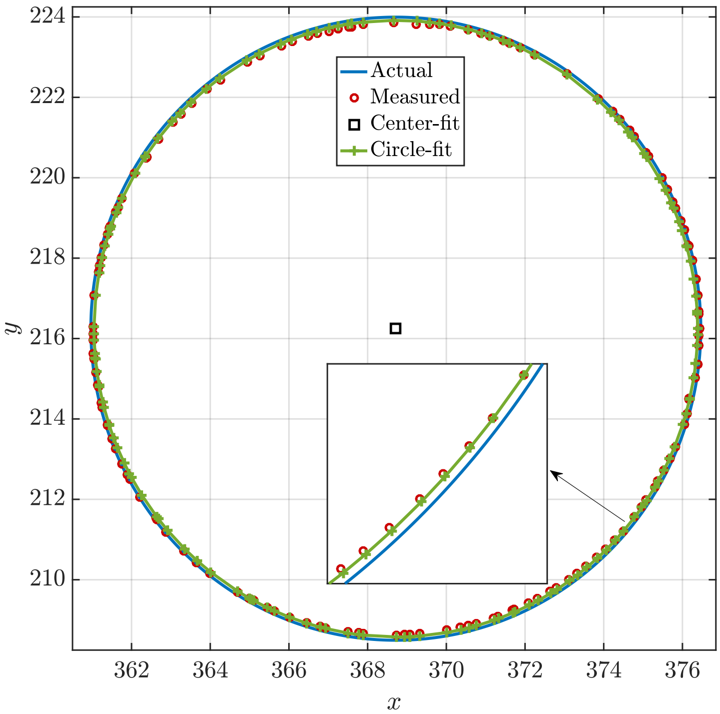


Figure 2. Comparison of actual, measured and fitted circle geometries

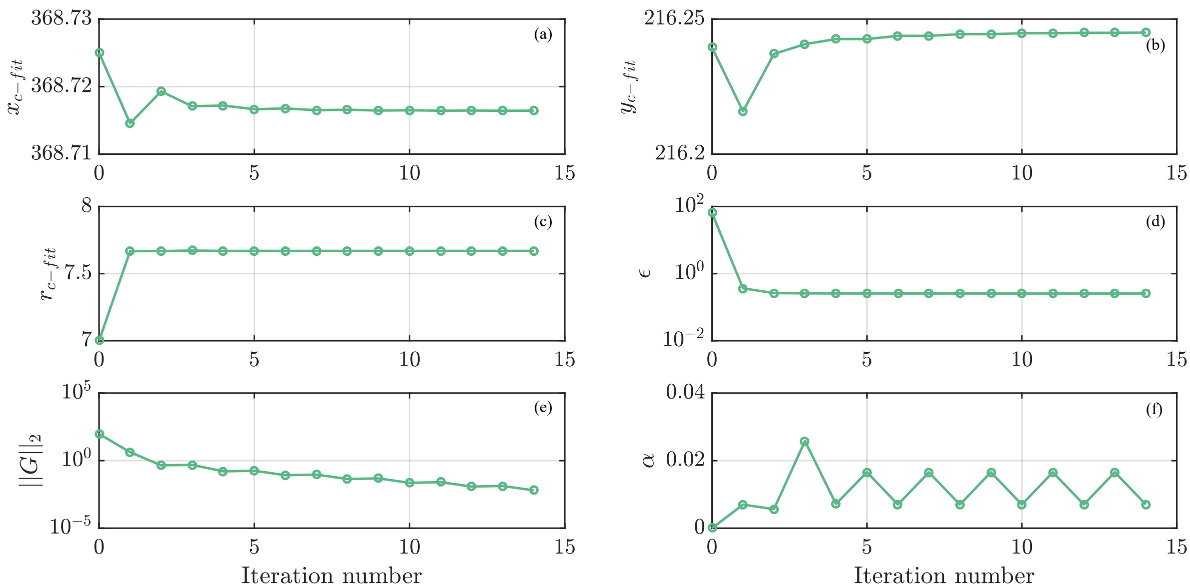


Figure 3. Fitting progress: Results versus iterations, (a) Circle center x-coordinate (b) Circle center y-coordinate (c) Circle radius (d) Sum of the squared error (e) Norm of the gradient of objective function (f) Step length

As mentioned before, the total number of function evaluations, when SD-line search condition combination being used converges, are set to be a performance measure. Therefore, the number of function evaluation at each iteration are also recorded. These results, corresponding to the one in Figure 3, are presented in Figure 4. From those figures, one can notice that even if number of iterations are quite reasonable, the number of function evaluations are remarkably high. This is due to computation of the gradient of the objective function at every iteration. As explained in Section 4, the step length computation methods strictly require to satisfy gradient related conditions during the fitting process so that the algorithm keeps calculating gradient of the objective function using finite difference approach until the condition is met. This is the reason behind those high number of function evaluations in the gradient related line search conditions.

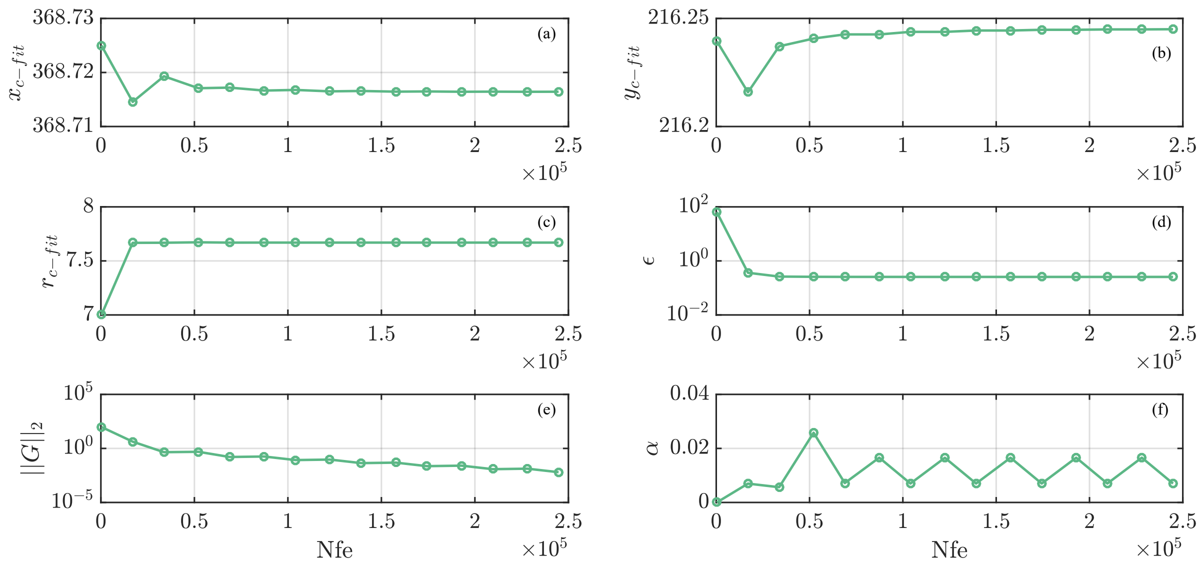


Figure 4. Fitting progress: Results versus number of function evaluations, (a) Circle center x-coordinate (b) Circle center y-coordinate (c) Circle radius (d) Sum of the squared error (e) Norm of the gradient of objective function (f) Step length

All above process shown in Figures 2 to 4 have been completed for all the geometries and line search conditions. The total number of function evaluations for all the line search conditions corresponding to the geometries are illustrated in Figure 5. Note that ∞ in this figure denotes that the line search condition fails to converge.

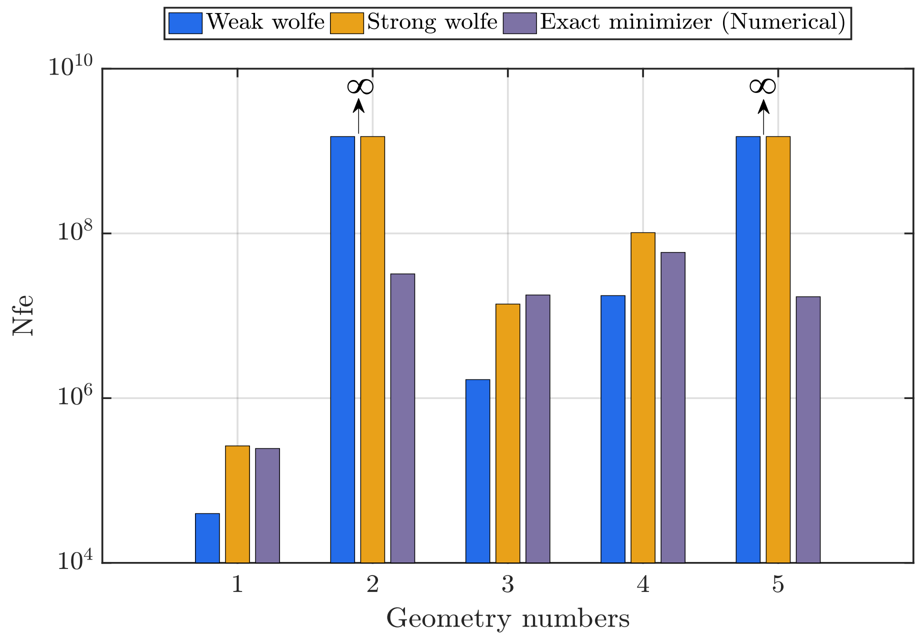


Figure 5. Total number of function evaluations for all the geometries and line search conditions

By a closer look at Figure 5, it must be stated that the line search condition has a considerable influence on the number of function evaluations. The WWC has the lowest number of function evaluations for geometries 1, 3 and 4. However, it fails on fitting of two geometries (i.e., 2 and 5). The same is also true for the SWC. On the other hand, the exact minimizer is the only one that is successful on all the geometries. All those interpretations seem a general evaluation of the effect of line search conditions on the SD method performance. However, the end-users might need more statistical evaluation results to choose an optimal line search condition for geometry fitting. Thus, we employ performance profiles [20] to perform reliable and efficient assessments and to determine the fastest, slowest and most robust line search conditions. Figure 6(a). shows the performance profiles of line search conditions. Those profiles are generated using the total number of function evaluations reported in Figure 5. In this study, the performance profiles, $P(\upsilon)$, basically provides the success probability of the line search conditions within the factor υ of the fastest line search condition. In other words, they give how many geometry fitting is completed within the factor υ of the fastest line search condition. For further details about the mathematical background of the performance profiles, the reader is referred to [20].

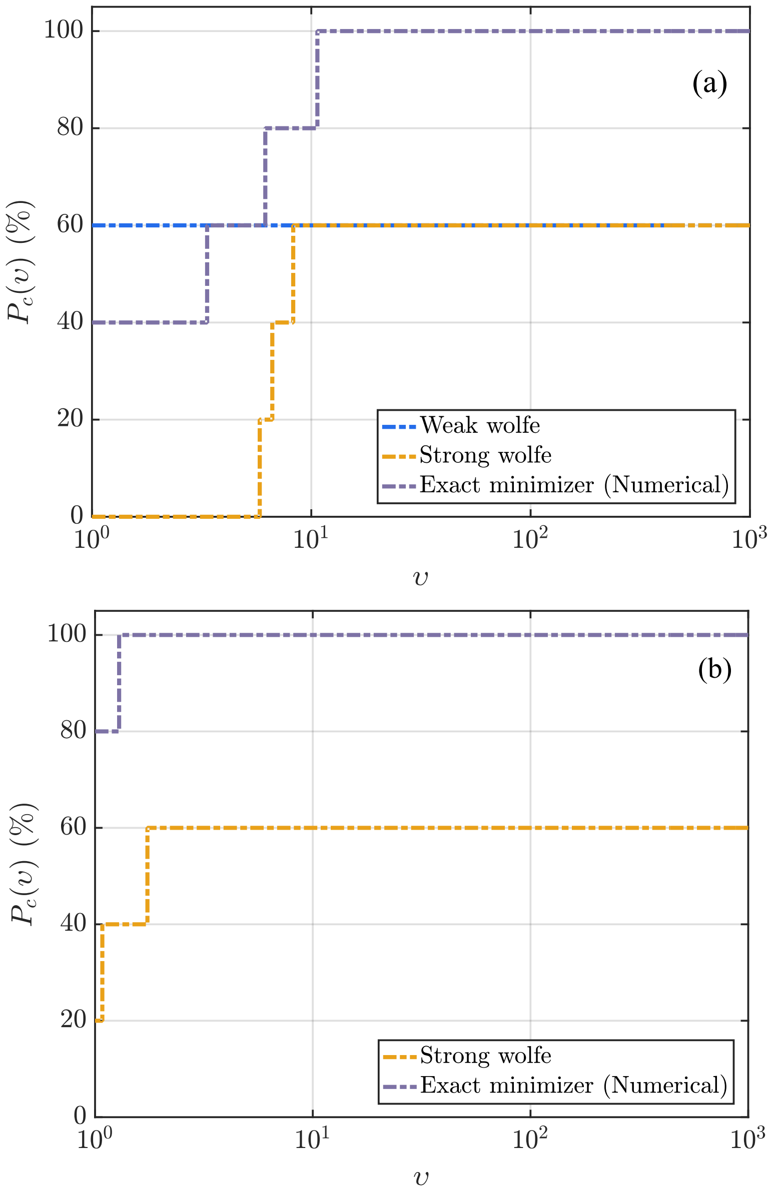


Figure 6. Performance profiles: (a) Step-1 (b) Step-2

From Figure 6(a)., by just looking at $P(10^0)$ values, it can be determined that the WWC is the fastest line search condition with the probability $P(10^0) = 60\%$. More specifically, the WWC is successful on 3 out of 5 geometries with the lowest number of function evaluations. Besides, it preserves being fastest one until $\upsilon \leq 3.35$. At that factor, the exact minimizer comes out with the probability $P(3.35) =$

60%. As the υ rises the success rate of the exact minimizer continuously increases and finally it reaches maximum probability, $P(\upsilon) = 100\%$, at the factor $\upsilon = 10.66$ of the fastest one. On the other hand, the SWC is slowest one and it is able to be successful on 60% of geometries (i.e., geometry number 1, 3 and 4) at the factor $\upsilon = 8.27$. In addition to these, we may rank the line search conditions with a successive excluding procedure. More clearly, by excluding first fastest line search condition, the WWC, we can determine the second fastest one which is the exact minimizer. This can be seen from Figure 6(b) (i.e., $P(10^0) = 80\%.$). Also, this figure shows that the SWC is the slowest one as mentioned before. From all those results, it is determined that the exact minimizer is the optimal choice for step length computation for geometry fitting in this study.

7. Conclusions

This paper has dealt with a performance evaluation of steepest descent method considering three well-known gradient related line search conditions in nonlinear least squares geometry fitting of 2D geometries. The CMM was used to obtain the 2D profiles of the primitive geometries. The geometry fitting processes for all those scanned data have been completed with three different line search conditions. This has provided us the best model parameters that represent the measured data. The total number of function evaluations to complete the fitting have been recorded for all the SD method-line search conditions combinations. By using these data, the performance profiles have generated for reliable and efficient assessment. From these profiles, the fastest and slowest line search conditions have been identified to be the WWC and SWC, respectively. For an optimal choice, it is determined that the exact minimizer is a great candidate. Considering all the evaluation results, the effect of the line search conditions on the SD method success and performance is significant in the geometry fitting procedure. Even if the approximation methods (i.e., the WWC and the SWC) are the first choices for calculating step length in general, because they might provide lower computational cost, the exact minimizer has proved itself to be an optimal choice for the geometry fitting process. This also shows that the line search conditions performance may differ from problem-to-problem. The approximation methods underperform in this study. The end-users might consider this fact. It is also noteworthy that the WWC and SWC parameters (i.e., c_1 and c_2) may affect the performance of the line search conditions. For future study, this could be elaborated.

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