A Finite-Differences Derivative-Descent Approach for Estimating Form Error in Precision-Manufactured Parts

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Background: Form-error measurement is mandatory for the quality assurance of manufactured parts and plays a critical role in precision engineering. There is now a significant literature on analytical methods of form-error measurement, which either use mathematical properties of the relevant objective function or develop a surrogate for the objective function that is more suitable in optimization. On the other hand, computational or numerical methods, which only require the numeric values of the objective function, are less studied in the literature on form-error metrology. Method of Approach: In this paper, we develop a methodology based on the theory of finite-differences derivative descent, which is of a computational nature, for measuring form error in a wide spectrum of features, including straightness, flatness, circularity, sphericity, and cylindricity. For measuring form-error in cylindricity, we also develop a mathematical model that can be used suitably in any computational technique. A goal of this research is to critically evaluate the performance of two computational methods, namely finite-differences and Nelder-Mead, in form-error metrology. Results: Empirically, we find encouraging evidence with the finite-differences approach. Many of the data sets used in experimentation are from the literature. We show that the finite-differences approach outperforms the Nelder-Mead technique in sphericity and cylindricity. Conclusions: Our encouraging empirical evidence with computational methods (like finite differences) indicates that these methods may require closer research attention in the future as the need for more accurate methods increases. A general conclusion from our work is that when analytical methods are unavailable, computational techniques form an efficient route for solving these problems.
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Keywords: form error, metrology, derivative descent, finite differences, cylindricity

1 Introduction

Quality assurance of parts manufactured in the industry usually requires that they conform to tolerance specifications, which may be internal or customer-specified. According to a modern perspective, quality is inversely proportional to variation [1]. To reduce variation, it becomes necessary to measure variation *accurately* in the first place. Measurement of *form errors* was carried out in the early days of manufacturing with mechanical instruments. In modern times, Coordinate Measuring Machines (CMMs) are used quite heavily, although for certain types of measurements mechanical devices such as gauges and V-blocks [2] are popular to this day. CMMs have made it possible to gather large sets of data—from the surface of the part to be measured—allowing increased accuracy in the measurement performed. This, and the fact that the power of modern-day computers has increased dramatically, have enabled the processing of large amounts of data with complex algorithms.

In this paper, we focus on *computational* methods for surface-metrology features belonging to the class of form errors. Examples of such features are: Straightness, flatness, circularity, sphericity, and cylindricity. While there has been a large volume of work in *analytical* methods for form-error measurement, computational methods have received less attention in the literature. Analytical methods exploit mathematical properties of the relevant objective function for optimization or optimize a surrogate objective function. Contrary to this approach, computational methods use numeric values of the objective function for optimization. Computational methods become attractive when it is difficult to obtain optimization-oriented, analytic properties of the objective function without tampering with it. In this paper, we introduce the method of derivative descent in the form of finite differences, which makes it a computational approach, for measurement of form errors. We also derive a model for measuring form error in cylindricity; the model can be used suitably in any computational technique. And finally, we test the performance of the finite-differences approach and a Nelder-Mead approach on numerous data sets—some of which are from the literature—related to all of the form-error features enumerated above. The empirical evidence that we have gathered suggests that for more complex features such as sphericity and cylindricity, the finite-difference approach outperforms the Nelder-Mead approach; of course, both techniques consistently outperform the least-squares technique that is widely used in industrial software.

The rest of this paper is organized as follows. Section 2 provides the background material for this subject along with the derivation of the form useful in determining cylindricity errors. Section 3 presents the finite-differences derivative-descent approach. Computational experiments are reported in Sec. 4. Section 5 concludes this paper with a discussion on topics related to future research.

2 Background

In this section, we will first define form-errors for straightness, flatness, circularity, and sphericity. For cylindricity, we will devise the closed form required for cylindricity error. Thereafter, we will also present the formulations used in least-squares techniques.

2.1 Form-Error Features. The ith data point on the surface being inspected will be denoted either by (x_i, y_i) or (x_i, y_i, z_i) depending on whether two-dimensional or three-dimensional data are required, where for the ith point, x_i, y_i, and z_i denote the x, y, and the z coordinates, respectively. To model the straightness error, we define a straight line using: $y = mx + c$ where m and c are the *defining parameters* of the equation. The vertical deviation of a point, (x_i, y_i), on the edge from the reference form is: $e_i = y_i - (mx_i + c)$. This deviation is measured along the y axis. The normal deviation of the same point from the reference edge is given by: $e_i = (y_i - (mx_i + c)) / \sqrt{1+m^2}$. Vertical deviations are *more easily* minimized than normal deviations using the popular least-squares method, which we will discuss later, and hence have been used extensively in commercial software. However, it is the normal deviation that measures the actual deviation according to Refs. [3–5]. Unfortunately, normality introduces nonlinearity in the definition of error, making its analysis more complicated.

Flatness is an extension of straightness to 3 dimensions. The

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Step 1: One is provided with data of the form (x_i, y_i) or (x_i, y_i, z_i) for $i = 1, 2, \ldots, n$. Determine the defining parameters of the reference surface so as to minimize some function of the deviations (the Euclidean norm, the max norm, or the zone).

Step 2: Use the defining parameters to compute the deviations at each point. Then declare the zone of the deviation vector to be the form error.

Fig. 1 A 2-step procedure in form-error measurement

equation of a plane is defined as: $z=mx+ly+c$. The normal deviation of any measured point, (x_i, y_i, z_i), from the reference plane is given by: $e_i=(z_i-(mx_i+ly_i+c))/\sqrt{(1+m^2+l^2)}$ and the vertical deviation is given by: $e_i=z_i-(mx_i+ly_i+c)$, which is measured along the z axis.

For defining *circularity* (or roundness), we need to define a circle whose equation is $(x-a)^2+(y-b)^2=R^2$ where R is the radius of circle and the coordinates of the center of the circle are: (a,b). The defining parameters of the equation of a circle are thus: a,b, and R. Unlike straightness or flatness, for circularity, only one type of deviation is of interest, which is called the *radial deviation*. The latter is measured *along the radius* from the circle center to the point in question. Hence the radial deviation for a point, (x_i, y_i), is: $e_i=\sqrt{(x_i-a)^2+(y_i-b)^2}-R$ in which the square-rooted term is the distance from (x_i, y_i) to the circle's center.

The equation of a sphere is given as: $(x-a)^2+(y-b)^2+(z-c)^2=R^2$, where R is the radius of the sphere and the sphere's center is: (a,b,c). The radial deviation for *sphericity*, which is an extension of the same for circularity to three dimensions, is defined as: $e_i=\sqrt{(x_i-a)^2+(y_i-b)^2+(z_i-c)^2}-R$. The defining parameters of the equation of a sphere are thus: a,b,c, and R. In the deviation, the square-rooted term is the distance from (x_i, y_i, z_i) to the center of the sphere.

For measuring *cylindricity*, we will employ a cylinder whose radius is R and whose axis is given by:

$$\frac{x-u}{m} = \frac{y-v}{l} = \frac{z-w}{k}. \tag{1}$$

Then the defining parameters of its equation are: l,m,k,u,v,w, and R. The deviation of any point on a real cylinder from a perfect cylinder can then be shown to be:

$$e_i = \sqrt{(x_i - mt_i - u)^2 + (y_i - lt_i - v)^2 + (z_i - kt_i - w)^2} - R, \tag{2}$$

$$\text{in which } t_i = \frac{(x_i - u)m + (y_i - v)l + (z_i - w)k}{m^2 + l^2 + k^2}. \tag{3}$$

In Eq. (2), the square-rooted term is the normal distance from a point, (x_i, y_i, z_i), on the surface of the cylinder, to the axis of the cylinder. We now provide a proof of the validity of the model presented above.

Derivation of Eq. (2) and (3): Let $\vec{\psi}$ denote a vector whose one end point is (x_i, y_i, z_i) and the other is on the axis of the cylinder, and the vector itself is perpendicular to the axis. Now, from the definition of the axis, i.e., Eq. (1), (m,l,k) is a vector on the axis. Hence the dot product of $\vec{\psi}$ and (m,l,k) has to be zero. Now, let the other end point of $\vec{\psi}$, which also lies on the axis, be parametrized by t_i. Then, from Eq. (1), $t_i=(x-u)/m=(y-v)/l=(z-w)/k$, which implies that the end point is defined as: (mt_i+u, lt_i+v, kt_i+w). Then, $\vec{\psi}=(x_i-mt_i-u, y_i-lt_i-v, z_i-kt_i-w)$. From the fact that $(m,l,k)\cdot\vec{\psi}=0$, it follows that: $0=m(x_i-mt_i-u)+l(y_i-lt_i-v)+k(z_i-kt_i-w)$ from which Eq. (3) follows. Now, the cylindricity error at (x_i, y_i, z_i) *is* the difference between the Euclidean norm of $\vec{\psi}$ and the radius of the cylinder. Therefore: $e_i=\sqrt{(x_i-mt_i-u)^2+(y_i-lt_i-v)^2+(z_i-kt_i-w)^2}-R$, and we are done.

Since the locus of any point on the cylinder satisfies the property that its perpendicular distance from the axis has to be R, we have that the equation of a cylinder is: $(x-mt-u)^2+(y-lt-v)^2+(z-kt-w)^2=R^2$ where t is defined in Eq. (3).

The *span seminorm* is the difference between the maximum and the minimum of the deviations, and can be expressed mathematically as:

$$sp(\vec{e}) \equiv (\max_i e_i - \min_i e_i) = |\max_i e_i| + |\min_i e_i|. \tag{4}$$

For the second equality to hold in (4), we assume that the deviations vector contains *both* positive and negative signs. When the span seminorm is minimized to obtain values for the defining parameters of the reference surface, the surface obtained is the so-called *minimum-zone* surface. The associated metric, span seminorm, is popularly called the "zone" in metrology, and we will refer to it as such in the remainder of this paper. What is to be noted is that according to Refs. [3–5] this metric measures the true error. Two other metrics, popularly used in metrology *for determining the defining parameters of the reference surface*, are the Euclidean norm and the max norm. The Euclidean norm is minimized in the least-squares techniques to obtain the defining parameters, while the max norm is minimized for the same purpose in *minimax* techniques. (Of course, the form error is always measured using the zone.) Their definitions are as follows:

$$\text{Euclidean norm} = \|\vec{e}\|_2 = \sqrt{\sum_{i=1} e_i^2} \text{ and the max norm}$$

$$= \|\vec{e}\|_\infty = \max_i |e_i|.$$

In Fig. 1, we describe a 2-step *generalized* procedure necessary in obtaining the form error of any feature. In this 2-step procedure, there are a number of factors that introduce a *bias* (error) on the measurand. The first factor arises from the fact that there is an infinite number of points on the actual surface and we use only a finite sample. This is called the *sampling* bias. This issue is beyond the scope of this paper, but the interested reader should read Refs. [6–11]. The second factor, discussed above, arises when the function used in Step 1 for finding the defining parameters is *not* the zone, but some other function, e.g., the Euclidean norm (used in least-squares techniques). In the case of straightness and flatness, using vertical distances in Step 1 but normal deviations in Step 2 can lead to an additional bias. A third type of bias can arise out of errors in measurement.

2.2 The Least-Squares Method. We will first consider straightness with vertical distances. Step 1 of the general procedure in Fig. 1 will require the minimization of the Euclidean norm, i.e., determine m and c to minimize $\Sigma_{i=1}^{n}(y_i-mx_i-c)^2$. The age-old algorithm of Gauss can be employed to solve this problem. The defining parameters can be determined by solving simultaneously the following two linear equations in which the unknowns are m and c: $\Sigma_{i=1}^{n} y_i = m\Sigma_{i=1}^{n} x_i + nc$ and $\Sigma_{i=1}^{n} x_i y_i = m\Sigma_{i=1}^{n} x_i^2 + c\Sigma_{i=1}^{n} x_i$. When we have values of m and c, we can compute the deviations at each point, and the form error is then calculated using Eq. (4).

For flatness measurement, Step 1 is: Find m, l, and c to minimize $\Sigma_{i=1}^{n}(z_i - mx_i - ly_i - c)^2$. The defining parameters can be determined by the simultaneous solution of the following three equations: $\Sigma_{i=1}^{n} z_i = m\Sigma_{i=1}^{n} x_i + l\Sigma_{i=1}^{n} y_i + nc$, $\Sigma_{i=1}^{n} x_i z_i = m\Sigma_{i=1}^{n} x_i^2 + l\Sigma_{i=1}^{n} x_i y_i + c\Sigma_{i=1}^{n} x_i$, and $\Sigma_{i=1}^{n} y_i z_i = m\Sigma_{i=1}^{n} x_i y_i + l\Sigma_{i=1}^{n} y_i^2 + c\Sigma_{i=1}^{n} y_i$. From m, l, and c, one can compute the deviations at each point, and the form error is then calculated using Eq. (4). It is to be noted that the least-squares approach for flatness and straightness involves *linear* least-squares, which have a straightforward solution. This does not carry over to circularity and sphericity, where the functions are nonlinear. A widely cited formula [12] in the literature for the defining parameters in circularity is $a = 2(\Sigma_{i=1}^{n} x_i / n)$, $b = 2(\Sigma_{i=1}^{n} y_i / n)$, and $R = (\Sigma_{i=1}^{n} \sqrt{x_i^2 + y_i^2})/n$. For this to work, one must collect data from *equally-spaced* points, i.e., points which have an equal angular spacing. For sphericity, the corresponding formula with equally-spaced data is: $a = 2(\Sigma_{i=1}^{n} x_i / n)$, $b = 2(\Sigma_{i=1}^{n} y_i / n)$, $c = 2(\Sigma_{i=1}^{n} z_i / n)$, and $R = (\Sigma_{i=1}^{n} \sqrt{x_i^2 + y_i^2 + z_i^2})/n$. Approximate least-squares solutions for cylindricity can be found in [13,14].

3 Finite-Differences Derivative Descent

In computational techniques, the objective function is used as it is, and this is in contrast to *many* analytical techniques that use approximations or surrogates. As mentioned above, the optimization algorithm uses only numeric values of the objective function. Hence the optimization algorithm in computational methods does not require any special structure, e.g., linear structure for linear programming / linear least-squares or a quadratic structure for sequential quadratic programming, etc. Consequently, the bias that arises from approximating the objective function disappears completely. This is an upside. Now the downside is that: the (computational) optimization technique is (i) not guaranteed to converge to the global optimum and (ii) may require numerous function evaluations and therefore a long time on the computer to provide a good solution. A large number of computational techniques are available in the literature. Some of the prominent ones are: The Hooke-Jeeves procedure [15], the Nelder-Mead [16] simplex procedure, derivative-based methods, and meta-heuristics, e.g., genetic algorithms, simulated annealing, and tabu search.

The lack of convergence guarantees of computational techniques may imply a rather poor solution at times. However, empirical evidence in metrology (see Refs. [17–20] for the use of the Nelder-mead method, [21] for a Hooke-Jeeves search, and [22] in the context of genetic algorithms) and application areas other than metrology [23] suggests that many computational techniques do provide good solutions in a robust manner. It is also to be noted that convergence guarantees in analytical optimization techniques are oftentimes for surrogate objective functions (e.g., a linearized function when the actual function is non-linear), and hence they may not signify a lot even in theory. The second disadvantage, i.e., significant time on the computer, is becoming less of an issue nowadays with the increasing power and availability of computers.

We now present a computational technique based on finite-difference approximations [24] of steepest descent (Cauchy [25]). To the best of our knowledge, this is the first use of finite-differences derivative (steepest) descent in form-error metrology. Derivative descent has been used in other works but in analytical methods [26–28]. The power of the derivative descent approach is that it is guaranteed to converge to a local optimum under certain conditions.

Step 1. Let D denote the number of decision variables (the defining parameters of the reference form). Further, let the solution for the ith decision variable in the pth iteration be denoted by q_i^p. Then: $\vec{q}^p = \{q_1^p, q_2^p, \ldots, q_D^p\}$. Set $p = 0$ and choose an arbitrary starting value for q_i^p for every $i = 1, 2, \ldots, D$. Select a stopping tolerance $\epsilon > 0$. Let $f(q_1, q_2, \ldots, q_D)$ denote the measurement criterion, which will equal the zone of the deviation vector computed with using $\vec{q}$ as the vector of defining parameters. Set Δ to a small positive value, e.g., 0.01, and the step-size μ also to a small size, e.g., 0.001.

Step 2. Compute the approximate value of the derivative for each $i = 1, 2, \ldots, D$ using:

$$\left.\frac{\partial f(.)}{\partial q_i}\right|_{\vec{q}=\vec{q}^p} \approx \frac{f(q_1^p, q_2^p, \ldots, q_i^p + \Delta, \ldots, q_D^p) - f(q_1^p, q_2^p, \ldots, q_i^p - \Delta, \ldots, q_D^p)}{2\Delta}.$$

Step 3. Check if the gradient norm is less than the stopping tolerance, i.e., check if:

$$\sqrt{\sum_{i=0}^{D}\left(\left.\frac{\partial f(.)}{\partial q_i}\right|_{\vec{q}=q^{\vec{p}}}\right)^2} < \epsilon.$$

If yes, stop and declare $\vec{q}^p$ to be the optimal solution. Otherwise, go to Step 4.

Step 4. Update the values for each $i = 1, 2, \ldots, D$,

$$q_i^{p+1} \leftarrow q_i^p - \mu \left.\frac{\partial f(.)}{\partial q_i}\right|_{\vec{q}=q^{\vec{p}}}.$$

Set $p \leftarrow p + 1$, and return to Step 2.

In the above step, we used a *central differences* [24] formula for computing the finite difference approximation of the partial derivative. With a *forward differences* formula, Step 2 would be:

Step 2. Compute the approximate value of the derivative for each $i = 1, 2, \ldots, D$ using:

$$\left.\frac{\partial f(.)}{\partial q_i}\right|_{\vec{q}=q^{\vec{p}}} \approx \frac{f(q_1^p, q_2^p, \ldots, q_i^p + \Delta, \ldots, q_D^p) - f(q_1^p, q_2^p, \ldots, q_i^p, \ldots, q_D^p)}{\Delta}.$$

It may be noted that in Step 2, the forward-differences formula requires only $(D+1)$ function evaluations as opposed to the $2D$ evaluations needed in central differences. However, the central-differences formula is shown [24] to have a reduction in the bias arising out of approximations employing a finite value of Δ, which theoretically is infinitely small.

4 Computational Results

We carried out numerous experiments on all the form-error features discussed above. There were many objectives behind the experimental study conducted. (1) We wanted to test how the computational methods, namely finite differences and Nelder-Mead, fared on existing data sets from the literature. We compared the performance in terms of the quality of solution obtained and the computational time. (2) The method of finite differences has a number of tuning parameters, which are: The step-size, μ, and the perturbation parameter Δ. Hence a computational study can reveal what values for these parameters can work well in practice. (3) The method of finite differences can also be used with a forward-differences formula instead of the central-differences formula. Hence an empirical comparison of the two formulas is essential in practice, which was also one goal of our study. Finally (4) we wanted to determine how the model derived for cylindricity performs in comparison to existing results.

The results of our computational experiments are summarized in Tables 1–5. In these tables, the data sets marked with asteriks are from the literature, whose sources are as follows: straightness: [29,30], flatness: [20], circularity: [31], sphericity: [32], and cylindricity [33]. All the experimental data sets can be found in Ref. [34].

The least-squares technique for straightness and flatness used vertical distances. For circularity and sphericity, the least-squares technique, which works well for equally spaced data, performs rather poorly when this condition is violated. Our computational

Table 1 Experiments with straightness

Data set	Sample Size	Finite-Differences	Least Squares	Nelder-Mead	Published
1*	5	2.121 333	2.400 98	2.121 32	2.66 [29]
2	5	0.147 067	0.147 462	0.147 053	-
3*	10	0.001 678	0.001 73	0.001 652	0.0017 [30]
4	10	0.084 808	0.089 51	0.084 695	-
5	5	0.172 363	0.174 39	0.172 22	-

experiments indicate that in *all cases* the least-squares technique is outperformed by Nelder-Mead search and finite-differences derivative descent in terms of the quality of the solution. In terms of computational time, Nelder-Mead takes an average of 4 times as much time as least-squares, and finite differences take 6 times as much time as least-squares. However, the maximum time in any of our computational experiments never exceeded 10 s on a UNIX Sun machine (SunBlade 150). Although the Nelder-Mead search does not have proven convergence properties, unlike derivative descent, its performance is on the average better than that of derivative descent for straightness, flatness, and circularity. A weakness of the Nelder-Mead approach is that for a large number of decision variables, its convergence properties deteriorate [35]. This is perhaps why it is outperformed by the finite difference derivative approach for sphericity and cylindricity. The numerical results demonstrate that computational methods have the potential of developing into robust and useful techniques in form-error metrology.

Ideally, the value of Δ should be the square root of 10^{-16}, which is typically the *unit round-off* in double precision arithmetic in most C compilers [24]. However, we were able to use a much larger value for Δ, which was 0.01. Larger values reduce the accuracy of the derivative, but increase the speed of the computer program. The value of μ was set at 0.001 in our experiments. Values of μ larger than 0.001 caused the algorithm to diverge from the solution produced by the least-squares technique, which indicated that all of these values must be chosen carefully if these computational techniques are to work.

The finite-differences method uses approximations of the derivatives, and hence may get into pathological situations where it cycles near the optimal point but fails to converge to it [35]. We did not encounter this problem in any of our experiments; we must also note that much of the data that we have used is from the literature. However, since this possibility cannot be ruled out, one

Table 2 Experiments with flatness. The best published results are with Nelder-Mead [20].

Data set	Sample Size	Finite-Differences	Least Squares	Nelder-Mead
1*	14	1.961 52	2.367 659	1.961 161
2*	20	4.858 402	5.895 094	4.857 338
3*	25	0.166 378	0.166 38	0.154 87
4*	20	0.043 934	0.043 96	0.041 33
5*	25	0.002 709	0.002 709	0.002 627
6*	9	14.296 734	16.476 041	14.295 217

Table 3 Experiments with circularity

Data set	Sample Size	Finite-Differences	Least Squares	Nelder-Mead	Published [31]
1*	8	2.2438	2.388 47	2.243 271	2.2432
2*	10	0.230 845	0.229 938	0.228 834	0.2288
3*	12	0.146 532	0.157 296	0.144 994	0.1449
4*	15	1.571 172	9.648 659	1.569 405	1.5694
5*	20	1.599 442	1.751 343	1.671 079	1.6711

Table 4 Experiments with sphericity

Data set	Sample Size	Finite-Differences	Least Squares	Nelder-Mead	Published [32]
1*	25	3.332663	3.543336	3.466298	3.32518
2	20	2.986749	12.848077	3.239792	-
3	15	3.192011	17.138677	3.386355	-
4	10	1.715243	20.624018	1.660672	-

Table 5 Experiments with cylindricity

Data set	Sample Size	Finite-Differences	Published [33]	Nelder-Mead
1*	24	0.002 789	0.002 788	0.008 124
2*	20	0.188 621	0.183 95	0.194 056
3*	22	0.619 088	0.8999	0.398
4	10	0.573 457	-	0.706 657
5*	10	0.004 334	0.015 089	0.005 393

must have alternative computational methods like Nelder-Mead or analytical methods like least-squares available in a software package that is expected to perform robustly.

The forward differences approach took less time because it required fewer function evaluations, but central differences invariably performed better than forward differences. As a result, we do not report results with forward differences. This is consistent with the behavior of forward differences in general, because, as stated above, the latter in comparison to central differences have a greater bias arising out of using a finite value for Δ [24].

Experiments with cylindricity demonstrate the true use of computational methods. The form-error in cylindricity is quite complex, and as such there is little work on analytical approximations. The performance of computational methods is very encouraging in this domain as well.

5 Conclusions

This paper introduced a new finite-differences derivative descent technique to form-error metrology. The technique was tested along with the Nelder-Mead technique on a large number of data sets on a wide spectrum of form-error features. In all the experiments performed, both techniques outperformed the least-squares technique which is widely used in industrial CMM software. A mathematical model was presented for measuring form error in cylindricity. This model can be used in any computational technique. Our work indicates that computational methods provide a simple route for solving these problems when analytical methods are unavailable. Although our experience with computational methods, which have a high computational burden, has been positive, we also believe that more research is needed to develop *provably convergent* analytical methods that exploit the derivative in a more accurate fashion. An important first task in these attempts will be to study continuity and differentiability properties of the error function. If such properties are established, a large number of superior optimization methods, e.g., methods which exploit the second derivative (Hessian), can be tried. Also, the method of simultaneous perturbation (see Spall [36]) can be employed in place of finite differences because the former has a lower computational burden in comparison to the latter.

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