ON COMBINING CHAOS SEARCH AND LEVENBERG-MARQUARDT ALGORITHM FOR NON-LINEAR SUBSTITUTED GEOMETRIC FITTING PROBLEMS

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Abstract:

Product quality is becoming a main concern in today manufacturing. As such, a dimensional metrology is strictly necessary. High accuracy result while reducing speed in measuring a product has to catch up with the improvement of metrology instrument which can capture many points in less time. Fitting algorithm of points cloud from measurement plays a critical role for the measurement accuracy and speed. In this study, non-linear least-square fitting of circle, sphere and cylinder are addressed without any prior knowledge of their nominal. These geometries have common use in practice, such as sphere for calibration and hole-shaft features in mechanical assembly application. The improvement of initial point guess for Levenberg-Marquardt (LM) algorithm by employing Chaos Optimization (CO) method is presented. The results show that, with this combination, higher quality of fitting results in term of smaller norm of the residuals can be obtained while preserving the computational cost.

Keywords: Metrology software, geometric fitting, non-linear optimization.

NOMENCLATURE

$\boldsymbol{x}$: A point in 2D *(x,y)* or 3D *(x,y,z)*.

$\boldsymbol{x_i}$: The i-*th* point of the point cloud.

$\boldsymbol{x_0}$: A point lies on the line/axis. For the initial guess, this point is the centroid (average) of the points.

d_i : The distance of point $\boldsymbol{x_i}$ to the fitted geometry.

M : A $n \times 3$ matrix of all the data points, defined as: $[x_1 \;\; y_1 \;\; z_1; \; ... \; .... \; ....; x_n \;\; y_n \;\; z_n]$

$\boldsymbol{n}$: The direction cosine (orientation) of a line or axis.

∇ : Scalar function gradient: $\nabla J = (\partial J/\partial x, \; \partial J/\partial y, \partial J/\partial z)$.

$\| \; . \; \|$: L_2-Norm of a vector: $\|x\| = \sqrt{x^2 + y^2 + z^2}$.

$\|r\|$: L_2-Norm of sum of the squared residuals.

MPE: Maximum Permissible Error.

1. INTRODUCTION

Quality of manufacturing product is one of the main concern in modern world to increase competitiveness [1]. As such quality inspection by dimensional metrology is necessary [2]. Fitting substitute geometry from obtained points is the first step before measurement [3-5] as shown in Fig. 1. Subsequently, fitting process is a critical step. This process becomes difficult without prior knowledge of the nominal geometry.

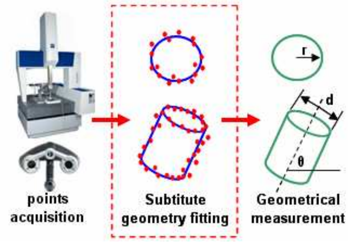

Fig. 1: geometrical fitting process in metrology.

In addition, fitting process should be non-computationally intensive since emerging instruments can obtain thousand-to-million points in short time, leading to faster and less expensive measurements [6]. Hence, an accurate and high speed fitting procedure is a strict requirement. In this article, Least-square (LS) fitting problem of non-linear geometry is addressed since it involves multi-modal function optimization task compared to the linear one. Particularly, initial point solution and its effect to the accuracy and computing time of non-linear LS geometric fitting will be addressed.

2. NON-LINEAR FITTING AND LEVENBERG-MARQUARDT ALGORITHM

Non-linear geometries are determined based on their description parameter which is not linear. In practice, the fitting processes are more difficult. LS fitting of circle, sphere and cylinder will be addressed in this study. Circle and sphere geometries have many applications as artefact geometry for calibration of dimensional metrology instrument [7-8]. Meanwhile, Cylinder is a geometry representation of shaft-hole assemblies features [9]. The fundamental of LS fitting is to minimize a function of errors which are defined as distance between measured points and ideal substitute geometry as illustrated in Fig. 2a:

$$\underset{param}{\arg\min} \sum d_i^2(param) \tag{1}$$

where *param* are parameters defining the geometric feature. For circle, the distance function is:

$$d_i(x_i, y_i) = \|\boldsymbol{x_i} - \boldsymbol{x_0}\| - r$$
$$= \sqrt{(x_i - x)^2 + (y_i - y)^2} - r \tag{2}$$

Meanwhile for sphere, the function is formulated as:

$$d_i(x_i, y_i, z_i) = \sqrt{(x_i - x)^2 + (y_i - y)^2 + (z_i - z)^2} - r \tag{3}$$

where x, y, z are the coordinates of the center of the sphere/circle and r is their radius. The Cylinder has a more complex distance function compared to the sphere and circle which is $d_i(x_i, y_i, z_i) = d_{i(3dp2Axis)} - r$. Variable $d_{i(3dp2Axis)}$ is defined as distance between 3D point $\boldsymbol{x_i}$ to the axis of cylinder (a straight line) which is estimated by its direction cosine and, based on Fig. 2b, is defined as:

$$d_{i(3dp2Axis)} = \left\|(\boldsymbol{x_i} - \boldsymbol{x_0}) \times \boldsymbol{n}\right\| \quad (4)$$

Finally, the distance function of a cylinder is:

$$d_i(x_i, y_i, z_i) = \left\|(\boldsymbol{x_i} - \boldsymbol{x_0}) \times \boldsymbol{n}\right\| - r \quad (5)$$

The parameters to estimate for a cylinder are a point $\boldsymbol{x_0}$ on the axis, having cosine direction $\boldsymbol{n}$, and its radius r. Fig. 2a describes the distance definition.

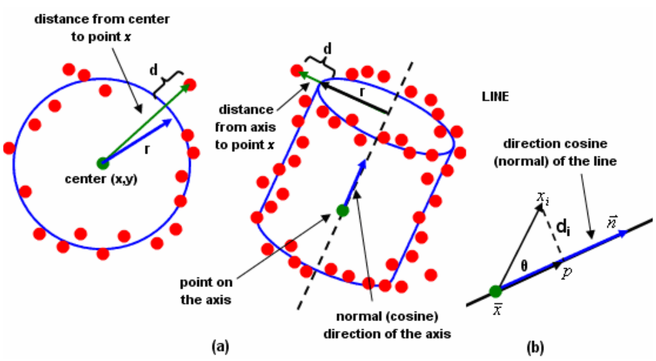

Fig. 2: (a) definition of point distance for circle (sphere) and cylinder, (b) definition of point distance of a line.

Levenberg-Marquardt (LM) algorithm is a well-known approximation method for solving non-linear least square estimation [10]. The recipe of LM algorithm is based on steepest-decent and Gauss-Newton method. The advantage of this method is when the searching process is far from the optimum, it uses steepest-decent step to move near the optimum region. On the other hand, when it is near optimum, it changes to Gauss-Newton step to find the optimum value. Subsequently, this method is robust for non-linear least square problem. The LM method used here is based on NIST [5] for their algorithm testing system, listed in **Algorithm 1**. λ is LM variable, which is increased and decreased by 10 and 0.04, respectively, based on NIST suggestion [5]. J_0 is a Jacobian matrix which elements on its ith row is $\nabla d_i(p_0)$, which is the partial derivatives of d_i respect to each parameter. The central idea of LM method lies on the variable $Hx = -v$, which is $J_0{}^T J_0 + \lambda(I + diag(J_0{}^T J_0))x = -J_0{}^T d(p_0)$, one can observe that if λ is zero or small, LM behaviour become Gauss-Newton method. In the opposite, it behaves like a steepest-decent method. The term $I + diag(J_0{}^T J_0)$ is used to obtain a positive definite matrix H.

Besides, LM iterative method has a drawback. It significantly depends on guess of initial solution, P_0 [11]. The function to be optimized is a multi-modal function as shown in Fig. 3. As a consequence, the risk exists that the search is trapped in a local minimum. Fig. 4 illustrates how initial guess as starting solution greatly affects the final results. If, the initial guess is far from optimum, an unexpected final result can be obtained (Fig. 4a). On the other hand, good initial guess can significantly improve the final solution (Fig. 4b).

Algorithm 1: Levenberg-Marquardt Algorithm

Input: Vector p_0 which is the initial guess for the parameter
Output: Vector p which is the fitted parameter

1: Set $\lambda = 0.0001$
2: DO { decrease λ
3: set $U = J_0^T J_0$
4: set $v = J_0^T d(p_0)$
5: set $F_0 = \sum_{i=0}^{N} d_i^2(p_0)$
6: DO { increase λ
7: set $H = U + \lambda(I + diag(U))$
8: solve $Hx = -v$ *for x*
9: set $p_{new} = p_0 + x$; *set* $F_{new} = \sum_{i=0}^{N} d_i^2(p_{new})$
10: IF converged THEN return $p_0 = p_{new}$
11: UNTIL $F_{new} < F_0$ or stop criterion is *true*
12: IF $F_{new} < F_0$ THEN $p_0 = p_{new}$
13: UNTIL stop criterion is *true*

3. CHAOS OPTIMIZATION

Chaos is defined as a semi-randomness property and generated by a nonlinear deterministic equation, creating a chaotic dynamic step which can escape from local optima. It has different behaviour of rejection-accepting in random-based heuristic search [12]**.** Searching through regularity of chaotic motion, represented by one-dimensional logistic map, is the central idea of CO with characteristics of ergodicity, stochastic property, and regularity [13]**.** The one-dimensional logistic map used is:

$$t_{(k+1)} = \lambda_c t_k (1 - t_k) \quad (6)$$

Where: $\lambda_c \in [3.56, 4]$ is the control arguments and k the is iteration number. From the Yang's report [14], $0 \le t_0 \le 1$ where $t_0 \notin \{0, 0.25, 0.5, 0.75, 1.0\}$ is recommended. This CO is used to improve the initial guess of LM method such that the initial guess can escape from local optima and is near the optimal by preserving the CPU time. The CO algorithm is presented in **Algorithm 2**. To adjust small ergodic ranges around p_i^*, we set γ = 0.45 [13]**,** λ = 4 [14]. The statement in line 11 and 12 are to encourage movement farther from the initial bounding area.

4. IMPLEMENTATION AND DISCUSSION

Random points with random error according to uniform distribution and normal distribution were generated as presented in Table 1. For Chaos-LM method, initial point guess of the initial solution of LM optimization iteration was improved by sending it to CO method. In LM algorithm, we set the stopping rule as maximum iteration = 1000 and half for the Chaos-LM method. The initial guess of the center of circle and sphere are their centroid location denoted as $\boldsymbol{x_0}$. The centroid location for each *x,y,z* is the average of the points $\sum x_i / N$. For the radius, its initial guess is: $r_0 = \frac{1}{2}\left(\frac{(\max x - \min x) + (\max y - \min y)}{2}\right)$.

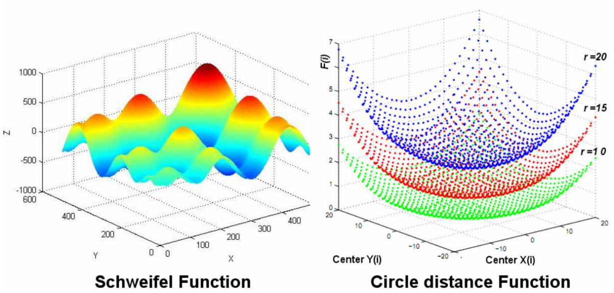

Fig. 3: Example of multi-modal function.

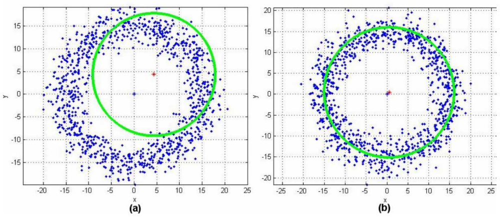

Fig. 4: (a) Initial guess is far from optimal, (b) near optimal.

Algorithm 2: Chaos search to improve the initial guess in LM method

Input: Vector p_0 is the initial guess for the parameter (1:*n-param*)

Goal: New vector p_0 is the improved initial guess by

$Min \sum d_i^2(p_i),\ p_i \in \{a_i, b_i\}\ Let\ \ p^k = (p^1 : p^k), t^k = (t^1 : t^k)$

1: Set $k = 0, r = 0$ Set $k_{\max} = 10, r_{\max} = 30$

2: Produce randomly $t_0 \in \{0,1\}\ and \notin \{0, 0.25, 0.5, 0.75, 1.0\}$

3: Set $t^k = t^0, t^* = t^0, a_i^0 = -MPE, b_i^0 = +MPE$

4: Set $p^* = p_0$ → **initial guess parameter**

5: DO WHILE { $r < r_{\max}$; DO WHILE { $k < k_{\max}$

6: Set $p_i = a_i^r + t_i^r(b_i^r - a_i^r)$; calculate $\sum d_i^2(p^k)$

7: IF $\sum d_i^2(p^k) < \sum d_i^2(p^*)$ THEN $\sum d_i^2(p^*) = \sum d_i^2(p^k),\ p^* = p^k, t^* = t^k$

8: $k = k+1;\ \ t_i^k = \lambda t_i^{k-1}(1 - t_i^{k-1}), \lambda \in \{3.56, 4\}$

9: }END *k*-th iteration; $r = r+1$

10: $a_i^{r+1} = p_i^* - \lambda(b_i^r - a_i^r)$ and $b_i^{r+1} = p_i^* + \lambda(b_i^r - a_i^r)$

11: IF $a_i^{r+1} > a_i^r$ THEN $a_i^{r+1} = a_i^r$, $\lambda \in \{0, 0.5\}$

12: IF $b_i^{r+1} > b_i^r$ THEN $b_i^{r+1} = b_i^r$, $\lambda \in \{0, 0.5\}$

13: IF $r < r_{\max}$ THEN produce $t_0 \in \{0,1\}$ by random, $k = 0,\ \ t^k = t^0$ GOTO(7)

14: ELSE CO is terminated, return $p_0 = p^*$;}END *r*-th iteration;

15: Insert the new p_0 into **Algorithm 1: LM algorithm**.

There is a special case for cylinder. Its initial guess for point on the axis and cosine direction of the axis is derived by fitting a 3D line to the point clouds according to NIST [5] method. According to this method, fitting a line is a case of constrained linear optimization problem. By using Lagrange multiplier method, the estimation of the cosine direction is obtained by finding the eigen-vector corresponding to the largest eigen-value derived from a matrix M which contains *n*-number of points obtained from the measurement. Two levels of sigma for the data deviation were chosen. Type 1 represents only the uncertainty of the instrument (Maximum Permissible Error/MPE) meanwhile type 2 simulates the uncertainty due to the part and the instrument.

Table 1: Details of data generation.

Type of Data		**Number of points and Nominal Parameter**		
		Circle	Sphere	Cylinder
Uniform	Range (μm)	*(x,y,r)*=(15,15,20) mm	*(x,y,z,r)*=(15,15,15,20) mm	(x,y,z,r)=(15,15,15,5) and ***n*** (1,1,1) mm
Type 1	[-2.2,2,2]	1000 pts	grid [30x30]	grid [25x25]
Type 2	[-5,5]	1000 pts	grid [30x30]	grid [25x25]
Normal	sigma σ			
Type 1	1.1	1000 pts	grid [30x30]	grid [25x25]
Type 2	2.5	1000 pts	grid [30x30]	grid [25x25]

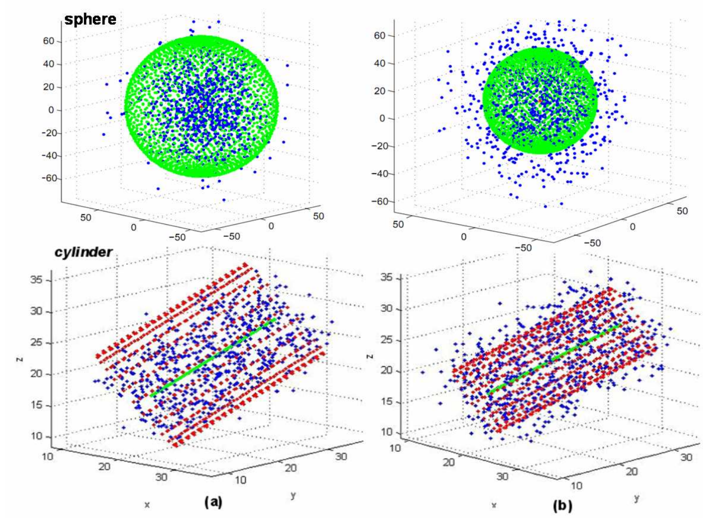

Fig. 5: Visualization of sphere and cylinder fitting. (a) LM Method and (b) Chaos-LM Method.

Results from 100 runs show that the combination of CO and LM methods increases accuracy of the fitting process. The indication is that the fitted geometry has a reduced residual error, in term of the magnitude of the norm of sum of the squared residuals $\|r\|$ while preserving the computation cost. Table 2 provides the complete results of the fitting results both with only LM method and Chaos-LM method. Chaos-LM encourages the initial guess of the solution to move to a better starting point thanks to the property of the chaotic motion which non-repeatedly searches through set of states in a certain bounded domain [15]. Sensitiveness of the final solution of LM method to where we put our guess is related to the Taylor approximation in the Gauss-Newton method, which highly depends on the non-linearity degree of the neighbourhood. Some visualizations of the fitting result for sphere and cylinder are depicted in Fig. 5. From this, we can observe that the Chaos-LM (Fig. 5b) fitting lies on the middle of the point cloud. It is coherent with the fundamental behaviour of least-square fitting which is an average over the whole data. Plot of the norm of residual and CPU time are presented in figure 6.

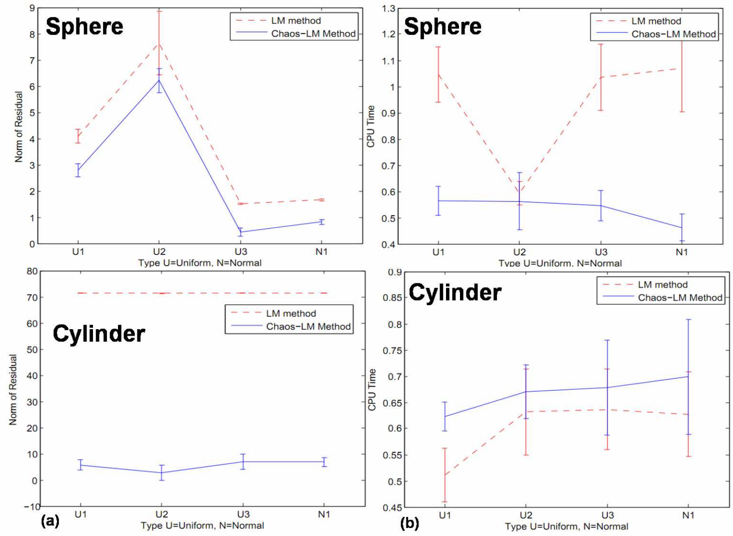

Fig. 6: (a) Norm of residual, (b) CPU time of the fitting.

Table 2: Simulation results of the geometric fitting.

Random Error Type (µm)	Levenberg-Marquardt Algorithm					
	Circle		Sphere		Cylinder	
	||r|| (µ±3σ)	CPU time (µ±3σ)	||r|| (µ±3σ)	CPU time (µ±3σ)	||r|| (µ±3σ)	CPU time (µ±3σ)
U [-2.2,2.2]	75.25 ±0.06	0.83 ±0.05	4.1 ±0.26	1.04 ± 0.10	71.42 ±0.06	0.51 ±0.05
U [-5,5]	75.26 ±0.05	0.8 ±0.02	7.65 ±1.21	0.59 ±0.04	71.43 ±0.12	0.63 ±0.08
N (σ=1.1)	75.22 ±0.016	0.82 ± .037	1.51 ±0.02	1.03 ±0.12	71.42 ±0.01	0.63 ±0.07
N (σ=2.5)	75.22 ±0.037	0.87 ±0.12	1.66 ±0.04	1.06 ±0.16	71.42 ±0.03	0.62 ±0.08
Random Error Type (µm)	**Chaos and Levenberg-Marquardt Algorithm**					
	Circle		Sphere		Cylinder	
	||r|| (µ±3σ)	CPU time (µ±3σ)	||r|| (µ±3σ)	CPU time (µ±3σ)	||r|| (µ±3σ)	CPU time (µ±3σ)
U [-2.2,2.2]	5.66 ±1.67	0.55 ±0.05	2.79 ±0.25	0.56 ±0.05	5.72 ±2.01	0.62 ±0.02
U [-5,5]	4.35 ±1.30	0.55 ±0.03	6.21 ±0.46	0.56 ±0.1	5.79 ±2.9	0.67 ±0.05
N (σ=1.1)	5.19 ±1.27	0.56 ±0.1	0.42 ±0.15	0.54 ± 0.05	6.93 ±2.96	0.67 ±0.09
N (σ=2.5)	5.4 ±1.46	0.54 ±0.08	0.81 ±0.09	0.46 ±0.05	6.91 ±1.65	0.69 ±0.11

5. CONCLUSIONS

The problem of fitting non-liner geometries of circle, sphere and cylinder, taking into account their common use has been addressed. This problem is critical in dimensional metrology to assure the quality of products. Results show that the use of chaos optimization to improve the initial guess for LM non-linear least square fitting has significantly improved the accuracy of the fitting by keeping the computational time.

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