Fitting two concentric spheres to data by orthogonal distance regression

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Abstract. *The problem of this research tackles the process of fitting two concentric spheres to data, which arises in computational metrology. There are also many fitting criteria that could be used effectively, and the most widely used one in metrology, for example, is that of the sum of squared minimal distance. However, a simple and robust algorithm assigned for using the orthogonal distance regression will be proposed in this paper. A common approach to this problem involves an iteration process which forces orthogonality to hold at every iteration and steps of Gauss-Newton type.*

Key words: *concentric spheres, orthogonal distance regression, Gauss-Newton method*

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1. Introduction

To find measured points in space two concentric spheres of the minimum difference in radii that contain all points between them is a problem in computational metrology [6, 9]. Let data $\mathbf{x}_i = (x_i, y_i, z_i), i = 1 \ldots, m$, be available. In order to make the problem of this paper more evident, it is recommended to assume that all points have errors. Moreover, to find two concentric spheres, it is suggested that such suitable criteria goes to its minimum level, where simultaneously each point has to be associated with one of the spheres [6].

The two concentric spheres are given in parametric representation as

$$\mathbf{x}(\mathbf{a}_p, \mathbf{t}) = \mathbf{c} + r \begin{bmatrix} \cos t_1 \sin t_2 \\ \sin t_1 \sin t_2 \\ \cos t_2 \end{bmatrix}, 0 \le t_1 < 2\pi, 0 < t_2 \le \pi \tag{1}$$

out of the smaller sphere, where $\mathbf{a}_p = (\mathbf{c}, r)^T$, $\mathbf{c} = (c_1, c_2, c_3)^T$ is the common centre, and r is the radius. Replacing $\mathbf{a}_p$ by $\mathbf{a}_q = (\mathbf{c}, R)^T$ in (1) gives the larger parametric

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sphere. The parametric representations are dependent upon the location parameter $\mathbf{t}$, which are independent of any coordinate system [11].

Fitting two concentric spheres to data is interpreted as a problem of orthogonal distance regression (ODR) in [6], which seems to have been the first suggested. The problem, in brief, is to find two subsets V and W of $1, \ldots, m$ with $V \cap W = \phi, V \cup W = \{1, \ldots, m\}, |V| \geq 4, |W| \geq 4$ such that the sum of squared minimal distances

$$S(V, W, \mathbf{a}) = \sum_{i \in V} \min_{\mathbf{t}} p_i^2(\mathbf{a}_p, \mathbf{t}) + \sum_{i \in W} \min_{\mathbf{t}} q_i^2(\mathbf{a}_q, \mathbf{t}) \tag{2}$$

is minimized, where $\mathbf{a} = (\mathbf{c}, r, R)^T$, V and W are the sets of given points associated with the smaller and larger spheres respectively, and where

$$\begin{aligned} p_i^2(\mathbf{a}_p, \mathbf{t}) &= (a + r\cos t_1 \sin t_2 - x_i)^2 + (b + r \sin t_1 \sin t_2 - y_i)^2 \\ &+ (c + r\cos t_2 - z_i)^2, \end{aligned}$$

and $q_i^2(\mathbf{a}_q, \mathbf{t})$ represent the larger sphere. The necessary condition, $\frac{\partial S}{\partial \mathbf{a}} = 0$, needs to solve a linear system of 5×5 equations for $\mathbf{a}$ at each iteration, until the tolerance is reduced to a sufficient small number. The algorithm of minimizing (2) for $\mathbf{t}$ is considered in section 4.

The purpose in this paper, is to fit two concentric spheres to data by an equivalent problem to [6], which becomes more appropriate when the data have independent identically distibuted errors [11]. The orthogonal distance regression problem, which is a nonlinear least squares problem, will be defined in next section. Further, the Jacobian matrix for the Gauss-Newton iteration and the starting points are defined in section 3. Furthermore, an algorithm and numerical results are considered in sections 4 and 5 respectively. In all cases in this paper, $\|.\|$ denotes the l_2 vector or matrix norm.

2. The ODR problem

The orthogonal distances vector represented in the following form

$$\boldsymbol{p}_i = \mathbf{x}_i - \mathbf{x}(\mathbf{a}_p, \mathbf{t}_i), \; i \in V,$$

refers to the smaller parametric sphere. Also, $\boldsymbol{q}_i, \; i \in W$ is used for the large one, which came as a result of replacing $\mathbf{a}_p$ by $\mathbf{a}_q$. Then the problem given in this paper is to find two subsets V, and W by minimizing

$$F(V, W, \mathbf{a}, \mathbf{t}) = \sum_{i \in V} \|\boldsymbol{p}_i(\mathbf{a}_p, \mathbf{t}_i)\|^2 + \sum_{i \in W} \|\boldsymbol{q}_i(\mathbf{a}_q, \mathbf{t}_i)\|^2, \tag{3}$$

with respect to $\mathbf{a} = (\mathbf{c}, r, R)^T \in R^5$ and $\mathbf{t}_i, \; i = 1, \ldots, m$.

Let $\mathbf{t}_i(\mathbf{a}_p), \; i \in V$ be such that for any $\mathbf{a}_p$, $\|\mathbf{x}_i - \mathbf{x}(\mathbf{a}_p, \mathbf{t}_i)\|$ is minimized with respect to $\mathbf{t}_i, i \in V$, and similarly for $\mathbf{t}_i(\mathbf{a}_q), i \in W$. Then the equivalent problem to (3) is the minimization with respect to $\mathbf{a} = (\mathbf{c}, r, R)^T \in R^5$ alone of

$$F(V, W, \mathbf{a}) = \sum_{i \in V} \|\boldsymbol{p}_i(\mathbf{a}_p, \mathbf{t}_i(\mathbf{a}_p))\|^2 + \sum_{i \in W} \|\boldsymbol{q}_i(\mathbf{a}_q, \mathbf{t}_i(\mathbf{a}_q))\|^2. \tag{4}$$

If we define, for simplicity, the vector $\boldsymbol{\delta} \in R^m$ which has ith component

$$\delta_i(\mathbf{a}) = \|\mathbf{x}_i - \mathbf{c} - r\boldsymbol{\alpha_i} - R\boldsymbol{\alpha_i}\|,$$

and $r = 0$ if $i \in W$, $R = 0$ if $i \in V$, where

$$\boldsymbol{\alpha_i} = \begin{bmatrix} \cos(t_{1i})\sin(t_{2i}) \\ \sin(t_{1i})\sin(t_{2i}) \\ \cos(t_{2i}) \end{bmatrix}.$$

Then the orthogonal distance regression problem is to find two subsets V, and W such as minimizing the objective function

$$F(V, W, \mathbf{a}) = \|\boldsymbol{\delta}\|^2. \tag{5}$$

This is a nonlinear problem which can be solved through the application of the Gauss-Newton method, or on of its variants, see for example [3, 4, 5, 10, 11, 12]. Then the subsets V and W can be determined by calculating, for each i, $\|\mathbf{p}_i\|$ and $\|\mathbf{q}_i\|$. If $\|\mathbf{p}_i\| < \|\mathbf{q}_i\|$, then $i \in V$, otherwise in W.

3. A Gauss-Newton step

The Gauss-Newton step $\mathbf{d}$ for minimizing (5) is given by finding

$$\min_{\mathbf{d}} \|\boldsymbol{\delta} + \nabla_{\mathbf{a}}\boldsymbol{\delta}\mathbf{d}\|^2,$$

where $\nabla_{\mathbf{a}}\delta \in R^{m\times 5}$ a Jacobian matrix has ith row, for any $\delta_i \neq 0$

$$\nabla_{\mathbf{a}}\delta_i = \begin{cases} -\frac{\mathbf{p}_i^T}{\|\mathbf{p}_i\|}\begin{bmatrix} I & \boldsymbol{\alpha}_i & \mathbf{0}\end{bmatrix} & \text{for } \; i \in V, \\ -\frac{\mathbf{q}_i^T}{\|\mathbf{q}_i\|}\begin{bmatrix} I & \mathbf{0} & \boldsymbol{\alpha}_i\end{bmatrix} & \text{for } \; i \in W, \end{cases} \tag{6}$$

by definition of $\mathbf{t}_i(\mathbf{a})$, and I signifies the identity matrix of order 3. Using the expression in the right-hand side of (6), the correct vector of partial derivatives of δ_i is easily calculated.

It is necessary to provide primary values for any iterative algorithm. Actually, it is preferable to minimize the procedures of determining the initial values of $\mathbf{a}^{(0)}$, which is considered in [6], in order to cut the long story short. The initial centre $\mathbf{c}$ can be determined by the data mean. The primary values assigned for radii can be found in the following equations

$$r^{(0)} = \frac{1}{f}h, \quad R^{(0)} = fH, \quad 0 < f < 1, \tag{7}$$

where h, H are the minimal and maximal distance of the data points to the starting centre, respectively. The scalar f is used on the basis of the assumption that not all points with errors are estimated to be lying between the inner and outer sphere, and for $R^{(0)} > r^{(0)}$.

4. An algorithm

The contents of the last two sections give the ingredients of algorithms which can be used to solve the orthogonal distance regression problem. For example, we could consider an algorithm as follows

STEP 0. Input: The data $\mathbf{x}_i$,$V^{(0)}$,$W^{(0)}$, and a tolerance (**Tol**).

STEP 1. Determine: the initial values of $\mathbf{a}^{(0)}$.

STEP 2. Determine:

- $\mathbf{t}_i(\mathbf{a}),\ i = 1, \ldots, m.$
- The nearest points on the two concentric spheres.
- $\boldsymbol{\delta}(\mathbf{a})$.
- The objective function: F.
- The Jacobian matrix:$\nabla_{\mathbf{a}}\boldsymbol{\delta}(\mathbf{a})$.

STEP 3. Solve: $\|\boldsymbol{\delta}(\mathbf{a}) + \nabla_{\mathbf{a}}\boldsymbol{\delta}(\mathbf{a})\mathbf{d}\|^2$ for $\mathbf{d}$.

- **if** $\|\mathbf{d}\|_\infty <$ **Tol** , **Then** Go to **STEP 7**.

STEP 4. Use line search.

STEP 5. Determine: $V^{(k)}$ and $W^{(k)}$.

STEP 6. Go to **STEP 2**.

STEP 7. The process of fitting the two concentric spheres using ODR has been completed.

The least squares solution is used to determine the values of $\mathbf{t}_i(\mathbf{a}),\ i = 1, \ldots, m$, see for example [6, 7], the algorithm [1]

$$t_{i1} = \arctan |\frac{y_i - c_2}{x_i - c_1}|.$$

- **If** $x_i - c_1 < 0$, **then** $t_{i1} = t_{i1} + \pi$.
- **If** $x_i - c_1 = 0$, **then**
  - $t_{i1} = \frac{\pi}{2}$, **if** $y_i - c_2 \geq 0$.
  - $t_{i1} = \frac{3}{2}\pi$, **if** $y_i - c_2 < 0$.

$$t_{i2} = \arctan |\frac{(x_i - c_1)\cos(t_{i1}) + (y_i - c_2)\sin(t_{i1})}{z_i - c_3}|$$

- **If** $z_i - c_3 < 0$, **then** $t_{i2} = t_{i2} + \pi$,.
- **If** $z_i - c_3 = 0$, **then**
  - $t_{i2} = \frac{\pi}{2}$, if $(x_i - c_1)\cos(t_{i1}) + (y_i - c_2)\sin(t_{i1}) > 0$.
  - $t_{i2} = \frac{3}{2}\pi$, if $(x_i - c_1)\cos(t_{i1}) + (y_i - c_2)\sin(t_{i1}) < 0$.

5. Numerical results

In order to verify the performance of the proposed algorithm, it is applied to some examples. Therefore, the plan adopted in this regard, is to compute a Gauss-Newton step $\mathbf{d}$ as indicated in the section 3, to be used as an approach to reduce the value of the objective function F, taking full steps, if possible. The performance shown in the examples is typical, with a second order rate of convergence usual. The factor $f = 0.8$ has been used to determine the initial radii, see (7). The symbol γ used in the following tables refers to the Gauss-Newton step $\mathbf{d}$'s length, and k refers to the iteration number.

Example 1 Consider the $\mathbf{x}_i,\ i = 1, \ldots, 16$ values given in Table 1, which has been considered in [6]. The Gauss-Newton method is applied with the line searching for fitting 16 points with two concentric spheres. The initial value of $\mathbf{a}^{(0)}$ was

$$\mathbf{a}^{(0)} = (1.6875, 2.1875, 1.3125, 2.9263, 5.5125)^T.$$

Table 2 shows the characterization of V and W, where an integer vector $\mathbf{f}$ with $f_i = 1$ if $i \in V$ and $f_i = 2$ if $i \in W$. This method gives $V = \{1, 2, \ldots, 8\}$ and $W = \{11, 12, \ldots, 16\}$ in 2 iterations, and converge to the global minimum in 6 iterations. Results are shown in Table 3. In the same time, the final sets of V and W by [6] take 35 iterations to determine, and 135 iterations to converge to the same minimum of applying the Gauss-Newton method with line search.

	1	-1	0	-1	2	2	4	5	1	-1	0	-1	3	2	5	6
x	2	1	3	4	2	3	1	1	2	1	3	5	2	3	1	1
	-1	0	-1	6	-1	-1	6	4	-2	-1	-2	7	-2	-2	6	5

Table 1: Example 1 data points

k	**f**															
0	1	1	1	2	1	1	2	2	1	1	1	2	1	1	2	2
1	1	1	1	1	1	1	2	1	2	2	2	2	2	2	2	2
2-6	1	1	1	1	1	1	1	1	2	2	2	2	2	2	2	2

Table 2: $\mathbf{f}$ within the iterations process

Example 2 The first subset, of size $|V|$, data points are generated, by taking a particular sphere. The second subset $|W|$ also generated in the same idea and same centre, but $R > r$, where $|V| = |W| = 50$. In other word, the data has been generated from the spheres $\mathbf{a} = (-2, 3, 1, 6, 7)^T$. Then random perturbations are introduced for these data. The initial subsets $V^{(0)}$ with $|V^{(0)}| = 70$ and $W^{(0)}$ with $|W^{(0)}| = 30$ have been determined by taking a random permutation of the integers from 1 to m, and the Matlab command "randperm" is used for this procedure. The initial approximation to $\mathbf{a}^{(0)}$ gives

$$\mathbf{a}^{(0)} = (-2.3853, 2.8976, -0.3254, 5.5841, 6.7438)^T.$$

k	a	b	c	r	R	F	$\|\mathbf{d}\|_\infty$	γ
1	1.4967	2.9712	2.6177	4.1826	4.7537	4.3229	1.3052	1
2	1.4439	3.0142	2.8949	4.1108	5.0542	0.59699	3.0056×10^{-1}	1
3	1.4480	2.7394	3.0126	4.1463	5.1282	0.18462	2.7484×10^{-1}	1
4	1.4452	2.7358	3.0125	4.1550	5.1357	0.18345	8.7263×10^{-3}	1
5	1.4452	2.7357	3.0125	4.1550	5.1357	0.18345	1.1021×10^{-5}	1
6	1.4452	2.7357	3.0125	4.1550	5.1357	0.18345	6.5115×10^{-8}	

Table 3: Example 1.

Results for fitting two concentric spheres to 100 points are shown in Table 4. The subsets V and W have been, as expected, with $V = \{1, 2, \ldots, 50\}$ and $W = \{51, 52, \ldots, 100\}$ in the second iteration. Other choices for $V^{(0)}$ and $W^{(0)}$ either sizes or data indexes give a similar behaviour.

k	a	b	c	r	R	F	$\|\mathbf{d}\|_\infty$	γ
1	-1.8617	3.0984	1.0791	6.3409	6.4127	25.498	1.4045	1
2	-1.8632	3.1113	1.1265	6.0087	6.9787	0.49438	5.6606×10^{-1}	1
3	-1.8633	3.1114	1.1266	6.0088	6.9789	0.49437	1.5797×10^{-4}	1
4	-1.8633e	3.1114	1.1266	6.0088	6.9789	0.49437	1.4517×10^{-7}	

Table 4: Example 2.

6. Conclusion

Fitting two concentric spheres to data by orthogonal distance regression is considered in this paper. One of the main differences between applying the Gauss-Newton method to the problem and the method which was applied by [6] is the number of linear equations need to solve at each iteration. Using the Gauss-Newton method needs to solve $m \times 5$ linear equations at each iteration. However, 5×5 linear equations at each iteration need to solve for applying [6].

Nevertheless, all the numerical results show that the use of the Gauss-Newton method with line search is very rigorous for solving ODR of two concentric spheres. It is worth noting that the number of iterations using the Gauss-Newton method with line search has proven to be small, when compared to [6] method. Moreover, The number of iterations on the orthogonal distance regression and the Gauss-Newton method with line search have been not generally affected by the value of m. The use of the results of [6] for starting point has proved to be crucial for the initial values of the problem.

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