

PERTURBATION ANALYSIS FOR CIRCLES, SPHERES, AND GENERALIZED HYPERSPHERES FITTED TO DATA BY GEOMETRIC TOTAL LEAST-SQUARES

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ABSTRACT. A continuous extension of the objective function to a projective space guarantees that for each data set there exists at least one hyperplane or hypersphere minimizing the average squared distance to the data. For data sufficiently close to a hypersphere, as the collinearity of the data increases, so does the sensitivity of the fitted hypersphere to perturbations of the data.

1. INTRODUCTION

The problem of fitting a circle to data arises in several applications, for instance, in archeology [19], engineering [14, p. 12], and particle physics [2], [5], [6], [13]. One class of methods of solution, called methods of *algebraic total least-squares* (ATLS), fits in the sense of linear least-squares the coefficients of some polynomial equation defining a circle [1, p. 358], [3], [4], [5], [8], [9], [10, pp. 191–198], [14], [16], [18]. The fitted circles are then called *algebraic fits*. However, some authors have found such algebraic methods unsatisfactory [8], [13]. A potentially more satisfactory class of methods, called “geometric” methods, minimizes a geometric objective. For instance, the method of *geometric total least-squares* (GTLS) minimizes the sum (or average) of the squared distances from the data to the fitted circle, which is called a *geometric fit* [1, p. 357], [8]. Unfortunately, this class of geometric methods “leads to intractable equations” [5, p. 223], [19, p. 750], [20]. Moreover, such methods can exhibit an unacceptable sensitivity to perturbations if the data cover only a short arc of a circle [5, p. 224]. At the limit such geometric methods fail for collinear data, because then there does not exist any best fitting circle. Furthermore, whereas algebraic methods lend themselves to every established perturbation analysis for linear (constrained, multiple, ordinary, or total) least-squares [1, §1.4], [12, §19.7], [15], [22, Ch. 7], the literature contains little information about the existence, uniqueness, and perturbation analyses for circles fitted geometrically.

Therefore, the following considerations extend such geometric methods seamlessly to circles and lines in the plane and provide a corresponding perturbation analysis. Thanks to a vectorial notation, the derivations and hence the results are

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exactly the same for spheres and planes in space and for hyperspheres and hyperplanes — collectively called *generalized hyperspheres* — of unit codimension in Euclidean spaces of any dimension.

2. LOCAL EXISTENCE AND UNIQUENESS OF GTLS HYPERSPHERES

For each positive integer L , denote by \mathbb{R}^L the L -dimensional Euclidean space, with its inner product $\langle \cdot, \cdot \rangle$ and norm $\|\cdot\|_2$. Also, for each point $\vec{z} \in \mathbb{R}^L$ and for each $r \geq 0$, denote by $\mathcal{S}^{L-1}(\vec{z}, r)$ the hypersphere with radius r and center at \vec{z} :

$$(1) \quad \mathcal{S}^{L-1}(\vec{z}, r) := \{\vec{x} \in \mathbb{R}^L : \|\vec{x} - \vec{z}\|_2 = r\}.$$

For each positive integer N , and for each data sequence $X := (\vec{x}_1, \dots, \vec{x}_N)$ of N distinct points in \mathbb{R}^L , the method of geometric total least-squares attempts to determine the hypersphere minimizing the sum of the squared distances to the data. The problem thus consists of minimizing the function $f : \mathbb{R}^{L+1} \rightarrow \mathbb{R}$ defined by

$$(2) \quad f(\vec{z}, r) := \sum_{k=1}^N (\|\vec{z} - \vec{x}_k\|_2 - r)^2.$$

An abbreviated notation will henceforth omit references to the center \vec{z} , the radius r , and the data X . For instance, the following quantities depend on \vec{z} , r , and X :

$$(3) \quad \vec{r}_k := \vec{z} - \vec{x}_k,$$

$$(4) \quad r_k := \|\vec{z} - \vec{x}_k\|_2,$$

$$(5) \quad \vec{\rho}_k := \frac{\vec{r}_k}{r_k},$$

$$(6) \quad \bar{r} := \frac{1}{N} \sum_{k=1}^N r_k,$$

$$(7) \quad \bar{\rho} := \frac{1}{N} \sum_{k=1}^N \vec{\rho}_k.$$

Lemma 1. *For all positive integers K and M , and for each finite sequence $W := (\vec{w}_1, \dots, \vec{w}_M) \in \mathbb{R}^{K \times M}$, the point that minimizes the sum of the squares of the distances to the elements of W is the mean $\bar{\vec{w}} = (1/M) \sum_{k=1}^M \vec{w}_k$.*

Proof. For each vector $\vec{w}_0 \in \mathbb{R}^K$, linear algebra gives

$$(8) \quad \sum_{k=1}^M \|\vec{w}_k - \vec{w}_0\|_2^2 = \sum_{k=1}^M \|(\vec{w}_k - \bar{\vec{w}})\|_2^2 + M \|(\bar{\vec{w}} - \vec{w}_0)\|_2^2 \geq \sum_{k=1}^M \|(\vec{w}_k - \bar{\vec{w}})\|_2^2,$$

with equality if and only if $\vec{w}_0 = \bar{\vec{w}}$. \square

Algebraic simplifications result from the following corollary, which eliminates r .

Corollary 2. *For each center \vec{z} , the radius r minimizing f is the mean \bar{r} .*

Proof. Apply Lemma 1 to $K := 1$, $M := N$, and $\vec{w}_k := r_k$. \square

Thus, if f has a minimum at (\vec{z}, r) , then $r = \bar{r}$, whence it suffices to determine the minimum of the objective function $g : \mathbb{R}^L \rightarrow \mathbb{R}$ defined by $g(\vec{z}) := f(\vec{z}, \bar{r})$:

$$(9) \quad g(\vec{z}) = \sum_{k=1}^N [r_k - \bar{r}]^2 = N \left[\overline{(r^2)} - (\bar{r})^2 \right].$$

With $I_{L \times L}$ denoting the $L \times L$ identity matrix and the superscript T denoting transposition, calculus gives the following expressions for the gradient $\vec{\nabla}g$, its partial derivatives $\partial(\vec{\nabla}g)/\partial\vec{x}_\ell$, the Laplacian Δg , and the Hessian $\mathcal{H}g$ of g :

$$(10) \quad \vec{\nabla}g = \frac{2}{N} \sum_{k=1}^N (r_k - \bar{r}) \vec{\rho}_k;$$

$$(11) \quad \frac{\partial(\vec{\nabla}g)}{\partial\vec{x}_\ell} = \left(\frac{\bar{r}}{r_\ell} - \frac{1}{N} \right) \vec{\rho}_\ell \vec{\rho}_\ell^T + \left(1 - \frac{\bar{r}}{r_\ell} \right) I_{L \times L};$$

$$(12) \quad \Delta g = 2N \left[L - \left\{ \|\vec{\rho}\|_2^2 + \bar{r} \cdot \left(\frac{1}{N} \sum_{\ell=1}^N \frac{1}{r_\ell} \right) \right\} \right];$$

$$(13) \quad \mathcal{H}g = \sum_{k=1}^N \left[(\vec{\rho}_k - \vec{\rho})(\vec{\rho}_k - \vec{\rho})^T + \left(1 - \frac{\bar{r}}{r_k} \right) (I_{L \times L} - \vec{\rho}_k \vec{\rho}_k^T) \right].$$

Every point, curve, surface, or manifold that minimizes the sum of the squared distances to a set of data will be abbreviated as a *GTLS* point, curve, surface, or manifold. By Lemma 1 a point is a GTLS point if and only if it is the mean, and by definition a hypersphere is a GTLS hypersphere if and only if it minimizes f or g .

In such applications as those mentioned in the introduction, the mathematical model constrains all the points to lie on a hypersphere S , and the data represent perturbations of the model. For sufficiently small perturbations of the model, the following results confirm that there exists exactly one GTLS hypersphere “near” S .

Theorem 3. *If the data $X := (\vec{x}_1, \dots, \vec{x}_N) \in \mathbb{R}^{L \times N}$ lie on exactly one hypersphere $S^{L-1}(\vec{z}, r)$ with $r > 0$, then there exist neighborhoods $U \subseteq \mathbb{R}^{L \times N}$ of X and $V \subseteq \mathbb{R}^L$ of \vec{z} such that for each perturbed data sequence $\tilde{X} \in U$, the Hessian matrix $\mathcal{H}g$ remains positive definite in V , and there exists exactly one GTLS hypersphere $S^{L-1}(\vec{z}, \tilde{r})$ with $\vec{z} \in V$ minimizing the sum of the squares of the distances to \tilde{X} .*

Proof. If every \vec{x}_k lies on the hypersphere $S^{L-1}(\vec{z}, r)$, then $r_k = \bar{r} = r$, whence

$$(14) \quad 1 - \frac{\bar{r}}{r_k} = 1 - \frac{r}{r} = 0$$

for every $k \in \{1, \dots, N\}$. Substituting equation (14) in equation (13) gives

$$(15) \quad \mathcal{H}g = \sum_{k=1}^N (\vec{\rho}_k - \vec{\rho})(\vec{\rho}_k - \vec{\rho})^T = \Gamma^T \Gamma,$$

with a matrix $\Gamma \in \mathbb{M}_{N \times L}(\mathbb{R})$ defined by

$$(16) \quad \Gamma^T := (\vec{\rho}_1 - \vec{\rho}, \dots, \vec{\rho}_N - \vec{\rho}).$$

The matrix Γ is singular if and only if there is a unit vector $\vec{v} \in \mathbb{R}^L$ with $\Gamma \vec{v} = \vec{0}$, so that all the normalized data $\vec{\rho}_k - \vec{\rho}$ lie on the hyperplane normal to \vec{v} through $\vec{\rho}$. If the data lie on exactly one hypersphere but not on two distinct hyperspheres, then they do not lie on a hyperplane, whence Γ is regular and $\mathcal{H}g = \Gamma^T \Gamma$ is positive definite. The conclusion follows from the Implicit-Function Theorem [7, p. 148]. \square

If the data lie on a hyperplane but not on any hypersphere, then the average squared distance from this hyperplane equals zero, but it remains positive for any hypersphere. For hyperspheres tangent to this hyperplane at the mean of the data and with centers diverging to infinity, the average squared distance tends to zero. In such a situation g has an infimum but no global minimum.

3. GLOBAL EXISTENCE OF GTLS GENERALIZED HYPERSPHERES

Extending g to a projective space including hyperspheres and hyperplanes guarantees the existence of at least one global minimum. To this end, let the real projective space $\mathbb{P}(\mathbb{R}^{L+1})$ consist of all the equivalence classes $[x_1, \dots, x_L, x_{L+1}]$ of points $(x_1, \dots, x_L, x_{L+1}) \in \mathbb{R}^{L+1} \setminus \{\vec{0}\}$. Then $(x_1, \dots, x_L, x_{L+1})$ and $(w_1, \dots, w_L, w_{L+1})$ are equivalent if and only if one of them is a nonzero multiple of the other.

Lemma 4. *The function g extends to a continuous function \check{g} on $\mathbb{P}(\mathbb{R}^{L+1})$, defined for every $[\vec{z}, z_{L+1}] \in \mathbb{P}(\mathbb{R}^{L+1})$ by*

$$(17) \quad \check{r}_k := \frac{2\langle \vec{x}_k, \vec{z} \rangle - z_{L+1} \|\vec{x}_k\|_2^2}{\|\vec{z}\|_2 + \sqrt{\sum_{\ell=1}^N (z_\ell - x_{k,\ell} \cdot z_{L+1})^2}},$$

$$(18) \quad \check{r} := \frac{1}{N} \sum_{k=1}^n \check{r}_k,$$

$$(19) \quad \check{g}([\vec{z}, z_{L+1}]) := \sum_{k=1}^N (\check{r}_k - \check{r})^2.$$

Proof. Homogenous coordinates and algebra show that

$$(20) \quad r_k = \|\vec{z} - \vec{x}\|_2 = \frac{\|\vec{z}\|_2}{|z_{L+1}|} + \frac{2\langle \vec{x}_k, \vec{z} \rangle - z_{L+1} \|\vec{x}_k\|_2^2}{\|\vec{z}\|_2 + \sqrt{\sum_{\ell=1}^N (z_\ell - x_{k,\ell} z_{L+1})^2}}.$$

Then all the terms $\|\vec{z}\|_2/|z_{L+1}|$ cancel one another in the formula (19) for \check{g} . □

The extension \check{g} provides a continuous transition from spheres to hyperplanes.

Theorem 5. *For each unit vector $\vec{u} \in \mathbb{R}^L$, if the center \vec{z} diverges to infinity in the direction \vec{u} , then $\check{g}([\vec{z}, 1])$ tends to the sum of the squared distances from the data to the hyperplane H normal to \vec{u} through the mean $\vec{\bar{x}} := (1/N) \sum_{k=1}^N \vec{x}_k$.*

Proof. If $\vec{z} = c\vec{u}$ and c diverges to infinity, then dividing $(z_1, \dots, z_L, z_{L+1})$ by c lets z_{L+1} tend to zero and keeps the first L coordinates equal to \vec{u} . Inserting this limit into the formulas (17), (18), (19) defining \check{g} gives

$$(21) \quad \lim_{z_{L+1} \rightarrow 0} \check{g}([\vec{z}, z_{L+1}]) = \sum_{k=1}^N \left(\frac{\langle \vec{x}_k, \vec{z} \rangle}{\|\vec{z}\|_2} - \frac{1}{N} \sum_{\ell=1}^N \frac{\langle \vec{x}_\ell, \vec{z} \rangle}{\|\vec{z}\|_2} \right)^2$$

$$(22) \quad = \sum_{k=1}^N \frac{\langle \vec{x}_k - \vec{\bar{x}}, \vec{u} \rangle^2}{\|\vec{u}\|_2^2},$$

which is the sum of the squared distances from the data to H . □

The preceding results lead to the existence of at least one global minimum.

Theorem 6. *For each sequence of distinct points $(\vec{x}_1, \dots, \vec{x}_N) \in \mathbb{R}^{L \times N}$, the objective function \check{g} has at least one global minimum at some $[\vec{z}; z_{L+1}] \in \mathbb{P}(\mathbb{R}^{L+1})$. Moreover, if $z_{L+1} = 0$ at a global minimum, then the global minimum corresponds to the hyperplane fitted to the data by geometric total least-squares.*

Proof. The existence follows from the continuity of \check{g} on the compact space $\mathbb{P}(\mathbb{R}^{L+1})$. If the minimum occurs at a point $[\vec{z}; z_{L+1}]$ where $z_{L+1} = 0$, then the formula (22) for the limit $\sum_{k=1}^N \langle \vec{x}_k - \vec{\bar{x}}, \vec{\bar{u}} \rangle^2 / \|\vec{\bar{u}}\|_2^2$ is precisely the sum of the squares of the distances to the hyperplane H with equation $\langle \vec{x} - \vec{\bar{x}}, \vec{\bar{u}} \rangle = 0$, where $\vec{\bar{u}} = (1/\|\vec{z}\|_2)\vec{z}$. \square

The global minimum of g need not be unique, however. For example, if the data lie on a circle in space, then there exists a continuum of spheres containing the circle, and for each such sphere g takes its global minimum value: zero.

4. GLOBAL UNIQUENESS OF GTLS GENERALIZED HYPERSPHERES

In such applications as those described in the introduction, the mathematical model constrains all the points to lie on a hypersphere, and the data represent perturbations of the model. For sufficiently small perturbations of the model, the following results confirm that there exists exactly one GTLS hypersphere anywhere.

Lemma 7. *The function g does not have a local minimum at any data point.*

Proof. At each data point \vec{x}_ℓ , expanding expression (9) for g and collecting all the terms that are differentiable at \vec{x}_ℓ leaves a single negative nondifferentiable term $(-2 \sum_{k \neq \ell} r_k) r_\ell$, where the sum $\sum_{k \neq \ell} r_k$ is either empty and hence equal to 0, or strictly positive because all the data points are distinct. Thus, if $\vec{z} = \vec{x}_\ell$, then $r_k = \|\vec{x}_\ell - \vec{x}_k\|_2 > 0$ for every $k \neq \ell$. Consequently, along every line through \vec{x}_ℓ , the restriction of g has a slope that changes by $-2 \sum_{k \neq \ell} r_k < 0$ at \vec{x}_ℓ . Hence this slope cannot pass from nonpositive values before to nonnegative values after \vec{x}_ℓ . \square

Lemma 8. *For each data sequence $(\vec{x}_1, \dots, \vec{x}_N) \in \mathbb{R}^{L \times N}$ with $N > L$, define*

$$(23) \quad m := \min\{\|\vec{x}_k - \vec{x}_\ell\|_2 : 1 \leq k < \ell \leq N\}.$$

Then g has no local minimum inside $S^{L-1}(\vec{x}_\ell, \lfloor N/2 \rfloor m / \lfloor NL \rfloor)$ for any $\ell \in \{1, \dots, N\}$.

Proof. For every pair of distinct indices $k \neq \ell$ in $\{1, \dots, N\}$,

$$(24) \quad r \leq \|\vec{x}_k - \vec{x}_\ell\|_2 \leq \|\vec{x}_k - \vec{z}\|_2 + \|\vec{z} - \vec{x}_\ell\|_2 = r_k + r_\ell.$$

Hence adding distances pairwise instead of recursively gives

$$(25) \quad \sum_{k=1}^N r_k \geq \sum_{\ell=1}^{\lfloor N/2 \rfloor} (r_{2\ell-1} + r_{2\ell}) = \lfloor N/2 \rfloor m.$$

If $r_\ell < \lfloor N/2 \rfloor m / (NL)$, then $1/r_\ell > NL / (\lfloor N/2 \rfloor m)$, whence

$$(26) \quad \left(\frac{1}{N} \sum_{k=1}^N r_k \right) \left(\frac{1}{N} \sum_{k=1}^N \frac{1}{r_\ell} \right) > \left(\frac{\lfloor N/2 \rfloor m}{N} \right) \left(\frac{1}{N} \frac{NL}{\lfloor N/2 \rfloor m} \right) = L.$$

Equation (12) for the Laplacian now shows that $\Delta g < 0$, so that g has no local minimum at any \vec{z} where $\|\vec{z} - \vec{x}_\ell\|_2 < \lfloor N/2 \rfloor m / (NL)$. \square

Thus g is differentiable near each minimum $\bar{\mathbf{z}}$. For sufficiently small perturbations, the next theorem guarantees the existence of exactly one GTLS hypersphere.

Theorem 9. *If the data $X := (\bar{\mathbf{x}}_1, \dots, \bar{\mathbf{x}}_N) \in \mathbb{R}^{L \times N}$ lie on exactly one hypersphere $\mathcal{S}^{L-1}(\bar{\mathbf{z}}, r)$ with radius $r > 0$, then there exists a neighborhood $W \subseteq \mathbb{R}^{L \times N}$ of X such that for each perturbed data sequence $\tilde{X} \in W$ there exists exactly one hypersphere $\mathcal{S}^{L-1}(\tilde{\mathbf{z}}, \tilde{r})$ minimizing the sum of the squares of the distances to \tilde{X} .*

Proof. If the data lie on exactly one hypersphere $\mathcal{S}^{L-1}(\bar{\mathbf{z}}, r)$, then $\bar{\mathbf{z}}$ is the unique zero of g . Also, there exist open neighborhoods $U \subseteq \mathbb{R}^{L \times N}$ of the data X , and $V \subseteq \mathbb{R}^L$ of the center $\bar{\mathbf{z}}$, such that for every data sequence $\tilde{X} \in U$, there exists a unique GTLS hypersphere $\mathcal{S}^{L-1}(\tilde{\mathbf{z}}, \tilde{r})$ with $\tilde{\mathbf{z}} = Z(\tilde{X}) \in V$, where $Z : U \rightarrow V$ is the implicit function from Theorem 3. Moreover, because the data do not lie on a hyperplane, $\liminf_{\bar{\mathbf{z}} \rightarrow \infty} g(\bar{\mathbf{z}}) = \sigma_L^2(\Gamma) > 0$ by Theorem 5. Consequently, by compactness of $\mathbb{P}(\mathbb{R}^{L+1}) \setminus (V \times \{1\})$, there exists a positive η such that $\check{g}(\bar{\mathbf{w}}, w_{L+1}) \geq \eta$ for every $[\bar{\mathbf{w}}, w_{L+1}]$ outside of $V \times \{1\}$. By the joint continuity of \check{g} relative to X and $\bar{\mathbf{z}}$, it follows that there exists a neighborhood $R \subseteq U$ of X with $g(\tilde{X}, \bar{\mathbf{w}}) \geq \eta/2$ for every $\tilde{X} \in R$ and $\bar{\mathbf{w}} \notin V$. Furthermore, from $(g \circ Z)(X) = g(\bar{\mathbf{z}}) = 0$, the Implicit-Function Theorem shows that there exists an open neighborhood $S \subseteq U$ of X such that $(g \circ Z)(\tilde{X}) < \eta/4$ for every $\tilde{X} \in S$. Let $W := R \cap S$. Then for each data sequence $\tilde{X} \in W$, the function \check{g} has a unique local minimum in V at $\tilde{\mathbf{z}} := Z(\tilde{X}) \in V$, where $g(\tilde{\mathbf{z}}) < \eta/4$, while $g(\bar{\mathbf{w}}) \geq \eta/2$ at every $\bar{\mathbf{w}} \notin V$. Consequently, $Z(\tilde{X})$ is also a global minimum of \check{g} , which thus has exactly one global minimum, at $Z(\tilde{X})$. \square

5. BACKWARD ANALYSIS FOR HYPERPLANES

For each data sequence $X := (\bar{\mathbf{x}}_1, \dots, \bar{\mathbf{x}}_N)$, a hyperplane H minimizes the sum of the squared distances to the data if and only if it passes through the mean $\bar{\bar{\mathbf{x}}}$ perpendicularly to a right-singular vector $\bar{\mathbf{v}}_L$ for the smallest singular value σ_L of the matrix $M(X)$ defined by centering the data around the mean [17]:

$$(27) \quad M(X)^T := (\bar{\mathbf{x}}_1 - \bar{\bar{\mathbf{x}}}, \dots, \bar{\mathbf{x}}_N - \bar{\bar{\mathbf{x}}}),$$

and σ_L^2 is the sum of the squared distances from the data to H . Data perturbations from X to $\tilde{X} := (\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_N)$ alter the mean from $\bar{\bar{\mathbf{x}}}$ to $\bar{\tilde{\mathbf{x}}}$ [11, p. 39] and alter the matrix from $M(X)$ to $M(\tilde{X})$. From Wedin’s “generalized $\sin(\theta)$ theorem” [23, p. 102], the change $\Delta \bar{\mathbf{v}}_L := \tilde{\mathbf{v}}_L - \bar{\mathbf{v}}_L$ in the unit normal is bounded above by

$$(28) \quad \|\Delta \bar{\mathbf{v}}_L\|_2 \leq \frac{\|M(X) - M(\tilde{X})\|_2}{\sigma_{L-1}[M(\tilde{X})] - \sigma_L[M(X)]}.$$

Also, a theorem of Weyl’s [21, p. 562] leads to an upper bound for the induced perturbation on the singular values, for every $j \in \{1, \dots, L\}$:

$$(29) \quad |\sigma_j[M(\tilde{X})] - \sigma_j[M(X)]| \leq \|M(X) - M(\tilde{X})\|_2.$$

With $\Delta M := M(X) - M(\tilde{X})$, $\|M(X)\|_2 = \sigma_1[M(X)]$, and $\|\bar{\mathbf{v}}_L\|_2 = 1$, it follows that the relative change $\|\Delta \bar{\mathbf{v}}_L\|_2 / \|\bar{\mathbf{v}}_L\|_2$ remains below the upper bound

$$(30) \quad \frac{\|\Delta \bar{\mathbf{v}}_L\|_2}{\|\bar{\mathbf{v}}_L\|_2} \leq \frac{\|\Delta M\|_2}{\|M(X)\|_2} \frac{\sigma_1[M(X)]}{\{\sigma_{L-1}[M(X)] - \|\Delta M\|_2\} - \sigma_L[M(X)]}.$$

Consequently,

$$(31) \quad \limsup_{\|\Delta M\|_2 \rightarrow 0} \frac{\|\Delta \vec{v}_L\|_2 / \|\vec{v}_L\|_2}{\|\Delta M\|_2 / \|M(X)\|_2} \leq \frac{\sigma_1[M(X)]}{\sigma_{L-1}[M(X)] - \sigma_L[M(X)]}.$$

Thus, the number

$$(32) \quad \kappa[M(X)] := \frac{\sigma_1[M(X)]}{\sigma_{L-1}[M(X)] - \sigma_L[M(X)]}$$

is a condition number [1, p. 38] for the sensitivity of GTLS hyperplanes. The vanishing of the denominator $\sigma_{L-1} - \sigma_L$ has the following geometric interpretation. All the data points lie on a hyperplane H_L if and only if $(\vec{x}_k - \bar{\vec{x}})^T \vec{v}_L = 0$ for every $k \in \{1, \dots, N\}$, which is equivalent to $M\vec{v}_L = \vec{0}$, which occurs if and only if $\sigma_L = 0$. Similarly, $\sigma_{L-1} = 0$ if and only if all the data also lie on another hyperplane H_{L-1} , normal to \vec{v}_{L-1} , and hence if and only if all the data lie along their intersection $H_L \cap H_{L-1}$. The following theorem generalizes this geometric interpretation to $\sigma_{L-1} \approx \sigma_L$ but not necessarily 0. To this end, for each point $\vec{x} \in \mathbb{R}^L$ and for each subset $C \subseteq \mathbb{R}^L$, define the distance from \vec{x} to C by

$$(33) \quad d(\vec{x}, C) := \inf\{d(\vec{x}, \vec{c}) : \vec{c} \in C\}.$$

Theorem 10. For each affine submanifold $C \subset \mathbb{R}^L$ of codimension 2,

$$(34) \quad \sum_{k=1}^N [d(\vec{x}_k, C)]^2 \geq \sigma_{L-1}^2 + \sigma_L^2.$$

Proof. Each affine submanifold $C \subset \mathbb{R}^L$ of codimension 2 is the intersection of two mutually perpendicular hyperplanes A and B . Moreover, for each point $\vec{x} \in \mathbb{R}^L$, the affine submanifold $C_{\vec{x}}^\perp$ through \vec{x} and perpendicular to C is a two-dimensional plane, which intersects A and B along two mutually perpendicular lines meeting at $C \cap C_{\vec{x}}^\perp$. In this plane $C_{\vec{x}}^\perp$, the Pythagorean Theorem shows that

$$(35) \quad [d(\vec{x}, C)]^2 = [d(\vec{x}, A)]^2 + [d(\vec{x}, B)]^2.$$

Consequently,

$$(36) \quad \sum_{k=1}^N [d(\vec{x}_k, C)]^2 = \sum_{k=1}^N [d(\vec{x}_k, A)]^2 + \sum_{k=1}^N [d(\vec{x}_k, B)]^2 \geq \sigma_{L-1}^2 + \sigma_L^2,$$

with equality if and only if $\{A, B\} = \{H_{L-1}, H_L\}$, possibly after reordering the singular spaces if $\sigma_{L-\ell} = \dots = \sigma_{L-1} = \sigma_L$ for some $\ell > 1$. \square

Theorem 10 thus reveals that $\sigma_{L-1} - \sigma_L = 0$ if and only if the GTLS affine manifold C of codimension 2 fits the data “exceptionally” well ($\sigma_{L-1}^2 + \sigma_L^2 = 2\sigma_L^2$), and then all the hyperplanes that contain C fit the data equally well. Therefore, the problem of determining “the” GTLS hyperplane is ill-conditioned for such data.

6. BACKWARD ANALYSIS FOR HYPERSPHERES

The present section derives upper bounds for the change in the fitted center \vec{z} caused by perturbations in the data $X = (\vec{x}_1, \dots, \vec{x}_N) \in \mathbb{R}^{L \times N}$. By its definition, the center \vec{z} minimizes the function g and hence solves the equation $\vec{\nabla}g(\vec{z}) = \vec{0}$. Thus \vec{z} is the value of a local implicit function $Z : \mathbb{R}^{L \times N} \rightarrow \mathbb{R}^L$ of the data $X = (\vec{x}_1, \dots, \vec{x}_N)$ (provided that the Hessian matrix $\mathcal{H}g$ is locally invertible). For the lack of any better notation, denote by $\partial\vec{z}/\partial\vec{x}_k \in \mathbb{M}_{L \times L}(\mathbb{R})$ the

matrix of partial derivatives of Z with respect to the coordinates of \vec{x}_k , so that $(\partial\vec{z}/\partial\vec{x}_k)_{p,q} = \partial(Z_p)/\partial(\vec{x}_k)_q$. The Implicit-Function Theorem then states that [7, p. 149]

$$(37) \quad \frac{\partial\vec{z}}{\partial\vec{x}_k} = (\mathcal{H}g)^{-1} \frac{\partial(\vec{\nabla}g)}{\partial\vec{x}_k}.$$

Any matrix-norm, for instance, the reciprocal $1/\lambda_L$ of the smallest singular value λ_L of $\mathcal{H}g$, measures the sensitivity of the fitted center to perturbations of the data:

$$(38) \quad \left\| \frac{\partial\vec{z}}{\partial\vec{x}_k} \right\|_2 \leq \left\| (\mathcal{H}g)^{-1} \right\|_2 \cdot \left\| \frac{\partial(\vec{\nabla}g)}{\partial\vec{x}_k} \right\|_2 = \frac{1}{\lambda_L} \left\| \frac{\partial(\vec{\nabla}g)}{\partial\vec{x}_k} \right\|_2.$$

For data that lie *on* a hypersphere, the Implicit-Function Theorem shows that the smallest singular-value of the Hessian matrix simultaneously measures the degree of collinearity of the data and the effect from perturbations of the data on the fitted hypersphere. (The perturbed data need not lie on any hypersphere.)

Theorem 11. *If $\vec{x}_k \in \mathcal{S}^{L-1}(\vec{z}, r)$ for every $k \in \{1, \dots, N\}$, then*

$$(39) \quad \left\| \frac{\partial\vec{z}}{\partial\vec{x}_k} \right\|_2 \leq \frac{1}{\sigma_L^2(\Gamma)}.$$

Proof. With $\vec{x}_k \in \mathcal{S}^{L-1}(\vec{z}, r)$ for every $k \in \{1, \dots, N\}$, substituting equation (14) in equation (11) shows that the norm of the term $\partial(\vec{\nabla}g)/\partial\vec{x}_k$ does not exceed unity:

$$(40) \quad \frac{\partial(\vec{\nabla}g)}{\partial\vec{x}_k} = \left(\frac{\bar{r}}{r_k} - \frac{1}{N} \right) \vec{\rho}_k \vec{\rho}_k^T + \left(1 - \frac{\bar{r}}{r_k} \right) I_{L \times L} = \left(1 - \frac{1}{N} \right) \vec{\rho}_k \vec{\rho}_k^T.$$

From $\|\vec{\rho}_k\|_2 = 1$, it follows that $|\langle \vec{x}, \vec{\rho}_k \rangle| \leq \|\vec{x}\|_2 \|\vec{\rho}_k\|_2 = \|\vec{x}\|_2$, with equality if and only if \vec{x} is a nonnegative multiple of $\vec{\rho}_k$. Hence, for the subordinate matrix norm,

$$(41) \quad \left\| \frac{\partial(\vec{\nabla}g)}{\partial\vec{x}_k} \right\|_2 = \left(1 - \frac{1}{N} \right).$$

Moreover, $\mathcal{H}g = \Gamma^T \Gamma$ with $\Gamma^T = (\vec{\rho}_1 - \vec{\bar{\rho}}, \dots, \vec{\rho}_N - \vec{\bar{\rho}})$ by Theorem 3, whence

$$(42) \quad \left\| \frac{\partial\vec{z}}{\partial\vec{x}_k} \right\|_2 \leq \left\| (\mathcal{H}g)^{-1} \right\|_2 \cdot \left\| \frac{\partial(\vec{\nabla}g)}{\partial\vec{x}_k} \right\|_2 = \frac{1}{\sigma_L^2(\Gamma)} \left(1 - \frac{1}{N} \right) \leq \frac{1}{\sigma_L^2(\Gamma)}.$$

□

Thus the sensitivity of the fitted center to data perturbations increases inversely proportionally to the sum of the squared distances to the GTLS hyperplane. In the foregoing considerations, the sequence $X := (\vec{x}_1, \dots, \vec{x}_k)$ can play the role of a mathematical model, or of data representing perturbations of the model. For each sequence of data $P := (\vec{p}_1, \dots, \vec{p}_N) \in \mathbb{R}^{L \times N}$ and *any* hypersphere $\mathcal{S}^{L-1}(\vec{z}, r) \subset \mathbb{R}^L$, the perturbation analysis proposed here uses a GTLS *line* as follows.

- (1) With $\vec{\rho}_k := (1/\|\vec{p}_k - \vec{z}\|_2)(\vec{p}_k - \vec{z})$, form the matrix Γ with columns $\vec{\rho}_k - \vec{\bar{\rho}}$.
- (2) Compute the reciprocal $1/\sigma_L$ of the smallest singular value σ_L of Γ .
- (3) Theorem 11 yields the estimate

$$(43) \quad \limsup_{\|\Delta X\| \rightarrow 0} \frac{\|\Delta\vec{z}\|}{\|\Delta X\|} \leq \frac{1}{\sigma_L^2(\Gamma)}.$$

(4) Let $Q := (\vec{\mathbf{q}}_1, \dots, \vec{\mathbf{q}}_N)$ denote the projections of the data P on $\mathcal{S}^{L-1}(\vec{\mathbf{z}}, r)$:

$$(44) \quad \vec{\mathbf{q}}_k = \vec{\mathbf{z}} + \frac{r}{\|\vec{\mathbf{p}}_k - \vec{\mathbf{z}}\|_2}(\vec{\mathbf{p}}_k - \vec{\mathbf{z}}).$$

(5) Substituting the norm of the perturbation of the data

$$(45) \quad \|\Delta X\| := \sum_{k=1}^N \|\vec{\mathbf{q}}_k - \vec{\mathbf{p}}_k\|_2$$

gives the first-order estimate

$$(46) \quad \|\Delta \vec{\mathbf{z}}\|_2 \approx \frac{1}{\sigma_L^2(\Gamma)} \|\Delta X\|.$$

The “backward analysis” is that the hypersphere $\mathcal{S}^{L-1}(\vec{\mathbf{z}}, r)$ is the unique exact solution to the problem of determining the GTLS hypersphere for the model $Q := (\vec{\mathbf{q}}_1, \dots, \vec{\mathbf{q}}_N)$, whereas the data $P := (\vec{\mathbf{p}}_1, \dots, \vec{\mathbf{p}}_N)$ represent perturbations of the model Q . Any subsequent perturbation of the data P to $\tilde{P} := (\tilde{\mathbf{p}}_1, \dots, \tilde{\mathbf{p}}_N)$ decomposes as a first perturbation from P to Q , followed by a second perturbation from Q to \tilde{P} , with $\|P - \tilde{P}\|_2 \leq 2\|\Delta X\|$. Thus, the factor $2\|\Delta X\|/\sigma_L^2(\Gamma)$ provides a differential estimate of the change in the center caused by data perturbations.

7. GEOMETRIC INTERPRETATION OF THE PERTURBATION ANALYSIS

Experiments show that the stability of the fitted circle diminishes as the circular arc λ containing the data decreases [5, p. 224], [13, p. 187]. The following results confirm that the condition number increases as $1/\lambda^2$. In higher dimensions, the same results apply to data confined to a spherical ring where the colatitude varies by at most λ . To this end, define a *slab* as a set bounded by two parallel hyperplanes.

Lemma 12. *Let ω denote the width of the thinnest slab that contains the normalized data $\vec{\rho}_1 - \vec{\rho}, \dots, \vec{\rho}_N - \vec{\rho}$ and is parallel to their GTLS hyperplane. Then*

$$(47) \quad \frac{\omega}{\sqrt{2}} \leq \sigma_L \leq \sqrt{N}\omega.$$

Proof. The distance $|\langle \vec{\rho}_k - \vec{\rho}, \vec{\mathbf{v}}_L \rangle|$ from each normalized point $\vec{\rho}_k$ to the GTLS hyperplane H_L does not exceed the width ω . Consequently,

$$(48) \quad \sigma_L^2 = \sum_{k=1}^N |\langle \vec{\rho}_k - \vec{\rho}, \vec{\mathbf{v}}_L \rangle|^2 \leq N\omega^2.$$

For an inequality in the reverse direction, set

$$(49) \quad p := \min_{1 \leq k \leq N} \langle \vec{\rho}_k - \vec{\rho}, \vec{\mathbf{v}}_L \rangle,$$

$$(50) \quad q := \max_{1 \leq k \leq N} \langle \vec{\rho}_k - \vec{\rho}, \vec{\mathbf{v}}_L \rangle.$$

Then $\omega = q - p$, whence

$$(51) \quad \omega^2 = (q - p)^2 \leq 2(p^2 + q^2) \leq 2 \sum_{k=1}^N |\langle \vec{\rho}_k - \vec{\rho}, \vec{\mathbf{v}}_L \rangle|^2 = 2\sigma_L^2. \quad \square$$

The sensitivity of the fitted circle to data perturbations is greater for data sets confined to the endpoints of an arc than for data sets nearly uniformly distributed along the arc. One method to distinguish between such distributions uses the intersection of the fitted hypersphere and the thinnest slab containing the data. For instance, data sets confined to the endpoints of an arc lie within a thin strip, whereas data sets nearly uniformly distributed along the arc require a wider strip.

Lemma 13. *If the thinnest slab containing the unit vectors $\vec{\rho}_1, \dots, \vec{\rho}_N$ intersects the unit hypersphere along a polar cap between the colatitudes 0 and $\lambda/2$, then*

$$(52) \quad \frac{1}{\sqrt{N}[\sin(\lambda/4)]^2} < \frac{1}{\sigma_L(\Gamma)} < \frac{1}{\sqrt{2}[\sin(\lambda/4)]^2}.$$

In the plane in particular, these inequalities hold if the thinnest strip containing the unit vectors $\vec{\rho}_1, \dots, \vec{\rho}_N$ intersects the unit circle along an arc of length λ .

Proof. The polar cap between the colatitudes 0 and $\lambda/2$ fits in a slab with width

$$(53) \quad w \geq 1 - \cos(\lambda/2) = 2[\sin(\lambda/4)]^2.$$

Therefore, the thinnest slab parallel to the GTLS hyperplane and containing the normalized data has width $\omega \geq w$. From Lemma 12, it follows that

$$(54) \quad \sigma_L^2 \geq \omega^2/2 \geq w^2/2 \geq 2[\sin(\lambda/4)]^4.$$

For an inequality in the reverse direction, consider the horizontal hyperplane H at height $[1 + \cos(\lambda/2)]/2$, midway into the polar cap. Then the distance from H to every point on the polar cap does not exceed $[1 - \cos(\lambda/2)]/2 = [\sin(\lambda/4)]^2$. Because the hyperplane of geometric total least-squares minimizes the sum of the squares of the distances, it follows that $\sigma_L^2 \leq N[\sin(\lambda/4)]^4$. Thus,

$$(55) \quad 2[\sin(\lambda/4)]^4 \leq \sigma_L^2 \leq N[\sin(\lambda/4)]^4. \quad \square$$

In contrast to data nearly uniformly distributed along an arc, data confined near the endpoints of an arc also lie near two shorter arcs about the same endpoints. In spaces of any dimensions, such data sets lie on a spherical ring.

Lemma 14. *If the thinnest slab containing the unit vectors $\vec{\rho}_1, \dots, \vec{\rho}_N$ intersects the unit hypersphere along a spherical ring between the colatitudes θ and $\theta + \lambda$, then*

$$(56) \quad \frac{1}{\sqrt{N} \sin[\theta + (\lambda/2)] \sin(\lambda/2)} < \frac{1}{\sigma_L(\Gamma)} < \frac{1}{\sqrt{2} \sin[\theta + (\lambda/2)] \sin(\lambda/2)}.$$

Proof. If the thinnest slab containing the data intersects the hypersphere along a spherical ring between the colatitudes θ and $\theta + \lambda$, which has width

$$(57) \quad w = \cos(\theta) - \cos(\theta + \lambda) = 2 \sin[\theta + (\lambda/2)] \sin(\lambda/2),$$

then from Lemma 12 it follows that

$$(58) \quad \sigma_L^2 \geq \omega^2/2 \geq w^2/2 \geq 2\{\sin[\theta + (\lambda/2)][\sin(\lambda/2)]\}^2.$$

For an inequality in the reverse direction, consider the hyperplane H at height $[\cos(\theta + \lambda) + \cos(\theta)]/2$, midway up the spherical ring. Then the distance from H to any data point does not exceed $[\cos(\theta + \lambda) - \cos(\theta)]/2 = \sin[\theta + (\lambda/2)] \sin(\lambda/2)$. Because the GTLS hyperplane minimizes the sum of the squares of the distances, it follows that $\sigma_L^2 \leq N\{\sin[\theta + (\lambda/2)] \sin(\lambda/2)\}^2$. Thus,

$$(59) \quad 2\{\sin[\theta + (\lambda/2)] \sin(\lambda/2)\}^2 \leq \sigma_L^2 \leq N\{\sin[\theta + (\lambda/2)] \sin(\lambda/2)\}^2. \quad \square$$

8. EXAMPLE

The following example illustrates an application of the foregoing analysis.

Example 15. Rorres and Romano fitted iteratively a GTLS circle to $N := 21$ data points on a starting line in an ancient Greek stadium in Corinth [19], as in Figure 1.

The first perturbation analysis (Theorem 11) uses the GTLS *line* fitted to the normalized projected data. For Rorres and Romano’s data P , the mean is $\bar{\rho} \approx (0.8220, 0.5655)$, and the unit normal to the GTLS line is $\bar{\nu}_2 \approx (0.8211, 0.5708)$, corresponding to $\sigma_2 = 0.008\,406\,9071$. Thus,

$$(60) \quad \frac{1}{\sigma_2^2} = \frac{1}{(0.008\,406\,9071)^2} \approx (118.950)^2 \approx 14149,$$

which means that perturbations of the data might be amplified by a factor of 14149 in the location of the center of the fitted GTLS *circle*. The much larger singular value $\sigma_1 = 0.30557536$ indicates that the GTLS *line* remains stable, with

$$(61) \quad \kappa = \frac{\sigma_1}{\sigma_1 - \sigma_2} = \frac{0.30557536}{0.30557536 - 0.008\,406\,9071} \approx 1.028,$$

so that perturbations of the data might cause changes of the same magnitude in the location and direction of the fitted GTLS line. Figure 1 shows the GTLS line (—), scaled to fit the projections $\bar{\mathbf{q}}_1, \dots, \bar{\mathbf{q}}_{21}$ (\times) instead of the normalized data $\bar{\rho}_k = (1/\|\bar{\mathbf{q}}_k - \bar{\mathbf{z}}\|_2)(\bar{\mathbf{q}}_k - \bar{\mathbf{z}})$, for comparison with the data $\bar{\mathbf{p}}_1, \dots, \bar{\mathbf{p}}_{21}$ ($+$).

The second perturbation analysis estimates the sensitivity factor $1/\sigma_L^2$ by means of the angle λ sustained by the projections of the data on the GTLS circle. For Rorres and Romano’s data, $\lambda \approx 0.211781$ radian (12 deg), whence Lemma 13 yields

$$(62) \quad 77.918 = \frac{1}{\sqrt{N}[\sin(\lambda/4)]^2} < \frac{1}{\sigma_L(\Gamma)} < \frac{1}{\sqrt{2}[\sin(\lambda/4)]^2} = 252.486.$$

This range contains the value already computed, 118.950, in equation (60).

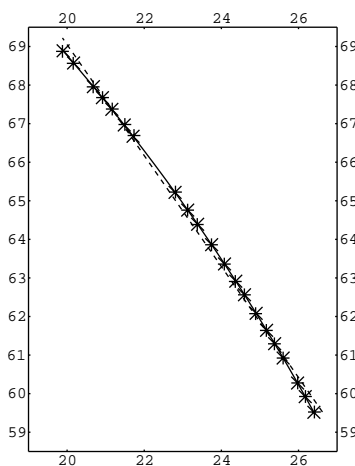


FIGURE 1. GTLS circle (—) [$\bar{\mathbf{z}} \approx (-21, 34)$, $r \approx 54$] fitted to data (+), from [19]; GTLS line (—) fitted to adjusted data (\times).

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