

PROBABILITY DISTRIBUTION OF THE MULTIVARIATE NONLINEAR LEAST SQUARES ESTIMATES

ANDREJ PÁZMAN

The nonlinear regression model $y_i = \eta_i(\theta_1, \dots, \theta_m) + \varepsilon_i$ with $(\varepsilon_1, \dots, \varepsilon_N) \sim N(0, \Sigma)$ and with $\eta_i(\cdot)$ twice continuously differentiable is considered. Under the assumption that the maximal curvature of the mean-values manifold $\{\eta(\theta) : \theta \in U\} \subset \mathbb{R}^N$ is bounded, an approximative probability density for the least squares estimates of $(\theta_1, \dots, \theta_m)$ is proposed. This density depends on the first form (= the information matrix) and on the second form of the mean-values manifold (Eq. (9)). The level of approximation depends on the probability that the sample goes beyond the nearest center of curvature of the mean-values manifold and it is expressed in the paper (Theorem 1).

1. INTRODUCTION AND MAIN RESULTS

As in [4], let us consider the gaussian nonlinear regression model

$$(1) \quad \mathbf{y} = \boldsymbol{\eta}(\boldsymbol{\theta}) + \boldsymbol{\varepsilon}$$

where $\mathbf{y} := (y_1, \dots, y_N)'$ is the vector of observed variables, $\boldsymbol{\theta} := (\theta_1, \dots, \theta_m)'$ is the vector of unknown parameters and $\boldsymbol{\varepsilon} := (\varepsilon_1, \dots, \varepsilon_N)'$ is the vector of random observations errors. It is supposed that $\boldsymbol{\theta} \in U \subset \mathbb{R}^m$, U open, and that $\boldsymbol{\varepsilon}$ is distributed normally, $N(0, \Sigma)$ with Σ known and nonsingular. The functions η_1, \dots, η_N are defined and have continuous second order derivatives $\partial^2 \eta_k / \partial \theta_i \partial \theta_j$ on U . Finally, it is supposed that the vectors $\partial \boldsymbol{\eta} / \partial \theta_1, \dots, \partial \boldsymbol{\eta} / \partial \theta_m$ are linearly independent for every $\boldsymbol{\theta} \in U$.

Eq. (1) could be also written in the more common form

$$y_i = \eta_{xi}(\boldsymbol{\theta}) + \varepsilon_{xi}; \quad (i = 1, \dots, N)$$

where x_1, \dots, x_N are the points of the design of the experiment. The dependence of $E(y_i)$ on x_i is of no importance in this paper, therefore we prefer the simpler Eq. (1).

Denote by $\langle \mathbf{a}, \mathbf{b} \rangle$, $\|\mathbf{a}\|$ the inner product and the norm defined by

$$\langle \mathbf{a}, \mathbf{b} \rangle = \mathbf{a}' \boldsymbol{\Sigma}^{-1} \mathbf{b}, \quad \|\mathbf{a}\|^2 = \langle \mathbf{a}, \mathbf{a} \rangle.$$

The probability density of \mathbf{y} is given by

$$(2) \quad f(\mathbf{y} \mid \boldsymbol{\eta}(\boldsymbol{\theta})) = \frac{1}{(2\pi)^{N/2} \det^{1/2}(\boldsymbol{\Sigma})} \exp \left\{ -\frac{1}{2} \|\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\theta})\|^2 \right\}.$$

The *least squares* (= l. s.) *estimate* for $\boldsymbol{\theta}$ is defined by

$$(3) \quad \hat{\boldsymbol{\theta}} := \hat{\boldsymbol{\theta}}(\mathbf{y}) := \operatorname{Arg} \min_{\boldsymbol{\theta} \in U} \|\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\theta})\|^2$$

(if it exists). Hence the l. s. estimate $\hat{\boldsymbol{\theta}}$ is one of the solutions of the equations

$$\frac{\partial}{\partial \theta_i} \|\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\theta})\|^2 = 0; \quad (i = 1, \dots, m),$$

or equivalently of

$$(4) \quad \left\langle \mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\theta}), \frac{\partial \boldsymbol{\eta}}{\partial \theta_i} \right\rangle = 0; \quad (i = 1, \dots, m).$$

Geometrically it means that the vector $\mathbf{y} - \boldsymbol{\eta}(\hat{\boldsymbol{\theta}})$ is orthogonal to the *mean values manifold* (the set of potentially possible mean values).

$$\mathcal{E} := \{\boldsymbol{\eta}(\boldsymbol{\theta}) : \boldsymbol{\theta} \in U\},$$

at the point $\boldsymbol{\eta}(\hat{\boldsymbol{\theta}})$. It means also that the vector \mathbf{y} is in the hyperplane $\kappa(\hat{\boldsymbol{\theta}})$ where

$$(5) \quad \kappa(\boldsymbol{\theta}) := \{\mathbf{z} : \mathbf{z} \in \mathbb{R}^N, \langle \mathbf{z} - \boldsymbol{\eta}(\boldsymbol{\theta}), \partial \boldsymbol{\eta} / \partial \theta_i \rangle = 0; (i = 1, \dots, m)\}.$$

Let us denote by r the minimal radius of curvature of the manifold \mathcal{E} . More exactly, we denote by $r(\boldsymbol{\eta})$ the minimal radius of curvature of a geodesics which contains the point $\boldsymbol{\eta} \in \mathcal{E}$ (see Appendix for the properties of geodesics), and we define

$$r := \inf \{r(\boldsymbol{\eta}) : \boldsymbol{\eta} \in \mathcal{E}\}$$

AS 1: We shall suppose in this paper that $r > 0$, i.e we consider models with bounded curvatures.

Let $\chi_N^2(p_0)$ be the $(1 - p_0)$ quantile of the χ^2 p.d. with N degrees of freedom. If $\chi_N^2(p_0) = r^2$, we say that $(1 - p_0)$ is the *level of regularity* of the model.

It means that

$$\mathbf{P}_{\boldsymbol{\eta}}\{\mathbf{y} : \mathbf{y} \in \mathbb{R}^N, \|\mathbf{y} - \boldsymbol{\eta}\| < r\} = 1 - p_0,$$

where $\mathbf{P}_{\boldsymbol{\eta}}$ is the p.d. with the density $f(\mathbf{y} \mid \boldsymbol{\eta})$.

We shall say that the regression model is *with a distant boundary* if for any expected $\boldsymbol{\eta} = \mathbf{E}(\mathbf{y})$ and any $\mathbf{y} \in \mathbb{R}^N$ such that $\|\mathbf{y} - \boldsymbol{\eta}\| < r$ there is a solution of Eq. (3). It means that we suppose that there is a set of expected values of the true vector $\boldsymbol{\theta}$, $U_0 \subset U$, which is sufficiently distant from “the boundary” of U .

AS 2: We suppose in this paper that the model is with a distant boundary.

The assumption AS 2 avoid to consider the “edges” of the manifold \mathcal{E} . Such an

assumption is usually adopted also in the linear regression model

$$(6) \quad \mathbf{y} = \mathbf{F}\boldsymbol{\theta} + \boldsymbol{\varepsilon}; \quad (\boldsymbol{\theta} \in U)$$

(\mathbf{F} = a given $N \times m$ matrix). Here it is commonly supposed that $U = \mathbb{R}^m$ although in reality the values of $\theta_1, \dots, \theta_m$ are always bounded a priori.

The model is called overlapping if for some $\mathbf{y} \in \mathbb{R}^N$ there are two solutions $\boldsymbol{\theta}^{(1)} \neq \boldsymbol{\theta}^{(2)}$ of Eqs. (4) such that

$$\|\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\theta}^{(1)})\| \leq r, \quad \|\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\theta}^{(2)})\| \leq r.$$

AS 3: We suppose in this paper that the considered model is not overlapping.

For any $\boldsymbol{\theta} \in U$ let us denote by

$$(7) \quad \{\mathbf{M}(\boldsymbol{\theta})\}_{ij} := \mathbb{E}_{\boldsymbol{\eta}(\boldsymbol{\theta})} \left\{ \frac{\partial \ln f(\mathbf{y} | \boldsymbol{\eta}(\boldsymbol{\theta}))}{\partial \theta_i} \frac{\partial \ln f(\mathbf{y} | \boldsymbol{\eta}(\boldsymbol{\theta}))}{\partial \theta_j} \right\} = \left\langle \frac{\partial \boldsymbol{\eta}}{\partial \theta_i}, \frac{\partial \boldsymbol{\eta}}{\partial \theta_j} \right\rangle;$$

$$(i, j = 1, \dots, m)$$

the (local) Fisher information matrix.

By

$$(8) \quad \mathbf{P}^\theta := \sum_{k,l} \frac{\partial \boldsymbol{\eta}}{\partial \theta_k} \{\mathbf{M}^{-1}(\boldsymbol{\theta})\}_{kl} \frac{\partial \boldsymbol{\eta}}{\partial \theta_l} \boldsymbol{\Sigma}^{-1}$$

we denote the matrix of projection onto the plane which is tangent to the manifold \mathcal{E} at the point $\boldsymbol{\eta}(\boldsymbol{\theta})$. Let us denote by $q(\boldsymbol{\theta} | \boldsymbol{\eta})$ the function

$$(9) \quad q(\boldsymbol{\theta} | \boldsymbol{\eta}) := \frac{\det \left[\left\{ \mathbf{M}(\boldsymbol{\theta}) \right\}_{ij} + \left\langle (\mathbf{I} - \mathbf{P}^\theta)(\boldsymbol{\eta}(\boldsymbol{\theta}) - \boldsymbol{\eta}), \frac{\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_i \partial \theta_j} \right\rangle_{i,j=1}^m \right]}{(2\pi)^{m/2} \det^{1/2} \mathbf{M}(\boldsymbol{\theta})} \times$$

$$\times \exp \left\{ -\frac{1}{2} \|\mathbf{P}^\theta(\boldsymbol{\eta}(\boldsymbol{\theta}) - \boldsymbol{\eta})\|^2 \right\}.$$

Let $f_{\theta^*}(\boldsymbol{\theta} | \boldsymbol{\eta})$ be the probability density* of the l.s. estimate $\hat{\boldsymbol{\theta}}$. The main result of the paper is expressed in Theorem 1 by the inequality

$$(10) \quad \left| \int_B f_{\theta^*}(\boldsymbol{\theta} | \boldsymbol{\eta}) d\boldsymbol{\theta} - \int_B q(\boldsymbol{\theta} | \boldsymbol{\eta}) d\boldsymbol{\theta} \right| \leq 2p_0$$

which is valid for every Borel set B which is a subset of $\{\boldsymbol{\theta} : \boldsymbol{\theta} \in U, \exists \mathbf{z} \in \mathbb{R}^N \|\mathbf{z} - \boldsymbol{\eta}\| < r, \boldsymbol{\eta}(\boldsymbol{\theta}) = \boldsymbol{\eta}[\hat{\boldsymbol{\theta}}(\mathbf{z})]\}$ ("the region of accessibility").

It follows that $q(\boldsymbol{\theta} | \boldsymbol{\eta})$ is an adequate approximative probability density of the l.s. estimates, the level of approximation being given by the level of regularity $(1 - p_0)$.

Especially, if $r \mapsto \infty$ (i.e. $p_0 \mapsto 0$), then we obtain the linear regression model (6). In that case

$$\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta}) / \partial \theta_i \partial \theta_j = 0, \quad \mathbf{P}^{\theta^*}[\boldsymbol{\eta}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta}(\boldsymbol{\theta})] = \boldsymbol{\eta}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta}(\boldsymbol{\theta}),$$

$$\partial \boldsymbol{\eta}(\boldsymbol{\theta}) / \partial \theta_j = \{\mathbf{F}\}_{ij}, \quad \mathbf{M}(\boldsymbol{\theta}) = \mathbf{F}' \boldsymbol{\Sigma}^{-1} \mathbf{F}.$$

* From typographical reasons we use θ^+ , θ^- instead of $\hat{\theta}$, $\bar{\theta}$ in superscript and subscript.

$$q(\hat{\theta} | \eta(\theta)) = \frac{\det^{1/2}(\mathbf{F}' \Sigma^{-1} \mathbf{F})}{(2\pi)^{m/2}} \exp \left\{ -\frac{1}{2}(\hat{\theta} - \theta)' (\mathbf{F}' \Sigma^{-1} \mathbf{F}) (\hat{\theta} - \theta) \right\}.$$

To clarify the ideas we shall construct heuristically the probability density of the l.s. estimate in the special case $m = 1, N = 2$. Without restrictions on generality we shall suppose in this section that the parameter θ is the “natural parameter” (= the distance measured from some fixed point along the curve $\theta \in U \mapsto \eta(\theta) \in \mathbb{R}^2$), i.e. that $\|\mathbf{d}\eta(\theta)/\mathbf{d}\theta\| = 1$.


$$(11) \quad \begin{aligned} \varphi(t) &= [2\pi]^{-1/2} \exp \{-t^2/2\}, \\ \Phi(x) &= \int_{-\infty}^x \varphi(t) dt, \end{aligned}$$
$$S(\theta) := \left\{ \mathbf{z} : \mathbf{z} \in \mathbb{R}^2, \left\langle \mathbf{z} - \boldsymbol{\eta}(\theta), \frac{d\boldsymbol{\eta}(\theta)}{d\theta} \right\rangle < 0 \right\}.$$
$$[S(\theta + \Delta) - S(\theta)] \cup [S(\theta) - S(\theta + \Delta)]$$

is the set of all points $\mathbf{y} \in \mathbb{R}^2$ which have a solution of Eq. (4) in the interval $(\theta, \theta + \Delta)$. Moreover, it can be seen from Fig. 1 that

$$(12) \quad \begin{aligned} P_{\eta}[S(\theta + \Delta) - S(\theta)] - P_{\eta}[S(\theta) - S(\theta + \Delta)] = \\ = P_{\eta}[S(\theta + \Delta)] - P_{\eta}[S(\theta)] \end{aligned}$$

where P_{η} is the probability distribution of the sample \mathbf{y} if η is its mean. Further evidently

$$P_{\eta}[S(\theta)] = \phi \left[\left\langle \eta(\theta) - \mathbf{y}, \frac{d\eta(\theta)}{d\theta} \right\rangle \right].$$

We shall show that with $\Delta \rightarrow 0$ for $\mathbf{y} \in S(\theta + \Delta) - S(\theta)$ (resp. for $\mathbf{y} \in S(\theta) - S(\theta + \Delta)$) the solution of Eq. (4) is a relative minimum (resp. a relative maximum) of the function $\theta \in U \mapsto \|\mathbf{y} - \eta(\theta)\|^2$.

To this purpose let us consider the second order derivative

$$(13) \quad \frac{1}{2} \frac{d^2}{d\theta^2} \|\eta(\theta) - \mathbf{y}\|^2 = 1 + \left\langle \eta(\theta) - \mathbf{y}, \frac{d^2\eta}{d\theta^2} \right\rangle.$$

The expression

$$\varrho_{\eta}(\theta) := \left\| \frac{d^2\eta}{d\theta^2} \right\|^{-1}$$

is the radius of curvature of the curve $\theta \in U \mapsto \eta(\theta)$, and the point

$$\eta(\theta) + \frac{d^2\eta}{d\theta^2}$$

is its centre of curvature, as known from elementary differential geometry [1]. Let us denote by

$$\mathbf{e}_{\eta}(\theta) := \varrho_{\eta}(\theta) \frac{d^2\eta}{d\theta^2}$$

the unit vector pointing from $\eta(\theta)$ to the centre of curvature. This allows to rewrite Eq. (13) as

$$(14) \quad \frac{1}{2} \frac{d^2}{d\theta^2} \|\eta(\theta) - \mathbf{y}\|^2 = \varrho_{\eta}^{-1}(\theta) \{ \varrho_{\eta}(\theta) + \langle \eta(\theta) - \mathbf{y}, \mathbf{e}_{\eta}(\theta) \rangle \}.$$

As seen from Fig. 1, the point $C(\Delta)$ (= the point of intersection of $\kappa(\theta)$ with $\kappa(\theta + \Delta)$) tends to the centre of curvature if Δ tends to zero. For $\Delta \rightarrow 0$ from $\mathbf{y} \in S(\theta + \Delta) - S(\theta)$ it follows that $\langle \mathbf{y} - \eta(\theta), \mathbf{e}_{\eta}(\theta) \rangle < \varrho_{\eta}(\theta)$, hence, according to Eq. (14), $d^2/d\theta^2 \|\eta(\theta) - \mathbf{y}\|^2 > 0$. Moreover, as supposed, θ is the solution of Eq. (4), hence θ is a relative minimum of $\|\eta(\theta) - \mathbf{y}\|^2$.

We proceed similarly in the case that $\mathbf{y} \in S(\theta) - S(\theta + \Delta)$. It follows that the

limit

$$q(\theta | \boldsymbol{\eta}) := \lim_{\Delta \rightarrow 0} \frac{P_{\boldsymbol{\eta}}[S(\theta + \Delta) - S(\theta)] - P_{\boldsymbol{\eta}}[S(\theta) - S(\theta + \Delta)]}{\Delta}$$

is the probability density of the relative minima minus the probability density of the relative maxima of the function $\theta \in U \mapsto \|\boldsymbol{\eta}(\theta) - \mathbf{y}\|^2$.

From (12) it follows

$$\begin{aligned} q(\theta | \boldsymbol{\eta}) &= \lim_{\Delta \rightarrow 0} \frac{\Phi \left[\left\langle \boldsymbol{\eta}(\theta + \Delta) - \boldsymbol{\eta}, \frac{d\boldsymbol{\eta}(\theta + \Delta)}{d\theta} \right\rangle \right] - \Phi \left[\left\langle \boldsymbol{\eta}(\theta) - \boldsymbol{\eta}, \frac{d\boldsymbol{\eta}(\theta)}{d\theta} \right\rangle \right]}{\Delta} = \\ (15) \quad &= \varphi \left(\left\langle \boldsymbol{\eta}(\theta) - \boldsymbol{\eta}, \frac{d\boldsymbol{\eta}(\theta)}{d\theta} \right\rangle \right) \frac{d}{d\theta} \left\langle \boldsymbol{\eta}(\theta) - \boldsymbol{\eta}, \frac{d\boldsymbol{\eta}(\theta)}{d\theta} \right\rangle. \end{aligned}$$

If $\Delta \rightarrow 0$ then $[S(\theta) - S(\theta + \Delta)] \cap \{\mathbf{y} : \|\mathbf{y} - \boldsymbol{\eta}\| > r\} \rightarrow \emptyset$. Hence if we neglect the set of samples $\{\mathbf{y} : \mathbf{y} \in \mathbb{R}^2, \|\mathbf{y} - \boldsymbol{\eta}\| > r\}$, the probability of which is less than p_0 , we can state that there are no relative maxima of $\|\boldsymbol{\eta}(\theta) - \mathbf{y}\|^2$ and that every relative minimum is an absolute minimum, i.e. it is the l.s. estimate $\hat{\theta}(\mathbf{y})$. Hence the expression in Eq. (15) is an approximative expression for the probability density of the l.s. estimate $\hat{\theta}$. To compare it with the expression in Eq. (9) we have just to use that in the special considered case $\mathbf{M}(\theta) = \|d\boldsymbol{\eta}/d\theta\|^2 = 1$ and that $\langle d\boldsymbol{\eta}/d\theta, d^2\boldsymbol{\eta}/d\theta^2 \rangle = 0$.

The derivative

$$\frac{d}{d\theta} \left\langle \boldsymbol{\eta}(\theta) - \boldsymbol{\eta}, \frac{d\boldsymbol{\eta}(\theta)}{d\theta} \right\rangle_{\theta(\mathbf{y})} = \varrho^{-1}(\theta) [\varrho(\theta) + \langle \boldsymbol{\eta}(\theta) - \boldsymbol{\eta}, \mathbf{e}_{\mathbf{y}}(\theta) \rangle]_{\theta(\mathbf{y})}$$

is positive (within our regularity assumptions). Hence, using the notation

$$(16) \quad v(\theta) := \left\langle \boldsymbol{\eta}(\theta) - \boldsymbol{\eta}, \frac{d\boldsymbol{\eta}(\theta)}{d\theta} \right\rangle,$$

the approximative probability density $q(\theta | \boldsymbol{\eta})$ in (15) can be expressed as

$$q(\theta | \boldsymbol{\eta}) = (2\pi)^{-1/2} \exp \left\{ -\frac{1}{2} v^2(\theta) \right\} \left| \frac{dv(\theta)}{d\theta} \right|.$$

It follows that the random variable $v(\hat{\theta})$ is (approximately) distributed $N(0, 1)$. Therefore, the interval

$$\left\{ \theta : \left[\left\langle \boldsymbol{\eta}(\hat{\theta}) - \boldsymbol{\eta}(\theta), \frac{d\boldsymbol{\eta}(\hat{\theta})}{d\theta} \right\rangle \right]^2 < \chi_1^2(\beta) \right\}$$

is a confidence interval for the true value of θ , with the confidence level depending on β and on p_0 .

Finally, let us compare the obtained probability density with the result in [4].

If $|\langle \boldsymbol{\eta}(\theta) - \boldsymbol{\eta}, \mathbf{e}_{\boldsymbol{\eta}}(\theta) \rangle|$ is much smaller than $\varrho_{\boldsymbol{\eta}}(\theta)$, then $|dv(\theta)/d\theta| \doteq 1$, and from (15) we obtain

$$q(\theta | \boldsymbol{\eta}) \doteq (2\pi)^{-1/2} \exp \left\{ -\frac{1}{2} \langle \boldsymbol{\eta}(\theta) - \boldsymbol{\eta}, d\boldsymbol{\eta}/d\theta \rangle^2 \right\}$$

which is the expression in Eq. (26) in [4] for the considered case that $\|d\boldsymbol{\eta}/d\theta\| = 1$.

3. THE MULTIVARIATE PROBABILITY DENSITY OF $\hat{\theta}$

In this section we proceed to the general case of arbitrary $m, N, N > m$. We define by $\boldsymbol{\eta}$ the (fixed) mean of the sample \mathbf{y} . We denote by

$$(17) \quad \mathcal{A}_{\boldsymbol{\eta}} := \{ \boldsymbol{\eta}[\hat{\theta}(\mathbf{y})] : \|\mathbf{y} - \boldsymbol{\eta}\| < r \}$$

the *region of accessibility* (cf. Eq. (A 13) and the assumption AS 2 in Section 1). We are interested in the probability density $f_{\boldsymbol{\theta}^*}(\theta | \boldsymbol{\eta})$ of the l.s. estimate $\hat{\theta}$. We shall show that it can be well approximated on the set $\{\theta : \boldsymbol{\eta}(\theta) \in \mathcal{A}_{\boldsymbol{\eta}}\}$ by the function $q(\theta | \boldsymbol{\eta})$ expressed in Eq. (9). The main aim of this section is to prove the following.

Theorem 1. Let B be a measurable subset of the set $\{\theta : \theta \in U, \boldsymbol{\eta}(\theta) \in \mathcal{A}_{\boldsymbol{\eta}}\}$. Then

$$\left| \int_B f_{\boldsymbol{\theta}^*}(\theta | \boldsymbol{\eta}) d\theta - \int_B q(\theta | \boldsymbol{\eta}) d\theta \right| \leq 2p_0.$$

To prove Theorem 1 it is necessary to do a stepwise approximation of $f_{\boldsymbol{\theta}^*}(\theta | \boldsymbol{\eta})$ by $q(\theta | \boldsymbol{\eta})$.

Take a fixed point $\bar{\theta} \in U$ such that $\boldsymbol{\eta}(\bar{\theta}) \in \mathcal{A}_{\boldsymbol{\eta}}$. According to Proposition A 5, there is a neighbourhood of $\bar{\theta}$, $U_{\bar{\theta}} \subset U$, such that $\boldsymbol{\eta}[U_{\bar{\theta}}] \subset \mathcal{A}_{\boldsymbol{\eta}}$. As explained in Appendix, if a neighbourhood $V_{\bar{\theta}} \subset U_{\bar{\theta}}$ is adequately chosen, we can introduce new local coordinates t_1, \dots, t_m in $V_{\bar{\theta}}$ and two sets of local coordinates x_1, \dots, x_N and z_1, \dots, z_N in the set $\mathcal{G}_{\bar{\theta}} := \{\mathbf{y} : \mathbf{y} \in \mathbb{R}^N, \mathbf{y} \in \mathcal{X}(\theta), \theta \in V_{\bar{\theta}}\}$ as follows. We take m geodesics in \mathcal{E} , $\gamma^{(1)}, \dots, \gamma^{(m)}$ such that $\gamma^{(i)}(0) = \boldsymbol{\eta}(\bar{\theta})$; ($i = 1, \dots, m$) and that $\langle \dot{\gamma}^{(i)}(0), \dot{\gamma}^{(j)}(0) \rangle = 0$ if $i \neq j$ (cf. Appendix for geodesics in \mathcal{E}). The coordinates $t_1 := \tau_1(\bar{\theta}), \dots, t_m := \tau_m(\bar{\theta})$ are defined by

$$(18) \quad \langle \boldsymbol{\eta}(\theta) - \gamma^{(i)}(t_i), \dot{\gamma}^{(i)}(t_i) \rangle = 0; \quad (i = 1, \dots, m)$$

i.e. by projecting $\boldsymbol{\eta}(\theta)$ onto the curves $\gamma^{(1)}, \dots, \gamma^{(m)}$. We define further

$$(19) \quad x_i = \xi_i(\mathbf{y}) := \tau_i[\boldsymbol{\theta}^*(\mathbf{y})]; \quad (i = 1, \dots, m),$$

where $\boldsymbol{\theta}^*(\mathbf{y})$ is the (unique) solution of Eqs. (4) which is in $V_{\bar{\theta}}$. The coordinates $x_{m+1} = \xi_{m+1}(\mathbf{y}), \dots, x_N = \xi_N(\mathbf{y})$ are complementary orthogonal coordinates defined by Eq. (A 22).

Projecting \mathbf{y} onto $\gamma^{(1)}, \dots, \gamma^{(m)}$, i.e. by the equations

$$(20) \quad \langle \mathbf{y} - \gamma^{(i)}(z_i), \dot{\gamma}^{(i)}(z_i) \rangle = 0; \quad (i = 1, \dots, m)$$

we define the coordinates $z_i = \zeta_i(\mathbf{y}), \dots, z_m = \zeta_m(\mathbf{y})$. The coordinates $z_{m+1} = \zeta_{m+1}(\mathbf{y}), \dots, z_N = \zeta_N(\mathbf{y})$ are again complementary orthogonal coordinates (cf. Eqs. (A 24)).

If $\Sigma = \mathbf{I}$, and if $\theta^*(\mathbf{y}) = \bar{\theta}$, the coordinates x_1, \dots, x_N and z_1, \dots, z_N are essentially the same. In that case we have namely: $x_i = z_i$; ($i = 1, \dots, N$) and $\partial z_i / \partial x_j = 0$; ($i \neq j$), $\partial z_i / \partial x_i = 1$ (cf. Eqs. (A 25) and Proposition A 7).

Let us introduce the notations

$$(21) \quad v_i(z_i) := \langle \gamma^{(i)}(z_i) - \eta, \dot{\gamma}^{(i)}(z_i) \rangle; \quad (i = 1, \dots, m)$$

and

$$Q_i^{\theta^-}(\mathbf{z}) := \{ \mathbf{y} : \mathbf{y} \in \mathbb{R}^N, v_i[\zeta_i(\mathbf{y})] < v_i(\mathbf{z}) \}$$

(cf. Eq. (A 17)).

Denote by $\zeta(\mathbf{y})$ the random vector

$$\zeta(\mathbf{y}) := (\zeta_1(\mathbf{y}), \dots, \zeta_m(\mathbf{y})),$$

and by $F_{\zeta}^{\theta^-}(z_1, \dots, z_m)$ its distribution function induced from the density of \mathbf{y} given by Eq. (2), and restricted to the set \mathcal{G}_{θ^-} . Because the functions v_1, \dots, v_m defined in Eqs. (21) are increasing (see Proposition A 3), the increase of $F_{\zeta}^{\theta^-}$ is given by

$$(22) \quad \Delta_{\varepsilon_1}^{(1)} \dots \Delta_{\varepsilon_m}^{(m)} F_{\zeta}^{\theta^-}(z_1, \dots, z_m) = P_{\eta} \left[\bigcap_{i=1}^m (Q_i^{\theta^-}(z_i) - Q_i^{\theta^-}(z_i - \varepsilon_i)) \right].$$

Here we used the notation

$$\Delta_{\varepsilon_k}^{(k)} h(z_1, \dots, z_m) := h(z_1, \dots, z_m) - h(z_1, \dots, z_{k-1}, z_k - \varepsilon_k, z_{k+1}, \dots, z_m),$$

(cf. [6], chpt. IV. 3). The density of $\zeta(\mathbf{y})$ is then

$$(23) \quad f_{\zeta}^{\theta^-}(z_1, \dots, z_m) := \frac{\partial^m}{\partial z_1 \dots \partial z_m} F_{\zeta}^{\theta^-}(z_1, \dots, z_m) = \\ = \lim_{\varepsilon_1 \rightarrow 0} \dots \lim_{\varepsilon_m \rightarrow 0} \frac{P_{\eta} \left[\bigcap_{i=1}^m (Q_i^{\theta^-}(z_i) - Q_i^{\theta^-}(z_i - \varepsilon_i)) \right]}{\varepsilon_1 \dots \varepsilon_m}.$$

Denote by $g(z_{m+1}, \dots, z_N | z_1, \dots, z_m)$ the conditional probability density of $\zeta_{m+1}(\mathbf{y}), \dots, \zeta_N(\mathbf{y})$ (induced again from $f(\mathbf{y} | \eta)$ in Eq. (2)). The joint density $f_{\zeta}^{\theta^-}(z_1, \dots, z_m) g(z_{m+1}, \dots, z_N | z_1, \dots, z_m)$ is transformed by the mapping (the change of coordinates) $(z_1, \dots, z_N) \mapsto (x_1, \dots, x_N)$ into the joint density of $(\xi_1(\mathbf{y}), \dots, \xi_N(\mathbf{y}))$. Denote by $f_{\xi}^{\theta^-}(x_1, \dots, x_m)$ the corresponding marginal density of the random vector

$$\xi(\mathbf{y}) := (\xi_1(\mathbf{y}), \dots, \xi_m(\mathbf{y})).$$

Then finally, according to Eqs. (19),

$$(24) \quad f_{\theta^*}(\bar{\theta} | \eta) = f_{\xi}^{\theta^-}(x_1, \dots, x_m) \left| \det \{ \partial \tau_{ij} / \partial \theta_j \}_{i,j=1}^m \right|$$

This complicated way to deduce $f_{\theta^*}(\bar{\theta} | \eta)$ from $f(\mathbf{y} | \eta)$ was chosen to make easy the comparison with $q(\bar{\theta} | \eta)$. Namely, we shall show that $q(\bar{\theta} | \eta)$ can be deduced in an analogous way, but from the distribution

$$(25) \quad \tilde{F}_{\xi}^{\theta^-}(z_1, \dots, z_m) := \mathbb{P}_{\eta} \left[\bigcap_{i=1}^m S_i^{\theta^-}(z_i) \right]$$

where

$$(26) \quad S_i^{\theta^-}(z_i) := \{ \mathbf{y} : \mathbf{y} \in \mathbb{R}^N, \langle \mathbf{y} - \gamma^{(i)}(z_i), \dot{\gamma}^{(i)}(z_i) \rangle < 0 \}$$

(cf. Eq. (A 16)). The corresponding density is given by

$$(27) \quad \tilde{f}_{\xi}^{\theta^-}(z_1, \dots, z_m) = \lim_{\varepsilon_1 \rightarrow 0} \dots \lim_{\varepsilon_m \rightarrow 0} \frac{\mathbb{P}_{\eta} \left[\bigcap_{i=1}^m (S_i^{\theta^-}(z_i) - S_i^{\theta^-}(z_i - \varepsilon_i)) \right]}{\varepsilon_1 \dots \varepsilon_m}$$

Again, the joint density $\tilde{f}_{\xi}^{\theta^-}(z_1, \dots, z_m) g(z_{m+1}, \dots, z_N | z_1, \dots, z_m)$ is transformed by the coordinate mapping $(z_1, \dots, z_N) \mapsto (x_1, \dots, x_N)$ into a joint density of $(\xi_1(\mathbf{y}), \dots, \xi_N(\mathbf{y}))$. Denote by $\tilde{f}_{\xi}^{\theta^-}(x_1, \dots, x_m)$ the corresponding marginal distribution of $\xi(\mathbf{y})$. We have the following important auxiliary proposition

Proposition 1. Let be $\Sigma = I$.

Then

$$\begin{aligned} \text{a)} \quad & \tilde{f}_{\xi}^{\theta^-}(0) = f_{\xi}^{\theta^-}(0), \tilde{f}_{\xi}^{\theta^-}(0) = \tilde{f}_{\xi}^{\theta^-}(0) \\ \text{b)} \quad & \tilde{f}_{\xi}^{\theta^-}(0) = \frac{1}{(2\pi)^{m/2}} \exp \left\{ -\frac{1}{2} (\eta(\bar{\theta}) - \eta)^T \sum_{i=1}^m \dot{\gamma}^{(i)}(0) \dot{\gamma}^{(i)}(0) (\eta(\bar{\theta}) - \eta) \right\} \times \\ (28) \quad & \times \prod_{i=1}^m [1 + (\eta(\bar{\theta}) - \eta)^T \dot{\gamma}^{(i)}(0)] \\ (29) \quad & \text{c)} \quad q(\bar{\theta} | \eta) = \tilde{f}_{\xi}^{\theta^-}(0) |\det \{ \{\partial \tau_i(\bar{\theta}) / \partial \theta_j\}_{i,j=1}^m \}|, \\ (30) \quad & f_{\theta^*}(\bar{\theta} | \eta) = f_{\xi}^{\theta^-}(0) |\det \{ \{\partial \tau_i(\bar{\theta}) / \partial \theta_j\}_{i,j=1}^m \}|. \end{aligned}$$

Proof. The statement a) follows from Eqs. (A 25) and from Proposition A 7 in Appendix.

From Eqs. (25), (26) and (21) it follows that

$$\tilde{F}_{\xi}^{\theta^-}(z_1, \dots, z_m) = \int_{-\infty}^{v_1(z_1)} \dots \int_{-\infty}^{v_m(z_m)} \frac{1}{(2\pi)^{m/2} \det^{1/2} \mathbf{K}} \exp \left\{ -\frac{1}{2} \mathbf{u}^T \mathbf{K}^{-1} \mathbf{u} \right\} du_1 \dots du_m,$$

where

$$\{\mathbf{K}\}_{ij} := \langle \dot{\gamma}^{(i)}(z_i), \dot{\gamma}^{(j)}(z_j) \rangle.$$

Therefore the corresponding density is

$$(31) \quad \tilde{f}_{\xi}^{\theta^-}(z_1, \dots, z_m) = \frac{1}{(2\pi)^{m/2} \det^{1/2} \mathbf{K}} \exp \left\{ -\frac{1}{2} \sum_{i,j=1}^m v_i(z_i) \{\mathbf{K}^{-1}\}_{ij} v_j(z_j) \right\} \prod_{i=1}^m (dv_i(z_i) / dz_i).$$

From (31) we obtain the expression in Eq. (28).

The equality in Eq. (30) follows directly from Eq. (24). It remains to prove Eq. (29).

First we can state that

$$(32) \quad \mathbf{P}^{\theta^-} = \sum_{l=1}^m \dot{\gamma}^{(l)}(0) \dot{\gamma}^{(l)'}(0).$$

To verify (32), put \mathbf{P}^{θ^-} according to Eq. (8) (for $\Sigma = \mathbf{I}$), and multiply Eq. (32) by $\partial \boldsymbol{\eta}'(\bar{\boldsymbol{\theta}})/\partial \theta_q$ from the left, and by $\partial \boldsymbol{\eta}(\bar{\boldsymbol{\theta}})/\partial \theta_h$ from the right ($q, h = 1, \dots, m$).

In the right side of Eq. (29) let us express $\tilde{f}_{\xi}^{\theta^-}(0)$ using Eq. (28), and $\partial \tau_i(\bar{\boldsymbol{\theta}})/\partial \theta_j$ using Eq. (A 27). We can write, according to Eq. (32),

$$(33) \quad [\boldsymbol{\eta}(\bar{\boldsymbol{\theta}}) - \boldsymbol{\eta}]' \sum_{l=1}^m \dot{\gamma}^{(l)}(0) \dot{\gamma}^{(l)'}(0) [\boldsymbol{\eta}(\bar{\boldsymbol{\theta}}) - \boldsymbol{\eta}] = \|\mathbf{P}^{\theta^-} [\boldsymbol{\eta}(\bar{\boldsymbol{\theta}}) - \boldsymbol{\eta}]\|^2.$$

Using Eq. (32) again, we obtain

$$(34) \quad \prod_{i=1}^m [1 + (\boldsymbol{\eta}(\bar{\boldsymbol{\theta}}) - \boldsymbol{\eta})' \dot{\gamma}^{(i)}(0)] |\det \{ \partial \tau_i(\bar{\boldsymbol{\theta}})/\partial \theta_j \}_{i,j=1}^m| = \\ = \det \left(\left\{ \frac{\partial}{\partial t_i} [(\gamma^{(i)}(t_i) - \boldsymbol{\eta})' \sum_{k=1}^m \dot{\gamma}^{(k)}(t_k) \dot{\gamma}^{(k)'}(t_k)]_{t_i=0} \frac{\partial \boldsymbol{\eta}(\bar{\boldsymbol{\theta}})}{\partial \theta_j} \right\}_{i,j=1}^m \right) = \\ = \det \left(\left\{ \mathbf{M}_{ij}(\bar{\boldsymbol{\theta}}) + [\boldsymbol{\eta}(\bar{\boldsymbol{\theta}}) - \boldsymbol{\eta}]' (\mathbf{I} - \mathbf{P}^{\theta^-}) \frac{\partial^2 \boldsymbol{\eta}(\bar{\boldsymbol{\theta}})}{\partial \theta_i \partial \theta_j} \right\}_{i,j=1}^m \right) \times \\ \times |\det^{-1} \{ \partial \tau_i(\bar{\boldsymbol{\theta}})/\partial \theta_j \}_{i,j=1}^m|.$$

From Eq. (A 27) we have

$$(35) \quad \det^2 \{ \partial \tau_i(\bar{\boldsymbol{\theta}})/\partial \theta_j \}_{i,j=1}^m = \det \mathbf{M}(\bar{\boldsymbol{\theta}}).$$

The validity of Eq. (29) follows from Eqs. (33)–(35). \square

From Proposition 1 it follows that the comparison of $f_{\theta}(\bar{\boldsymbol{\theta}} | \boldsymbol{\eta})$ with $q(\bar{\boldsymbol{\theta}} | \boldsymbol{\eta})$, needed in Theorem 1, reduces to the comparison of $f_{\xi}^{\theta^-}(0)$ with $\tilde{f}_{\xi}^{\theta^-}(0)$.

Proposition 2. For sufficiently small $\varepsilon_1 > 0, \dots, \varepsilon_m > 0$ we have the inequality

$$(36) \quad |A_{\varepsilon_1}^{(1)} \dots A_{\varepsilon_m}^{(m)} [F_{\xi}^{\theta^-}(z_1, \dots, z_m) - \tilde{F}_{\xi}^{\theta^-}(z_1, \dots, z_m)]| \leq \\ \leq \mathbf{P}_{\boldsymbol{\eta}}[(\mathcal{R}^N - W_r) \cap (\mathcal{Q}_i^{\theta^-}(z_i) - \mathcal{Q}_i^{\theta^-}(z_i - \varepsilon_i))] + \\ + \mathbf{P}_{\boldsymbol{\eta}}[(\mathcal{R}^N - W_r) \cap (\mathcal{S}_i^{\theta^-}(z_i) - \mathcal{S}_i^{\theta^-}(z_i - \varepsilon_i))] \\ \text{where}$$

$$W_r := \{\boldsymbol{\gamma} : \boldsymbol{\gamma} \in \mathbb{R}^N, \|\boldsymbol{\gamma} - \boldsymbol{\eta}\| < r\}.$$

Proof. From (25) we obtain

$$\begin{aligned} \Delta_{\varepsilon_1}^{(1)} \dots \Delta_{\varepsilon_m}^{(m)} \bar{F}_{\zeta}^{\theta^-}(z_1, \dots, z_m) &= \mathbf{P}_{\boldsymbol{\eta}}[(\mathbb{R}^N - W_r) \cap \bigcap_{i=1}^m (S_i^{\theta^-}(z_i) - S_i^{\theta^-}(z_i - \varepsilon_i))] + \\ &+ \mathbf{P}_{\boldsymbol{\eta}}[W_r \cap \bigcap_{i=1}^m (S_i^{\theta^-}(z_i) - S_i^{\theta^-}(z_i - \varepsilon_i))]. \end{aligned}$$

Analogically, from (22) we obtain

$$\begin{aligned} \Delta_{\varepsilon_1}^{(1)} \dots \Delta_{\varepsilon_m}^{(m)} F_{\zeta}^{\theta^-}(z_1, \dots, z_m) &= \mathbf{P}_{\boldsymbol{\eta}}[(\mathbb{R}^N - W_r) \cap \bigcap_{i=1}^m (Q_i^{\theta^-}(z_i) - Q_i^{\theta^-}(z_i - \varepsilon_i))] + \\ &+ \mathbf{P}_{\boldsymbol{\eta}}[W_r \cap \bigcap_{i=1}^m (Q_i^{\theta^-}(z_i) - Q_i^{\theta^-}(z_i - \varepsilon_i))]. \end{aligned}$$

Hence, we prove the inequality (36) if we use that, according to Proposition A 6,

$$W_r \cap \bigcap_{i=1}^m [Q_i^{\theta^-}(z_i) - Q_i^{\theta^-}(z_i - \varepsilon_i)] = W_r \cap \bigcap_{i=1}^m [S_i^{\theta^-}(z_i) - S_i^{\theta^-}(z_i - \varepsilon_i)],$$

for $\varepsilon_1, \dots, \varepsilon_m$ sufficiently small. \square

Proof of Theorem 1. We shall write $\boldsymbol{\theta}$ instead of $\bar{\boldsymbol{\theta}}$ in this proof. Without lack of generality we shall do the proof for $\boldsymbol{\Sigma} = \mathbf{I}$.

According to Proposition 1 we have

$$\begin{aligned} D &:= \left| \int_B f_{\boldsymbol{\theta}}(\boldsymbol{\theta} \mid \boldsymbol{\eta}) d\boldsymbol{\theta} - \int_B q(\boldsymbol{\theta} \mid \boldsymbol{\eta}) d\boldsymbol{\theta} \right| \leq \\ &\leq \int_B |f_{\zeta}^{\boldsymbol{\theta}}(0) - \bar{f}_{\zeta}^{\boldsymbol{\theta}}(0)| |\det(\{\partial \tau_i / \partial \theta_j\}_{i,j=1}^m)| d\boldsymbol{\theta}. \end{aligned}$$

Hence, using Proposition 2, we obtain

$$\begin{aligned} (37) \quad D &\leq \int_B \frac{\partial^m}{\partial z_1 \dots \partial z_m} \{ \mathbf{P}_{\boldsymbol{\eta}}[(\mathbb{R}^N - W_r) \cap \bigcap_{i=1}^m S_i^{\boldsymbol{\theta}}(z_i)] + \\ &+ \mathbf{P}_{\boldsymbol{\eta}}[(\mathbb{R}^N - W_r) \cap \bigcap_{i=1}^m Q_i^{\boldsymbol{\theta}}(z_i)] \}_{\mathbf{z}=\mathbf{0}} |\det(\{\partial \tau_i / \partial \theta_j\}_{i,j=1}^m)| d\boldsymbol{\theta} = \\ &= \int_B \frac{\partial^m}{\partial z_1 \dots \partial z_m} \int_{\mathbb{R}^N - W_r} \prod_{i=1}^m [\chi(\mathbf{y}; S_i^{\boldsymbol{\theta}}(z_i)) + \chi(\mathbf{y}; Q_i^{\boldsymbol{\theta}}(z_i))] \times \\ &\quad d\mathbf{P}_{\boldsymbol{\eta}}(\mathbf{y})|_{\mathbf{z}=\mathbf{0}} |\det(\{\partial \tau_i / \partial \theta_j\}_{i,j=1}^m)| d\boldsymbol{\theta} \end{aligned}$$

where $\chi(\mathbf{y}; T)$ denotes the indicator of a set T .

For fixed \mathbf{y} , $\boldsymbol{\theta}$ the functions $z_i \mapsto \chi(\mathbf{y}; S_i^{\boldsymbol{\theta}}(z_i))$; ($i = 1, \dots, m$) have unit jumps at $\mathbf{z} = \mathbf{0}$ iff $\boldsymbol{\theta} = \boldsymbol{\theta}^*(\mathbf{y})$. As a consequence, from (37) it follows

$$D \leq 2 \int_{\mathbb{R}^N - W_r} \chi(\boldsymbol{\theta}^*(\mathbf{y}); B) d\mathbf{P}_{\boldsymbol{\eta}}(\mathbf{y}) \leq 2p_0. \quad \square$$

Corollary. Let A be an arbitrary measurable subset of U . Then

$$\left| \int_A f_{\theta^*}(\theta | \eta) d\theta - \int_{A \cap \mathcal{B}_\eta} q(\theta | \eta) d\theta \right| \leq 3p_0$$

where $\mathcal{B}_\eta := \{\theta : \eta(\theta) \in \mathcal{A}_\eta\}$.

Proof. We have

$$\left| \int_A f_{\theta^*}(\theta | \eta) d\theta - \int_{A \cap \mathcal{B}_\eta} f_{\theta^*}(\theta | \eta) d\theta \right| \leq \int_{\mathbb{R}^N - W_r} f(y | \eta) dy = p_0. \quad \square$$

4. CONFIDENCE REGIONS FOR $\hat{\theta}$

Let us choose for every $\bar{\theta} \in U_0$ a set $I_{\bar{\theta}} \subset \{\theta : \eta(\theta) \in \mathcal{A}_{\eta(\bar{\theta})}\}$ such that

$$\int_{I_{\bar{\theta}}} q(\theta | \eta(\bar{\theta})) d\theta \geq 1 - \beta.$$

Then, according to Theorem 1,

$$\int_{I_{\bar{\theta}}} f_{\theta^*}(\theta | \eta(\bar{\theta})) d\theta \geq 1 - \beta - 2p_0.$$

Hence the set

$$\mathcal{J}_{\theta^*} := \{\theta : \theta \in U_0, \hat{\theta} \in I_{\theta}\}$$

is a confidence region with the level of significance equal at least to $1 - \beta - 2p_0$.

Theorem 2. If for every $\theta \in U$ there is a (differentiable) orthonormal basis $I_1(\theta), \dots, I_m(\theta)$ of the tangent space to \mathcal{E} at the point $\eta(\theta)$, such that

$$(38) \quad \frac{\partial I_i(\theta)}{\partial \theta_j} I_k(\theta) = 0; \quad (i, j, k = 1, \dots, m)$$

then we can take

$$\mathcal{J}_{\theta^*} = \{\theta : \theta \in U_0, \|\mathbf{P}^\theta[\eta(\hat{\theta}) - \eta(\theta)]\|^2 < \chi_m^2(\beta)\}$$

where $\chi_m^2(\beta)$ is the $(1 - \beta)$ quantile of the χ^2 probability distribution with m degrees of freedom.

Proof. Take $\Sigma = \mathbf{I}$. The expression in Eq. (9) can be written as

$$(39) \quad q(\theta | \eta) = \frac{1}{(2\pi)^{m/2}} \exp\left(-\frac{1}{2}\|\mathbf{P}^\theta[\eta(\theta) - \eta]\|^2\right) \frac{\det\left(\left\{\frac{\partial \eta'}{\partial \theta_j} \frac{\partial}{\partial \theta_k} (\mathbf{P}^\theta[\eta(\theta) - \eta])\right\}_{j,k=1}^m\right)}{\det^{1/2}\left(\left\{\frac{\partial \eta'}{\partial \theta_j} \frac{\partial \eta}{\partial \theta_k}\right\}_{j,k=1}^m\right)}.$$

Define

$$v_i(\theta) := I'_i(\theta) [\eta(\theta) - \eta] ; \quad (i = 1, \dots, m).$$

Evidently

$$(40) \quad \sum_{i=1}^m v_i^2(\theta) = \|\mathbf{P}^0[\eta(\theta) - \eta]\|^2.$$

Further, from (38) it follows that

$$\frac{\partial v_i(\theta)}{\partial \theta_k} = I'_i(\theta) \frac{\partial}{\partial \theta_k} (\mathbf{P}^0[\eta(\theta) - \eta]).$$

Hence

$$(41) \quad \frac{\partial \eta'}{\partial \theta_j} \frac{\partial}{\partial \theta_k} (\mathbf{P}^0[\eta(\theta) - \eta]) = \sum_{i=1}^m \frac{\partial \eta'}{\partial \theta_j} I_i I'_i \frac{\partial}{\partial \theta_k} (\mathbf{P}^0[\eta(\theta) - \eta]) = \sum_{i=1}^m \frac{\partial \eta'}{\partial \theta_j} I_i \frac{\partial v_i}{\partial \theta_k}.$$

From Eqs. (39)–(41) we obtain that

$$q(\theta | \eta) = \frac{1}{(2\pi)^{m/2}} \exp\left(-\frac{1}{2} \sum_i v_i^2(\theta)\right) \left| \det \left(\left\{ \frac{\partial v_i(\theta)}{\partial \theta_j} \right\}_{i,j=1}^m \right) \right|,$$

hence the random vector (v_1, \dots, v_m) is distributed $N(0, \mathbf{I})$. The needed statement follows. \square

Example 1. Take $m = 1$,

$$I(\theta) = \frac{d\eta(\theta)/d\theta}{\|d\eta(\theta)/d\theta\|}.$$

Then

$$0 = \frac{d}{d\theta} (I' I) = 2 \frac{dI'}{d\theta} I,$$

hence the assumption (38) is valid.

Example 2. Take \mathcal{E} a subset of the cylinder

$$\{\mathbf{z} : \mathbf{z} \in \mathbb{R}^N, z_1^2 = 1\}.$$

Evidently Eq. (38) can be satisfied.

APPENDIX A

In this section we present some necessary geometrical statements. We start by some definitions.

A (regular) *curve* in U is a mapping

$$\mathbf{g} : t \in (a, b) \mapsto \mathbf{g}(t) \in U$$

such that the vector of second order derivatives $d^2 \mathbf{g}/dt^2$ exists and it is continuous

on (a, b) . To the curve \mathbf{g} we can associate a curve

$$\gamma : t \in (a, b) \mapsto \gamma(t) \in \mathcal{E}$$

according to

$$(A\ 1) \quad \gamma(t) = \boldsymbol{\eta}[\mathbf{g}(t)].$$

The curve γ is called a *geodesics in the manifold* \mathcal{E} (and correspondingly \mathbf{g} is called a *geodesics in* U) iff

a) the parameter t is normed so that

$$(A\ 2) \quad \left\| \frac{d\gamma}{dt} \right\| = 1 ; \quad (t \in (a, b))$$

b) the *vector of curvature* $d^2\gamma/dt^2$ is orthogonal to \mathcal{E} i.e.

$$(A\ 3) \quad \left\langle \frac{d^2\boldsymbol{\eta}[\mathbf{g}(t)]}{dt^2}, \frac{\partial \boldsymbol{\eta}[\mathbf{g}(t)]}{\partial \theta_i} \right\rangle = 0 ; \quad (i = 1, \dots, m)$$

As known from differential geometry [3, 7], every nonzero solution \mathbf{g} of the differential equations (A 3) (=the Euler-Lagrange equations) is a geodesics in U . Moreover, for every point $\bar{\theta} \in U$ and every nonzero vector $\mathbf{u} \in \mathbb{R}^m$ there is a geodesics \mathbf{g} such that for some \bar{t}

$$(A\ 4) \quad \mathbf{g}(\bar{t}) = \bar{\theta}, \quad d\mathbf{g}(\bar{t})/dt \approx \mathbf{u}.$$

Correspondingly, to every point $\boldsymbol{\eta}(\bar{\theta}) \in \mathcal{E}$ and to every unit vector $\mathbf{w} \in \mathbb{R}^N$ which is tangent to \mathcal{E} at $\boldsymbol{\eta}(\bar{\theta})$ (i.e. \mathbf{w} is a linear combination of the vectors $\partial \boldsymbol{\eta}(\bar{\theta})/\partial \theta_1, \dots, \partial \boldsymbol{\eta}(\bar{\theta})/\partial \theta_m$) there is a geodesics γ such that

$$(A\ 5) \quad \gamma(\bar{t}) = \boldsymbol{\eta}(\bar{\theta}), \quad d\gamma(\bar{t})/dt = \mathbf{w}.$$

We shall use the abbreviated notations

$$\begin{aligned} \dot{\gamma}(\bar{t}) &= d\gamma(t)/dt|_{t=\bar{t}} \\ \ddot{\gamma}(\bar{t}) &= d^2\gamma(t)/dt^2|_{t=\bar{t}} \end{aligned}$$

We denote further

$$(A\ 6) \quad \begin{aligned} \varrho_\gamma(t) &:= \|\ddot{\gamma}(t)\|^{-1} \\ \mathbf{e}_\gamma(t) &:= \ddot{\gamma}(t) \varrho_\gamma(t) \end{aligned}$$

the *radius of curvature* and the unit vector oriented from the point $\gamma(t)$ toward the centre of curvature. By

$$(A\ 7) \quad \mathcal{N}_\gamma(t) := \{\mathbf{y} : \mathbf{y} \in \mathbb{R}^N, \langle \gamma(t) - \mathbf{y}, \dot{\gamma}(t) \rangle = 0\}$$

we denote the hyperplane orthogonal to the curve γ .

Denote by $B(\theta, \mathbf{y})$ (or simply by B) the $m \times m$ symmetric matrix with the entries

$$(A\ 8) \quad B_{ij}(\theta, \mathbf{y}) := \left\langle \frac{\partial \boldsymbol{\eta}}{\partial \theta_i}, \frac{\partial \boldsymbol{\eta}}{\partial \theta_j} \right\rangle + \left\langle \boldsymbol{\eta}(\theta) - \mathbf{y}, \frac{\partial^2 \boldsymbol{\eta}}{\partial \theta_i \partial \theta_j} \right\rangle.$$

Proposition A 1. Let be $\mathbf{y} \in \mathbb{R}^N$ and let $\bar{\boldsymbol{\theta}}$ be a solution of Eqs. (4). $B(\bar{\boldsymbol{\theta}}, \mathbf{y})$ is positive semidefinite (= p.s.) iff for every geodesics γ such that $\gamma(\bar{t}) = \boldsymbol{\eta}(\bar{\boldsymbol{\theta}})$ for some \bar{t} , we have the inequality

$$(A\ 9) \quad \langle \mathbf{y} - \boldsymbol{\eta}(\bar{\boldsymbol{\theta}}), \mathbf{e}_\gamma(\bar{t}) \rangle \leq \varrho_\gamma(\bar{t}).$$

There is the equality sign in (A 9) for some geodesics γ iff $\det B(\bar{\boldsymbol{\theta}}, \mathbf{y}) = 0$.

Proof. Let $\gamma = \boldsymbol{\eta} \circ \mathbf{g}$ be a geodesics and let us denote $\mathbf{c} := \dot{\mathbf{g}}(\bar{t})$. From (A 8) we obtain

$$(A\ 10) \quad \mathbf{c}' \mathbf{B} \mathbf{c} = 1 - \langle \mathbf{y} - \boldsymbol{\eta}(\bar{\boldsymbol{\theta}}), \mathbf{e}_\gamma(\bar{t}) \rangle \varrho_\gamma^{-1}(\bar{t}).$$

i) If \mathbf{B} is p.s. then from Eq. (A 10) follows Eq. (A 9). Conversely, if Eq. (A 9) is valid for every geodesics γ then Eq. (A 10) implies that $\mathbf{c}' \mathbf{B} \mathbf{c} \geq 0$ for every $\mathbf{c} \in \mathbb{R}^n$, such that $\mathbf{c} = \dot{\mathbf{g}}(\bar{t})$ for some geodesics \mathbf{g} . That means, according to Eqs. (A 2) and (A 4), $\mathbf{c}' \mathbf{B} \mathbf{c} \geq 0$ for every \mathbf{c} which is a solution of

$$(A\ 11) \quad \mathbf{c}' \mathbf{M}(\bar{\boldsymbol{\theta}}) \mathbf{c} = 1.$$

Since $\mathbf{M}(\bar{\boldsymbol{\theta}})$ is positive definite it follows that \mathbf{B} is p.s.

ii) If $\det \mathbf{B} = 0$ then $\mathbf{B} \mathbf{c} = 0$ for some $\mathbf{c} \in \mathbb{R}^m$, $\mathbf{c} \neq \mathbf{0}$. Leg \mathbf{g} be the geodesics in U , such that $\mathbf{g}(\bar{t}) = \bar{\boldsymbol{\theta}}$ and that $\dot{\mathbf{g}}(\bar{t}) \approx \mathbf{c}$. Take $\gamma = \boldsymbol{\eta} \circ \mathbf{g}$. From (A 10) it follows that

$$\langle \mathbf{y} - \boldsymbol{\eta}(\bar{\boldsymbol{\theta}}), \mathbf{e}_\gamma(\bar{t}) \rangle = \varrho_\gamma(\bar{t}).$$

Conversely, if this equality is valid for some geodesics $\gamma = \boldsymbol{\eta} \circ \mathbf{g}$ then, according to (A 10), $\mathbf{c}' \mathbf{B} \mathbf{c} = 0$ for some $\mathbf{c} \neq \mathbf{0}$. Since \mathbf{B} is p.s. there is a matrix \mathbf{A} such that $\mathbf{B} = \mathbf{A}' \mathbf{A}$. Therefore $\|\mathbf{A} \mathbf{c}\|^2 = \mathbf{c}' \mathbf{B} \mathbf{c} = 0$. Thus $\mathbf{B} \mathbf{c} = 0$, and $\det \mathbf{B} = 0$. \square

Corollary A 1. Let $\bar{\boldsymbol{\theta}}$ be a solution of Eqs. (4) and let $\|\mathbf{y} - \boldsymbol{\eta}(\bar{\boldsymbol{\theta}})\| < r$. Then $\bar{\boldsymbol{\theta}}$ is the l.s. estimate $\hat{\boldsymbol{\theta}}(\mathbf{y})$.

Proof. We have

$$\langle \mathbf{y} - \boldsymbol{\eta}(\bar{\boldsymbol{\theta}}), \mathbf{e}_\gamma(\bar{t}) \rangle \leq \|\mathbf{y} - \boldsymbol{\eta}(\bar{\boldsymbol{\theta}})\| < r \leq \varrho_\gamma(\bar{t}).$$

Hence the matrix with entries

$$\frac{\partial^2}{\partial \theta_i \partial \theta_j} \|\boldsymbol{\eta}(\bar{\boldsymbol{\theta}}) - \mathbf{y}\|^2 = 2 \mathbf{B}_{ij}(\bar{\boldsymbol{\theta}}, \mathbf{y})$$

is p.d. and $\bar{\boldsymbol{\theta}}$ is a relative minimum. The equality $\bar{\boldsymbol{\theta}} = \hat{\boldsymbol{\theta}}(\mathbf{y})$ then follows from the assumption AS 3. \square

Let us fix a point $\boldsymbol{\eta} \in \mathcal{E}$. Let us denote

$$(A\ 12) \quad \begin{aligned} \mathcal{W}_r &:= \{\mathbf{y} : \mathbf{y} \in \mathbb{R}^N, \|\mathbf{y} - \boldsymbol{\eta}\| < r\}, \\ \bar{\mathcal{W}}_r &:= \{\mathbf{y} : \mathbf{y} \in \mathbb{R}^N, \|\mathbf{y} - \boldsymbol{\eta}\| \leq r\}. \end{aligned}$$

Cf. Eqs. (5), (A 7) and (17) for the definitions of $\kappa(\boldsymbol{\theta})$, $\kappa_\gamma(t)$ and \mathcal{A}_η . From Corollary

A 1 and from the assumptions AS 2, AS 3 it follows that we can write

$$(A\ 13) \quad \mathcal{A}_\eta = \{\eta(\theta) : \theta \in U, \exists \mathbf{z} \in \mathcal{K}(\theta), \|\mathbf{z} - \eta\| < r, \|\mathbf{z} - \eta(\theta)\| < r\}.$$

Proposition A 2. If $\mathbf{y} \in W_r \cap \mathcal{K}(\bar{\theta})$ and $\eta(\bar{\theta}) \in \mathcal{A}_\eta$ then $\|\mathbf{y} - \eta(\bar{\theta})\| < r$.

Proof. According to (A 13) there is a point $\mathbf{z} \in \mathcal{K}(\bar{\theta}) \cap W_r$ such that $\|\mathbf{z} - \eta(\bar{\theta})\| < r$. Suppose that $\|\mathbf{y} - \eta(\bar{\theta})\| \geq r$. Consider the N -dimensional open sphere

$$\mathcal{S} := \{\mathbf{w} : \mathbf{w} \in \mathbb{R}^N, \|\mathbf{w} - \mathbf{c}\| < r\}$$

which is tangent to \mathcal{E} at the point $\eta(\bar{\theta})$ and is such that \mathbf{c} is on the straight line connecting \mathbf{y} with \mathbf{z} . Evidently \mathbf{c} is on the abscissa with the endpoints \mathbf{y}, \mathbf{z} , hence $\|\mathbf{c} - \eta\| < r$. It follows that $\eta \in \mathcal{S}$. But $\mathcal{S} \cap \mathcal{A}_\eta = \emptyset$. This is a contradiction to $\eta \in \mathcal{A}_\eta$. \square

Proposition A 3. Let γ be a geodesics and $\gamma(t) \in \mathcal{A}_\eta$ for some t . Then

$$\frac{d^2 \|\gamma(t) - \eta\|^2}{dt^2} > 0.$$

Proof. Take $\theta \in U$ such that $\eta(\theta) = \gamma(t)$. Denote by η_θ the point of projection of η onto $\mathcal{K}(\theta)$. From Eqs. (5) and (A 3) we obtain

$$(A\ 14) \quad \langle \eta_\theta - \eta, \ddot{\gamma}(t) \rangle = 0$$

According to (A 13) take $\mathbf{y} \in \mathbb{R}^N$ such that $\|\mathbf{y} - \eta\| < r$, $\|\mathbf{y} - \eta(\theta)\| < r$, $\mathbf{y} \in \mathcal{K}(\theta)$. We have $\|\eta - \eta_\theta\| \leq \|\eta - \mathbf{y}\| < r$, hence from Proposition A 2 we obtain $\|\eta_\theta - \gamma(t)\| < r$. Therefore using (A 14) we can write

$$\frac{1}{2} \frac{d^2}{dt^2} \|\gamma(t) - \eta\|^2 = 1 + \langle \gamma(t) - \eta_\theta, \ddot{\gamma}(t) \rangle \geq 1 - \|\eta_\theta - \gamma(t)\|/q_\gamma(t) > 0. \quad \square$$

Proposition A 4. Let be $\eta(\theta^{(1)}) \in \mathcal{A}_\eta$, $\eta(\theta^{(2)}) \in \mathcal{A}_\eta$. Then $\mathcal{K}(\theta^{(1)}) \cap \mathcal{K}(\theta^{(2)}) \cap W_r = \emptyset$.

Proof. According to the assumption AS 3, $\mathbf{z} \in \mathcal{K}(\theta^{(1)}) \cap \mathcal{K}(\theta^{(2)})$ implies $\|\mathbf{z} - \eta(\theta^{(1)})\| > r$ or $\|\mathbf{z} - \eta(\theta^{(2)})\| > r$. Hence, according to Proposition A 2, $\mathbf{z} \notin W_r$. \square

Proposition A 2. Let γ be a geodesics, $\gamma(\bar{i}) = \eta(\bar{\theta}) \in \mathcal{A}_\eta$. Then there is a neighbourhood of $\bar{\theta}$, $U_{\theta^-} \subset U$, such that $\eta(U_{\theta^-}) \subset \mathcal{A}_\eta$.

Proof. Let η_θ be the point of projection of η onto $\mathcal{K}(\theta)$, i.e. the solution of the equations

$$\left\langle \eta_\theta - \eta(\theta), \frac{\partial \eta}{\partial \theta_i} \right\rangle = 0; \quad (i = 1, \dots, m),$$

which satisfies the equality

$$\eta_\theta - \eta = \sum_{j=1}^m k_j^{(\theta)} \frac{\partial \eta(\theta)}{\partial \theta_j}$$

for some $k_1^{(\theta)}, \dots, k_m^{(\theta)}$. Using the implicit function theorem (cf. [2], Theorem 211) we may verify that the mapping $\theta \mapsto \eta_\theta$ is continuous in a neighbourhood V_{θ^-} of $\bar{\theta}$.

We have $\|\eta - \eta_{\theta^-}\| = \min \{\|\eta - \mathbf{z}\| : \mathbf{z} \in \mathcal{K}(\bar{\theta})\} < r$, because $\eta(\bar{\theta}) \in \mathcal{A}_\eta$. Hence $\|\eta_{\theta^-} - \eta(\bar{\theta})\| < r$ (Proposition A 2). From the continuity of the mappings $\theta \mapsto \eta(\theta)$, $\theta \mapsto \eta_\theta$ we have a neighbourhood $U_{\theta^-} \subset V_{\theta^-}$ such that

$$\|\eta_\theta - \eta\| < r, \quad \|\eta_\theta - \eta(\theta)\| < r; \quad (\theta \in U_{\theta^-}).$$

Therefore, according to (A 13) we have $\eta(\theta) \in \mathcal{A}_\eta; (\theta \in U_{\theta^-})$. \square

Let us denote

$$(A 15) \quad t(\mathbf{y}) := \underset{t}{\text{Arg min}} \|\gamma(t) - \mathbf{y}\|,$$

$$(A 16) \quad S_\gamma(t) := \left\{ \mathbf{y} : \mathbf{y} \in \mathbb{R}^N, \frac{d}{dt} \|\gamma(t) - \mathbf{y}\|^2 > 0 \right\}$$

$$(A 17) \quad Q_\gamma(t) := \left\{ \mathbf{y} : \mathbf{y} \in \mathbb{R}^N, \frac{d}{dt} \|\gamma(t) - \eta\|_{t(\mathbf{y})}^2 < \frac{d}{dt} \|\gamma(t) - \eta\|^2 \right\}.$$

Proposition A 6. Let γ be a geodesics, $\gamma(\bar{t}) = \eta(\bar{\theta}) \in \mathcal{A}_\eta$, $\eta(U_{\theta^-}) \subset \mathcal{A}_\eta$, $\gamma(t) \in (U_{\theta^-})$, $t < \bar{t}$.

Then

$$(A 18) \quad W_r \cap [S_\gamma(\bar{t}) - S_\gamma(t)] = W_r \cap [Q_\gamma(\bar{t}) - Q_\gamma(t)].$$

Proof. From Proposition A 3 it follows that the function $t \mapsto (d/dt) \|\gamma(t) - \eta\|^2$ is increasing as long as $\gamma(t) \in U_{\theta^-}$. Evidently $(d/dt) \|\gamma(t) - \mathbf{y}\|_{t(\mathbf{y})}^2 = 0$. Hence, for $t < \bar{t}$, $\gamma(t) \in U_{\theta^-}$ we have

$$(A 19) \quad \mathbf{y} \in Q_\gamma(\bar{t}) - Q_\gamma(t) \Leftrightarrow t \leq t(\mathbf{y}) < \bar{t}.$$

The halfspaces $S_\gamma(\bar{t})$, resp. $S_\gamma(t)$, are limited by the hyperplanes $\mathcal{K}_\gamma(\bar{t})$, resp. $\mathcal{K}_\gamma(t)$. Therefore from Proposition A 4 it follows that

$$\langle t, \bar{t} \rangle = \{t(\mathbf{y}) : \mathbf{y} \in W_r \cap [S_\gamma(\bar{t}) - S_\gamma(t)]\}.$$

Comparing this with Eq. (A 19) we obtain Eq. (A 18). \square

Take a point $\bar{\theta} \in U$ such that $\eta(\bar{\theta}) \in \mathcal{A}_\eta$. In the remaining part of the Appendix we shall introduce adequate local coordinates on \mathcal{E} and local coordinates on \mathbb{R}^N in a neighbourhood of the point $\eta(\bar{\theta})$.

Take m geodesics $\gamma^{(1)}, \dots, \gamma^{(m)}$ such that

$$(A 20) \quad \begin{aligned} \gamma^{(i)}(0) &= \eta(\bar{\theta}); \quad (i = 1, \dots, m). \\ \dot{\gamma}^{(i)}(0), \dot{\gamma}^{(j)}(0) &\rangle = 0; \quad (i \neq j). \end{aligned}$$

We introduce new local coordinates on \mathcal{E} , $t_1 = \tau_1(\theta), \dots, t_m = \tau_m(\theta)$ by the

equations

$$(A\ 21) \quad \langle \eta(\theta) - \gamma^{(i)}(t_i), \dot{\gamma}^{(i)}(t_i) \rangle = 0; \quad (i = 1, \dots, m).$$

From the implicit function theorem (cf. [2]) it follows that the functions $\tau_1(\theta), \dots, \tau_m(\theta)$ are one-to-one and differentiable in a neighbourhood $V_{\theta^-} \subset U_{\theta^-}$.

Analogically, we define new coordinates $x_1 = \xi_1(\mathbf{y}), \dots, x_N = \xi_N(\mathbf{y})$ in the set $\mathcal{G}_{\theta^-} := \{\mathbf{y} : \mathbf{y} \in \mathbb{R}^N, \mathbf{y} \in \mathcal{K}(\theta), \theta \in V_{\theta^-}\}$ by the equations

$$(A\ 22) \quad \langle \eta[\theta^*(\mathbf{y})] - \gamma^{(i)}(x_i), \dot{\gamma}^{(i)}(x_i) \rangle = 0; \quad (i = 1, \dots, m)$$

$$\xi_i(\mathbf{y}) := \langle \mathbf{y} - \eta[\theta^*(\mathbf{y})], \mathbf{w}^{(i)}[\theta^*(\mathbf{y})] \rangle; \quad (i = m+1, \dots, N),$$

where $\mathbf{w}^{(m+1)}(\theta), \dots, \mathbf{w}^{(N)}(\theta)$ is an orthonormal basis of $\{\mathbf{y} - \eta(\theta) : \mathbf{y} \in \mathcal{K}(\theta)\}$ and $\theta^*(\mathbf{y})$ is the solution of Eq. (4) which is in V_{θ^-} .

Other coordinates $z_1 = \zeta_1(\mathbf{y}), \dots, z_N = \zeta_N(\mathbf{y})$ can be introduced as follows. First we define z_1, \dots, z_m by

$$(A\ 23) \quad \langle \mathbf{y} - \gamma^{(i)}(z_i), \dot{\gamma}^{(i)}(z_i) \rangle = 0; \quad (i = 1, \dots, m).$$

Further we denote by $\bar{\theta}(\mathbf{y}) \in U$ the vector defined by

$$\{\eta[\bar{\theta}(\mathbf{y})]\} = \mathcal{A}_{\eta} \cap \bigcap_{i=1}^m \mathcal{K}_i[\zeta_i(\mathbf{y})]$$

(cf. Eq. (A 7) for the definition of $\mathcal{K}_i(t) := \mathcal{K}_{\gamma^{(i)}}(t)$). Denote by $\mathbf{r}^{(m+1)}(\mathbf{y}), \dots, \mathbf{r}^{(N)}(\mathbf{y})$ an orthonormal basis of $\bigcap_{i=1}^m \mathcal{K}_i[\zeta_i(\mathbf{y})]$. Let us define

$$(A\ 24) \quad \zeta_j(\mathbf{y}) := \langle \mathbf{y} - \eta[\bar{\theta}(\mathbf{y})], \mathbf{r}^{(j)}(\mathbf{y}) \rangle; \quad (j = m+1, \dots, N).$$

Evidently

$$(A\ 25) \quad \theta^*(\mathbf{y}) = \bar{\theta} \Rightarrow \bar{\theta}(\mathbf{y}) = \bar{\theta}, \quad \mathbf{r}^{(j)}(\mathbf{y}) = \mathbf{w}^{(j)}[\bar{\theta}(\mathbf{y})] = \mathbf{w}^{(j)}(\bar{\theta}),$$

$$x_1 = \dots = x_m = 0, \quad z_1 = \dots = z_m = 0, \quad x_{m+1} = z_{m+1}, \dots, x_N = z_N.$$

The functions ζ_1, \dots, ζ_N are one-to-one and differentiable in the set \mathcal{G}_{θ^-} with V_{θ^-} choosen adequately. Evidently

$$(A\ 26) \quad \xi_i(\mathbf{y}) = \tau_i[\theta^*(\mathbf{y})],$$

$$\zeta_i(\mathbf{y}) = \tau_i[\bar{\theta}(\mathbf{y})]; \quad (i = 1, \dots, m)$$

We shall compute the Jacobi matrices of the mappings $\theta \mapsto \mathbf{t}, \mathbf{x} \mapsto \mathbf{y}, \mathbf{y} \mapsto \mathbf{z}$.

Differentiating Eqs. (A 21) with respect to θ_j we obtain

$$\left\langle \frac{\partial \eta(\theta)}{\partial \theta_j}, \gamma^{(i)}(t_i) \right\rangle + \sum_{k=1}^m \frac{\partial}{\partial t_k} \langle \eta(\theta) - \gamma^{(i)}(t_i), \dot{\gamma}^{(i)}(t_i) \rangle \frac{\partial \tau_k}{\partial \theta_j} = 0.$$

Hence

$$(A\ 27) \quad \left. \frac{\partial \tau_i}{\partial \theta_j} \right|_{\theta=\bar{\theta}} = \left\langle \frac{\partial \eta(\bar{\theta})}{\partial \theta_j}, \dot{\gamma}^{(i)}(0) \right\rangle; \quad (i, j = 1, \dots, m).$$

Analogously, from Eqs. (A 23) we obtain

$$(A\ 28) \quad \left. \frac{\partial \zeta_i}{\partial y_j} \right|_{\theta^*(\mathbf{y}) = \bar{\theta}} = \frac{\dot{\gamma}_j^{(i)}(0)}{\frac{1}{2} \frac{d^2}{dt^2} \|\mathbf{y}^{(i)}(t) - \mathbf{y}\|_{t=0}^2}; \quad (i = 1, \dots, m, \ j = 1, \dots, N)$$

From (A 24) and (A 26) we obtain

$$\zeta_i(\mathbf{y}) = \langle \mathbf{y} - \boldsymbol{\eta}[\boldsymbol{\tau}^{-1}(\zeta_1(\mathbf{y}), \dots, \zeta_m(\mathbf{y}))], \mathbf{r}^{(i)}(\mathbf{y}) \rangle; \quad (i = m + 1, \dots, N).$$

Hence

$$(A\ 29) \quad \left. \frac{\partial \zeta_i}{\partial y_j} \right|_{\theta(\mathbf{y}) = \bar{\theta}} = r_j^{(i)}(\mathbf{y}) + \sum_{s=1}^m Q_{is} \frac{\partial \zeta_s}{\partial y_j} = w_j^{(i)}; \\ (i = m + 1, \dots, N, \ j = 1, \dots, N)$$

where

$$Q_{is} := \frac{\partial}{\partial z_s} \langle \mathbf{y} - \boldsymbol{\eta}[\boldsymbol{\tau}^{-1}(z_1, \dots, z_m), \mathbf{w}^{(i)}(\bar{\theta})] \rangle|_{z_1 = \dots = z_m = 0} = 0.$$

From Eqs. (A 22) and (A 26) we obtain

$$\mathbf{y} = \boldsymbol{\eta}[\boldsymbol{\tau}^{-1}(x_1, \dots, x_m) + \sum_{j=m+1}^N x_j \mathbf{w}^{(j)}[\boldsymbol{\tau}^{-1}(x_1, \dots, x_m)]] .$$

It follows that for $i = 1, \dots, N$

$$(A\ 30) \quad \left. \frac{\partial y_i}{\partial x_j} \right|_{\theta^*(\mathbf{y}) = \bar{\theta}} = \left. \frac{\partial \eta_i[\boldsymbol{\tau}^{-1}(x_1, \dots, x_m)]}{\partial x_j} \right|_{x_1 = \dots = x_m = 0}; \quad (j = 1, \dots, m) \\ = w_{(j)}^i(\bar{\theta}); \quad (j = m + 1, \dots, N).$$

Proposition A 7. If $\Sigma = \mathbf{I}$ then

$$\{\mathbf{J}\}_{ij} := \left. \frac{\partial z_i}{\partial x_j} \right|_{x_1 = \dots = x_m = 0} \begin{cases} = 1; & i = j, \\ = 0; & i \neq j; \end{cases} \quad (i, j = 1, \dots, N).$$

Proof. Let us denote $\mathbf{d}^{(i)} := \dot{\gamma}^{(i)}(0)/\frac{1}{2}(d^2/dt^2) \|\mathbf{y}^{(i)}(t) - \mathbf{y}\|_0^2$.

We have $\{\mathbf{J}\}_{ij} = \sum_k (\partial z_i / \partial y_k) (\partial y_k / \partial x_j)$. Hence from Eqs. (A 28)–(A 30) we obtain

$$(A\ 31) \quad \mathbf{J} = \begin{pmatrix} \mathbf{d}^{(1)} \\ \vdots \\ \mathbf{d}^{(m)} \\ \mathbf{w}'_{m+1}(\theta) \\ \vdots \\ \mathbf{w}'_N(\theta) \end{pmatrix} \left(\left. \frac{\partial \eta[\boldsymbol{\tau}^{-1}(\mathbf{x})]}{\partial x_1} \right|_{\mathbf{x}=\theta}, \dots, \left. \frac{\partial \eta[\boldsymbol{\tau}^{-1}(\mathbf{x})]}{\partial x_m} \right|_{\mathbf{x}=\theta}, \mathbf{w}_{m+1}(\theta), \dots, \mathbf{w}_N(\theta) \right) = \mathbf{I}$$

since, if $\theta^*(\mathbf{y}) = \bar{\theta}$ then $\partial \boldsymbol{\eta}[\boldsymbol{\tau}^{-1}(\mathbf{x})] / \partial x_i = \dot{\gamma}^{(i)}(0)$. □

APPENDIX B (COMPUTATION)

It may be useful to consider the computational aspect when computing the density $q(\hat{\theta} | \theta)$ and the level of regularity $1 - p_0$. To be concrete, let us consider the following example.

Take

$$\eta_x(\theta) = e^{\theta_1 x} \sin \theta_2 x; \quad \theta_1 \in (0, 10) \\ \theta_2 \in (0, 2\pi),$$

take $\Sigma = \mathbf{I}$, and take 4 design points $x_1 = 1, x_2 = 2, x_3 = 3, x_4 = 4$.

The program for the computation of $f(\hat{\theta} | \theta)$:

Input variables: $\theta_1, \theta_2, \hat{\theta}_1, \hat{\theta}_2$ (4 numbers)

Subroutines:

(A) $\eta_i(\theta) = e^{i\theta_1} \sin i\theta_2; \quad (i = 1, 2, 3, 4)$

(B) $\frac{\partial \eta_i(\theta)}{\partial \theta_1} = i e^{i\theta_1} \sin i\theta_2$

(C) $\frac{\partial \eta_i(\theta)}{\partial \theta_2} = i e^{i\theta_1} \cos i\theta_2$

(D) $\frac{\partial^2 \eta_i(\theta)}{\partial \theta_1^2} = i^2 e^{i\theta_1} \sin i\theta_2$

(E) $\frac{\partial^2 \eta_i(\theta)}{\partial \theta_1 \partial \theta_2} = i^2 e^{i\theta_1} \cos i\theta_2$

(F) $\frac{\partial^2 \eta_i(\theta)}{\partial \theta_2^2} = -i^2 e^{i\theta_1} \sin i\theta_2$

Subroutines for matrices:

(G) $M_{jk}(\theta) = \sum_{i=1}^4 \frac{\partial \eta_i(\theta)}{\partial \theta_j} \frac{\partial \eta_i(\theta)}{\partial \theta_k}; \quad (j, k = 1, 2)$

(H) $\mathbf{M}(\theta) \mapsto \mathbf{M}^{-1}(\theta)$

(I) $P_{jk}^{\theta} = \sum_{p,q=1}^2 \frac{\partial \eta_j(\theta)}{\partial \theta_p} \{M^{-1}(\theta)\}_{pq} \frac{\partial \eta_k(\theta)}{\partial \theta_q}$

Use the subroutines (A)–(I) for $\theta = (\hat{\theta}_1, \hat{\theta}_2)$, the subroutine (A) for $\theta = (\theta_1, \theta_2)$ and compute Eq. (9) for different inputs $\theta_1, \theta_2, \hat{\theta}_1, \hat{\theta}_2$.

The program for the computation of $(1 - p_0)$:

The main idea of the algorithm is that through any point $\theta = (\theta_1, \theta_2) \in (0, 10) \times (0, 2\pi)$ and in any direction given by $\hat{\theta} := d\theta/dt$ we can draw a unique geodesics

which is a solution if Eqs. (A 3), but for the natural parameter t_{nat} , where $dt_{\text{nat}}/dt = \|\mathbf{d}\boldsymbol{\eta}/d\mathbf{t}\|$ (cf. Eq. (A 2)).

Input: $\theta_1, \theta_2, \theta_1, \theta_2$ (4 numbers)

Subroutines: (B)–(F)

Subroutine “derivatives”:

$$(J) \quad \frac{d\boldsymbol{\eta}}{dt} = \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_1} \dot{\theta}_1 + \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_2} \dot{\theta}_2$$

$$(K) \quad \frac{d^2 \boldsymbol{\eta}}{dt^2} [v, w] = \frac{\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_1^2} (\dot{\theta}_1)^2 + 2 \frac{\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_1 \partial \theta_2} \dot{\theta}_1 \dot{\theta}_2 + \\ + \frac{\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_2^2} (\dot{\theta}_2)^2 + \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_1} v + \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_2} w$$

where v, w are unknown input variables (interpreted as $v = \ddot{\theta}_1, w = \ddot{\theta}_2$),

$$(L) \quad \frac{d\boldsymbol{\eta}}{dt_{\text{nat}}} = \frac{d\boldsymbol{\eta}}{dt} / \left\| \frac{d\boldsymbol{\eta}}{dt} \right\|$$

$$(M) \quad \frac{d^2 \boldsymbol{\eta} [v, w]}{dt_{\text{nat}}^2} = \frac{\frac{d^2 \boldsymbol{\eta}}{dt^2} [v, w] - \frac{d\boldsymbol{\eta}}{dt} \left(\frac{d}{dt} \left\| \frac{d\boldsymbol{\eta}}{dt} \right\| \right) / \left\| \frac{d\boldsymbol{\eta}}{dt} \right\|}{\left\| \frac{d\boldsymbol{\eta}}{dt} \right\|^2}$$

Linear equations: Compute v, w as the solution of the linear equations

$$(EQ) \quad \sum_{i=1}^4 \frac{d^2 \eta_i [v, w]}{dt_{\text{nat}}^2} \frac{\partial \eta_i(\boldsymbol{\theta})}{\partial \theta_1} = 0 \\ \sum_{i=1}^4 \frac{d^2 \eta_i [v, w]}{dt_{\text{nat}}^2} \frac{\partial \eta_i(\boldsymbol{\theta})}{\partial \theta_2} = 0$$

(cf. Eqs. (A 3))

Put v, w into (K), (M) and compute

$$\varrho(\theta_1, \theta_2, \theta_1, \theta_2) = \left\| \frac{d^2 \boldsymbol{\eta} [v, w]}{dt_{\text{nat}}^2} \right\|^{-1}.$$

For different inputs $\theta_1, \theta_2, \theta_1, \theta_2$ compute

$$r = \min \{ \varrho(\theta_1, \theta_2, \theta_1, \theta_2) : \theta_1 \in (0, 10), \theta_2 \in (0, 2\pi),$$

$$\dot{\theta}_1 \in \langle 0, 1 \rangle, \dot{\theta}_2 \in \langle 0, 1 \rangle, \dot{\theta}_1^2 + \dot{\theta}_2^2 = 1 \}.$$

Compute p_0 from

$$\chi_4^2(p_0) = r^2$$

where $\chi_4^2(p_0)$ is the $(1 - p_0)$ quantile of the χ^2 p.d. with 4 degrees of freedom.

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REFERENCES

- [1] B. Hostinský: Diferenciální geometrie křivek a ploch (Differential geometry of curves and surfaces). Přírodovědecké nakladatelství JČSMF, Praha 1950.
- [2] V. Jarník: Diferenciální počet II (Differential calculus). NČSAV, Praha 1956.
- [3] J. Milnor: Morse Theory. Princeton Univ. Press, Princeton, N. J. 1963.
- [4] A. Pázman: Geometry of gaussian nonlinear regression — parallel curves and confidence intervals. *Kybernetika* 18 (1982), 376—396.
- [5] A. Pázman: Nonlinear least squares — uniqueness versus ambiguity. *Math. Operationsforsch. Statist. Ser. Statistics* 14 (1984) (to appear.)
- [6] A. Rényi: Teorie pravděpodobnosti (Probability theory). Academia, Praha 1972.
- [7] S. Sternberg: Lectures on Differential Geometry. Second printing. Prentice-Hall, Englewood Cliffs 1965.

RNDr. Andrej Pázman, DrSc., Matematický ústav SAV (Mathematical Institute — Slovak Academy of Sciences), ul. Obrancov mieru 49, 814 73 Bratislava. Czechoslovakia.