

DISTRIBUTION OF THE WEIGHTED L.S. ESTIMATES IN NONLINEAR MODELS WITH SYMMETRICAL ERRORS

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The nonlinear regression model $\mathbf{y} = \boldsymbol{\eta}(\boldsymbol{\theta}) + \boldsymbol{\varepsilon}$ with the error vector $\boldsymbol{\varepsilon}$ having an elliptically symmetrical probability distribution is considered. An approximative formula for the non-asymptotical (= small sample) probability density of the weighted L. S. estimates of $\boldsymbol{\theta}$ is obtained by geometrical methods. The considered weights are general (i.e. not related to the variance matrix $\boldsymbol{\Sigma}$ of $\boldsymbol{\varepsilon}$). The difference between the true and the approximative densities is evaluated. Earlier author's results are thus extended from the case of normal errors, and of weights depending on $\boldsymbol{\Sigma}$, to a more general case.

1. INTRODUCTION

Let

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

be a nonlinear regression model. Here $\mathbf{y} := (y_1, \dots, y_N)^T$ is the vector of the observed data, $\boldsymbol{\theta} := (\theta_1, \dots, \theta_m)^T$ is the vector of unknown parameters, $m < N$, $\boldsymbol{\theta} \in \Theta$ where Θ is the (given) parameter space which is an open subset of \mathbb{R}^m . The mapping $\boldsymbol{\eta}: \Theta \in \overline{\Theta} \mapsto \boldsymbol{\eta}(\boldsymbol{\theta}) \in \mathbb{R}^N$, defined and finite on the closure $\overline{\Theta}$ of the set Θ , is supposed to be known, continuous, and to have continuous second order derivatives on Θ . The vectors of the first order derivatives $\partial \boldsymbol{\eta}(\boldsymbol{\theta}) / \partial \theta_1, \dots, \partial \boldsymbol{\eta}(\boldsymbol{\theta}) / \partial \theta_m$ are supposed to be linearly independent for every $\boldsymbol{\theta} \in \Theta$ (i.e. the model is regular).

In this paper we consider the case when the probability density of the error vector $\boldsymbol{\varepsilon}$ is elliptically symmetrical, with a zero mean $\mathbf{E}(\boldsymbol{\varepsilon}) = 0$, and a positive definite variance matrix $\boldsymbol{\Sigma}$, $\text{Var}(\boldsymbol{\varepsilon}) = \boldsymbol{\Sigma}$, defining the elliptical symmetry. Such a probability density (with respect to the Lebesgue measure in \mathbb{R}^N) is given by the formula (cf. [5])

$$(2) \quad f(\boldsymbol{\varepsilon}) := \det^{-1/2}(\boldsymbol{\Sigma}) h(\boldsymbol{\varepsilon}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\varepsilon})$$

where $h: \langle 0, \infty \rangle \mapsto \langle 0, \infty \rangle$ is a function such that

$$\int_0^\infty z^{N/2} h(z) dz < \infty.$$

To ensure that $f(\boldsymbol{\varepsilon})$ is a probability density and that $\text{Var}(\boldsymbol{\varepsilon}) = \boldsymbol{\Sigma}$ we have to suppose that

$$\int_{\mathbb{R}^N} h(\|\mathbf{v}\|^2) d\mathbf{v} = 1$$

$$\int_{\mathbb{R}^N} h(\|\mathbf{v}\|^2) \|\mathbf{v}\|^2 d\mathbf{v} = N.$$

If the function h does not satisfy these two norming conditions, we can always find two positive numbers α and β such that the function $\mathbf{z} \mapsto \alpha h(\beta \mathbf{z})$ has the required properties. (We note that, like in Section 2, these two N -dimensional integrals can be changed to two onedimensional integrals when using spherical coordinates in \mathbb{R}^N .)

The set $\{\boldsymbol{\varepsilon}: f(\boldsymbol{\varepsilon}) = \text{const}\}$ is an ellipsoid in \mathbb{R}^N , therefore we speak about the elliptical symmetry. In the case of $\boldsymbol{\Sigma} = \mathbf{I}$, $f(\boldsymbol{\varepsilon})$ is spherically symmetrical. Another equivalent definition of the spherical symmetry is that $f(\boldsymbol{\varepsilon}) = f(\mathbf{U}\boldsymbol{\varepsilon})$ for every orthogonal $m \times m$ matrix \mathbf{U} (i.e. such that $\mathbf{U}^T \mathbf{U} = \mathbf{I}$). Thus spherically symmetrical densities are invariant to every rotation of the sample space of $\boldsymbol{\varepsilon}$.

Elliptically symmetrical distributions are studied in several papers [2, 5, 6], and we resume their properties in Section 2.

A special case of an elliptically symmetrical density is the normal density $N(\mathbf{0}, \boldsymbol{\Sigma})$ with

$$h(t) = (2\pi)^{-N/2} \exp\{-t/2\}.$$

Other choices of the function $h(\cdot)$ are presented in Section 2.

A standard estimator of the vector $\boldsymbol{\theta}$ is the weighted least squares (= L. S.) estimator given by

$$(3) \quad \hat{\boldsymbol{\theta}} := \hat{\boldsymbol{\theta}}(\mathbf{y}) := \arg \min [\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\theta})]^T \mathbf{V}^{-1} [\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\theta})],$$

where $\boldsymbol{\theta} \in \bar{\Theta}$ and \mathbf{V} is some given positive definite (= p.d.) matrix. Usually (if possible) the matrix \mathbf{V} is proportional to the covariance matrix $\boldsymbol{\Sigma}$. This leads to an optimal unbiased estimator of $\boldsymbol{\theta}$ when the model (1) is linear (i.e. $\boldsymbol{\eta}(\boldsymbol{\theta}) = \mathbf{A}\boldsymbol{\theta} + \boldsymbol{\alpha}$) (cf. [6]), and such a \mathbf{V} is considered as preferable also in the nonlinear case. However, if $\boldsymbol{\Sigma}$ is unknown, the matrix \mathbf{V} is to be chosen ad hoc. Since the estimate (3) is not influenced by setting a matrix $c\mathbf{V}$ ($c > 0$) instead of \mathbf{V} , we can always choose \mathbf{V} such that it dominates the matrix $\boldsymbol{\Sigma}$, i.e. that

$$\boldsymbol{\alpha}^T \mathbf{V}^{-1} \boldsymbol{\alpha} \leq \boldsymbol{\alpha}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\alpha}; \quad (\boldsymbol{\alpha} \in \mathbb{R}^N)$$

(see Proposition 3).

The normal equations corresponding to (3) are

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

hence, if $\hat{\boldsymbol{\theta}}(\mathbf{y}) \in \Theta$, it is a solution of

$$(4) \quad [\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\theta})]^T \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^T} = \mathbf{0}.$$

In this paper we present an approximative nonasymptotical probability density

of $\hat{\theta}$, and we present a formula for the upper bound for the difference between the true and the approximative densities. Earlier author's results [7, 8] are thus extended from the case of normal errors to the case of elliptically symmetrical errors, and from the case of $\mathbf{V} = \mathbf{\Sigma}$ to the case of arbitrary, p.d. matrices \mathbf{V} and $\mathbf{\Sigma}$. However, the main geometrical ideas remain unchanged since the elliptical symmetry has been important also in the investigation presented in [7, 8].

The approximative nonasymptotical probability density of $\hat{\theta}$ proposed in this paper is equal to

$$(5) \quad q(\hat{\theta} | \bar{\theta}) := \frac{\det \mathbf{Q}(\hat{\theta}, \bar{\theta})}{\det^{1/2} \mathbf{B}(\bar{\theta})} h_m(\|\mathbf{P}^0[\boldsymbol{\eta}(\hat{\theta}) - \boldsymbol{\eta}]\|_{\bar{\mathbf{z}}}^2)$$

where

$$\boldsymbol{\eta} := \boldsymbol{\eta}(\bar{\theta})$$

is the true mean of \mathbf{y} ,

$$(6) \quad \mathbf{B}(\bar{\theta}) := \frac{\partial \boldsymbol{\eta}^T(\bar{\theta})}{\partial \bar{\theta}} \mathbf{V}^{-1} \boldsymbol{\Sigma} \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\bar{\theta})}{\partial \bar{\theta}^T},$$

$$\mathbf{Q}(\hat{\theta}, \bar{\theta}) := \mathbf{M}(\bar{\theta}) + [(\mathbf{I} - \mathbf{P}^0)(\boldsymbol{\eta}(\hat{\theta}) - \boldsymbol{\eta})]^T \mathbf{V}^{-1} \frac{\partial^2 \boldsymbol{\eta}(\bar{\theta})}{\partial \bar{\theta} \partial \bar{\theta}^T}$$

$$\mathbf{M}(\bar{\theta}) := \frac{\partial \boldsymbol{\eta}^T(\bar{\theta})}{\partial \bar{\theta}} \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\bar{\theta})}{\partial \bar{\theta}^T},$$

$$(7) \quad \mathbf{P}^0 := \boldsymbol{\Sigma} \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\bar{\theta})}{\partial \bar{\theta}^T} \mathbf{B}^{-1}(\bar{\theta}) \frac{\partial \boldsymbol{\eta}^T(\bar{\theta})}{\partial \bar{\theta}} \mathbf{V}^{-1}$$

(\mathbf{P}^0 is a projector),

$$\|\boldsymbol{\alpha}\|_{\bar{\mathbf{z}}}^2 := \boldsymbol{\alpha}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\alpha}; \quad (\boldsymbol{\alpha} \in \mathbb{R}^N),$$

and where $h_m: \langle 0, \infty \rangle \mapsto \langle 0, \infty \rangle$ is defined by the formula

$$(8) \quad h_m(t) := \frac{\pi^{(N-m)/2}}{\Gamma\left(\frac{N-m}{2}\right)} \int_0^\infty u^{(N-m)/2-1} h(t+u) du.$$

The expression in (5) becomes simpler when $\boldsymbol{\Sigma} = \mathbf{V}$. Then $\mathbf{M}(\bar{\theta}) = \mathbf{B}(\bar{\theta}) =$ the Fisher information matrix for the case of normal errors, and $\mathbf{Q}(\hat{\theta}, \bar{\theta})$ is the information matrix $\mathbf{M}(\bar{\theta})$ corrected by a term reflecting the curvature of the model (1). ($\mathbf{Q}(\hat{\theta}, \bar{\theta})$ is a measure of the observed information gained from the experiment when $\hat{\theta} = \hat{\theta}(\mathbf{y})$ is obtained from the observation and $\bar{\theta}$ is the true value of θ (cf. [9]).)

In the case that the model (1) is linear, $\boldsymbol{\eta}(\theta) = \mathbf{A}\theta$, $q(\hat{\theta} | \bar{\theta})$ is equal to the exact probability density of $\hat{\theta}$. In the case that $\mathbf{V} = \boldsymbol{\Sigma}$, it is equal to

$$q(\hat{\theta} | \bar{\theta}) = \det^{1/2}(\mathbf{M}) h_m[(\hat{\theta} - \bar{\theta})^T \mathbf{M}(\hat{\theta} - \bar{\theta})],$$

where $\mathbf{M} := \mathbf{A}\boldsymbol{\Sigma}^{-1}\mathbf{A}^T$ is the information matrix. In the normal case we obtain the

well known formula

$$q(\hat{\theta} | \bar{\theta}) = (2\pi)^{m/2} \det^{1/2}(\mathbf{M}) \exp \left\{ -\frac{1}{2}(\hat{\theta} - \bar{\theta})^T \mathbf{M}(\hat{\theta} - \bar{\theta}) \right\}.$$

In the general case the approximative density $q(\hat{\theta} | \bar{\theta})$ is invariant to the change of parameters $\beta = \beta(\theta)$, i.e.

$$q(\hat{\theta} | \bar{\theta}) = \left| \det \left(\frac{\partial \beta(\theta)}{\partial \theta^T} \Big|_{\theta = \hat{\theta}} \right) \right| q(\hat{\beta} | \bar{\beta}),$$

where $q(\hat{\beta} | \bar{\beta})$ is obtained by putting into the expression (5) the function $v(\beta) := \eta[\theta^{-1}(\beta)]$ and its derivatives instead of the function $\eta(\theta)$.

Example. (The contaminated normal nonlinear regression.)

Suppose that the probability density of ε is equal to

$$f(\varepsilon) = (2\pi)^{-N/2} \left[(0.9) \exp \left\{ -\frac{1}{2} \|\varepsilon\|^2 \right\} + \frac{(0.1)}{10^{N/2}} \exp \left\{ -\frac{1}{20} \|\varepsilon\|^2 \right\} \right]$$

and consider the non-weighted L. S. estimates. Hence $\mathbf{V} = \Sigma = \mathbf{I}$, and

$$h(t) = (2\pi)^{-N/2} \left[(0.9) \exp \left\{ -\frac{1}{2} t \right\} + 10^{-N/2-1} \exp \left\{ -\frac{1}{20} t \right\} \right].$$

Consequently

$$h_m(t) = (2\pi)^{-m/2} \left[(0.9) \exp \left\{ -\frac{1}{2} t \right\} + 10^{-m/2-1} \exp \left\{ -\frac{1}{20} t \right\} \right]$$

because $h_m(\sum_{i=1}^m \varepsilon_i^2)$ is the m -dimensional marginal of $f(\varepsilon)$ (see Section 2). Further

$$\mathbf{P}^0 = \frac{\partial \eta(\theta)}{\partial \theta^T} \mathbf{M}^{-1}(\theta) \frac{\partial \eta^T(\theta)}{\partial \theta},$$

$$\mathbf{M}(\theta) = \mathbf{B}(\theta) = \frac{\partial \eta^T(\theta)}{\partial \theta} \frac{\partial \eta(\theta)}{\partial \theta^T},$$

and

$$q(\hat{\theta} | \bar{\theta}) = (2\pi)^{-m/2} \frac{\det \left[\mathbf{M}(\hat{\theta}) + [\eta(\hat{\theta}) - \bar{\eta}]^T (\mathbf{I} - \mathbf{P}^0) \frac{\partial^2 \eta(\theta)}{\partial \theta \partial \theta^T} \right]}{\det^{1/2} \mathbf{M}(\hat{\theta})} \times$$

$$\times \left[(0.9) \exp \left\{ -\frac{1}{2} \|\mathbf{P}^0[\eta(\hat{\theta}) - \bar{\eta}]\|^2 \right\} + 10^{-m/2-1} \exp \left\{ -\frac{1}{20} \|\mathbf{P}^0[\eta(\hat{\theta}) - \bar{\eta}]\|^2 \right\} \right]$$

Computing point by point both components of $q(\hat{\theta} | \bar{\theta})$, we can evaluate the influence of the contamination on the least squares in a gaussian nonlinear model.

2. PROPERTIES OF ELLIPTICALLY (SPHERICALLY) SYMMETRICAL DENSITIES

We write: $\mathbf{y} \sim S_N(\boldsymbol{\eta}, \Sigma, h)$ iff \mathbf{y} has the density

$$(9) \quad f_{\mathbf{r}}(\mathbf{y}) = \det^{-1/2}(\Sigma) h[(\mathbf{y} - \boldsymbol{\eta})^T \Sigma^{-1}(\mathbf{y} - \boldsymbol{\eta})].$$

This density has all moments up to the k th order iff

$$(10) \quad \int_0^\infty u^{\frac{N+k}{2}-1} h(u) \, du < \infty$$

(cf. [5]). If $k \geq 1$, we have $E(\mathbf{y}) = \boldsymbol{\eta}$. If $k \geq 2$, we have $\text{Var}(\mathbf{y}) = \boldsymbol{\Sigma}$. (See Section 1 for the norming conditions on h .)

If $\mathbf{z} = \mathbf{A}\mathbf{y}$, where \mathbf{A} is an $N \times N$ nonsingular matrix, then

$$\mathbf{z} \sim S_N(\mathbf{A}\boldsymbol{\eta}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T, h)$$

(cf. [5]). Consequently, if $\mathbf{y} \sim S_N(\boldsymbol{\eta}, \boldsymbol{\Sigma}, h)$, then there is a matrix \mathbf{A} such that $\mathbf{z} = \mathbf{A}(\mathbf{y} - \boldsymbol{\eta}) \sim S_N(\mathbf{0}, \mathbf{I}, h)$.

If $\mathbf{y} \sim S_N(\boldsymbol{\eta}, \boldsymbol{\Sigma}, h)$, then

$$\mathbf{y} = \boldsymbol{\eta} + l\boldsymbol{\Sigma}^{1/2}\mathbf{u},$$

where the vector \mathbf{u} is uniformly distributed on the unit sphere $\{\mathbf{z} \in \mathbb{R}^N, \|\mathbf{z}\| = 1\}$, and where l is a nonnegative random variable which is independent of \mathbf{u} (cf. [6]).

If $\boldsymbol{\varepsilon} \sim S_N(\mathbf{0}, \mathbf{I}, h)$, then the marginal density of $(\varepsilon_1, \dots, \varepsilon_m)$ is equal to

$$h_m\left(\sum_{k=1}^m \varepsilon_k^2\right)$$

where

$$h_m(t) := \int_{\mathbb{R}^{N-m}} h(t + \|\mathbf{v}\|^2) \, d\mathbf{v}$$

(cf. [5]). Using spherical coordinates in \mathbb{R}^{N-m} (like [5], p. 427) we obtain the formula (8).

Suppose that $\boldsymbol{\varepsilon} \sim S_N(\mathbf{0}, \mathbf{I}, h)$. Denote $J := \{i_1, \dots, i_m\}$. The conditional density of $\{\varepsilon_j; j \notin J\}$ given $\{\varepsilon_j; j \in J\}$ is evidently equal to

$$k_{N-m}\left(\sum_{i \notin J} \varepsilon_i^2 \mid \sum_{j \in J} \varepsilon_j^2\right)$$

where

$$(11) \quad k_{N-m}(t \mid u) := \frac{h(t + u)}{h_m(u)}.$$

Hence this density is spherically symmetrical.

Let $\boldsymbol{\varepsilon} \sim S_N(\mathbf{0}, \mathbf{I}, h)$. Then the probability density of the random variable $u := \|\boldsymbol{\varepsilon}\|^2$ is equal to

$$(12) \quad \frac{\pi^{N/2}}{\Gamma\left(\frac{N}{2}\right)} u^{\frac{N}{2}-1} h(u)$$

(cf. [5]).

Evidently, if $\boldsymbol{\varepsilon} \sim S_N(\mathbf{0}, \mathbf{I}, h)$, then $\varepsilon_1, \dots, \varepsilon_N$ are uncorrelated random variables. They are independent if and only if $f(\boldsymbol{\varepsilon})$ is the normal density (cf. [5] or [10], chpt. 3a.1).

We have a large choice for the function $h(t)$ in the expression (9). Some examples of $h(t)$ are (cf. [2]):

a)

$$h(t) = \alpha(2\pi)^{N/2} \int_0^\infty \exp\{-\frac{1}{2}\beta tu\} G(du),$$

where G is a probability distribution on $\langle 0, \infty \rangle$ and $\alpha > 0, \beta > 0$. The corresponding densities are mixed normal densities.

b)

$$h(t) = ct^{k-1} \exp\{-rt^{\lambda}\}$$

for some $c > 0, \lambda > 0, r > 0$ and k such that $2k + N > 2$ (the generalized gamma densities).

c)

$$h(t) = c\sqrt{\pi/2} \exp\{-\sqrt{t}/s\},$$

where c, s are positive constants (the spherical Laplace density), etc.

3. THE GEOMETRY OF THE MODEL

The set

$$(13) \quad \mathcal{E} := \{\boldsymbol{\eta}(\boldsymbol{\theta}); \boldsymbol{\theta} \in \Theta\}$$

is the "expectation surface" of the nonlinear regression model (1). The point $\boldsymbol{\eta} = \boldsymbol{\eta}(\boldsymbol{\theta})$ is a fixed point of \mathcal{E} . Take $r > 0$. Denote by

$$(14) \quad G_n(r) := \{\boldsymbol{y} \in \mathbb{R}^N, \|\boldsymbol{y} - \boldsymbol{\eta}\|_2 < r\}$$

a sphere centred at $\boldsymbol{\eta}$ (see Fig. 1). Further denote by $A_n(r)$ a subset of the extended parameter space Θ defined by

$$A_n(r) := \{\boldsymbol{\theta}(\boldsymbol{y}); \boldsymbol{y} \in G_n(r)\}.$$

For every $\boldsymbol{\theta} \in \Theta$ denote by

$$\mathcal{N}(\boldsymbol{\theta}) := \left\{ \boldsymbol{z} \in \mathbb{R}^N, \boldsymbol{z}^T \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^T} = 0 \right\}$$

the subspace of \mathbb{R}^N which is \mathbf{V} -orthogonal to the tangent plane to \mathcal{E} (the later being generated by the vectors $\partial \boldsymbol{\eta}(\boldsymbol{\theta})/\partial \theta_1, \dots, \partial \boldsymbol{\eta}(\boldsymbol{\theta})/\partial \theta_m$).

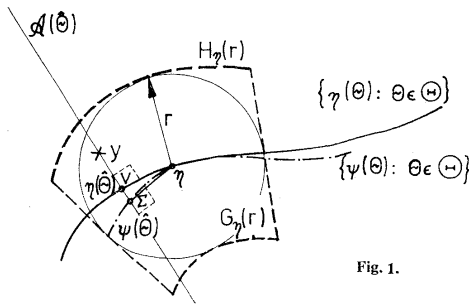


Fig. 1.

Denote by $\mathbf{w}_1(\boldsymbol{\theta}), \dots, \mathbf{w}_{N-m}(\boldsymbol{\theta})$ a Σ -orthogonal basis of $\mathcal{N}(\boldsymbol{\theta})$. It is \mathbf{V} -orthogonal to the tangent plane, i.e.

$$(15) \quad \begin{aligned} \mathbf{w}_i^T(\boldsymbol{\theta}) \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_j} &= 0; \quad \begin{cases} i = 1, \dots, N-m \\ j = 1, \dots, m \end{cases} \\ \mathbf{w}_i^T(\boldsymbol{\theta}) \Sigma^{-1} \mathbf{w}_j(\boldsymbol{\theta}) &= 0 \quad \text{if } i \neq j \\ &= 1 \quad \text{if } i = j \end{aligned}$$

Evidently, the Σ -orthogonal projector onto $\mathcal{N}(\boldsymbol{\theta})$ is equal to the matrix

$$\mathbf{R}^0 := \mathbf{W}(\boldsymbol{\theta}) \mathbf{W}^T(\boldsymbol{\theta}) \Sigma^{-1}$$

where $\mathbf{W}(\boldsymbol{\theta}) := (\mathbf{w}_1(\boldsymbol{\theta}), \dots, \mathbf{w}_{N-m}(\boldsymbol{\theta}))$. Let us denote by

$$(16) \quad \boldsymbol{\psi}(\boldsymbol{\theta}) := \boldsymbol{\eta}(\boldsymbol{\theta}) + \mathbf{R}^0 [\boldsymbol{\eta} - \boldsymbol{\eta}(\boldsymbol{\theta})]$$

the Σ -orthogonal projection of the point $\boldsymbol{\eta}$ onto the set

$$\mathcal{A}(\boldsymbol{\theta}) := \mathcal{N}(\boldsymbol{\theta}) + \boldsymbol{\eta}(\boldsymbol{\theta})$$

(see Fig. 1 for $\mathbf{V} = \mathbf{I}$). We introduce the vector $\boldsymbol{\psi}(\boldsymbol{\theta})$ because $\boldsymbol{\psi}(\hat{\boldsymbol{\theta}})$ is equal to a conditional mean of \mathbf{y} (see Section 4). We have

$$\boldsymbol{\psi}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta} = [\mathbf{I} - \mathbf{R}^{\hat{\boldsymbol{\theta}}}] (\boldsymbol{\eta}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta}),$$

and from (4) we obtain

$$\mathbf{y} - \boldsymbol{\eta}(\hat{\boldsymbol{\theta}}) \in \mathcal{A}(\hat{\boldsymbol{\theta}}).$$

Hence we have the Pythagorean relation

$$(17) \quad \|\mathbf{y} - \boldsymbol{\eta}\|_{\Sigma}^2 = \|\mathbf{y} - \boldsymbol{\psi}(\hat{\boldsymbol{\theta}})\|_{\Sigma}^2 + \|\boldsymbol{\psi}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta}\|_{\Sigma}^2.$$

Denote by

$$(18) \quad H_{\boldsymbol{\eta}}(r) := \{\mathbf{y}: \mathbf{y} \in \mathbb{R}^N, \hat{\boldsymbol{\theta}}(\mathbf{y}) \in A_{\boldsymbol{\eta}}(r), \|\mathbf{y} - \boldsymbol{\psi}[\hat{\boldsymbol{\theta}}(\mathbf{y})]\|_{\Sigma} < r\}$$

a ‘‘tube’’ in the sample space around the surface $\{\boldsymbol{\psi}(\boldsymbol{\theta}): \boldsymbol{\theta} \in A_{\boldsymbol{\eta}}(r)\}$ (see Fig. 1).

We have

$$(19) \quad G_{\boldsymbol{\eta}}(r) \subset H_{\boldsymbol{\eta}}(r).$$

In Section 4 we shall consider samples belonging to $H_{\boldsymbol{\eta}}(r)$, but only such that the corresponding L. S. estimates are not on the boundary of $\bar{\Theta}$. Therefore we assume that:

A1:

$$A_{\boldsymbol{\eta}}(r) \subset \Theta$$

(i.e. the point $\boldsymbol{\eta}$ is ‘‘sufficiently distant’’ from the boundary of $\bar{\Theta}$).

To avoid complications with the nonidentifiability of the parameter $\boldsymbol{\theta}$ we shall suppose that

A2: The mapping $\boldsymbol{\theta} \in A_{\boldsymbol{\eta}}(r) \mapsto \boldsymbol{\eta}(\boldsymbol{\theta}) \in \mathcal{E}$ is one-to-one.

To avoid that the expectation surface \mathcal{E} could overlap the neighbourhood of its subset $\{\boldsymbol{\eta}(\boldsymbol{\theta}): \boldsymbol{\theta} \in A_{\boldsymbol{\eta}}(r)\}$, we require that r is such that

A3: If

- i) $\boldsymbol{y} \in H_{\boldsymbol{\eta}}(r)$
 - ii) $\boldsymbol{\theta}^*$ is a solution of (4)
 - iii) $\|\boldsymbol{y} - \boldsymbol{\eta}(\boldsymbol{\theta}^*)\|_{\mathbf{E}} < r$
- then $\boldsymbol{\theta}^* \in A_{\boldsymbol{\eta}}(r)$ and $\boldsymbol{\theta}^* = \hat{\boldsymbol{\theta}}(\boldsymbol{y})$.

Finally we shall suppose that

A4: The surface $\{\boldsymbol{\eta}(\boldsymbol{\theta}): \boldsymbol{\theta} \in A_{\boldsymbol{\eta}}(r)\}$ has no centre of curvature which is a point of $H_{\boldsymbol{\eta}}(r)$.

How to compute numerically curvatures of the expectation surface is explained in [1] and in the appendix of [7]. For a further use we present the definition of a geodesics on \mathcal{E} , like in [8].

By definition, a curve

$$\gamma: (-\delta, \delta) \mapsto \mathcal{E}$$

is a \mathbf{V} -geodesics on \mathcal{E} through the point $\gamma(0) = \boldsymbol{\eta}(\boldsymbol{\theta})$ if there is a twice continuously differentiable mapping

$$\boldsymbol{\kappa}: (-\delta, \delta) \mapsto \Theta$$

such that for every $t \in (-\delta, \delta)$

- i) $\gamma(t) = \boldsymbol{\eta} \circ \boldsymbol{\kappa}(t)$
- ii) $\left\| \frac{d\gamma(t)}{dt} \right\|_{\mathbf{V}} = 1$
- iii) $\frac{d^2\gamma^T(t)}{dt^2} \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^T} \Big|_{\boldsymbol{\theta}=\boldsymbol{\kappa}(t)} = \mathbf{0}$

i.e. the parameter t is the length of the curve γ ,

i.e. the "vector of curvature" $d^2\gamma^T(t)/dt^2$ is always orthogonal to \mathcal{E} .

The radius of curvature of $\gamma(t)$ at $t = 0$ is equal to

$$r_{\gamma}(0) := \left[\left\| \frac{d^2\gamma(t)}{dt^2} \right\|_{\mathbf{V}}^{-1} \right]_{t=0}$$

and it is the radius of a circle which is "as tangent as possible" to the curve $\gamma(t)$. According to iii) this circle with centre (= the centre of curvature)

$$\boldsymbol{\eta}(\boldsymbol{\theta}) + \frac{d^2\gamma(t)}{dt^2} \Big|_{t=0}$$

is also tangent to the expectation surface \mathcal{E} at the point $\boldsymbol{\eta}(\boldsymbol{\theta})$, and its radius-vector is \mathbf{V} -orthogonal to the tangent plane. The centre of curvature of γ is considered as a centre of curvature of the surface \mathcal{E} at the point $\boldsymbol{\eta}(\boldsymbol{\theta})$. Since there are many \mathbf{V} -

geodesics on \mathcal{E} going through the same point $\boldsymbol{\eta}(\boldsymbol{\theta})$, we define the minimal radius of curvature

$$\varrho(\boldsymbol{\theta}) := \inf_{\gamma} r_{\gamma}(0).$$

Instead of A4 we can assume equivalently

$$\mathbf{A4}^*: \quad r < \varrho(\boldsymbol{\theta}); \quad (\boldsymbol{\theta} \in A_n(r))$$

The assumptions A1 – A4 are slight modifications of the assumptions formulated in [7, 8]. A heuristic discussion is in [7].

The vector $\mathbf{y} - \boldsymbol{\Psi}(\boldsymbol{\theta})$ is \mathbf{V} -orthogonal to the tangent plane (Eqs. (4) and (16)), hence we can write

$$\mathbf{y} = \boldsymbol{\Psi}(\boldsymbol{\theta}) + \sum_{l=1}^{N-m} b_l \mathbf{w}_l(\boldsymbol{\theta})$$

where

$$b_l := [\mathbf{y} - \boldsymbol{\Psi}(\boldsymbol{\theta})]^T \boldsymbol{\Sigma}^{-1} \mathbf{w}_l(\boldsymbol{\theta}).$$

It follows that $\hat{\theta}_1, \dots, \hat{\theta}_m, b_1, \dots, b_{N-m}$ can be used as new coordinates of the point $\mathbf{y} \in H_n(r)$. The corresponding coordinate transformation will be denoted by $\mathbf{g}(\hat{\boldsymbol{\theta}}, \mathbf{b})$, i.e.

$$(20) \quad \mathbf{g}(\hat{\boldsymbol{\theta}}, \mathbf{b}) := \boldsymbol{\Psi}(\hat{\boldsymbol{\theta}}) + \sum_{l=1}^{N-m} b_l \mathbf{w}_l(\hat{\boldsymbol{\theta}})$$

Its Jacobi matrix $\nabla \mathbf{g}$ is equal to

$$\begin{aligned} \nabla \mathbf{g}(\hat{\boldsymbol{\theta}}, \mathbf{b}) &:= \left(\frac{\partial \mathbf{g}}{\partial \hat{\boldsymbol{\theta}}^T}, \frac{\partial \mathbf{g}}{\partial \mathbf{b}^T} \right) \\ &= \left(\frac{\partial \mathbf{g}}{\partial \hat{\boldsymbol{\theta}}^T}, \mathbf{W}(\hat{\boldsymbol{\theta}}) \right) \end{aligned}$$

Proposition 1. We have

$$(21) \quad |\det [\nabla \mathbf{g}(\hat{\boldsymbol{\theta}}, \mathbf{b})]| = \frac{\det [\mathbf{Q}(\hat{\boldsymbol{\theta}}, \bar{\boldsymbol{\theta}}) + \mathbf{D}(\mathbf{b}, \hat{\boldsymbol{\theta}})]}{\det^{1/2} \mathbf{B}(\hat{\boldsymbol{\theta}})} \det^{1/2} \boldsymbol{\Sigma}$$

where $\mathbf{Q}(\hat{\boldsymbol{\theta}}, \bar{\boldsymbol{\theta}})$ and $\mathbf{B}(\hat{\boldsymbol{\theta}})$ are defined in (6), and $\mathbf{D}(\mathbf{b}, \hat{\boldsymbol{\theta}})$ is an $m \times m$ matrix

$$\{\mathbf{D}(\mathbf{b}, \hat{\boldsymbol{\theta}})\}_{ij} := - \sum_{l=1}^{N-m} b_l \mathbf{w}_l^T(\hat{\boldsymbol{\theta}}) \mathbf{V}^{-1} \frac{\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \theta_i \partial \theta_j}.$$

The proof is in the Appendix.

If we compare the right-hand side of Eq. (21) with the first term in the right-hand side of Eq. (5) we see that we omitted the matrix $\mathbf{D}(\mathbf{b}, \hat{\boldsymbol{\theta}})$ in the determinant in (5). To evaluate the influence of this omission we shall need the following Proposition 2.

Let us use the notation

$$\mathbf{e} := (b_1, \dots, b_{N-m})^T / \|\mathbf{b}\|.$$

We can write

$$(22) \quad \mathbf{D}(\mathbf{b}, \hat{\boldsymbol{\theta}}) = \|\mathbf{b}\| \mathbf{D}(\mathbf{e}, \hat{\boldsymbol{\theta}}).$$

For every $m \times m$ matrix \mathbf{A} , and $s \leq m$, denote by $\mathbf{A}^{(s)}$ the matrix of all $s \times s$ minors of \mathbf{A} ; hence $\text{tr}[\mathbf{A}^{(s)}]$ is the sum of all $s \times s$ principal minors of \mathbf{A} (cf. [3]).

Proposition 2. For every $\hat{\boldsymbol{\theta}} \in A_n(r)$ we have

$$|\text{tr}[\mathbf{D}(\mathbf{e}, \hat{\boldsymbol{\theta}}) \mathbf{Q}^{-1}(\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\theta}})]^{(s)}| \leq \binom{m}{s} \frac{2^s}{r^s}.$$

Proposition 3. If the matrix \mathbf{V} is dominating $\boldsymbol{\Sigma}$, i.e., $\|\boldsymbol{\alpha}\|_{\boldsymbol{\Sigma}} \geq \|\boldsymbol{\alpha}\|_{\mathbf{V}}$; ($\boldsymbol{\alpha} \in \mathbb{R}^N$), then for every $\hat{\boldsymbol{\theta}} \in A_n(r)$ the matrix $\mathbf{Q}(\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\theta}})$ is positive definite.

The proofs of both propositions are in the Appendix.

4. THE PROBABILITY DENSITY OF $\hat{\boldsymbol{\theta}}$

The probability density of \mathbf{y} is given in Eq. (9). In the sequel we shall not take into account those samples \mathbf{y} which belong to the set $\mathbb{R}^N - H_n(r)$. From (12) and (19) it follows that the probability of this set is bounded above by the number

$$1 - \int_{G_n(r)} f_r(\mathbf{y}) \, d\mathbf{y} = \int_r^\infty \frac{\pi^{N/2}}{\Gamma(N/2)} u^{N/2-1} h(u) \, du.$$

For points inside the set $H_n(r)$ we shall use the coordinate transformation (20), to obtain the joint density of $\hat{\boldsymbol{\theta}}$ and \mathbf{b} :

$$p_n(\hat{\boldsymbol{\theta}}, \mathbf{b}) := |\det[\nabla \mathbf{g}(\hat{\boldsymbol{\theta}}, \mathbf{b})]| \det^{-1/2}(\boldsymbol{\Sigma}) h(\|\mathbf{b}\|^2 + \|\boldsymbol{\psi}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta}\|_{\boldsymbol{\Sigma}}^2)$$

where we used Eq. (17) and the equality $\|\mathbf{b}\|^2 = \|\mathbf{y} - \boldsymbol{\psi}(\hat{\boldsymbol{\theta}})\|_{\boldsymbol{\Sigma}}^2$. Denote $I(r) := \langle -r, r \rangle^{N-m}$. The density of $\hat{\boldsymbol{\theta}}$ is the marginal density

$$(23) \quad \begin{aligned} \tilde{p}_n(\hat{\boldsymbol{\theta}}) &:= \int_{I(r)} p_n(\hat{\boldsymbol{\theta}}, \mathbf{b}) \, d\mathbf{b} = \\ &= \int_{I(r)} \frac{\det[\mathbf{Q}(\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\theta}}) + \mathbf{D}(\mathbf{b}, \hat{\boldsymbol{\theta}})]}{\det^{1/2} \mathbf{B}(\hat{\boldsymbol{\theta}})} h(\|\mathbf{b}\|^2 + \|\boldsymbol{\psi}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta}\|_{\boldsymbol{\Sigma}}^2) \, d\mathbf{b} \text{ (Proposition 1)} = \\ &= q(\hat{\boldsymbol{\theta}} | \bar{\boldsymbol{\theta}}) \int_{I(r)} \det[\mathbf{I} + \mathbf{D}(\mathbf{b}, \hat{\boldsymbol{\theta}}) \mathbf{Q}^{-1}(\hat{\boldsymbol{\theta}}, \bar{\boldsymbol{\theta}})] k_{N-m}(\|\mathbf{b}\|^2 | \|\boldsymbol{\psi}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta}\|_{\boldsymbol{\Sigma}}^2) \, d\mathbf{b} \end{aligned}$$

Here we used Eq. (11) and the equality

$$\boldsymbol{\psi}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta} = \mathbf{P}^{\hat{\boldsymbol{\theta}}}[\boldsymbol{\eta}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta}]$$

which follows from Eq. (16) and (A2).

Denote by $E_{\hat{\boldsymbol{\theta}}}^*$ the (conditional) mean with respect to the density

$$\mathbf{b} \in I(r) \mapsto \varphi(\mathbf{b} | \hat{\boldsymbol{\theta}}) := k_{N-m}(\|\mathbf{b}\|^2 | \|\boldsymbol{\psi}(\hat{\boldsymbol{\theta}}) - \boldsymbol{\eta}\|_{\boldsymbol{\Sigma}}^2).$$

Instead of Eq. (23) we can write

$$(24) \quad \tilde{p}_n(\hat{\boldsymbol{\theta}}) = q(\hat{\boldsymbol{\theta}} | \bar{\boldsymbol{\theta}}) E_{\hat{\boldsymbol{\theta}}}^*\{\det[\mathbf{I} + \mathbf{D}(\mathbf{b}, \hat{\boldsymbol{\theta}}) \mathbf{Q}^{-1}(\hat{\boldsymbol{\theta}}, \bar{\boldsymbol{\theta}})]\}.$$

From [4], III, §7 we obtain

$$(25) \quad \det [\mathbf{I} + \mathbf{D}(\mathbf{b}, \hat{\theta}) \mathbf{Q}^{-1}(\hat{\theta}, \bar{\theta})] = 1 + \sum_{s=1}^m \text{tr} [\mathbf{D}(\mathbf{b}, \hat{\theta}) \mathbf{Q}^{-1}(\hat{\theta}, \bar{\theta})]^{(s)}$$

According to the definition of $\mathbf{D}(\mathbf{b}, \hat{\theta})$, each term in the right-hand side of Eq. (25) is a homogeneous polynomial in the variables b_1, \dots, b_{N-r} . Consequently, if s is odd, then

$$\mathbf{E}_{\hat{\theta}}^*[\mathbf{D}(\mathbf{b}, \hat{\theta}) \mathbf{Q}^{-1}(\hat{\theta}, \bar{\theta})]^{(s)} = \mathbf{0},$$

because $\varphi(\mathbf{b} | \hat{\theta})$ is a spherically symmetrical density. It follows that

$$(26) \quad \begin{aligned} & \mathbf{E}_{\hat{\theta}}^*\{\det [\mathbf{I} + \mathbf{D}(\mathbf{b}, \hat{\theta}) \mathbf{Q}^{-1}(\hat{\theta}, \bar{\theta})]\} \leq \\ & \leq 1 + \sum_{s=1}^{\text{INT}(m/2)} \mathbf{E}_{\hat{\theta}}^*\{\text{tr} [\mathbf{D}(\mathbf{b}, \hat{\theta}) \mathbf{Q}^{-1}(\hat{\theta}, \bar{\theta})]^{(2s)}\} \leq \\ & \leq 1 + \sum_{s=1}^{\text{INT}(m/2)} \mathbf{E}_{\hat{\theta}}^*(\|\mathbf{b}\|^{2s}) \binom{m}{2s} \left(\frac{2}{r}\right)^{2s} \end{aligned}$$

(Eq. (22) and Proposition 2.).

Similarly we obtain

$$(27) \quad \begin{aligned} & \mathbf{E}_{\hat{\theta}}^*\{\det [\mathbf{I} + \mathbf{D}(\mathbf{b}, \hat{\theta}) \mathbf{Q}^{-1}(\hat{\theta}, \bar{\theta})]\} \geq \\ & \geq 1 - \sum_{s=1}^{\text{INT}(m/2)} \mathbf{E}_{\hat{\theta}}^*(\|\mathbf{b}\|^{2s}) \binom{m}{2s} \left(\frac{2}{r}\right)^{2s}. \end{aligned}$$

Further, we have from Eqs. (8) and (12)

$$\begin{aligned} \mathbf{E}_{\hat{\theta}}^*(\|\mathbf{b}\|^{2s}) & \leq \int_{\|\mathbf{b}\|^2 \leq (N-m)r^2} \|\mathbf{b}\|^{2s} \frac{h(\|\mathbf{b}\|^2 + \|\Psi(\hat{\theta}) - \mathbf{\eta}\|_{\Sigma}^2)}{h_m(\|\Psi(\hat{\theta}) - \mathbf{\eta}\|_{\Sigma}^2)} d\mathbf{b} = \\ & = \frac{\int_0^{(N-m)r^2} u^s u^{(N-m)/2-1} h(u + \|\Psi(\hat{\theta}) - \mathbf{\eta}\|_{\Sigma}^2) du}{\int_0^{\infty} u^{(N-m)/2-1} h(u + \|\Psi(\hat{\theta}) - \mathbf{\eta}\|_{\Sigma}^2) du}. \end{aligned}$$

Consequently, if h is a nonincreasing function, then from $\|\Psi(\hat{\theta}) - \mathbf{\eta}\|_{\Sigma} < r$ we obtain

$$(28) \quad \mathbf{E}_{\hat{\theta}}^*(\|\mathbf{b}\|^{2s}) \leq \frac{\int_0^{(N-m)r^2} u^{(N-m)/2+s-1} h(u) du}{\int_0^{(N-m)r^2} u^{(N-m)/2-1} h(r^2 + u) du}.$$

From Eqs (24)–(28) follows the proof of the following theorem.

Theorem. If $h: \langle 0, \infty \rangle \mapsto \langle 0, \infty \rangle$ is non-increasing then

$$\frac{\bar{p}_{\mathbf{\eta}}(\hat{\theta}) - q(\hat{\theta} | \bar{\theta})}{q(\hat{\theta} | \bar{\theta})} \leq \sum_{s=1}^{\text{INT}(m/2)} \binom{m}{2s} \left(\frac{2}{r}\right)^{2s} \frac{\int_0^{(N-m)r^2} u^{(N-m)/2+s-1} h(u) du}{\int_0^{(N-m)r^2} u^{(N-m)/2-1} h(r^2 + u) du}$$

APPENDIX

Proof of Proposition 1. We shall write θ instead of $\hat{\theta}$. We have

$$\begin{aligned}
 (A1) \quad \frac{\det^2 [\nabla \mathbf{g}(\theta, \mathbf{b})]}{\det \Sigma} &= \det \begin{pmatrix} \frac{\partial \mathbf{g}^T}{\partial \theta} \Sigma^{-1} \frac{\partial \mathbf{g}}{\partial \theta^T}, & \frac{\partial \mathbf{g}^T}{\partial \theta} \Sigma^{-1} \mathbf{W} \\ \mathbf{W}^T \Sigma^{-1} \frac{\partial \mathbf{g}}{\partial \theta^T}, & \mathbf{I} \end{pmatrix} = \\
 &= \det \left(\frac{\partial \mathbf{g}^T}{\partial \theta} \Sigma^{-1} [\mathbf{I} - \mathbf{W} \mathbf{W}^T \Sigma^{-1}] \frac{\partial \mathbf{g}}{\partial \theta^T} \right) \quad ([4], \text{II}, \S 5) \\
 &= \det \left(\frac{\partial \mathbf{g}^T}{\partial \theta} \Sigma^{-1} [\mathbf{I} - \mathbf{R}^0] \frac{\partial \mathbf{g}}{\partial \theta^T} \right).
 \end{aligned}$$

From the equation

$$\mathbf{R}^0 \Sigma \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\theta)}{\partial \theta^T} = \mathbf{W}(\theta) \mathbf{W}^T(\theta) \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\theta)}{\partial \theta^T} = \mathbf{0}$$

we see that the linearly independent vectors

$$\mathbf{t}_i := \Sigma \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\theta)}{\partial \theta_i}; \quad (i = 1, \dots, m)$$

span the linear space $\{\mathbf{z} \in \mathbb{R}^N, (\mathbf{I} - \mathbf{R}^0) \mathbf{z} = \mathbf{z}\}$. Hence the Σ -orthogonal projector onto this space is equal to

$$\mathbf{I} - \mathbf{R}^0 = \sum_{i,j=1}^m \mathbf{t}_i \{\mathbf{T}^{-1}\}_{ij} \mathbf{t}_j^T \Sigma^{-1}$$

where $\{\mathbf{T}\}_{ij} := \mathbf{t}_i^T \Sigma^{-1} \mathbf{t}_j$. It is easy to verify that $\mathbf{T} = \mathbf{B}(\theta)$, and that

$$(A2) \quad \mathbf{I} - \mathbf{R}^0 = \mathbf{P}^0,$$

where \mathbf{P}^0 is defined in Eq. (7). Putting the expression for \mathbf{P}^0 into (A1) we obtain

$$\begin{aligned}
 \frac{\det^2 [\nabla \mathbf{g}(\theta, \mathbf{b})]}{\det \Sigma} &= \frac{\det^2 \left(\frac{\partial \mathbf{g}^T}{\partial \theta} \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}}{\partial \theta^T} \right)}{\det [\mathbf{B}(\theta)]} = \\
 &= \frac{\det^2 \left[\frac{\partial \Psi^T}{\partial \theta} \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}}{\partial \theta^T} + \sum_l b_l \frac{\partial \mathbf{w}_l^T}{\partial \theta} \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}}{\partial \theta^T} \right]}{\det [\mathbf{B}(\theta)]}.
 \end{aligned}$$

From

$$\Psi(\theta) - \boldsymbol{\eta}(\theta) = \mathbf{R}^0 [\boldsymbol{\eta} - \boldsymbol{\eta}(\theta)] \in \mathcal{N}(\theta)$$

we obtain that

$$(A3) \quad [\Psi(\theta) - \boldsymbol{\eta}(\theta)]^T \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\theta)}{\partial \theta^T} = \mathbf{0}.$$

We differentiate this equality, and obtain

$$(A4) \quad \frac{\partial \Psi^T(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^T} = \mathbf{M}(\boldsymbol{\theta}) + [\boldsymbol{\eta}(\boldsymbol{\theta}) - \boldsymbol{\psi}(\boldsymbol{\theta})]^T \mathbf{V}^{-1} \frac{\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T} = \mathbf{Q}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}).$$

Further, differentiating the first equations in (15) we obtain

$$\mathbf{D}(\mathbf{b}, \boldsymbol{\theta}) = \sum_t b_t \frac{\partial \mathbf{w}_t^T(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \mathbf{V}^{-1} \frac{\partial \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^T}.$$

Finally, from (3) it follows that the matrix $\frac{\partial^2}{\partial \boldsymbol{\theta}} \frac{\partial \boldsymbol{\theta}^T}{\partial \boldsymbol{\theta}} \{\frac{1}{2} \|\boldsymbol{\eta}(\boldsymbol{\theta}) - \mathbf{y}\|_{\Sigma}^2\}_{\boldsymbol{\theta}=\bar{\boldsymbol{\theta}}}$ is p.d., and we can verify that it is equal to $\mathbf{Q}(\bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\theta}}) + \mathbf{D}(\mathbf{b}, \bar{\boldsymbol{\theta}})$ when putting $\mathbf{y} = \mathbf{g}(\bar{\boldsymbol{\theta}}, \mathbf{b})$. \square

The matrix $\mathbf{M}(\boldsymbol{\theta})$ is positive definite. Therefore, there is a nonsingular matrix \mathbf{U} such that

$$\mathbf{U}^T \mathbf{M}(\boldsymbol{\theta}) \mathbf{U} = \mathbf{I}.$$

Denote

$$\begin{aligned} \mathbf{D}^*(\mathbf{e}) &:= \mathbf{D}^*(\mathbf{e}, \boldsymbol{\theta}) := \mathbf{U}^T \mathbf{D}(\mathbf{e}, \boldsymbol{\theta}) \mathbf{U} \\ \mathbf{Q}^* &:= \mathbf{Q}^*(\boldsymbol{\theta}) := \mathbf{U}^T \mathbf{Q} \mathbf{U}. \end{aligned}$$

For any eigenvalue λ of the matrix $\mathbf{D}(\mathbf{e}, \boldsymbol{\theta})$ we have the inequality

$$(A5) \quad |\lambda| \leq \frac{1}{\varrho(\boldsymbol{\theta})}$$

(cf. [7], Proposition 2).

Proof of Proposition 2. For any matrices \mathbf{A}, \mathbf{B} we have (cf. [3], theorem 6.13)

$$\mathbf{A}^{(s)} \mathbf{B}^{(s)} = (\mathbf{A} \mathbf{B})^{(s)}.$$

Hence

$$(A6) \quad \begin{aligned} \text{tr} [\mathbf{D}^*(\mathbf{e}) \mathbf{Q}^{*-1}]^{(s)} &= \text{tr} \{ (\mathbf{U}^T)^{(s)} [\mathbf{D}(\mathbf{e}) \mathbf{Q}^{-1}]^{(s)} (\mathbf{U}^T)^{(s)} \} \\ &= \text{tr} [\mathbf{D}(\mathbf{e}) \mathbf{Q}^{-1}]^{(s)} \end{aligned}$$

Denote by $\mathbf{C} := (\mathbf{c}^{(1)}, \dots, \mathbf{c}^{(m)})$ and by $\boldsymbol{\Lambda} := \text{diag}(\lambda_1, \dots, \lambda_m)$ the matrices of the orthonormal eigenvectors and of the eigenvalues of $\mathbf{D}^*(\mathbf{e})$. From $\mathbf{D}^*(\mathbf{e}) = \mathbf{C} \boldsymbol{\Lambda} \mathbf{C}^T$ we obtain

$$\text{tr} [\mathbf{D}^*(\mathbf{e}) \mathbf{Q}^{*-1}]^{(s)} = \text{tr} [\boldsymbol{\Lambda}^{(s)} (\mathbf{C}^T)^{(s)} (\mathbf{Q}^{*-1})^{(s)} \mathbf{C}^{(s)}].$$

The matrix $\boldsymbol{\Lambda}^{(s)}$ is diagonal, having diagonal entries of the form $\lambda_{i_1}, \dots, \lambda_{i_s}$; ($i_1 < \dots < i_s$). Hence from (A5) we obtain

$$(A7) \quad \begin{aligned} |\text{tr} [\mathbf{D}^*(\mathbf{e}) \mathbf{Q}^{*-1}]^{(s)}| &\leq [\varrho(\boldsymbol{\theta})]^{-s} \text{tr} [(\mathbf{C}^T)^{(s)} (\mathbf{Q}^{*-1})^{(s)} \mathbf{C}^{(s)}] = \\ &= [\varrho(\boldsymbol{\theta})]^{-s} \text{tr} (\mathbf{Q}^{*-1})^{(s)} \end{aligned}$$

since $\mathbf{C}^{(s)} (\mathbf{C}^T)^{(s)} = (\mathbf{C} \mathbf{C}^T)^{(s)} = \mathbf{I}^{(s)} = \mathbf{I}$.

From (A3) we obtain

$$\mathbf{Q} = \mathbf{I} + \mathbf{U}^T [\boldsymbol{\eta}(\boldsymbol{\theta}) - \boldsymbol{\psi}(\boldsymbol{\theta})]^T \mathbf{V}^{-1} \frac{\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T} \mathbf{U}.$$

According to Eq. (A3) we can write

$$\boldsymbol{\eta}(\boldsymbol{\theta}) - \boldsymbol{\psi}(\boldsymbol{\theta}) = - \sum_{i=1}^{N-m} d_i \mathbf{w}_i(\boldsymbol{\theta}),$$

where $d_i := [\boldsymbol{\psi}(\boldsymbol{\theta}) - \boldsymbol{\eta}(\boldsymbol{\theta})]^T \boldsymbol{\Sigma}^{-1} \mathbf{w}_i(\boldsymbol{\theta})$. Hence

$$[\boldsymbol{\eta}(\boldsymbol{\theta}) - \boldsymbol{\psi}(\boldsymbol{\theta})]^T \mathbf{V}^{-1} \frac{\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T} = \mathbf{D}(\mathbf{d}, \boldsymbol{\theta}).$$

Thus

$$\mathbf{Q}^* = \mathbf{I} + \|\boldsymbol{\psi}(\boldsymbol{\theta}) - \boldsymbol{\eta}(\boldsymbol{\theta})\|_{\mathbf{z}} \mathbf{D}^*(\mathbf{f})$$

where $\mathbf{f} := \mathbf{d}/\|\mathbf{d}\|$.

Using once more the inequality (A4) we obtain that the eigenvalues μ_1, \dots, μ_m of the matrix \mathbf{Q}^* are bounded according to the inequalities

$$1 - \|\boldsymbol{\psi}(\boldsymbol{\theta}) - \boldsymbol{\eta}(\boldsymbol{\theta})\|_{\mathbf{z}} \varrho^{-1}(\boldsymbol{\theta}) \leq \mu_i \leq 1 + \|\boldsymbol{\psi}(\boldsymbol{\theta}) - \boldsymbol{\eta}(\boldsymbol{\theta})\|_{\mathbf{z}} \varrho^{-1}(\boldsymbol{\theta}).$$

Denote by $\mathbf{Z} := (\mathbf{z}_1, \dots, \mathbf{z}_m)$ the matrix of the orthonormal eigenvectors of \mathbf{Q}^* . We have

$$\begin{aligned} \text{(A8)} \quad \text{tr}(\mathbf{Q}^{*-1})^{(s)} &= \text{tr}[(\mathbf{Z}^{-1}(\mathbf{Z}^T)^{-1})^{(s)}(\mathbf{Q}^{*-1})^{(s)}] = \text{tr}[(\mathbf{Z}^T \mathbf{Q}^* \mathbf{Z})^{-1}]^{(s)} = \\ &= \sum_{i_1 < \dots < i_s} \mu_{i_1}^{-1} \dots \mu_{i_s}^{-1} \leq \binom{m}{s} \left[\frac{\varrho(\boldsymbol{\theta})}{\varrho(\boldsymbol{\theta}) - \|\boldsymbol{\psi}(\boldsymbol{\theta}) - \boldsymbol{\eta}(\boldsymbol{\theta})\|_{\mathbf{z}}} \right]^s. \end{aligned}$$

From (A6)–(A8) we have

$$|\text{tr}[\mathbf{D}(\mathbf{e}, \boldsymbol{\theta}) \mathbf{Q}^{-1}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}})]^{(s)}| \leq \binom{m}{s} [\varrho(\boldsymbol{\theta}) - \|\boldsymbol{\psi}(\boldsymbol{\theta}) - \boldsymbol{\eta}(\boldsymbol{\theta})\|_{\mathbf{z}}]^{-s}.$$

We obtain the required inequality from $[\boldsymbol{\psi}(\boldsymbol{\theta}) - \boldsymbol{\eta}(\boldsymbol{\theta})]_{\mathbf{z}} \leq \varrho(\boldsymbol{\theta})/2$ which follows from the assumption A4. \square

Proof of Proposition 3. Take $\boldsymbol{\theta} \in \mathcal{A}_n(r)$. It is sufficient to show that for every geodesics $\gamma = \boldsymbol{\eta} \circ \boldsymbol{x}$ going through the point $\boldsymbol{\theta}$ the inequality

$$\frac{d\boldsymbol{x}^T(0)}{dt} \mathbf{Q}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) \frac{d\boldsymbol{x}(0)}{dt} > 0$$

holds. From Eqs. (A4) and (16) we obtain

$$\frac{d\boldsymbol{x}^T}{dt} \mathbf{Q}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) \frac{d\boldsymbol{x}}{dt} = \frac{d\boldsymbol{\gamma}^T(0)}{dt} \mathbf{V}^{-1} \frac{d\boldsymbol{\gamma}(0)}{dt} + \frac{d\boldsymbol{x}^T(0)}{dt} \left\{ [\mathbf{R}^0(\boldsymbol{\eta}(\boldsymbol{\theta}) - \boldsymbol{\eta})]^T \mathbf{V}^{-1} \frac{\partial^2 \boldsymbol{\eta}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T} \right\} \frac{d\boldsymbol{x}(0)}{dt}.$$

Hence from the definition of the V-geodesics $\boldsymbol{\gamma}$ (Section 3) we have

$$\begin{aligned} \frac{d\boldsymbol{x}^T}{dt} \mathbf{Q}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) \frac{d\boldsymbol{x}}{dt} &= 1 + [\mathbf{R}^0(\boldsymbol{\eta}(\boldsymbol{\theta}) - \boldsymbol{\eta})]^T \mathbf{V}^{-1} \frac{d^2 \boldsymbol{\gamma}(0)}{dt^2} = \\ &= 1 - [\boldsymbol{\psi}(\boldsymbol{\theta}) - \boldsymbol{\eta}(\boldsymbol{\theta})]^T \mathbf{V}^{-1} \frac{d^2 \boldsymbol{\gamma}(0)}{dt^2}. \end{aligned}$$

Therefore, from the Schwarz inequality and from the definition of $r_\gamma(\mathbf{0})$ (Section 3) we obtain that it is sufficient to prove that

$$\|\psi(\mathbf{0}) - \eta(\mathbf{0})\|_{\mathbf{V}} < r_\gamma(\mathbf{0}).$$

Since $\mathbf{0} \in A_n(r)$, there is a point $\mathbf{y} \in G_n(r)$, i.e.

$$\|\mathbf{y} - \eta\|_{\Sigma} < r < r_\gamma(\mathbf{0}),$$

such that $\mathbf{y} \in \mathcal{A}(\mathbf{0})$ (see the definition of $A_n(r)$). Consequently

$$\|\psi(\mathbf{0}) - \eta\|_{\Sigma} = \|\mathbf{P}^0(\mathbf{y} - \eta)\|_{\Sigma} < \|\mathbf{y} - \eta\|_{\Sigma} < r_\gamma(\mathbf{0}).$$

It follows that $\psi(\mathbf{0}) \in G_n(r)$. Evidently $\psi(\mathbf{0}) \in \mathcal{A}(\mathbf{0})$. Consequently, according to the property A3, $\mathbf{0}$ solves Eq. (3) for $\mathbf{y} = \psi(\mathbf{0})$. It follows that $\|\psi(\mathbf{0}) - \eta(\mathbf{0})\|_{\mathbf{V}} \leq \|\psi(\mathbf{0}) - \eta\|_{\mathbf{V}} \leq \|\psi(\mathbf{0}) - \eta\|_{\Sigma} < r_\gamma(\mathbf{0})$ since \mathbf{V} is dominating Σ . \square

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