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A CANONICAL DEFINITION OF SHAPE

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Abstract

Very general concepts of scatter, extending the traditional notion of covariance matrices, have become classical tools in robust multivariate analysis. In many problems of practical importance (principal components, canonical correlation, testing for sphericity), only homogeneous functions of the scatter matrix are of interest, and the latter thus is relevant up to a positive scalar factor only. In line with this fact, scatter functionals (such as, e.g., Tyler (1987)'s matrix) often are only defined up to a positive scalar factor, yielding a family of scatter matrices rather than a uniquely defined one. In such families, it is natural to single out one representative by imposing a normalization constraint: this normalized scatter is called a *shape matrix*. In the particular case of elliptical families, this constraint in turn induces a concept of scale; along with a location center and a standardized radial density, the shape and scale parameters entirely characterize an elliptical density. In this paper, we show that, among all possible normalizations, one and only one has the additional properties that (i) the resulting Fisher information matrices for shape and scale, in locally asymptotically normal (LAN) elliptical families, are block-diagonal, and (ii) that the semiparametric elliptical families indexed by location, shape, and completely unspecified radial densities are adaptive. This particular normalization, which consists in imposing that the determinant of the shape matrix be equal to one, therefore can be considered canonical.

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1 Introduction.

The multivariate concepts of location and scatter, extending to the multivariate context the traditional concepts of location and scale are generally characterized via their behavior under affine transformations of the observation space. More precisely, denoting by \mathbf{X} a k-variate random vector with probability distribution $P^{\mathbf{X}}$, consider a couple $(\boldsymbol{\theta}, \boldsymbol{\Sigma})$ of functionals defined over $\{P^{\mathbf{AX}+\mathbf{b}}: \mathbf{A} \text{ an invertible } k \times k \text{ real matrix}, \mathbf{b} \in \mathbb{R}^k\}$ mapping $P^{\mathbf{X}}$ onto $(\boldsymbol{\theta}^{\mathbf{X}}, \boldsymbol{\Sigma}^{\mathbf{X}}) \in \mathbb{R}^k \times S_k$, where S_k denotes the set of symmetric positive definite real $k \times k$ matrices—throughout, $k \geq 2$. This couple is called a location-scatter functional iff

$$(\boldsymbol{\theta}^{\mathbf{AX+b}}, \ \boldsymbol{\Sigma}^{\mathbf{AX+b}}) = (\mathbf{A}\boldsymbol{\theta}^{\mathbf{X}} + \mathbf{b}, \ \mathbf{A}\boldsymbol{\Sigma}^{\mathbf{X}}\mathbf{A}')$$
 (1.1)

for any invertible $k \times k$ matrix **A** and any $\mathbf{b} \in \mathbb{R}^k$. The traditional example of such a couple of course is the mean and the covariance matrix, but many other solutions exist, and the problem

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of defining robust counterparts to means and covariances has generated a huge literature which we do not attempt to review here—see (11) or (19) for recent surveys.

In many problems in multivariate analysis, it is sufficient to know—or to estimate—normalized versions of scatter matrices to be able to perform the analysis (see below). In line with this fact, scatter matrices often are only defined up to a positive factor—see, for instance, (17) and (18). In such families of scatter matrices, it is natural to pick up one representative by imposing a normalization constraint. More specifically, let $S : S_k \to \mathbb{R}^+_0$ be a homogeneous function—i.e., satisfying $S(\lambda \Sigma) = \lambda S(\Sigma)$ for all $\lambda > 0$ —and define $\mathcal{V}_k^S := \{\mathbf{V} \in \mathcal{S}_k : S(\mathbf{V}) = 1\}$: the elements of \mathcal{V}_k^S are called shape matrices, and $\mathbf{V}_S^{\mathbf{X}} := \Sigma^{\mathbf{X}} / S(\Sigma^{\mathbf{X}})$ is called the shape matrix of \mathbf{X} .

The choice of S is arbitrary and, to some extent, inessential (see the comments below). Classical choices include

- (i) $S(\mathbf{\Sigma}) = \Sigma_{11}$ ((6), (7), (9), and (13)),
- (ii) $S(\mathbf{\Sigma}) = (\operatorname{tr} \mathbf{\Sigma})/k$ ((5), (12), and (18)), and
- (iii) $S(\mathbf{\Sigma}) = |\mathbf{\Sigma}|^{1/k}$ ((4), (14), (15), and (16)).

Now consider the particular case of a k-variate *elliptical* random vector **X**, that is, letting $d(\mathbf{x}, \boldsymbol{\theta}; \boldsymbol{\Sigma}) := ((\mathbf{x} - \boldsymbol{\theta})' \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\theta}))^{1/2}$, assume that $P^{\mathbf{X}}$ admits the density

$$\mathbf{x} \mapsto \frac{c_{k,f_1}}{|\mathbf{\Sigma}|^{1/2}} f_1(d(\mathbf{x}, \boldsymbol{\theta}; \mathbf{\Sigma})), \tag{1.2}$$

where $\boldsymbol{\theta}$, the center of symmetry, is a k-dimensional real vector, $\boldsymbol{\Sigma}$ belongs to \mathcal{S}_k , and $f_1 : \mathbb{R}_0^+ \longrightarrow \mathbb{R}_0^+$, the standardized radial density is such that $\mu_{k-1,f_1} := \int_0^\infty r^{k-1} f_1(r) dr < \infty$ (c_{k,f_1} is a normalization factor). To ensure identifiability of $\boldsymbol{\Sigma}$ and $c_{k,f_1} \times f_1$ without imposing any moment conditions, the pdf of $d(\mathbf{X}, \boldsymbol{\theta}; \boldsymbol{\Sigma})$ under (1.2) (that is, $r \mapsto f_{1k}(r) := (\mu_{k-1,f_1})^{-1} r^{k-1} f_1(r) I_{[r>0]}$) is assumed to have median one.

Under this elliptical setting, the unique solutions of (1.1) are the couples $(\boldsymbol{\theta}, \lambda \boldsymbol{\Sigma})$, with arbitrary $\lambda > 0$. It follows that the shape $\mathbf{V}_S = \boldsymbol{\Sigma}/S(\boldsymbol{\Sigma})$ is uniquely defined for any homogeneous function S, and that $\sigma_S := (S(\boldsymbol{\Sigma}))^{1/2}$, as the median of $d(\mathbf{X}, \boldsymbol{\theta}; \mathbf{V}_S)$, has the interpretation of a scale parameter. This allows for rewriting (1.2) as

$$\mathbf{x} \mapsto \frac{c_{k,f_1}}{\sigma_S^k |\mathbf{V}_S|^{1/2}} f_1\left(\frac{1}{\sigma_S} d(\mathbf{x}, \boldsymbol{\theta}; \mathbf{V}_S)\right) = \frac{c_{k,f}}{|\mathbf{V}_S|^{1/2}} f\left(d(\mathbf{x}, \boldsymbol{\theta}; \mathbf{V}_S)\right).$$
(1.3)

This latter density is indexed by $\boldsymbol{\theta}$, \mathbf{V}_S , and the *(non-standardized) radial density f*. Under finite second-order moments, of course, $\boldsymbol{\Sigma}$ reduces to a multiple of $\text{Cov}[\mathbf{X}]$, and hence $\mathbf{V}_S = \text{Cov}[\mathbf{X}]/S(\text{Cov}[\mathbf{X}])$.

Whatever the choice of S, the shape matrix \mathbf{V}_S is a parameter of primary interest in a number of standard problems in multivariate analysis. Principal component analysis (PCA), canonical correlation analysis (CCA), and the problem of testing for sphericity, among others, only depend on shape—rather than on scatter or covariance matrices; see, for instance, (3), (6), and (15). Inference on shape is thus an essential issue in the domain.

The choice of S so far is still arbitrary. The objective of this paper is to show that decisiontheoretic arguments, involving the structure of Fisher information and semiparametric efficiency, strongly suggest adopting the determinant-based normalization $S(\mathbf{\Sigma}) = |\mathbf{\Sigma}|^{1/k}$. This particular choice indeed is the only one for which

- (a) the Fisher information matrices for scale and shape, in locally asymptotically normal (LAN) elliptical families, are block-diagonal, and
- (b) the semiparametric elliptical families indexed by location $\boldsymbol{\theta}$, shape \mathbf{V}_S , and completely unspecified radial densities f (see (1.3)) are adaptive; this adaptivity result is much stronger than the one established in (1) (see Section 2 for a discussion).

These two properties considerably simplify the structure of information, and in principle allow for parametrically efficient inference for shape, under unspecified ($\boldsymbol{\theta}, f$) (equivalently, unspecified ($\boldsymbol{\theta}, \sigma_S, f_1$)). The determinant-based concepts of shape and scale therefore can be considered canonical.

2 Assumptions, notation, and local asymptotic normality.

The following notation will be used. For any $k \times k$ matrix **A**, let vec **A** be the k^2 -vector resulting from stacking the columns of **A** on top of each other. If **A** moreover is symmetric, write vech $\mathbf{A} := (A_{11}, (\text{vech } \mathbf{A})')'$ for the (K+1)-vector (throughout, K = k(k+1)/2 - 1) obtained by stacking the upper-triangular elements of $\mathbf{A} = (A_{ij})$: vech **A** thus stands for vech **A** deprived of its first component A_{11} . On the scale functional S we make the following assumption.

ASSUMPTION (A1). The scale functional $S : S_k \to \mathbb{R}_0^+$ (i) is homogeneous (see Section 1), (ii) is differentiable, with $\frac{\partial S}{\partial \Sigma_{11}}(\mathbf{\Sigma}) \neq 0$ for all $\mathbf{\Sigma} \in S_k$, and (iii) satisfies $S(\mathbf{I}_k) = 1$, where \mathbf{I}_k denotes the k-dimensional identity matrix.

Clearly, one can also look at $\Sigma \mapsto S(\Sigma)$ as a function of vech Σ : with a slight abuse of notation, we indifferently write $S(\Sigma)$ or $S(\text{vech }\Sigma)$ in the sequel, and denote by $\nabla S(\text{vech }\Sigma)$ the gradient grad_{vech Σ} $S(\text{vech }\Sigma)$. Under Assumption (A1), $(\mathbf{V}_S)_{11}$, for any $\mathbf{V}_S \in \mathcal{V}_k^S$, can be recovered from (vech \mathbf{V}_S). Also note that the special role of Σ_{11} in Assumption (A1) could have been played by any other entry of Σ . Assuming that some other component of ∇S is non-zero would allow, for instance, for dealing with scale functionals such as $S(\Sigma) = \Sigma_{12}$ or $S(\Sigma) = (\prod_{i=2}^k \Sigma_{ii})^{1/(k-1)}$ with appropriate redefinition of the vech operator. As the extension of our results to such cases is trivial, we stick to Assumption (A1) in the sequel.

Denote by $P_{\boldsymbol{\theta},\boldsymbol{\Sigma},f_1}^n$ or equivalently (for any given S) $P_{\boldsymbol{\theta},\sigma_S^2,\mathbf{V}_S,f_1}^n$ the distribution of an i.i.d. n-tuple $(\mathbf{X}_1,\ldots,\mathbf{X}_n)$ with density (1.2) or (1.3). For given S satisfying Assumption (A1), the scatter parameter $\boldsymbol{\Sigma}$ (in vector form, vech $\boldsymbol{\Sigma}$) decomposes into scale and shape parameters through $\boldsymbol{\Sigma} = \sigma_S^2 \mathbf{V}_S$, where $\sigma_S^2 = S(\boldsymbol{\Sigma})$ and $\mathbf{V}_S := \boldsymbol{\Sigma}/S(\boldsymbol{\Sigma}) \in \mathcal{V}_k^S$. In vector form, dropping $(\mathbf{V}_S)_{11}$, the new parameter is thus $\boldsymbol{\vartheta}_S := (\boldsymbol{\theta}', \sigma_S^2, (\operatorname{vech} \mathbf{V}_S)')' \in \boldsymbol{\Theta}_S (:= \mathbb{R}^k \times \mathbb{R}_0^+ \times \operatorname{vech} \mathcal{V}_k^S)$. Theorem 2.1 below states that, under mild regularity conditions on f_1 , the families of distributions $\mathcal{P}_{S;f_1}^n :=$ $\{P_{\boldsymbol{\vartheta}_S,f_1}^n : \boldsymbol{\vartheta}_S \in \boldsymbol{\Theta}_S\}$ are locally asymptotically normal (LAN; see (10)). This theorem extends to an arbitrary scale functional S the result obtained for $S(\boldsymbol{\Sigma}) = \boldsymbol{\Sigma}_{11}$ in (6), where minimal assumptions are given; here, for the sake of simplicity, we rather provide the following sufficient one.

ASSUMPTION (A2). The standardized radial density f_1 belongs to the collection \mathcal{F} of absolutely continuous functions, with a.e.-derivative \dot{f}_1 , and, letting $\varphi_{f_1} := -\dot{f}_1/f_1$, the quantities $\mathcal{I}_k(f_1) := \int_0^\infty (\varphi_{f_1}(r))^2 \tilde{f}_{1k}(r) \, dr$ and $\mathcal{J}_k(f_1) := \int_0^\infty r^2 (\varphi_{f_1}(r))^2 \tilde{f}_{1k}(r) \, dr$ are finite.

The finiteness of the radial Fisher informations for location $\mathcal{I}_k(f_1)$ and scale $\mathcal{J}_k(f_1)$ does not imply any moment conditions. Hence, Assumption (A2) is extremely mild and turns out to be satisfied at Gaussian densities as well as at all Student and power-exponential densities (see (6)).

The following notation is needed in the statement of LAN. Denoting by \mathbf{e}_{ℓ} the ℓ th vector of the canonical basis of \mathbb{R}^k , let $\mathbf{K}_k := \sum_{i,j=1}^k (\mathbf{e}_i \mathbf{e}'_j) \otimes (\mathbf{e}_j \mathbf{e}'_i)$ be the $k^2 \times k^2$ commutation matrix, and put $\mathbf{J}_k := (\text{vec } \mathbf{I}_k)(\text{vec } \mathbf{I}_k)'$. Write also $\mathbf{A}^{\otimes 2}$ for the Kronecker product $\mathbf{A} \otimes \mathbf{A}$. Finally, for any $\mathbf{\Sigma} \in \mathcal{S}_k$ and S satisfying (A1), let $\mathbf{M}_S^{\mathbf{\Sigma}} := \mathbf{M}_{S,k}^{\mathbf{\Sigma}}$ be the $K \times k^2$ matrix such that $(\mathbf{M}_S^{\mathbf{\Sigma}})'(\text{vech } \mathbf{v}) = \text{vec } \mathbf{v}$ for any symmetric $k \times k$ matrix \mathbf{v} satisfying $(\nabla S(\text{vech } \mathbf{\Sigma}))'(\text{vech } \mathbf{v}) = 0$. Note that $(\nabla S(\text{vech } \mathbf{\Sigma}))'(\text{vech } \mathbf{v}) = 0$ holds for $S(\mathbf{\Sigma}) = \Sigma_{11}, S(\mathbf{\Sigma}) = (\text{tr } \mathbf{\Sigma})/k$, and $S(\mathbf{\Sigma}) = |\mathbf{\Sigma}|^{1/k}$, iff $(\mathbf{v})_{11} = 0$, tr $\mathbf{v} = 0$, and tr $(\mathbf{\Sigma}^{-1}\mathbf{v}) = 0$, respectively.

Theorem 2.1 Under Assumptions (A1) and (A2), the family $\mathcal{P}_{S;f_1}^n = \{P_{\vartheta_S,f_1}^n : \vartheta_S \in \Theta_S\}$ is LAN. More precisely, for any $\vartheta_S = (\theta', \sigma_S^2, (\text{vech} \mathbf{V}_S)')'$ and any bounded sequence $\boldsymbol{\tau}_n \in \mathbb{R}^{k+K+1}$, we have that (i) under P_{ϑ_S,f_1}^n ,

$$\log\left(dP_{\boldsymbol{\vartheta}_{S}+n^{-1/2}\boldsymbol{\tau}_{n},f_{1}}^{n}/dP_{\boldsymbol{\vartheta}_{S},f_{1}}^{n}\right)=\boldsymbol{\tau}_{n}^{\prime}\boldsymbol{\Delta}_{\boldsymbol{\vartheta}_{S},f_{1}}^{n}-\frac{1}{2}\boldsymbol{\tau}_{n}^{\prime}\boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1}}\boldsymbol{\tau}_{n}+o_{P}(1),$$

where, letting $d_i := d(\mathbf{X}_i, \boldsymbol{\theta}; \mathbf{V}_S)$ and $\mathbf{U}_i := \mathbf{V}_S^{-1/2} (\mathbf{X}_i - \boldsymbol{\theta})/d_i$ (throughout, $\mathbf{V}_S^{1/2}$ is taken symmetric), $\boldsymbol{\Delta}_{\boldsymbol{\theta}_S, f_1}^n := ((\boldsymbol{\Delta}_{\boldsymbol{\theta}_S, f_1; 1}^n)', \boldsymbol{\Delta}_{\boldsymbol{\theta}_S, f_1; 2}^n, \boldsymbol{\Delta}_{\boldsymbol{\theta}_S, f_1; 3}^n)')'$, with

$$\boldsymbol{\Delta}_{\boldsymbol{\vartheta}_{S},f_{1};1}^{n} := \frac{1}{\sigma_{S}\sqrt{n}} \sum_{i=1}^{n} \varphi_{f_{1}}\left(\frac{d_{i}}{\sigma_{S}}\right) \mathbf{V}_{S}^{-1/2} \mathbf{U}_{i},$$
$$\Delta_{\boldsymbol{\vartheta}_{S},f_{1};2}^{n} := \frac{1}{2\sigma_{S}^{2}\sqrt{n}} \sum_{i=1}^{n} \left(\varphi_{f_{1}}\left(\frac{d_{i}}{\sigma_{S}}\right) \frac{d_{i}}{\sigma_{S}} - k\right),$$
(2.4)

and

$$\boldsymbol{\Delta}_{\boldsymbol{\vartheta}_{S},f_{1};3}^{n} := \frac{1}{2\sqrt{n}} \mathbf{M}_{S}^{\mathbf{V}_{S}} (\mathbf{V}_{S}^{\otimes 2})^{-1/2} \sum_{i=1}^{n} \operatorname{vec} \left(\varphi_{f_{1}} \left(\frac{d_{i}}{\sigma_{S}} \right) \frac{d_{i}}{\sigma_{S}} \mathbf{U}_{i} \mathbf{U}_{i}' - \mathbf{I}_{k} \right),$$
(2.5)

and that (ii) the *central sequence* $\Delta_{\vartheta_S,f_1}^n$, still under P_{ϑ_S,f_1}^n , is asymptotically normal with mean zero and covariance matrix

$$\boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1}} := \begin{pmatrix} \boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};11} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};22} & \boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};32} \\ \boldsymbol{0} & \boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};32} & \boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};33} \end{pmatrix},$$
(2.6)

with

$$\begin{split} \mathbf{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};11} &:= \frac{\mathcal{I}_{k}(f_{1})}{k\sigma_{S}^{2}} \mathbf{V}_{S}^{-1}, \\ \Gamma_{\boldsymbol{\vartheta}_{S},f_{1};22} &:= \frac{\mathcal{J}_{k}(f_{1}) - k^{2}}{4\sigma_{S}^{4}}, \quad \mathbf{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};32} := \frac{\mathcal{J}_{k}(f_{1}) - k^{2}}{4k\sigma_{S}^{2}} \mathbf{M}_{S}^{\mathbf{V}_{S}} \left(\operatorname{vec} \mathbf{V}_{S}^{-1} \right), \end{split}$$

and

$$\Gamma_{\vartheta_{S},f_{1};33} := \frac{1}{4} \mathbf{M}_{S}^{\mathbf{V}_{S}} (\mathbf{V}_{S}^{\otimes 2})^{-1/2} \left[\frac{\mathcal{J}_{k}(f_{1})}{k(k+2)} \left(\mathbf{I}_{k^{2}} + \mathbf{K}_{k} + \mathbf{J}_{k} \right) - \mathbf{J}_{k} \right] (\mathbf{V}_{S}^{\otimes 2})^{-1/2} (\mathbf{M}_{S}^{\mathbf{V}_{S}})'.$$
(2.7)

The block-diagonal structure of the information matrix (2.6) implies that the non-specification of the location centre $\boldsymbol{\theta}$ does not affect optimal parametric performances when estimating \mathbf{V}_S and/or σ_S^2 , or when performing tests about the same; more precisely, when estimating \mathbf{V}_S for instance, the optimal asymptotic covariance matrix that can be achieved (at $P_{\boldsymbol{\theta},\sigma_S^2,\mathbf{V}_S,f_1}^n$) by an estimator of \mathbf{V}_S is the same in $\mathcal{P}^n_{S;\sigma_S^2,f_1} := \{P^n_{\boldsymbol{\theta},\sigma_S^2,\mathbf{V}_S,f_1} : \boldsymbol{\theta} \in \mathbb{R}^k, \mathbf{V}_S \in \mathcal{V}_k^S\}$ as in $\mathcal{P}^n_{S;\boldsymbol{\theta},\sigma_S^2,f_1} := \{P^n_{\boldsymbol{\theta},\sigma_S^2,\mathbf{V}_S,f_1} : \mathbf{V}_S \in \mathcal{V}_k^S\}$, where $\boldsymbol{\theta}$ is specified, and is actually given by $(\boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_S,f_1;33})^{-1}$. Since the latter does only depend on \mathbf{V}_S and f_1 , so does this optimal performance.

On the contrary, the non-zero covariance between the scale and shape parts of the central sequences implies that, when estimating \mathbf{V}_S , the non-specification of σ_S^2 affects the optimal parametric performance at f_1 . The latter actually is given by the f_1 -efficient Fisher information for shape

$$\boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};33}^{\star} := \boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};33} - \boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};32} \boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};22}^{-1} \boldsymbol{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};32}^{\prime}$$

$$= \frac{\mathcal{J}_{k}(f_{1})}{4k(k+2)} \mathbf{M}_{S}^{\mathbf{V}_{S}} (\mathbf{V}_{S}^{\otimes 2})^{-1/2} \left[\mathbf{I}_{k^{2}} + \mathbf{K}_{k} - \frac{2}{k} \mathbf{J}_{k} \right] (\mathbf{V}_{S}^{\otimes 2})^{-1/2} (\mathbf{M}_{S}^{\mathbf{V}_{S}})^{\prime}, \qquad (2.8)$$

that is, the asymptotic covariance matrix, under P_{ϑ_S,f_1}^n , of the f_1 -efficient central sequence for shape

$$\begin{aligned} \mathbf{\Delta}_{\boldsymbol{\vartheta}_{S},f_{1};3}^{\star n} &:= \mathbf{\Delta}_{\boldsymbol{\vartheta}_{S},f_{1};3}^{n} - \mathbf{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};32} \Gamma_{\boldsymbol{\vartheta}_{S},f_{1};22}^{-1} \Delta_{\boldsymbol{\vartheta}_{S},f_{1};22}^{n} \\ &= \frac{1}{2\sqrt{n}} \mathbf{M}_{S}^{\mathbf{V}_{S}} (\mathbf{V}_{S}^{\otimes 2})^{-1/2} \sum_{i=1}^{n} \varphi_{f_{1}} \left(\frac{d_{i}}{\sigma_{S}}\right) \frac{d_{i}}{\sigma_{S}} \operatorname{vec} \left(\mathbf{U}_{i}\mathbf{U}_{i}' - \frac{1}{k}\mathbf{I}_{k}\right); \end{aligned}$$

as explained in a general parametric setup in, e.g, section 2.4 of (2), locally optimal inference on shape—under unspecified σ_S^2 —should be based on $\Delta_{\vartheta_S,f_1;3}^{\star n}$.

Note that, unlike the original central sequence for shape in (2.5), $\Delta_{\boldsymbol{\vartheta}_{S},f_{1};3}^{\star n}$ remains centered under any $P_{\boldsymbol{\vartheta}_{S},g_{1}}^{n}$, $g_{1} \neq f_{1}$. Actually, letting $K_{f_{1}}(u) = \varphi_{f_{1}}(\tilde{F}_{1k}^{-1}(u)) \times \tilde{F}_{1k}^{-1}(u)$ $(u \in (0,1))$, where \tilde{F}_{1k} stands for the cdf associated with the pdf \tilde{f}_{1k} , and denoting by $R_{i} = R_{i}(\boldsymbol{\theta}, \mathbf{V}_{S})$ the rank of $d_{i} = d(X_{i}, \boldsymbol{\theta}; \mathbf{V}_{S})$ among d_{1}, \ldots, d_{n} , a trivial extension of the proof of Lemma 4.1 in (6) (which is restricted to $S(\boldsymbol{\Sigma}) = \Sigma_{11}$) yields that, under $P_{\boldsymbol{\vartheta}_{S},f_{1}}^{n}$, as $n \to \infty$,

$$\boldsymbol{\Delta}_{\boldsymbol{\vartheta}_{S},f_{1};3}^{\star n} = \frac{1}{2\sqrt{n}} \mathbf{M}_{S}^{\mathbf{V}_{S}} (\mathbf{V}_{S}^{\otimes 2})^{-1/2} \sum_{i=1}^{n} K_{f_{1}} \left(\frac{R_{i}}{n+1}\right) \operatorname{vec} \left(\mathbf{U}_{i} \mathbf{U}_{i}^{\prime} - \frac{1}{k} \mathbf{I}_{k}\right) + o_{P}(1),$$

which shows that $\Delta_{\vartheta_S,f_1;3}^{\star n}$ admits an asymptotically equivalent version based on the ranks R_i and the multivariate signs \mathbf{U}_i . This asymptotic equivalence, along with the invariance properties of the families $\cup g_1\{P_{S;\vartheta_S,g_1}\}$ (see, for $S(\mathbf{\Sigma}) = \Sigma_{11}$, section 4.1 in (6)) and a general result by (8), shows that the (semiparametrically) optimal performance (at P_{ϑ_S,f_1}^n), when performing inference on shape in $\mathcal{P}_S^n = \{P_{\vartheta_S,g_1}^n : \vartheta_S \in \Theta_S, g_1 \in \mathcal{F}\}$ concides with the optimal performance achievable in the parametric model $\mathcal{P}_{S;f_1}^n = \{P_{\vartheta_S,f_1}^n : \vartheta_S \in \Theta_S\}$ (as characterized by the efficient information matrix $\Gamma_{\vartheta_S,f_1;33}^{\star}$ in (2.8)). This confirms the adaptivity result first obtained in Example 4 of (1), where it is shown that the non-specification of f_1 has no cost when estimating *the inverse shape matrix* $\mathbf{V}^{-1} := \mathbf{\Sigma}^{-1}/(\operatorname{tr} \mathbf{\Sigma}^{-1})$; note that although this adaptivity result restricts to what is called there a "most general" normalization (the one based on the trace), its proof actually holds for an arbitrary scale functional S.

Summing up, when estimating the shape \mathbf{V}_S in $\mathcal{P}_S^n = \{P_{\boldsymbol{\vartheta}_S,g_1}^n : \boldsymbol{\vartheta}_S \in \boldsymbol{\Theta}_S, g_1 \in \mathcal{F}\}$, the non-specification of σ_S^2 alone is responsible for a loss of efficiency (as already mentioned, the non-specification of $\boldsymbol{\theta}$ does not play any role). This property—call it *Bickel adaptivity*—actually holds for an arbitrary scale functional S. In this paper, we consider a stronger adaptivity concept—full adaptivity, say—under which $\boldsymbol{\theta}, \sigma_S^2$ and f_1 (rather than f_1 alone) lie in the nuisance space of the semiparametric model. The next section shows that full adaptivity holds for one and only one scale functional S, which therefore can be considered canonical.

3 A canonical definition of shape.

We are now ready to state the main result of the paper, which shows that there exists a *unique* scale functional S (thus a unique definition of the shape \mathbf{V}_S) for which the non-specification of σ_S^2 does not cause any loss of efficiency when performing inference on \mathbf{V}_S , hence, for which inference on \mathbf{V}_S in \mathcal{P}_S^n and $\mathcal{P}_{S;\sigma_S^2,f_1}^n$ (equivalently, $\mathcal{P}_{S;\theta,\sigma_S^2,f_1}^n$) yield the same optimal performance.

Theorem 3.1 Let Assumptions (A1) and (A2) hold. Then $\Gamma_{\vartheta_S, f_1; 32} = \mathbf{0}$ for all $\vartheta_S \in \Theta_S$ iff $S = S_d$, where $S_d(\Sigma) := |\Sigma|^{1/k}$.

The decomposition of scatter into scale and shape through the functional S_d is thus the only one that guarantees (a) mutual orthogonality of the scale and shape parts of the central sequence (hence, independence in the asymptotic multinormal distribution), and, consequently, (b) full adaptivity (see above) in the estimation of shape.

For this canonical parametrization, the shape part of the central sequence and Fisher information matrix take the simple form

$$\boldsymbol{\Delta}_{\boldsymbol{\vartheta}_{S},f_{1};3}^{n} = \frac{1}{2\sqrt{n}} \mathbf{M}_{S}^{\mathbf{V}_{S}} (\mathbf{V}_{S}^{\otimes 2})^{-1/2} \sum_{i=1}^{n} \varphi_{f_{1}} \left(\frac{d_{i}}{\sigma_{S}}\right) \frac{d_{i}}{\sigma_{S}} \operatorname{vec} \left(\mathbf{U}_{i}\mathbf{U}_{i}^{\prime}\right) = \boldsymbol{\Delta}_{\boldsymbol{\vartheta}_{S},f_{1};3}^{\star n},$$

and

$$\mathbf{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};33} = \frac{\mathcal{J}_{k}(f_{1})}{4k(k+2)} \mathbf{M}_{S}^{\mathbf{V}_{S}} \left[\mathbf{I}_{k^{2}} + \mathbf{K}_{k} \right] \left(\mathbf{V}_{S}^{\otimes 2} \right)^{-1} \left(\mathbf{M}_{S}^{\mathbf{V}_{S}} \right)' = \mathbf{\Gamma}_{\boldsymbol{\vartheta}_{S},f_{1};33}^{\star}$$
(3.9)

(note indeed that the proof of Theorem 3.1 shows that $\mathbf{M}_{S}^{\mathbf{V}_{S}}(\text{vec }\mathbf{V}_{S}^{-1}) = \mathbf{0}$ for all $\mathbf{V}_{S} \in \mathcal{V}_{k}^{S}$, which entails that $\mathbf{M}_{S}^{\mathbf{V}_{S}}(\mathbf{V}_{S}^{\otimes 2})^{-1/2}\mathbf{J}_{k} = \mathbf{0}$). Theorem 3.1 shows that the determinant-based definition of scale/shape is the only one for which parametric and semiparametric efficiency bounds do coincide (hence, no other choice of S is such that $\Delta_{\boldsymbol{\vartheta}_{S},f_{1};3}^{\star n}$ and $\Delta_{\boldsymbol{\vartheta}_{S},f_{1};3}^{n}$ are equal up to $o_{P}(1)$ terms). Also note that, since $\mathcal{J}_{k}(f_{1}) = k(k+2)$ at the multinormal, the canonical parametrization of shape is also the only one for which the information matrix for shape (either in its original or efficient version) in (3.9) has at any f_{1} the same structure as that of the parametric information matrix (2.7) at the multinormal.

4 Proofs.

In this final section, we prove Theorems 2.1 and 3.1.

For any S satisfying Assumption (A1), consider the mapping V_{11}^S : vech $\mathcal{S}^k \to \mathbb{R}$ defined by $S((V_{11}^S(\text{vech}\mathbf{V}), (\text{vech}\mathbf{V})')') = 1$, the existence of which—locally around any $\mathbf{V}_S \in \mathcal{V}_k^S$ —is guaranteed by Assumption (A1) and the implicit function Theorem. We then start with the following lemma.

Lemma 4.1 Let Assumption (A1) hold and fix $\mathbf{V}_S \in \mathcal{V}_k^S$. Let also \mathbf{P}_k be the $(K+1) \times k^2$ matrix such that $\mathbf{P}'_k(\operatorname{vech} \mathbf{v}) = \operatorname{vec} \mathbf{v}$ for any symmetric $k \times k$ matrix \mathbf{v} . Then, $\mathbf{M}_S^{\mathbf{V}_S} = (\nabla V_{11}^S(\operatorname{vech} \mathbf{V}_S) \vdots \mathbf{I}_K) \mathbf{P}_k$.

PROOF OF LEMMA 4.1. Differentiating (at vech \mathbf{V}_S) both sides of $S((V_{11}^S(\text{vech}\mathbf{V}), (\text{vech}\mathbf{V})')') = 1$ with respect to vech \mathbf{V} , we obtain

$$\nabla V_{11}^S(\operatorname{vech}^{S} \mathbf{V}_S) = -\frac{\nabla_2 S(\operatorname{vech}^{S} \mathbf{V}_S)}{\nabla_1 S(\operatorname{vech}^{S} \mathbf{V}_S)},$$
(4.1)

where $\nabla S(\operatorname{vech} \mathbf{V}_S) = (\nabla_1 S(\operatorname{vech} \mathbf{V}_S), (\nabla_2 S(\operatorname{vech} \mathbf{V}_S))')' \in \mathbb{R} \times \mathbb{R}^K$. Now, $\mathbf{M}_S^{\mathbf{V}_S}$ is such that $(\mathbf{M}_S^{\mathbf{V}_S})'(\operatorname{vech} \mathbf{v}) = (\operatorname{vec} \mathbf{v})$ for any symmetric $k \times k$ matrix $\mathbf{v} = (v_{ij})$ satisfying $(\nabla S(\operatorname{vech} \mathbf{V}_S))'$ $(\operatorname{vech} \mathbf{v}) = (\nabla_1 S(\operatorname{vech} \mathbf{V}_S)) \times v_{11} + (\nabla_2 S(\operatorname{vech} \mathbf{V}_S))'(\operatorname{vech} \mathbf{v}) = 0$, that is, any \mathbf{v} satisfying $(\operatorname{see}(4.1))$

$$(\nabla V_{11}^S(\operatorname{vech} \mathbf{V}_S))'(\operatorname{vech} \mathbf{v}) = v_{11}.$$

The result follows since, for any such \mathbf{v} , one also has $((\nabla V_{11}^S(\operatorname{vech} \mathbf{V}_S) \colon \mathbf{I}_K)\mathbf{P}_k)'(\operatorname{vech} \mathbf{v}) = \mathbf{P}'_k(v_{11}, (\operatorname{vech} \mathbf{v})')' = \mathbf{P}'_k(\operatorname{vech} \mathbf{v}) = \operatorname{vec} \mathbf{v}.$

PROOF OF THEOREM 2.1. As shown in the proof of Proposition 2.1 in (6), the family $\mathcal{P}_{f_1}^n := \{P_{\boldsymbol{\xi},f_1}^n = P_{\boldsymbol{\theta},\boldsymbol{\Sigma},f_1}^n : \boldsymbol{\xi} = (\boldsymbol{\theta}', (\operatorname{vech} \boldsymbol{\Sigma})')' \in \boldsymbol{\Xi} := \mathbb{R}^k \times (\operatorname{vech} \mathcal{S}_k)\}, \text{ under Assumption (A2), is LAN.}$ Now, for any scale functional *S* satisfying Assumption (A1), consider the function $h^S : \boldsymbol{\Theta}_S \to \boldsymbol{\Xi}$ that maps $\boldsymbol{\vartheta}_S$ onto the corresponding value of $\boldsymbol{\xi}$, namely onto $\boldsymbol{\xi} = h^S(\boldsymbol{\vartheta}_S) = (\boldsymbol{\theta}', \sigma_S^2(\operatorname{vech} \mathbf{V}_S)')' = (\boldsymbol{\theta}', \sigma_S^2 V_{11}^S(\operatorname{vech} \mathbf{V}_S), \sigma_S^2(\operatorname{vech} \mathbf{V}_S)')'$. Since h^S is a diffeomorphism, $\mathcal{P}_{S;f_1}^n = \{P_{\boldsymbol{\vartheta}_S,f_1}^n : \boldsymbol{\vartheta}_S \in \boldsymbol{\Theta}_S\}$ is also LAN, and the corresponding central sequence is given by

$$\boldsymbol{\Delta}^{n}_{\boldsymbol{\vartheta}_{S},f_{1}} = \left(Dh^{S}(\boldsymbol{\vartheta}_{S})\right)' \bar{\boldsymbol{\Delta}}^{n}_{h(\boldsymbol{\vartheta}_{S}),f_{1}},\tag{4.2}$$

where

$$Dh^{S}(\boldsymbol{\vartheta}_{S}) = \begin{pmatrix} \mathbf{I}_{k} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & V_{11}^{S}(\text{vech}\mathbf{V}_{S}) & \sigma_{S}^{2}(\nabla V_{11}^{S}(\text{vech}\mathbf{V}_{S}))' \\ \mathbf{0} & \text{vech}\mathbf{V}_{S} & \sigma_{S}^{2}\mathbf{I}_{K} \end{pmatrix}$$

is the jacobian matrix of h^S at $\boldsymbol{\vartheta}_S$ and where, letting $d_i(\boldsymbol{\xi}) = d(\mathbf{X}_i, \boldsymbol{\theta}; \boldsymbol{\Sigma})$ and $\mathbf{U}_i(\boldsymbol{\xi}) = \boldsymbol{\Sigma}^{-1/2}(\mathbf{X}_i - \boldsymbol{\theta})/d_i(\boldsymbol{\xi})$ (where $\boldsymbol{\Sigma}^{1/2}$ denotes the symmetric root of $\boldsymbol{\Sigma}$),

$$\bar{\boldsymbol{\Delta}}_{\boldsymbol{\xi},f_1}^n := \begin{pmatrix} \frac{1}{\sqrt{n}} \sum_{i=1}^n \varphi_{f_1}(d_i(\boldsymbol{\xi})) \boldsymbol{\Sigma}^{-1/2} \mathbf{U}_i(\boldsymbol{\xi}) \\ \frac{1}{2\sqrt{n}} \mathbf{P}_k \left(\boldsymbol{\Sigma}^{\otimes 2} \right)^{-1/2} \sum_{i=1}^n \operatorname{vec} \left(\varphi_{f_1}(d_i(\boldsymbol{\xi})) d_i(\boldsymbol{\xi}) \mathbf{U}_i(\boldsymbol{\xi}) \mathbf{U}_i'(\boldsymbol{\xi}) - \mathbf{I}_k \right) \end{pmatrix}$$

is the central sequence in the LAN family $\mathcal{P}_{f_1}^n = \{P_{\boldsymbol{\xi},f_1}^n : \boldsymbol{\xi} \in \boldsymbol{\Xi}\}$ (see the proof of Proposition 2.1 in (6)). The result then readily follows from (4.2), since (i) the scale part $\Delta_{\boldsymbol{\vartheta}_S,f_1;2}^n$ of $\Delta_{\boldsymbol{\vartheta}_S,f_1}^n$ can be written as in (2.4) by noting that $(\operatorname{vech} \mathbf{V}_S)'\mathbf{P}_k(\mathbf{V}_S^{\otimes 2})^{-1/2}\operatorname{vec} \mathbf{v} = (\operatorname{tr} \mathbf{v})$ for any $k \times k$ symmetric matrix \mathbf{v} , and since (ii) the shape part $\Delta_{\boldsymbol{\vartheta}_S,f_1;3}^n$ of $\Delta_{\boldsymbol{\vartheta}_S,f_1}^n$ can be directly put under the form (2.5) by using Lemma 4.1.

Now, for any $\Sigma \in S_k$ and S satisfying Assumption (A1), define $\mathbf{C}_S^{\Sigma} := \mathbf{C}_{S,k}^{\Sigma}$ as the uppertriangular $k \times k$ matrix such that vech $\mathbf{C}_S^{\Sigma} := \nabla S(\operatorname{vech} \Sigma)$, and let $\mathbf{D}_S^{\Sigma} := (\mathbf{C}_S^{\Sigma} + (\mathbf{C}_S^{\Sigma})')/2$. Clearly, $(\operatorname{vec} \mathbf{D}_S^{\Sigma})'(\operatorname{vec} \mathbf{v}) = (\operatorname{vech} \mathbf{C}_S^{\Sigma})'(\operatorname{vech} \mathbf{v})$ for any symmetric $k \times k$ matrix \mathbf{v} . The matrix \mathbf{M}_S^{Σ} is then such that $(\mathbf{M}_S^{\Sigma})'(\operatorname{vech} \mathbf{v}) = (\operatorname{vec} \mathbf{v})$ for any symmetric $k \times k$ matrix \mathbf{v} satisfying $(\operatorname{vec} \mathbf{D}_S^{\Sigma})'(\operatorname{vec} \mathbf{v}) = 0$ (equivalently, satisfying tr $(\mathbf{D}_S^{\Sigma}\mathbf{v}) = 0$). For $S(\Sigma) = \Sigma_{11}$, $S(\Sigma) = (\operatorname{tr} \Sigma)/k$, and $S(\Sigma) = |\Sigma|^{1/k}$, one has $\mathbf{D}_S^{\Sigma} = \mathbf{e}_1\mathbf{e}_1'$, $\mathbf{D}_S^{\Sigma} = \frac{1}{k}\mathbf{I}_k$, and $\mathbf{D}_S^{\Sigma} = \frac{1}{k}|\Sigma|^{1/k}\Sigma^{-1}$, respectively. The following result states some important properties of \mathbf{M}_S^{Σ} and \mathbf{D}_S^{Σ} , which are needed in the proof of Theorem 3.1.

Lemma 4.2 Let Assumption (A1) hold and fix $\Sigma \in S_k$. Then, (i) $\mathbf{D}_S^{\Sigma} = \mathbf{D}_S^{\lambda\Sigma}$ for all $\lambda > 0$; (ii) $S(\Sigma) = \operatorname{tr}(\mathbf{D}_S^{\Sigma}\Sigma)$; (iii) letting $\Sigma_{\lambda} := (1-\lambda)\mathbf{I}_k + \lambda\Sigma$, $S(\Sigma) = \exp\left[\int_0^1 \operatorname{tr}((\Sigma - \mathbf{I}_k)\mathbf{D}_S^{\Sigma_{\lambda}}/S(\Sigma_{\lambda})) d\lambda\right]$; (iv) \mathbf{M}_S^{Σ} has (maximal) rank K; (v) denoting by ker \mathbf{A} the null space of a matrix \mathbf{A} , (ker \mathbf{M}_S^{Σ}) \cap (vec S_k) = { λ (vec \mathbf{D}_S^{Σ}) : $\lambda \in \mathbb{R}$ }.

PROOF OF LEMMA 4.2. (i) The claim readily follows from the definition of \mathbf{D}_{S}^{Σ} and the homogeneity of S, which implies that the gradient of S is constant along half lines of the form $\{\lambda \Sigma : \lambda > 0\}$. (ii) By taking derivatives at $\lambda = 1$ of both sides of the equality $\lambda S(\operatorname{vech} \Sigma) =$ $S(\lambda (\operatorname{vech} \Sigma))$, one obtains that $S(\Sigma) = (\operatorname{vech} \mathbf{C}_{S}^{\Sigma})'(\operatorname{vech} \Sigma) = (\operatorname{vec} \mathbf{D}_{S}^{\Sigma})'(\operatorname{vec} \Sigma) = \operatorname{tr} (\mathbf{D}_{S}^{\Sigma} \Sigma)$. (iii) The result follows by integrating between 0 and 1 the mapping $\lambda \mapsto d\log S(\Sigma_{\lambda})/d\lambda =$ $(\operatorname{vech} (\Sigma - \mathbf{I}_{k}))'(\operatorname{vech} \mathbf{C}_{S}^{\Sigma_{\lambda}})/S(\Sigma_{\lambda}) = (\operatorname{vec} (\Sigma - \mathbf{I}_{k}))'(\operatorname{vec} \mathbf{D}_{S}^{\Sigma_{\lambda}})/S(\Sigma_{\lambda}) = \operatorname{tr} ((\Sigma - \mathbf{I}_{k})\mathbf{D}_{S}^{\Sigma_{\lambda}}/S(\Sigma_{\lambda}))$. (iv) It is clear from the definition of \mathbf{M}_{S}^{Σ} that $(\mathbf{M}_{S}^{\Sigma})'$ maps the canonical basis of \mathbb{R}^{K} into a collection of linearly independent vectors (in $(\operatorname{vec} S_{k})$, actually). Hence, $\operatorname{rank}(\mathbf{M}_{S}^{\Sigma}) = K$. (v) It follows from the definition of \mathbf{M}_{S}^{Σ} that, for any symmetric $k \times k$ matrix \mathbf{v} satisfying $(\operatorname{vec} \mathbf{D}_{S}^{\Sigma})_{11} = \frac{\partial S}{\partial \Sigma_{11}}(\Sigma) \neq 0$ for all $\Sigma \in S_{k}$, this entails that $\mathbf{M}_{S}^{\Sigma}(\operatorname{vec} \mathbf{D}_{S}^{\Sigma}) = \mathbf{0}$. Now, the proof of (ii) shows that the restriction (L, say) to $(\operatorname{vec} S_{k})$ of the linear mapping from $\mathbb{R}^{k^{2}}$ to \mathbb{R}^{K} with matrix \mathbf{M}_{S}^{Σ} has rank K. Hence, the null space of L has dimension 1, which establishes the result. \Box

We are now able to prove Theorem 3.1.

PROOF OF THEOREM 3.1. Assume that $\Gamma_{\vartheta_S,f_1;32} = \mathbf{0}$ for all $\vartheta_S \in \Theta_S$. Since Assumption (A2) guarantees that $\mathcal{J}_k(f_1) > k^2$ (see (6)), we must have that $\mathbf{M}_S^{\mathbf{V}_S}(\operatorname{vec} \mathbf{V}_S^{-1}) = \mathbf{0}$ for all $\mathbf{V}_S \in \mathcal{V}_k^S$. Lemma 4.2(v) shows that, for all $\mathbf{V}_S \in \mathcal{V}_k^S$, there exists some $\lambda(\mathbf{V}_S) \neq 0$ such that $\mathbf{V}_S^{-1} = \lambda(\mathbf{V}_S) \mathbf{D}_S^{\mathbf{V}_S}$. Lemma 4.2(ii) then yields that $1 = S(\mathbf{V}_S) = \operatorname{tr}((\lambda(\mathbf{V}_S))^{-1}\mathbf{I}_k) = (\lambda(\mathbf{V}_S))^{-1}k$, so that $\lambda(\mathbf{V}_S) = k$ for all $\mathbf{V}_S \in \mathcal{V}_k^S$. Hence, Lemma 4.2(i) entails that, for any $\mathbf{\Sigma} \in \mathcal{S}_k, \mathbf{D}_S^{\mathbf{\Sigma}}/S(\mathbf{\Sigma}) = \mathbf{D}_S^{\mathbf{\Sigma}/S(\mathbf{\Sigma})}/S(\mathbf{\Sigma}) = \frac{1}{k}(\mathbf{\Sigma}/S(\mathbf{\Sigma}))^{-1}/S(\mathbf{\Sigma}) = \frac{1}{k}\mathbf{\Sigma}^{-1}$. Since we also have that $\mathbf{D}_{S_d}^{\mathbf{\Sigma}}/S_d(\mathbf{\Sigma}) = S_d(\mathbf{\Sigma})$ for any $\mathbf{\Sigma} \in \mathcal{S}_k$, which establishes the result. \Box

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