

On UMVU Estimator of the Generalized Variance for Natural Exponential Families

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Abstract

For any given natural exponential family (NEF), the existence is proven for the uniformly minimum variance and unbiased (UMVU) estimator of the generalized variance, i.e. the determinant of the covariance matrix. This result provides a unification and a general extension of those appearing in recent literature. In order to compare the UMVU estimator with an unbiased maximum likelihood (ML) estimator, the necessary and sufficient condition will be given. Finally, a characterization of the Poisson-Gaussian laws in \mathbb{R}^d will be given.

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1 Introduction

The problem of estimating the determinant of a covariance matrix, referred to as the *generalized variance*, has received much attention in literature (e.g., Shorrocks and Zidek, 1976; Gupta and Ofori-Nyarko, 1995). Let $\mathbf{M}_n(\mathbf{X}) = (\mathbf{X}_1, \dots, \mathbf{X}_n)$ be a $d \times n$ random matrix with i.i.d. columns to the random vector \mathbf{X} such that $\mathbf{m} = \mathbb{E}(\mathbf{X})$ is the mean and $\Sigma = Cov(\mathbf{X})$ is the covariance matrix. Assume that \mathbf{m} is unknown and Σ is known to be a positive definite (i.e., $|\Sigma| > 0$, where $|\Sigma|$ denotes the determinant of Σ). All the usual statistics are based on the sample generalized variance

$$|\mathbf{S}_n| = \left| \frac{1}{n-1} \sum_{i=1}^n (\mathbf{X}_i - \bar{\mathbf{X}}) \otimes (\mathbf{X}_i - \bar{\mathbf{X}}) \right|,$$

where $\bar{\mathbf{X}} = n^{-1} \sum_{i=1}^n \mathbf{X}_i$ is the random sample mean vector, and $\mathbf{X}_i \otimes \mathbf{X}_j$ denotes the matrix $\mathbf{X}_i \mathbf{X}_j^t$. Generally $|\mathbf{S}_n|$ is a biased estimator. Some of their properties are known for \mathbf{X} distributed as normal via Wishart distribution (e.g., Iliopoulos and Kourouklis, 1998, also for some references on the developments of this purpose) or for \mathbf{X} distributed as elliptic (see Iwashita and Siotani, 1994). In the literature of multivariate data analysis, that is $|\mathbf{S}_n|$ which is very often used without distribution hypothesis to detect outliers (e.g., Rousseeuw and Van Driessen, 1999, also for some references). In addition, the *maximum likelihood* (ML) estimator can be used to exploit the (asymptotical) advantages of this method.

The present paper is devoted to the *uniformly minimum variance and unbiased* (UMVU) estimator of $|\Sigma|$ for \mathbf{X} distributed as a probability $P(\mathbf{m}, F)$ in a *natural exponential family* (NEF) F on \mathbb{R}^d with mean \mathbf{m} and covariance matrix $\Sigma := \mathbf{V}_F(\mathbf{m})$, depending on \mathbf{m} (see Kotz *et al.*, 2000, Chapter 54, for more details). It is indicated that the generalized variance $|\mathbf{V}_F(\mathbf{m})|$ is a measure of the variability within a population. In general, we can use it to compare covariance matrices between themselves. Naturally, it appears in the matrix inversion problems. But one can find it in other situations (e.g., Butler *et al.*, 1992). Finally, it can be seen as the determinant of the Fisher Information matrix.

Motivated by the partial results of the literature (e.g., Kokonendji and Seshadri (1996) for $n = d + 1$; Pommeret (1998) for the class of simple quadratic NEFs of Casalis (1996); Kokonendji and Pommeret (2001a) for infinitely divisible NEFs), the main aim of this paper is to point out the UMVU estimator for all NEFs and for any $n (> d)$ observations. In Section 2 the result will be shown and connected to an unbiased ML estimator under any necessary and sufficient condition. Finally, in Section 3, we investigate two applications: the first provides the way to improve the Gaussian case via Wishart NEF. The second application is a new characterization of the Poisson-Gaussian NEFs on \mathbb{R}^d .

2 Basic Results

First, let us briefly recall the notations of NEFs. Let μ be a generating measure of $F := F(\mu)$, and $\Theta(\mu)$ defined as the non-empty interior of the domain of the Laplace transform $L_\mu(\theta) := \int_{\mathbb{R}^d} \exp\langle \theta, \mathbf{x} \rangle \mu(d\mathbf{x})$ of μ . We will denote by k_μ'' the $d \times d$ Hessian matrix of the cumulant function $k_\mu(\theta) := \log L_\mu(\theta)$ and by ψ_μ the inverse map of $\theta \mapsto k_\mu'(\theta) =: \mathbf{m}$ from $\Theta(\mu)$ into $M_F := k_\mu'(\Theta(\mu))$ referred to as the mean domain of F . The covariance matrix of the probability measure $P(\mathbf{m}, F)(d\mathbf{x}) := \exp\{\langle \psi_\mu(\mathbf{m}), \mathbf{x} \rangle - k_\mu(\psi_\mu(\mathbf{m}))\} \mu(d\mathbf{x})$ can be written $\mathbf{V}_F(\mathbf{m}) = k_\mu''(\psi_\mu(\mathbf{m}))$. Note that $\mathbf{V}_F(\mathbf{m})$, defined on M_F , is so-called the *variance function* of $F := \{P(\mathbf{m}, F); \mathbf{m} \in M_F\}$. An important feature of \mathbf{V}_F is that it characterizes the NEF F , and it presents an expression far simpler than $P(\mathbf{m}, F)$.

We now present the UMVU estimator of $|\mathbf{V}_F(\mathbf{m})|$ and then compare it to the ML estimator.

2.1 UMVU estimator

Let us first state an important preliminary result, which guarantees the existence of the UMVU estimator of the generalized variance for all NEFs.

Theorem 2.1 *Let μ be a generating measure of a NEF on \mathbb{R}^d . Then for all integer $n > d$, there exists a positive measure ν_n on \mathbb{R}^d verifying the three following statements:*

(i) ν_n is the image measure of

$$\frac{1}{(d+1)!} \left| \left[\begin{array}{cccc} 1 & 1 & \cdots & 1 \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_{d+1} \end{array} \right] \right|^2 \mu(d\mathbf{x}_1) \cdots \mu(d\mathbf{x}_{d+1}) \cdots \mu(d\mathbf{x}_n)$$

by the map $(\mathbf{x}_1, \dots, \mathbf{x}_n) \mapsto \mathbf{x}_1 + \cdots + \mathbf{x}_n$;

(ii) its Laplace transform is

$$L_{\nu_n}(\theta) = |k''_{\mu}(\theta)| (L_{\mu}(\theta))^n \quad (1)$$

for all $\theta \in \Theta(\mu)$;

(iii) there exists $C_n : \mathbb{R}^d \rightarrow \mathbb{R}$ such that

$$\nu_n(d\mathbf{x}) = C_n(\mathbf{x}) \mu^{*n}(d\mathbf{x}). \quad (2)$$

For the proof we can refer to Kokonendji and Pommeret (2001b).

Note that, first, ν_n is invariant by the choice of the first $d+1$ components among n . Second, if μ is an infinitely divisible measure then there exists a positive measure $\rho(\mu)$ on \mathbb{R}^d such that $|k''_{\mu}(\theta)| = L_{\rho(\mu)}(\theta)$ for all $\theta \in \Theta(\mu)$ (see Hassairi, 1999; Theorem 2.1), and, hence, we have the following interpretation: $\nu_n = \rho(\mu) * \mu^{*n}$. This observation was at the origin of the Kokonendji and Pommeret (2001a) Note.

We can now show the main result of this paper, which has no restriction either for the sample size $n > d$ or for a kind of NEF.

Theorem 2.2 *Let $F = F(\mu)$ be a NEF on \mathbb{R}^d generated by μ and let $\mathbf{X}_1, \dots, \mathbf{X}_n$ be n -random variables i.i.d. as $P(\mathbf{m}, F) \in F$. Then for all $n \geq d+1$, the UMVU estimator of the generalized variance $|\mathbf{V}_F(\mathbf{m})|$ is*

$$T_n = C_n(n\bar{\mathbf{X}}), \quad (3)$$

where C_n is defined in (2) of Theorem 2.1 and $\bar{\mathbf{X}} = n^{-1} \sum_{i=1}^n \mathbf{X}_i$.

Proof: By Rao-Blackwell theorem (e.g., Lehmann and Casella, 1998, page 47) it suffices to observe the following fact. From Theorem 2.1 we have, for each $\mathbf{m} = k'_{\mu}(\theta) \in M_F$,

$$|\mathbf{V}_F(\mathbf{m})| = |k''_{\mu}(\theta)| = L_{\nu_n}(\theta) / L_{\mu^{*n}}(\theta) = \mathbb{E}_{\theta(\mathbf{m})}(C_n(n\bar{\mathbf{X}}))$$

$$= \int_{(\mathbb{R}^d)^n} C_n(\mathbf{y}_1 + \cdots + \mathbf{y}_n) P(\mathbf{m}, F)(d\mathbf{y}_1) \cdots P(\mathbf{m}, F)(d\mathbf{y}_n). \square$$

Comment. Theorem 2.2 is a unification and extension of results in Kokonendji and Pommeret (2001a; Theorem 2), Kokonendji and Seshadri (1996; Theorem 3.3), and also Pommeret (1998; with its real function $g(\mathbf{m})$ as $|\mathbf{V}_F(\mathbf{m})|$). Further, Theorem 2.1 guarantees the existence of C_n (for $n \geq d + 1$), which the first two papers above do not give. For practical reasons, if C_n could be calculated then it is possible to consider T_n given by (3) for the small sample sizes $n \leq d$, which loses its UMVU property. See Kokonendji and Pommeret (2001b) for more details concerning the *simple quadratic* NEFs in \mathbb{R}^d of Casalis (1996) with variance functions having the form

$$\mathbf{V}_F(\mathbf{m}) = \alpha \mathbf{m} \otimes \mathbf{m} + \mathbf{B}(\mathbf{m}) + \mathbf{C} \quad (4)$$

where $\alpha \in \mathbb{R}$, $\mathbf{B}(\mathbf{m})$ is a $(d \times d)$ matrix of linear elements in \mathbf{m} , and \mathbf{C} is a $(d \times d)$ symmetric positive matrix of constants.

Remark 1. If $\mathbf{X}_1, \dots, \mathbf{X}_{n_1}$ and $\mathbf{Z}_1, \dots, \mathbf{Z}_{n_2}$ are two independents i.i.d. samples with distributions $P(\mathbf{m}_1, F_1) \in F_1$ and $P(\mathbf{m}_2, F_2) \in F_2$, respectively, then the joint distribution $P(\mathbf{m}_1, F_1) \times P(\mathbf{m}_2, F_2)$ belongs to the NEF $F = F_1 \times F_2$. Since F_1 and F_2 are independent, then

$$|\mathbf{V}_F(\mathbf{m})| = |\mathbf{V}_{F_1}(\mathbf{m}_1)| |\mathbf{V}_{F_2}(\mathbf{m}_2)|,$$

where $\mathbf{m} = (\mathbf{m}_1, \mathbf{m}_2)$. Thus the UMVU estimator of $|\mathbf{V}_F(\mathbf{m})|$ is the product of the two UMVU estimators of $|\mathbf{V}_{F_1}(\mathbf{m}_1)|$ and $|\mathbf{V}_{F_2}(\mathbf{m}_2)|$ respectively.

Remark 2. The asymptotic efficiency of T_n can be obtained by using some results of Portnoy (1977), restricted to lattice and infinitely divisible distributions.

2.2 Comparing UMVU and ML estimators

Let $\mathbf{X}_1, \dots, \mathbf{X}_n$ be n -random variables i.i.d. as $P(\mathbf{m}, F) \in F(\mu)$. Then it is easily seen that the ML estimator of the generalized variance $|\mathbf{V}_F(\mathbf{m})|$ is $|\mathbf{V}_F(\bar{\mathbf{X}})|$ and generally biased. By completeness, there can be only one unbiased estimator function of $\bar{\mathbf{X}}$. Thus, the comparison (between UMVU and ML estimators) should be based on the mean squared error as risk; one of which is more complicated in this general situation. However, through the construction of the UMVU estimator (3), we have the following result.

Theorem 2.3 *Let $\mathbf{X}_1, \dots, \mathbf{X}_n$ be n -random variables i.i.d. as $P(\mathbf{m}, F) \in F(\mu)$, $\bar{\mathbf{X}} = n^{-1} \sum_{i=1}^n \mathbf{X}_i$, and C_n as defined in (2) of Theorem 2.1. Then there exists $(a, \mathbf{b}, c) \in \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}$ such that*

$$|k''_\mu(\theta)| = \exp\{ak_\mu(\theta) + \langle \mathbf{b}, \theta \rangle + c\} \quad (5)$$

for all $\theta \in \Theta(\mu)$ if and only if there exists $\lambda_n > 0$ such that

$$C_n(\mathbf{X}_1 + \cdots + \mathbf{X}_n) = \lambda_n |\mathbf{V}_F(\bar{\mathbf{X}})|. \quad (6)$$

Comment. The condition (5) has already appeared in Gutiérrez-Peña and Smith (1995) related to the equality of two conjugate prior distribution families of a NEF $F(\mu)$. Also, it is satisfied for all homogeneous and simple quadratic NEFs (Casalis, 1991, 1996), but it does not provide their characterization for $d > 1$.

As for one part of the proof, we can just observe the following fact.

Proposition 2.4 *Let $F = F(\mu)$ be a NEF generated by μ satisfying (5). Let ν_n be defined from μ as in Theorem 2.1. Then $F(\nu_n)$ and $F(\mu)$ are of the same type (i.e., up to affinity and power). More precisely, one has $\nu_n = (\exp c) A_* \mu^{*(n+a)}$ where $A : \mathbf{x} \mapsto \mathbf{x} + \mathbf{b}$.*

Proof: From (1) of Theorem 2.1 and (5) of Theorem 2.3 we have

$$k_{\nu_n}(\theta) = (n + a)k_{\mu}(\theta) + \langle \theta, \mathbf{b} \rangle + c.$$

Letting $\bar{\mathbf{m}} = k'_{\nu_n}(\theta)$, $\mathbf{m} = k'_{\mu}(\theta)$ and $\bar{a}_n = n + a$, we have $\bar{\mathbf{m}} = \bar{a}_n \mathbf{m} + \mathbf{b}$ and $\mathbf{V}_{F(\nu_n)}(\bar{\mathbf{m}}) = \bar{a}_n \mathbf{V}_F((\bar{\mathbf{m}} - \mathbf{b})/\bar{a}_n)$. This shows that $F(\nu_n)$ and $F(\mu)$ are of the same type, because $\bar{\mathbf{m}}$ and \mathbf{m} are linked by an affinity transformation. \square

3 Applications

We now present two applications of the previous results.

3.1 Wishart and Gaussian families

Since in the Gaussian NEF the variance Σ does not depend on the mean \mathbf{m} , we need a good estimator of Σ in the Wishart family.

Let E be the space of $(r \times r)$ real symmetric matrices and S be the cone in E of positive definite matrices. Consider the standard Wishart distribution $W_r(2p, \Sigma)$ concentrated on \bar{S} (closure of S) with Σ in S and p in

$$\Lambda = \{1/2, 1, 3/2, \dots, (r-1)/2\} \cup ((r-1)/2, \infty). \quad (7)$$

Then it is known that the NEF

$$F_p = \{W_r(2p, \Sigma); \Sigma \in S\} \quad (8)$$

has a homogeneous quadratic variance (Letac, 1989a; Casalis, 1991).

The key to the UMVU estimator of the generalized variance in the Wishart NEF is provided by the following result, without proof here.

Proposition 3.1 Let $\mu \in M(E)$ such that $F(\mu) = F_p$ with F_p given by (8) and p in Λ given by (7). Let ν_n be defined from μ as in Theorem 2.1. Then $F(\nu_n) = F_{\bar{p}_n}$, where $\bar{p}_n = np + r + 1$ with $n \geq 1 + r(r + 1)/2$; that is, $F(\nu_n)$ and $F(\mu)$ are of the same type.

Furthermore for

$$p > (r - 1)/2 \text{ and } n \geq 1 + r(r + 1)/2, \quad (9)$$

the function $C_n(X) = \nu_n(dX)/\mu^{*n}(dX)$ is explicitly given by

$$C_n(\mathbf{X}) = 2^{r(r+1)} p^{r(r+1)/2} \frac{\Gamma_r(np)}{\Gamma_r(np + r + 1)} |\mathbf{X}|^{r+1} \quad (10)$$

where

$$\Gamma_r(q) = 2^{rq} \pi^{r(r-1)/4} \prod_{k=0}^{r-1} \Gamma(q - k/2). \quad (11)$$

Now, our estimator $T_n = C_n(\mathbf{X}_1 + \dots + \mathbf{X}_n)$ is the best, concerning UMVU, to estimate the generalized variance $|k''_{\mu_p}(\theta(\Sigma))| = 2^{r(r+1)} p^{r(r+1)/2} |\Sigma|^{r+1}$ in the Wishart family $W_r(2p, \Sigma)$ for any $n \geq 1 + r(r + 1)/2$, where C_n is given by (10).

The direct calculation of $Var_{\theta(\Sigma)}(T_n)$, using (10) and

$$\mathbb{E}_{\theta}(|\mathbf{X}_1 + \dots + \mathbf{X}_n|^q) = \frac{\Gamma_r(q + np)}{\Gamma_r(np)} | - 2\theta |^{-q}$$

(see Muirhead, 1982; page 101) for all sample size n , where $\mathbf{X}_1, \dots, \mathbf{X}_n$ are i.i.d. random variables with Wishart distribution $W_r(2p, \Sigma)$ with $\theta = -\Sigma^{-1}/2$, shows that

$$Var_{\Sigma}(T_n) = 2^{2r(r+1)} p^{r(r+1)} |\Sigma|^{2(r+1)} \left[\frac{\Gamma_r(np) \Gamma_r(np + 2r + 2)}{\Gamma_r^2(np + r + 1)} - 1 \right],$$

where Γ_r is defined in (11). Thus, the following remark could improve some properties of the generalized variance in the Gaussian case, for which both mean \mathbf{m} and variance Σ are unknown.

Remark 3. The traditional notation of the Wishart distribution generated by n independent centred Gaussian variables with covariance matrix Σ' is $W_r(n, \Sigma')$, where r is the dimension of Σ' . The correspondence between this notation and the one $W_r(2p, \Sigma)$ we adopt in this paper is immediate: $p = n/2$ and $\Sigma = 2\Sigma'$.

3.2 Characterization of Poisson-Gaussian Laws in \mathbb{R}^d

Let $\mathbf{X} \in \mathbb{R}^d$ be a Poisson-Gaussian $(PG)_{k=0,1,\dots,d}$ vector such that the first k (in $\{0, 1, \dots, d\}$) components have Poisson distributions independent to the $d - k$ components which are Gaussian distributions (see Casalis, 1996). The corresponding generating measure μ of this type is

$$\mu(d\mathbf{x}) = \left\{ \sum_{j \in \mathbb{N}^k} \frac{\delta_j(dx_1, \dots, dx_k)}{j!} \right\} \frac{\exp \left\{ - \sum_{i=k+1}^d x_i^2 / 2 \right\}}{(2\pi)^{(d-k)/2}} (dx_{k+1}, \dots, dx_d),$$

where δ_j is the Dirac mass at j , $k_\mu(\theta) = \sum_{i=1}^k e^{\theta_i} + \sum_{i=k+1}^d (\theta_i^2/2)$, $|k_\mu''(\theta)| = \exp(\theta_1 + \dots + \theta_k)$, $\Theta(\mu) = \mathbb{R}^d$ and $\mathbf{V}_F(\mathbf{m}) = \mathbf{diag}(m_1, \dots, m_k, 1, \dots, 1)$ on $M_F = (0, \infty)^k \times \mathbb{R}^{d-k}$.

By symmetry conditions on variance functions, Letac (1989b) described that all NEFs with variance function as the form (4) where $\alpha = 0$ are of the type $(PG)_{k=0,1,\dots,d}$. The new characterization of the Poisson-Gaussian NEFs on \mathbb{R}^d is given by the following theorem and its interpretation is from Theorem 2.1 (i) and Proposition 2.4 for all interger $n > d$.

Theorem 3.2 *Let μ be a generating measure of a NEF on \mathbb{R}^d . Then μ generates one of the $d + 1$ types of $(PG)_{k=0,1,\dots,d}$ if and only if $a = 0$ in (5).*

Comments. (i) For $k = 0$ and hence $(a = 0, \mathbf{b} = \mathbf{0})$ in (5), we obtain here a new interpretation for the Gaussian distribution given in Kokonendji and Seshadri (1996) only for $n = d + 1$. Note also that for $k \in \{1, \dots, d\}$, we have $\lambda_n = 1$ in (6).

(ii) The set of NEFs generating by μ satisfying (5) is neither only the simple quadratic NEFs, nor the quadratic ones; it is an open problem for $a \neq 0$ with $d > 1$.

(iii) The “if” part of Theorem 3.2 is established. For the “only if” part of the proof, first take the complex result of Pogorelov (1978; page 90) reformulated as follows:

Lemma 3.3 *Let f be a C^∞ convex function on \mathbb{R}^d such that the determinant of the Hessian matrix f'' is a constant. Then f'' itself is a constant.*

Then apply Lemma 3.3 to f so that $|f''(\theta)| = |\exp\{-\langle \mathbf{b}, \theta \rangle / d\} k_\mu''(\theta)|$.

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