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DETECTION OF MULTIVARIATE OUTLIERS IN ELLIPTICALLY SYMMETRIC DISTRIBUTIONS[1]

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An extension of Ferguson's (*Fourth Berkeley Symposium on Probability and Mathematical Statistics*, 1961, Volume 1) univariate normal results and Schwager and Margolin's (1982) multivariate normal results for detection of outliers is made to the multivariate elliptically symmetric case with mean slippage. The main result can be viewed as a robustness property of the use of Mardia's multivariate kurtosis statistic as a locally optimum test statistic to detect outliers against nonnormal multivariate distributions.

1. Introduction. Ferguson (1961) did a pioneering work on the detection and rejection of outliers in samples from a univariate normal distribution with either mean or variance slippage. Later much work followed on the problem of estimation of parameters and tests of hypotheses of parameters in particular probability models, assuming the presence of outliers in the data. These two aspects of the problem of outliers, as mentioned clearly in Schwager and Margolin (1982), are entirely different. Generally, one needs one kind of techniques to determine if outliers are present and to identify them. However, a different kind of techniques is required to suitably modify a statistical analysis for purposes of inferences to incorporate the information regarding the presence and identity of outlying observations.

The motivation for the present investigation lies in a recent paper of Schwager and Margolin (1982) who derive a locally optimum procedure for detection of multivariate normal outliers arising from mean slippage. The paper has some very interesting features. First, this seems to be the only paper attempting successfully to generalize the concept and techniques of Ferguson to the multinormal case. Second, interestingly enough, it turns out that the locally best invariant test for outliers (under a suitable group of transformations) against mean slippage alternatives is based on Mardia's (1970) multivariate sample kurtosis. We will show that the assumption of multinormality of the error components can be dispensed with without any essential difficulty.

In this paper we extend the results of Schwager and Margolin (1982) to nonnormal elliptically symmetric multivariate populations and in the process provide a simpler derivation of the main optimality result. This derivation of

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course depends mostly on the existing calculations of Schwager and Margolin (1982). The class of nonnormal multivariate populations we consider is well known in the context of robust tests for multivariate problems (see Kariya and Eaton, 1977; Kariya, 1981a, 1981c; and Sinha and Drygas, 1982, for a univariate problem). The main tool we use is a representation theorem due to Wijsman (1967). The multivariate outlier problem is formulated in Section 2, while Section 3 contains the main result.

2. The multivariate outlier problem. Let $\mathscr{O}(n)$ and $\mathscr{S}(p)$ denote the set of $n \times n$ orthogonal matrices and the set of $p \times p$ positive definite matrices respectively. For an $n \times p$ random matrix U, we denote by $\mathscr{L}(U)$ the distribution of U. We call U elliptically symmetric about M with scale matrix $\Sigma \in \mathscr{S}(p)$ if $\mathscr{L}(gY) = \mathscr{L}(Y)$ for all $g \in \mathscr{O}(np)$, where $Y = (\mathbf{Y}_1, \cdots, \mathbf{Y}_n)$, $\mathbf{Y}_i$ is the ith row of $Y = (U - M)\Sigma^{-1/2}$. Let $\mathscr{X} = \{U\colon n \times p \mid \text{rank}\ (U) = p\}$. Throughout the paper, $n \geq p + 1$ is assumed. Moreover, we denote by $\mathscr{F}(M, I_n \otimes \Sigma)$ the class of np-dimensional elliptically symmetric distributions about M with scale matrix $\Sigma \in \mathscr{S}(p)$ such that $P\{U - M \in \mathscr{X}\} \equiv 1$. We assume that $\mathscr{L}(U) \in \mathscr{F}(M, I_n \otimes \Sigma)$ has a density (with respect to the Lebesgue measure) which is expressible as

$$f(U \mid M, \Sigma) = |\Sigma|^{-n/2}\phi(\text{tr}\ \Sigma^{-1}(U - M)'(U - M)) \tag{2.1}$$

where $\phi\colon [0, \infty) \to [0, \infty)$.

Consider a random sample of size n from a multivariate distribution. We will denote the sample by $X\colon n \times p$ and assume that the following model holds:

$$X = \mathbf{1}\mu' + U\Sigma^{-1/2} \tag{2.2}$$

where $\mathbf{1}$ is the unit vector $(n \times 1)$, μ is the unknown common mean vector $(p \times 1)$ of the rows of X and the random error component U has a distribution $\mathscr{L}(U) \in \mathscr{F}(0, I_n \otimes I_p)$ with a density given in (2.1) with $M = 0$ and $\Sigma = I_p$. This is equivalent to the specification that $\mathscr{L}(X) \in \mathscr{F}(\mathbf{1}\mu', I_n \otimes \Sigma)$. It is clear that our formulation is more general than Schwager and Margolin's (1982) in that ϕ is arbitrary. Some mild regularity conditions on ϕ which will be needed in the sequel are presented later.

In this paper we consider the possibility of outliers with mean slippage. For any matrix $A = (a_{ij})\colon n \times p$, extending Ferguson's (1961) formulation and proceeding as in Schwager and Margolin (1982), this can be incorporated by considering the model

$$X = \mathbf{1}\mu' + \Delta A\Sigma^{-1/2} + U\Sigma^{-1/2}. \tag{2.3}$$

Here Δ is a nonzero scalar and A is an arbitrary matrix such that some of the rows of A are zero. In this formulation, unless $\Delta = 0$, the observation X_i corresponding to the ith row of X is an outlier if the ith row of A is nonzero.

The general multivariate outlier problem then consists of the model (2.3), the distributional assumption about U: $\mathscr{L}(U) \in \mathscr{F}(0, I_n \otimes I_p)$, and the null hypothesis H_0: $\Delta = 0$ versus the alternative hypothesis H_1: $\Delta \neq 0$. In what follows we will derive a locally optimum test of H_0 against H_1 employing invariance arguments through the use of a group of transformations keeping the testing problem invariant. It may be noted that rejection of H_0 implies a decision to act as if there are outliers in the data according to the assumed structure of A. However, as will be seen later, the optimum test obtains for a wide variety of outliers structures (see Remark 3.1). Moreover, the test is null robust in the sense that the null distribution of the test statistic remains the same for any $\mathscr{L}(X) \in \mathscr{F}(\mathbf{1}\boldsymbol{\mu}', I_n \otimes \Sigma)$ (see Remark 3.3).

Following Schwager and Margolin (1982), it is clear that the above testing problem remains invariant under the action of the group $\mathscr{G} = \mathscr{P} \times Gl(p) \times \mathbb{R}^p$ where $\mathscr{P}$ denotes the group of all $n \times n$ permutation matrices with elements Γ_α, $Gl(p)$ the group of $p \times p$ nonsingular matrices with elements C and $\mathbb{R}^p$ the Euclidean p-space. The three (sub)group operations are defined by: (1) addition of an arbitrary vector $\boldsymbol{\mu}^* \in \mathbb{R}^p$ to each row of X; (2) postmultiplication of X by any nonsingular matrix $C \in Gl(p)$ and (3) permutation of the rows of X by premultiplying X by $\Gamma_\alpha \in \mathscr{P}$. For details see Schwager and Margolin (1982). In the next section we derive the distribution of a maximal invariant statistic, applying Wijsman's (1967) theorem. This method does not require an explicit evaluation of a maximal invariant statistic although this is available in Schwager and Margolin (1982). It may be pointed out that the null distribution of a maximal invariant statistic is independent of any parameter and, as stated earlier, is independent of any $\mathscr{L} \in \mathscr{F}$.

3. Main results. Without loss of generality, by invariance of the problem, we may assume $\boldsymbol{\mu} = \mathbf{0}$ and $\Sigma = I_p$. To obtain a formal expression of the distribution of a maximal invariant $T(X)$, we use the following version of Wijsman's (1967) theorem.

LEMMA 3.1. *Let $h(x \mid \Delta) = \phi(\mathrm{tr}(x - \Delta A)'(x - \Delta A))$ be the pdf of X, let $T = t(X)$ be a maximal invariant under the transformation $\mathscr{G}$ and let P_Δ^T be the distribution induced by T under Δ. Then the pdf of T with respect to P_0^T evaluated at $T = t(X)$ is given by*

$$\frac{dP_\Delta^T}{dP_0^T}(t(X)) = \frac{\int_{\mathscr{G}} h(g \cdot X \mid \Delta) \mid C'C \mid^{n/2} d\nu(g)}{\int_{\mathscr{G}} h(g \cdot X \mid \Delta = 0) \mid C'C \mid^{n/2} d\nu(g)} \tag{3.1}$$

where ν is a left invariant measure on $\mathscr{G}$.

Conditions under which (3.1) holds are stated in Wijsman (1967); the details are omitted here.

We now proceed to evaluate (3.1) explicitly. The transformation $g \cdot x$ is given by (see Schwager and Margolin, 1982)

$$g \cdot x = \Gamma_\alpha x C + \mathbf{1}\boldsymbol{\mu}^{*\prime}, \quad \Gamma_\alpha \in \mathscr{P}, \quad C \in Gl(p), \quad \boldsymbol{\mu}^* \in \mathbb{R}^p \tag{3.2}$$

and we take $\nu = \nu_1 \times \nu_2 \times \nu_3$ where ν_1 is the discrete uniform probability measure with mass $1/n!$ at each of the $n!$ elements $\Gamma_\alpha \in \mathscr{P}$, $d\nu_2(C) = dC/ \mid C'C \mid^{p/2}$ and $d\nu_3(\boldsymbol{\mu}^*)$ is the Lebesgue measure on $\mathbb{R}^p$.

LEMMA 3.2. *The ratio of the pdfs in expression* (3.1) *is evaluated as*

$$\frac{\sum_\alpha \int_{G1(p)} \tilde{\phi}\left[\operatorname{tr}\left(C'C - 2\Delta C'S^{-1/2}(\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}')'A + \Delta^2\left(A'A - \frac{A'\mathbf{1}\mathbf{1}'A}{n}\right)\right)\right] |C'C|^{(n-p)/2}\, dC}{\sum_\alpha \int_{G1(p)} \tilde{\phi}[\operatorname{tr}(C'C)]\, |C'C|^{(n-p)/2}\, dC} \tag{3.3}$$

for some $\tilde{\phi}$: $[0, \infty) \to [0, \infty)$, *where* $\sum_\alpha$ *denotes the summation over* $n!$ *terms representing permutations of the rows of* x, $\bar{\mathbf{x}}$ *the sample mean vector and* $S = x'x - n\bar{\mathbf{x}}\bar{\mathbf{x}}'$.

PROOF. The numerator N_Δ (say) of (3.1) can be written as

$$N_\Delta = \frac{1}{n!} \sum_\alpha \int_{G1(p)} \int_{\mathbb{R}^p} \phi(\operatorname{tr}(x'x - \Delta x'A - \Delta A'x + \Delta^2 A'A \mid x \to g \cdot x)) \cdot |C'C|^{(n-p)/2}\, dC\, d\nu_3(\mu^*). \tag{3.4}$$

Here $\phi(\operatorname{tr}(\cdots \mid x \to g \cdot x))$ stands for the value of ϕ evaluated when x is replaced by $g \cdot x$ provided by (3.2). The argument of ϕ, after the substitution $x = g \cdot x$, simplifies to

$$\begin{aligned}
\operatorname{tr}[(\Gamma_\alpha xC + \mathbf{1}\mu^{*\prime})'(\Gamma_\alpha xC + \mathbf{1}\mu^{*\prime}) &- 2\Delta A'(\Gamma_\alpha xC + \mathbf{1}\mu^{*\prime}) + \Delta^2 A'A] \\
&= \operatorname{tr}(C'x'\Gamma_\alpha'\Gamma_\alpha xC + 2nC'\bar{\mathbf{x}}\mu^{*\prime} + n\mu^*\mu^{*\prime} \\
&\qquad - 2\Delta A'\Gamma_\alpha xC - 2\Delta A'\mathbf{1}\mu^{*\prime} + \Delta^2 A'A) \\
&= \operatorname{tr}\Big(C'x'xC - 2\Delta A'\Gamma_\alpha xC + \Delta^2 A'A \\
&\qquad - n\left(C'\bar{\mathbf{x}} - \frac{\Delta}{n} A'\mathbf{1}\right)\left(\bar{\mathbf{x}}'C - \frac{\Delta}{n}\mathbf{1}'A\right) + n\mathbf{c}^*\mathbf{c}^{*\prime}\Big) \\
&= \operatorname{tr}\Big(C'(x'x - n\bar{\mathbf{x}}\bar{\mathbf{x}}')C - 2\Delta C'(\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}')'A \\
&\qquad + \Delta^2\left(A'A - \frac{A'\mathbf{1}\mathbf{1}'A}{n}\right) + n\mathbf{c}^*\mathbf{c}^{*\prime}\Big).
\end{aligned} \tag{3.5}$$

In the equalities above, $\mathbf{c}^* = \mu^* - (\Delta/n)A'\mathbf{1} + C'\bar{\mathbf{x}}$ and we have used the fact that $x'\Gamma_\alpha'\Gamma_\alpha x = x'x$, $\forall \Gamma_\alpha \in \mathscr{P}$. Since $d\nu_3(\mu^*) = d\nu_3(\mathbf{c}^*)$, using a result of Dawid (1977), integration with respect to $\mathbf{c}^*$ over $\mathbb{R}^p$ yields

$$N_\Delta = \frac{1}{n!} \sum_\alpha \int_{G1(p)} \tilde{\phi}\left[\operatorname{tr}\left(C'(x'x - n\bar{\mathbf{x}}\bar{\mathbf{x}}')C - 2\Delta C'(\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}')'A + \Delta^2\left(A'A - \frac{A'\mathbf{1}\mathbf{1}'A}{n}\right)\right)\right] |C'C|^{(n-p)/2}\, dC \tag{3.6}$$

for $\tilde{\phi}$: $[0, \infty) \to [0, \infty)$ given by $\tilde{\phi}(Z) \equiv \int_{\mathbb{R}^p} \phi(Z + n\mathbf{u}'\mathbf{u})\, d\mathbf{u}$.

Now $x'x - n\bar{\mathbf{x}}\bar{\mathbf{x}}' = S$, the sample sum of squares and products matrix, is p.d. by our assumption $n \geq p + 1$. Writing $S = S^{1/2}S^{1/2}$ where $S^{1/2}$ is the positive square root of S and making the transformation $C \to S^{1/2}C$, N_Δ reduces to

$$N_\Delta = \frac{|S|^{-n/2}}{n!} \sum_\alpha \int_{G1(p)} \tilde{\phi}\Big[\operatorname{tr}\Big(C'C - 2\Delta C'S^{-1/2}(\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}')'A + \Delta^2\Big(A'A - \frac{A'\mathbf{1}\mathbf{1}'A}{n}\Big)\Big)\Big] |C'C|^{(n-p)/2}\, dC. \tag{3.7}$$

Since the denominator of (3.1) corresponds to N_Δ with $\Delta = 0$, the lemma follows. □

We now proceed to evaluate the expression in (3.3). An exact evaluation of the expression is difficult but its Taylor series expansion up to a few terms evaluated at $\Delta = 0$, which is all we need to derive a locally best invariant test, is not so. Making a transformation from C to $-C$, it is clear from (3.3) that the ratio of the pdfs depends only on Δ^2. We show that the coefficient δ_2 of Δ^2 in this ratio

$$\delta_2 = \sum_\alpha \int_{G1(p)} [\operatorname{tr}\{AC'S^{-1/2}(\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}')'\}]^2 \tilde{\phi}^{(2)}(\operatorname{tr} C'C)\, |C'C|^{(n-p)/2}\, dC, \tag{3.8}$$

apart from another constant term depending only on A, is a constant, and that the coefficient δ_4 of Δ^4 in the ratio

$$\delta_4 = \sum_\alpha \int_{G1(p)} [\operatorname{tr}\{AC'S^{-1/2}(\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}')'\}]^4 \tilde{\phi}^{(4)}(\operatorname{tr} C'C)\, |C'C|^{(n-p)/2}\, dC, \tag{3.9}$$

apart from other terms including (3.8) which are constants, is of the form $K_1(\tilde{\phi})T(x)L(A) + K_2(\tilde{\phi})$ where $K_1(\tilde{\phi})$, $K_2(\tilde{\phi})$ are constants, $\tilde{\phi}^{(i)}(u) = (d^i/du^i)\tilde{\phi}(u)$, $i = 2, 4$, $\bar{\mathbf{a}} = (1/n)\sum_1^n \mathbf{a}_i$,

$$T(x) = b_{2,p} \equiv n \sum_1^n \{(\mathbf{x}_i - \bar{\mathbf{x}})'S^{-1}(\mathbf{x}_i - \bar{\mathbf{x}})\}^2 \tag{3.10}$$

and

$$L(A) = (n^3 + n^2)\sum_{i=1}^n \|\gamma_i\|^4 - (n^2 - n)[2\sum_{i,j=1}^n (\gamma_i'\gamma_j)^2 + (\sum_{i=1}^n \|\gamma_i\|^2)^2], \tag{3.11}$$

with $\gamma_i = (\mathbf{a}_i - \bar{\mathbf{a}})$, $\|\gamma_i\|^2 = \gamma_i'\gamma_i$, $x' = (\mathbf{x}_1, \cdots, \mathbf{x}_n)$ and $A' = (\mathbf{a}_1, \cdots, \mathbf{a}_n)$.

EVALUATION OF δ_2. This is based on the following elementary result whose proof is omitted. $\sum_\alpha$ below is over $n!$ permutations obtained by permuting the columns of A_α, and A_α satisfies $A_\alpha\mathbf{1} = \mathbf{0}$ and $A_\alpha A_\alpha' = A_0$ (independent of α) for all α.

LEMMA 3.3. $\sum_\alpha \{\operatorname{tr}(BA_\alpha)\}^2 = n(n-2)!(\operatorname{tr} BA_0B') - (n-2)!(\mathbf{1}'BA_0B'\mathbf{1})$.

Taking $B = AC'S^{-1/2}$, $A_\alpha = (\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}')'$ and using the fact that $(\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}')'(\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}') = S$ for any α, it follows that

$$\delta_2 = \int_{G1(p)} \{n(n-2)!(\operatorname{tr} AC'CA') - (n-2)!(1'AC'CA'\mathbf{1})\} \cdot \phi^{(2)}(\operatorname{tr} C'C)\,|C'C|^{(n-p)/2}\,dC \tag{3.12}$$

which is a constant.

EVALUATION OF δ_4. This is primarily based on some results derived by Schwager and Margolin (1982). Write

$$\operatorname{tr}\{AC'S^{-1/2}(\Gamma_\alpha x - \mathbf{1}\bar{\mathbf{x}}')'\} = \operatorname{tr}\{\Gamma_\alpha' AC'S^{-1/2}(x - \mathbf{1}\bar{\mathbf{x}}')'\} = \textstyle\sum_{i=1}^n \xi_i' C\mathbf{a}_{i\alpha}$$

where $\xi_i = S^{-1/2}\delta_i$, δ_i is the ith column vector of $(x - \mathbf{1}\bar{\mathbf{x}}')'$ and $\mathbf{a}_{i\alpha}$ is the ith column vector of $A'\Gamma_\alpha$. Since $\sum_{i=1}^n \xi_i$ is a null vector, in the last equality above we can replace $\mathbf{a}_{i\alpha}$ by $\gamma_{i\alpha}$ = the ith column vector of $(A'\Gamma_\alpha - \bar{\mathbf{a}}\mathbf{1}')$. We now use the results of Section 5 of Schwager and Margolin (1982). Their Theorem 5.1 is applicable directly and their Lemmas 5.1 and 5.2 and Theorem 5.2 are used with Φ suitably redefined as

$$\Phi = \int_{G1(p)} c_{11}^4 \tilde{\phi}^{(4)}(\operatorname{tr} C'C)\,|C'C|^{(n-p)/2}\,dC. \tag{3.13}$$

The justification follows easily because the above results are independent of any particular structure of the underlying probability distribution and actually depend on the invariance of the associated measure under orthogonal transformations. This yields

$$\delta_4 = (n-4)!\Phi L(A)\{\textstyle\sum_{i=1}^n \|\xi_i\|^4\} + k(\tilde{\phi}) \tag{3.14}$$

where $L(A)$ is as defined in (3.11). This completes our demonstration since $\|\xi_i\|^2 = (\mathbf{x}_i - \bar{\mathbf{x}})'S^{-1}(\mathbf{x}_i - \bar{\mathbf{x}})$ and $k(\tilde{\phi})$ is a constant.

Our main result is the following.

THEOREM 3.1. *Assume that $\tilde{\phi}$ satisfies* (i) $\Phi < \infty$, (ii) $\tilde{\phi}(x+y)$ *admits a Taylor expansion in y for every x with continuous fourth order derivative, and* (iii) *that the first four derivatives of the power function of an invariant test with respect to Δ can be carried out beneath the integral sign. The locally best invariant locally unbiased test, conditionally on A, rejects H_0: $\Delta = 0$ for large values of $b_{2,p}$ if $\Phi \cdot L(A) > 0$ and small values of $b_{2,p}$ if $\Phi \cdot L(A) < 0$.*

PROOF. An application of Lemma 3.2 and the generalized Neyman–Pearson Lemma along with the quantities δ_2, δ_4 completes the proof of the theorem. The routine details are omitted (see, for example, Kariya, 1981b). □

REMARK 3.1. As mentioned in Schwager and Margolin (1982), the local optimality of the $b_{2,p}$-test obtains for a specific A and a universal optimality (local) result holds whenever the fraction of nonzero rows of A is at most 21%.

REMARK 3.2. The class of nonnormal distributions ϕ considered in (2.1) contains the (np-dimensional) multivariate t-distribution, the multivariate Cauchy distribution, the contaminated normal distribution and more generally continuous normal mixtures of the type $f = \int_0^\infty N(U \mid M, a\Sigma)\, dG(a)$ where N is the normal density and G is a distribution function on $(0, \infty)$. For such an f, it is easy to justify the conditions in Theorem 3.1 (see Ferguson, 1961) and it turns out that $\Phi > 0$.

REMARK 3.3. It is easy to verify that the locally optimum test statistic $T(x) = b_{2,p}$ satisfies (i) $T((x - \mathbf{1}\boldsymbol{\mu}')\Sigma^{-1/2}) = T(x)$ for all $\boldsymbol{\mu} \in \mathbb{R}^p$, $\Sigma \in \mathscr{S}(p)$, and (ii) $T(\alpha x) = T(x)$ for all scalars $\alpha > 0$. This establishes the null robustness of the locally optimum test (vide Corollary 2.1, Kariya, 1981c).

REMARK 3.4. It may be noted that the conditions in Theorem 3.1 are stated in terms of the intermediate function $\tilde{\phi}(x) \equiv \int_{\mathbb{R}^p} \phi(x + n\mathbf{u}'\mathbf{u})\, d\mathbf{u}$. Stated in terms of ϕ, the following are sufficient:

(i) $$\int_{G1(p)} \left| \int_{\mathbb{R}^p} \frac{\partial^4}{\partial x^4} \phi(x + n\mathbf{u}'\mathbf{u})\, d\mathbf{u} \right|_{x=\mathrm{tr}C'C} c_{11}^4 \, |C'C|^{(n-p)/2}\, dC < \infty;$$

(ii) $\phi(x + y)$ admits a Taylor expansion in y for every x with continuous fourth order derivative and

$$\frac{\partial^i}{\partial x^i}\left[\int_{\mathbb{R}^p} \phi(x + n\mathbf{u}'\mathbf{u})\, d\mathbf{u}\right] = \int_{\mathbb{R}^p} \frac{\partial^i}{\partial x^i} \phi(x + n\mathbf{u}'\mathbf{u})\, d\mathbf{u}, \quad i = 1, 2, 3, 4.$$

It is remarked that these conditions are satisfied for a large class of pdfs especially in the case of normal mixture: $\phi(x) = \int_0^\infty e^{-ax}\, dF(a)$ provided

$$\int_0^\infty a^{2-p(n+1)/2}\, dF(a) < \infty \quad \text{and} \quad \int_0^\infty a^{i-(p/2)}\, dF(a) < \infty, \quad i = 1, 2, 3, 4.$$

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