On complex Gaussian random fields, Gaussian quadratic forms and sample distance multivariance

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Abstract

The paper contains results in three areas: First we present a general estimate for tail probabilities of Gaussian quadratic forms with known expectation and variance. Thereafter we analyze the distribution of norms of complex Gaussian random fields (with possibly dependent real and complex part) and derive representation results, which allow to find efficient estimators for the moments of the associated Gaussian quadratic form. Finally, we apply these results to sample distance multivariance, which is the test statistic corresponding to distance multivariance – a recently introduced multivariate dependence measure. The results yield new tests for independence of multivariate random vectors. These are less conservative than the classical tests based on a general quadratic form estimate and they are (much) faster than tests based on a resampling approach. As a special case this also improves independence tests based on distance covariance, i.e., tests for independence of two random vectors.

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1 Introduction

Recently distance multivariance and total distance multivariance were introduced as measures of dependence for multiple random vectors \[ \text{(Székely, Rizzo and Bakirov [26])}, \] these extend the concept of distance covariance introduced by Székely, Rizzo and Bakirov \[ \text{[26]} \]. For random vectors \( X_i \) with values in \( \mathbb{R}^d \), \( 1 \leq i \leq n \), the total distance multivariance \( \mathcal{M}(X) \) of \( X := (X_1, \ldots, X_n) \) is zero if and only if the random variables are independent. See \[ \text{[4]} \] for a practical guide to distance multivariance, as well as many examples and a comparison to other dependence measures. In \[ \text{[7]} \] conservative tests of independence based on distance multivariance were presented. Using a resampling approach less conservative but computationally more expensive tests are possible, \[ \text{[4]} \]. In this paper we analyze the proposed test statistics in more detail, in order to derive

Other dependence measures. In \[ \text{[7]} \] conservative tests of independence based on distance multivariance were presented. Using a resampling approach less conservative but computationally more expensive tests are possible, \[ \text{[4]} \]. In this paper we analyze the proposed test statistics in more detail, in order to derive

the (performance of the) tests for the basic case \( (n = 2) \) of distance covariance \[ \text{[26]} \], this is due to the fact that our method provides in this case p-value estimates without the use of a resampling technique, see, e.g., Examples \[ \text{5.2} \] and \[ \text{5.4} \]. The derived methods are implemented in the R package multivariance \[ \text{[4]} \].

Along the way at least two results which are also of general interest – without the context of distance multivariance – are proved:

- A general tail estimate for Gaussian quadratic forms: Let \( 0 \leq \alpha_i \leq \alpha \leq 1 \) for \( i \in \mathbb{N} \) with \( \sum_{i=1}^{\infty} \alpha_i = 1 \) and \( Z_i \) be independent standard normal random variables then
  \[
  \Pr \left( \sum \alpha_i Z_i^2 \geq x \right) \leq \Pr \left( \alpha Y_\frac{x}{\alpha} \geq x \right) \quad \text{for all } x \geq x_0, \tag{1.1}
  \]
  where \( Y_\alpha \) is a chi-squared distributed random variable with (fractional) \( \frac{\alpha}{2} \) degree of freedom and \( x_0 \) depends on \( \alpha \) and is bounded from above by 1.5365, see Theorem \[ \text{2.1} \]. This result extends the special case \( \alpha = 1 \) which was treated in \[ \text{[26]} \]. Their estimate was based on the first moment only, other estimates require at least the knowledge of moments up to order 3, e.g. \[ \text{[13]} \]. Thus in a sense our estimate fills the gap, since it can be applied if only the first two moments are known, cf. Remark \[ \text{2.2} \]. For further references and a comparison with other estimates for Gaussian quadratic forms see Equation \[ \text{2.6} \].

- A representation of the squared \( L^2(\rho) \)-norm \( \|G\|_\rho^2 \) of a complex Gaussian random field \( G \) – with possibly dependent real and imaginary parts – as positive Gaussian quadratic form:
  \[
  \|G\|_\rho^2 = \sum_{i \in I} \alpha_i Z_i^2,
  \]
  where \( \alpha_i, i \in I \subseteq \mathbb{N} \), are the eigenvalues of the covariance operator associated to the random field and \( Z_i \) are independent standard normally distributed random variables, see Theorem \[ \text{3.9} \].

Certainly similar results are known (see, e.g., \[ \text{[14]} \]), but we are not aware of a citable proof for our setting. Moreover – for applications most important – we present explicit representations of the sums \( \mu^{(k)} = \sum_{i \in I} \alpha_i^k \) of the coefficients in terms of the covariance kernel of the random field \( G \), see Proposition \[ \text{3.12} \].

In the setting of distance multivariance (see Section \[ \text{3} \] for the underlying definitions) it is known that the limit (as the sample size \( N \) increases to \( \infty \)) of sample distance multivariance \( N^{-\gamma} \mathcal{M}_\gamma^2 \) is distributed as a Gaussian quadratic form which is obtained as the \( L^2 \)-norm of a Gaussian random field. It is denoted by \( \|G\|_\rho^2 \), and it (obviously) fits into the above framework. So far its exact distribution was intangible. In Section \[ \text{4} \] we will derive many useful results about it, e.g., an explicit representation in Proposition \[ \text{4.5} \] which simplifies the previously known representation \[ \text{[7]} \text{ Eq. (4.20) ff.} \]. But here in the introduction we just want to mention the results which seem of major practical importance. First of all we derive explicit estimators for the moments of the limiting distribution (analogous results for total- and \( m \)-multivariance are also proved in Section \[ \text{4.4} \].

\[ ^1 \text{The methods will be included in the next release of the package multivariance (current version: 1.1.0).} \]
Theorem (Corollary 4.12). Let \( (x^{(1)}, \ldots, x^{(N)}) \) be samples of \( (X_1, \ldots, X_n) \) (with possibly dependent components!) and let \( \|G\|^2_\rho \) be the distributional limit of the test statistic \( N \cdot \nu M^2_\rho \) under the hypothesis of independence. Set \( S := \{1, \ldots, n\} \), then

\[
\begin{align*}
\frac{\nu M_\rho^{(1)}}{\|G\|^2_\rho} & \xrightarrow{N \to \infty} \mathbb{E}(\|G\|^2_\rho), \\
2 \cdot \frac{\nu M_\rho^{(2)}}{\|G\|^2_\rho} & \xrightarrow{N \to \infty} \mathbb{V}(\|G\|^2_\rho), \\
8 \cdot \frac{\nu M_\rho^{(3)}}{\|G\|^2_\rho} & \xrightarrow{N \to \infty} \mathbb{E} \left[ (\|G\|^2_\rho - \mathbb{E}(\|G\|^2_\rho))^2 \right], \\
48 \nu M_\rho^{(4)} + 12 \left( \frac{\nu M_\rho^{(2)}}{\|G\|^2_\rho} \right)^2 & \xrightarrow{N \to \infty} \mathbb{E} \left[ (\|G\|^2_\rho - \mathbb{E}(\|G\|^2_\rho))^4 \right],
\end{align*}
\]

where the \( \nu M_\rho^{(k)} \) can be computed directly from the (possibly dependent) samples. The formulas are given in Corollary 4.13 on page 22. (See also Remark 4.13 for the corresponding unbiased estimators.)

It turns out that for the case of \( n = 2 \) and \( n = 3 \) the above provides also good estimates for the distribution of sample distance multivariance \( N \cdot \nu M^2_\rho \) for small sample sizes \( N \) (cf. Example 5.7). But beware, in general for larger \( n \) the parameters of the distribution of \( N \cdot \nu M^2_\rho \) are not well approximated by the above result – this is true even for reasonable sample sizes like \( N = 100 \). In particular the variance of the limit can be much lower than the variance of the finite sample estimator \( N \cdot \nu M^2_\rho \) (cf. Theorem 4.14 and Example 5.7). Nevertheless, also for the finite sample case we derive by careful analysis the following explicit formulas (which again can be estimated directly from possibly dependent samples).

Theorem (Theorem 4.14). Let \( X_1, \ldots, X_n \) be independent. Then

\[
\begin{align*}
\mathbb{E}(N \cdot \nu M^2_\rho(X^{(1)}, \ldots, X^{(N)})) & = \frac{(N - 1)^n + (-1)^n(N - 1)}{N^n} \prod_{i=1}^{n} \mathbb{E}(\psi_i(X_i - X'_i)), \\
\mathbb{E}([N \cdot \nu M^2_\rho(X^{(1)}, \ldots, X^{(N)})]^2) & = \frac{1}{N^2} \sum_{k=1}^{7} C(N, k) \prod_{i=1}^{n} \left[ \frac{b(N, k)b_i + c(N, k)c_i + d(N, k)d_i}{N^4} \right],
\end{align*}
\]

where \( b_i := \mathbb{E}(\psi_i(X_i - X'_i))^2 \), \( c_i := \mathbb{E}(\psi_i(X_i - X'_i)\psi_i(X'_i - X''_i)) \), \( d_i := [\mathbb{E}(\psi_i(X_i - X'_i))]^2 \) and the coefficients \( C(\ldots), b(\ldots), c(\ldots), d(\ldots) \) are given in Table 1 on page 36. (For the estimators see Remarks 4.15 and 4.13.)

Finally, recall that in [1] [7] [20] for the independence tests the so-called normalized sample distance multivariance \( N \cdot \nu M^2_\rho \) was used (which is just a scaled version of \( N \cdot \nu M^2_\rho \), see Section 4). But note that the scaling therein also depends on the sample and thus for finite samples the distribution has to be analyzed jointly with the scaling factor. This is done in Theorem 4.16.

The methods can also be extended to total- and \( m \)-multivariance, see Section 4.4. Moreover the explicit knowledge of the expectation and variances can also be used to construct further (new) tests of \( m \)-independence using the central limit theorem (see Remark 4.19).

For readers with an interest to apply our results in the context of distance multivariance we recommend the overview of the methods in Section 4.5 and the examples in Section 5. Based on the examples, especially using the extensive study in Example 5.10 we have the following remarks and recommendations for performing independence tests based on distance multivariance:

- Estimate 4.61 provides more powerful tests than the classical estimate 4.62. Moreover, the tests show (at least in all of our examples) conservative behavior when used with the unbiased finite sample estimators for the parameters.

- Using any of the proposed methods to estimate the p-value is faster than the resampling approach (Example 5.4).
• Using the unbiased finite sample estimators for the mean and variance of normalized (total-, \(m\)-) multivariance (Theorem 4.16, Corollary 4.22) together with the unbiased estimator for the skewness (Corollaries 4.12, 4.18) in Pearson’s estimate (4.64) provides p-value estimates which have the smallest relative mean squared error in comparison to the benchmark. (This holds for the samples and methods studied in Example 5.10 which are so rich that it seems to be reasonable to generalize this statement.)

• Also for the special case of distance multivariance \((n = 2)\) the above method is recommended.

• For the case of analyzing pairwise or triple dependence of identically distributed marginals with \(m\)-multivariance the central limit theorem based method (4.65) performs very similarly to the above method (cf. Figure 21 in the Appendix).

• If the marginal distributions are known, one can compute the required parameters apriori (Example 5.6).

• Using normalized multivariance instead of multivariance without normalization is always recommended (see the discussion before Remark 4.24 and their performance in Example 5.10).

• All methods discussed rely on the existence of certain moments, if this existence is in doubt there are the fundamental options, but also these require some basic moment conditions (Remark 4.2). Nevertheless there is some indication for robust behavior (Example 5.9), but in our opinion it requires further investigation.

2 Gaussian quadratic forms

We start with a general tail estimate for Gaussian quadratic forms. See (2.6) for a comparison with other existing methods.

**Theorem 2.1.** Let \(Z_i\) be independent standard normal random variables and \((\alpha_i)_{i \in \mathbb{N}}\) be a sequence in \(\mathbb{R}\) with \(0 \leq \alpha_i \leq \alpha \leq 1\) and \(\sum \alpha_i = 1\). Then there exists \(x_0 = x_0(\alpha, (\alpha_i)_{i \in \mathbb{N}}) \geq 0\) such that

\[
P \left( \sum \alpha_i Z_i^2 \geq x \right) \leq P \left( \alpha Y_\frac{1}{\alpha} \geq x \right) \quad \text{for all} \ x \geq x_0, \tag{2.1}
\]

where \(Y_\frac{1}{\alpha}\) is a chi-squared distributed random variable with (fractional) \(\frac{1}{\alpha}\) degree of freedom.

The value \(x_0(\alpha) := \sup \{x_0(\alpha, (\alpha_i)_{i \in \mathbb{N}}) \mid 0 \leq \alpha_i \leq \alpha \leq 1, \ \sum \alpha_i = 1\}\) is bounded from above by 1.5365, i.e., inequality (2.1) holds uniformly for all \(x \geq 1.5365\), all \(\alpha < 1\) and all \(\alpha_i\) with \(0 \leq \alpha_i \leq \alpha\) and \(\sum \alpha_i = 1\).

**Remark 2.2.**

1. To use this bound a suitable \(\alpha\) has to be known or estimated. A simple choice is

\[
\alpha := \sqrt{\frac{1}{2} \left( \sum \alpha_i Z_i^2 \right)},
\]

cf. Lemma 2.3. Note that \(\alpha = \max_{i \in \mathbb{N}} \alpha_i\) is the optimal choice – this is nothing but the spectral radius of the associated integral operator \(T_K\), see (3.2).

2. For \(\alpha \in (0, 1]\) let \(x_0(\alpha)\) be such that \(0 < \mathbb{P}(|\frac{1}{\sqrt{\alpha}} Y_\frac{1}{\alpha}| \leq x_0(\alpha)) = \mathbb{P}(\frac{1}{\sqrt{\alpha}} Y_\frac{1}{\alpha} \leq x_0(\alpha)) < 1\).

By [25] Prop. 1.1 \(x_0(\alpha)\) is unique, and in our setting \(x_0(\alpha)\) is an upper bound for \(x_0(\alpha)\) of Theorem 2.1. For all \(\alpha \in (0, 1]\) the corresponding tail probability \(1 - \mathbb{P}(\alpha Y_\frac{1}{\alpha} \geq x_0(\alpha))\) is larger than 0.215, which is well above any commonly used significance level (for details see Section 6.1 in the Appendix, especially Figure 18). Thus the estimate is proper for hypothesis testing.
3. The special case \( \alpha = 1 \), i.e.,
\[
P\left( \sum \alpha_i Z_i^2 \geq x \right) \leq P(Y_1 \geq x) \quad \text{for all } x \geq x_0,
\]
was proved in [25]. Therein also bounds for smaller \( x \) can be found. These bounds are of the form
\[
P\left( \frac{1}{n} Y_n \geq x \right) \text{ for some } n = n(x) \in \mathbb{N}.
\]

4. Recall that for \( \alpha, \beta > 0 \) and \( Y_{\frac{1}{\alpha}} \sim \chi^2(\frac{1}{\alpha}) \) (i.e., chi-squared distributed with parameter \( \frac{1}{\alpha} \)) the density and characteristic function of \( \beta Y_{\frac{1}{\alpha}} \) are
\[
p_{\beta Y_{\frac{1}{\alpha}}}(x) = \frac{1}{\beta 2^{\frac{\alpha}{2}} \Gamma\left(\frac{\alpha}{2}\right)} \left( \frac{x}{\beta} \right)^{-\frac{\alpha}{2} - 1} e^{-\frac{x}{\beta}} I_{(0, \infty)}(x) \quad \text{and} \quad f_{\beta Y_{\frac{1}{\alpha}}}(t) = (1 - 2i\beta t)^{-\frac{\alpha}{2}}.
\]

The density of \( \beta Y_{\frac{1}{\alpha}} \) is strictly monotonically decreasing for \( \frac{1}{\alpha} \leq 2 \), and for independent \( Y_{\frac{1}{\alpha}} \sim \chi^2(\frac{1}{\alpha}) \) with \( \frac{1}{\alpha_i} > 0 \)
\[
\sum_{i=1}^{\infty} Y_{\frac{1}{\alpha_i}} = Y_{\sum_{i=1}^{\infty} \frac{1}{\alpha_i}}
\]
holds.

Proof of Theorem [27]. Let the assumptions of the theorem hold. Without loss of generality we assume that \((\alpha_n)_{n \in \mathbb{N}}\) is monotonically decreasing and denote by \( n_1 \) the largest \( n \in \mathbb{N} \) such that \( \alpha_1 = \alpha_n \).

If \( \alpha_1 = \frac{1}{n_1} \) then the statement is trivial, since in this case \( \sum \alpha_i Z_i \overset{d}{=} \alpha_1 Y_{n_1} = \alpha_1 Y_{\frac{1}{\alpha}} \) by (2.3), and its tail distribution is dominated by \( \alpha Y_{\frac{1}{\alpha}} \) for any \( \alpha > \alpha_1 \). The latter is a direct consequence of \( \frac{1}{n_1} > \frac{1}{\alpha} \)
and thus
\[
p_{\alpha_1 Y_{\frac{1}{n_1}}}(x) = c_{\alpha_1, \alpha} x^{-\frac{1}{n_1} - \frac{1}{\alpha}} e^{-\frac{x}{\alpha_1}} \left( \frac{x}{\alpha_1} \right)^{-\frac{1}{n_1} - \frac{1}{\alpha}} \xrightarrow{x \to \infty} 0.
\]

It remains to consider the case \( \alpha_1 < \frac{1}{n_1} \). By [29] Equation (5)] the density of \( \sum_{i=1}^{\infty} \alpha_i Z_i^2 \) has the form
\[
p(x) = c \frac{x^{-\frac{n_1}{\alpha}} e^{-\frac{x}{\alpha_1}} (1 + \varepsilon(x))}{\Gamma\left(\frac{\alpha}{2}\right)}
\]
with \( \varepsilon(x) \xrightarrow{x \to \infty} 0 \) and some constant \( c \). Thus
\[
p_{\alpha Y_{\frac{1}{n_1}}}(x) = c x^{-\left(n_1 - \frac{1}{\alpha} + \frac{1}{\alpha_1} \right)} e^{\left(-\frac{x}{\alpha_1} - \frac{x}{\alpha} + \frac{1}{\alpha_1} + \frac{1}{\alpha} \varepsilon(x)\right)} \xrightarrow{x \to \infty} 0
\]
since either \( \alpha_1 < \alpha \), and hence \( \frac{1}{\alpha_1} - \frac{1}{\alpha} > 0 \) implies the limit in (2.4), or \( \alpha_1 = \alpha \) and thus the exponential term is equal to \( 1 \) and \( n_1 - \frac{1}{\alpha} = n_1 - \frac{1}{\alpha} < 0 \) implies the limit in (2.4).

Finally, note that (2.4) implies that the density of \( \sum \alpha_i Z_i^2 \) is dominated by the density of \( \alpha Y_{\frac{1}{\alpha}} \) for sufficiently large values, and thus (2.1) holds. This method proves the existence of \( x_0 \) but it does not provide a bound.

To get a bound for \( x_0 \) one can follow exactly the proof of [25] Theorem 1] with the additional restriction: \( \lambda_i \leq \beta \leq 1 \) for all \( i \) (where the \( \lambda_i \) are the coefficients of the quadratic form in their notation). Their proof is technical, long and uses many auxiliary results. It seems reasonable to omit a replication of the details here. In essence, differential calculus yields
\[
\inf_{0 \leq \alpha_i \leq \beta, \sum \alpha_i = 1} P\left( \sum \alpha_i Z_i^2 \leq x \right) = \min \left\{ \inf_{n \in \mathbb{N}, \frac{1}{n} \leq \beta} P\left( \frac{1}{n} Y_n \leq x \right), P\left( \beta Y_{\frac{1}{n_1}} \right) + (1 - \beta \frac{1}{\alpha_1}) Y_{\frac{1}{\alpha}} \right\},
\]
where $Y_n \sim \chi^2(n)$ and $Y^{(i)}_n \sim \chi^2(r_i)$ for $i = 1, 2$ are independent. Furthermore, let $x_0(\alpha)$ be such that $0 < P(\frac{1}{1+\alpha} Y^{(1)}_n \leq x_0(\alpha)) = P(\frac{1}{1+\alpha} Y^{(2)}_n + 1 \leq x_0(\alpha)) < 1$. Then by [23] Prop. 1', p. 189] the function $\alpha \mapsto x_0(\alpha)$ is increasing on $(0, 1]$, bounded by $x_0(1) \approx 1.536404$ and for all $x \geq x_0(\beta)$
\[
P(\frac{1}{1+\beta} Y^{(2)}_n \leq x) = \inf_{n \in N, 0 \leq \beta} P(\frac{1}{1+\beta} Y_n \leq x).
\]
Finally, it can be verified (numerically; for details and discussion see Section 6.1 in the Appendix), that
\[
\min \{ P(\frac{1}{1+\beta} Y^{(2)}_n \leq x), P(\beta Y^{(1)}_n + (1 - \beta) Y^{(2)}_n \leq x) \} \geq P(\alpha Y_n \leq x)
\]
(2.5)
for all $x \geq x_0(\alpha)$ and all $\beta \leq \alpha$.

On can summarize the available options to estimate the tails of positive Gaussian quadratic forms as follows (here $Y_i \sim \chi^2(r)$ and the random variables $Z_i$ are independent standard normally distributed):
\[
P\left( \sum_{i \in N} \alpha_i Z_i^2 \geq x \right) \begin{cases} 
\leq P(Y_i \geq x) & \text{for } x \geq x_0, \ \sum_{i \in N} \alpha_i = 1, \text{ cf. } 25 \\
\leq P(\alpha Y_i \frac{1}{\alpha} \geq x) & \text{for } x \geq x_0, \ \sum_{i \in N} \alpha_i = 1, \ \alpha_i \leq \alpha, \text{ see Theorem 2.1} \\
\approx P(Y_{\alpha(i, \epsilon)} \geq h(x, (\alpha_i)_{i \in N}) & \text{if } \sum_{i \in N} \alpha_i^k \text{ known for } k = 1, \ldots, 4, \text{ cf. } 15, \text{ i.e., first four moments known, see Lemma 2.3} \\
\approx \text{Series} & \text{if some of the } \alpha_i \text{ are known, e.g., } 13 \text{ 20} \\
\approx \text{Fourier inversion} & \text{if some of the } \alpha_i \text{ are known, e.g., } 8 \text{ 11} \\
\approx \text{explicit} & \text{if all } \alpha_i \text{ are known, e.g., } 27
\end{cases}
\]
(2.6)
Implementations of some of the methods are available in the R package CompQuadForm [9]. Furthermore, quantile asymptotics have also been investigated by Jaschke et al. [12]. For further representations of the distribution we refer to [16] Chapter 4 and the references within.

In Section 5 these estimates will be compared for the Gaussian quadratic forms related to distance multivariate. In the next section the $\alpha_i$ are computed explicitly for the case that the Gaussian quadratic form is the $L^2$-norm of a complex Gaussian random field.

For the approximation by Liu et al. [15] the first four moments of the quadratic form are required. Here the following lemma is useful.

Lemma 2.3 (compare [16] Theorem 3.2b.2]). With the notation from Theorem 2.1 let $Q := \sum_{i \in N} \alpha_i Z_i^2$. Then
\[
\mathbb{E}(Q) = \sum_{i \in N} \alpha_i, \quad \mathbb{E}((Q - \mathbb{E}(Q))^3) = 8 \sum_{i \in N} \alpha_i^3,
\]
\[
\mathbb{V}(Q) = \mathbb{E}((Q - \mathbb{E}(Q))^2) = 2 \sum_{i \in N} \alpha_i^2, \quad \mathbb{E}((Q - \mathbb{E}(Q))^4) = 48 \sum_{i \in N} \alpha_i^4 + 3 \mathbb{V}(Q)^2.
\]

Proof. Since $Z_i \sim N(0, 1)$ implies $Z_i^2 \sim \chi^2(1)$ and thus
\[
\mathbb{E}(Z_i^2) = 1, \quad \mathbb{V}(Z_i^2) = 2, \quad \mathbb{E}((Z_i^2 - \mathbb{E}(Z_i^2))^3) = 8, \quad \mathbb{E}((Z_i^2 - \mathbb{E}(Z_i^2))^4) = 60.
\]
Furthermore $\mathbb{E}(Q) = \sum_{i \in N} \alpha_i$ implies, using independence,
\[
\mathbb{V}(Q) = \mathbb{E}((Q - \mathbb{E}(Q))^2) = \mathbb{E} \left( \left( \sum_{i \in N} \alpha_i (Z_i^2 - 1) \right)^2 \right) = \sum_{i,k \in N} \alpha_i \alpha_k \mathbb{Cov}(Z_i^2, Z_k^2) = \sum_{i \in N} \alpha_i^2 \mathbb{V}(Z_i^2) = 2 \sum_{i \in N} \alpha_i^2.
\]
Analogously, for the third central moment one finds
\[
\mathbb{E}((Q - \mathbb{E}(Q))^3) = \mathbb{E}\left(\left(\sum_{i \in \mathbb{N}} \alpha_i (Z_i^2 - 1)^3\right)\right) = \sum_{i,k,l \in \mathbb{N}} \alpha_i \alpha_k \alpha_l \mathbb{E}((Z_i^2 - 1)(Z_k^2 - 1)(Z_l^2 - 1)) = \sum_{i \in \mathbb{N}} \alpha_i^3 \mathbb{E}((Z_i^2 - 1)^3) = 8 \sum_{i \in \mathbb{N}} \alpha_i^3.
\]

Finally, for the fourth central moment we find
\[
\mathbb{E}((Q - \mathbb{E}(Q))^4) = \mathbb{E}\left(\left(\sum_{i \in \mathbb{N}} \alpha_i (Z_i^2 - 1)^4\right)\right) = \sum_{i \in \mathbb{N}} \alpha_i^4 \mathbb{E}((Z_i^2 - 1)^4) + 3 \sum_{i \in \mathbb{N}} \sum_{k \neq i} \alpha_i^2 \alpha_k^2 \mathbb{E}((Z_i^2 - 1)^2) \mathbb{E}((Z_k^2 - 1)^2)
\]
\[
= 60 \sum_{i \in \mathbb{N}} \alpha_i^4 + 12 \sum_{i \in \mathbb{N}} \sum_{k \neq i} \alpha_i^2 \alpha_k^2 = 48 \sum_{i \in \mathbb{N}} \alpha_i^4 + 12 \sum_{i,k \in \mathbb{N}} \alpha_i^2 \alpha_k^2
\]
\[
= 48 \sum_{i \in \mathbb{N}} \alpha_i^4 + 3V(Q)^2.
\]

\[
\square
\]

3 Complex Gaussian random fields

This section is devoted to establishing a connection between complex Gaussian random fields and positive Gaussian quadratic forms. Main tools will be a Mercer representation of the covariance kernel and an associated Karhunen-Loève type expansion of the random field. Results linking moments of quadratic Gaussian quadratic forms and sample distance multivariance.

\[
\text{Proposition 3.1 (see, e.g., [21, Chapter 2]). Let } \mathbb{G} \text{ be a complex second-order random field with mean } \mu, \text{ covariance kernel } K \text{ and pseudo-covariance kernel } C \text{.}
\]

1. The covariance kernel is positive definite, i.e., for all choices of finitely many points \( t_1, \ldots, t_m \in \mathbb{R}^d \) and coefficients \( c_1, \ldots, c_m \in \mathbb{C} \)
\[
\sum_{i,j=1}^m c_i \overline{c_j} K(t_i, t_j) = \mathbb{E}\left(\left|\sum_{i=1}^m c_i (\mathbb{G}(t_i) - \mu(t_i))\right|^2\right) \geq 0.
\]

This implies that \( K \) is hermitian, i.e., \( K(s,t) = \overline{K(t,s)} \).

The pseudo-covariance kernel is symmetric, i.e., \( C(s,t) = C(t,s) \).
2. If \( \mu \equiv 0 \), and \( G(t) = \overline{G(t)} \) (or the weaker requirement \( K(s, t) = C(s, -t) \) for all \( s, t \in \mathbb{R}^d \)) then the field is a hermitian, centered complex second-order field. Note that in this case
\[
K(s, t) = C(s, -t) = C(-t, s) = K(-t, -s) = K(-s, -t), \quad s, t \in \mathbb{R}^d.
\]

3. If \( G \) is a strongly continuous second-order random field, i.e., for all \( t_0 \in \mathbb{R}^d \),
\[
\lim_{t \to t_0} \mathbb{E}(|G(t) - G(t_0)|^2) = 0,
\]
the functions \( \mu, K, \) and \( C \) are continuous.

In order to link random fields to quadratic forms discussed in Section 2 we assume \( \rho \) to be a non-negative, symmetric, \( \sigma \)-finite Borel measure on \( \mathbb{R}^d \). For notational simplicity we write \( L^2(\rho) := L^2(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d), \rho) \), denote the inner product in \( L^2(\rho) \) by
\[
\langle u, v \rangle = \langle u, v \rangle_\rho := \int_{\mathbb{R}^d} u(t) \overline{v(t)} \rho(dt),
\]
and the norm by \( \|u\|_\rho = \sqrt{\langle u, u \rangle_\rho} \), for all \( u, v \in L^2(\rho) \).

All statements in this section are made under the following assumptions.

**Assumption 3.2.** Let \( d \in \mathbb{N} \) and \( G : \mathbb{R}^d \to L^2(\Omega, \mathcal{A}, \mathbb{P}) \) be a hermitian, centered, strongly continuous complex second-order random field. Denote by \( K \) its covariance kernel and let \( \rho \) be a non-negative, symmetric, \( \sigma \)-finite Borel measure satisfying
\[
\int_{\mathbb{R}^d} K(t, t) \rho(dt) < \infty. \tag{3.1}
\]

Note that in the statements of the results, below, all necessary assumptions will be repeated. Moreover we want to point out that in fact all results do hold under the weaker requirement of measurability instead of strong continuity.

Positive-definiteness of the covariance kernel \( K \) implies \( |K(s, t)|^2 \leq K(s, s) K(t, t) \). Therefore, the integrability condition (3.1) directly gives
\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} |K(s, t)|^2 (\rho \otimes \rho)(ds, dt) \leq \left( \int_{\mathbb{R}^d} K(t, t) \rho(dt) \right)^2 < \infty,
\]
making
\[
T_K : L^2(\rho) \to L^2(\rho), \quad u \mapsto \int_{\mathbb{R}^d} K(\cdot, t) u(t) \rho(dt), \tag{3.2}
\]
a well-defined, positive, compact and self-adjoint operator on \( L^2(\rho) \). Using Mercer’s theorem (see, e.g., [24]), there exists an index set \( I \subseteq \mathbb{N} \), a monotonically decreasing sequence \( (\alpha_i)_{i \in I} \) of positive – not necessarily distinct – real numbers and an orthonormal system \( (e_i)_{i \in I} \) in \( L^2(\rho) \) such that
\[
T_K e_i = \alpha_i e_i, \quad i \in I, \quad \text{Range } T_K = \text{span}\{e_i : i \in I\},
\]
and Mercer’s representation holds:
\[
K(s, t) = \sum_{i \in I} \alpha_i e_i(s) \overline{e_i(t)}, \quad s, t \in \mathbb{R}^d, \tag{3.3}
\]
where the convergence is absolute and uniform on compact subsets. Under the integrability condition (3.1),
\[
\sum_{i \in I} \alpha_i = \sum_{i \in I} \alpha_i \int_{\mathbb{R}^d} e_i(t) \overline{e_i(t)} \rho(dt) = \int_{\mathbb{R}^d} K(t, t) \rho(dt) < \infty,
\]
which implies that \( T_K \) is a nuclear – or trace-class – operator (see, e.g., [19]).

Define \( e_i^*(t) := e_i(-t), \; t \in \mathbb{R}^d, \; i \in I \). Symmetry of \( \rho \) and hermiticity of \( G \) allow to deduce that with \( (e_i)_{i \in I} \) also \( (e_i^*)_{i \in I} \) is an orthonormal system of Range \( T_K \). In particular, we find
\[
T_K e_i^* = \alpha_i e_i^*, \quad i \in I.
\]
Remark 3.3. In the situation of matching product structures of the measure \( \rho \) and the kernel \( K \), i.e., \( \rho = \bigotimes_{j=1}^n \rho_j \) and \( K(s,t) = \prod_{j=1}^n K_j(s_j,t_j) \) on \( \mathbb{R}^d = \mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_n} \), the eigenvalues and eigenvectors of the operator \( T_K \) arise as products of the eigenvalues and eigenvectors of the operators \( T_{K_j} \), \( 1 \leq j \leq n \), respectively. In fact, from the orthogonal eigensystems \( (e_i^{(j)})_{i \in I_j} \) of \( T_{K_j} \) in \( L^2(\rho_j) \) associated to the eigenvalues \( \alpha_i^{(j)} > 0 \), \( i \in I_j \), \( 1 \leq j \leq n \), we obtain by setting for each multi-index \( i \in I_1 \times \cdots \times I_n \)

\[
\alpha_i = \prod_{j=1}^n \alpha_{i_j}^{(j)}, \quad e_i(t) = \prod_{j=1}^n e_{i_j}^{(j)}(t_j), \quad t = (t_j)_{j=1,...,n} \in \mathbb{R}^d,
\]

an orthonormal eigensystem \( (e_i)_{i \in I_1 \times \cdots \times I_n} \) of \( T_K \) associated to the eigenvalues \( \alpha_i > 0 \), \( i \in I_1 \times \cdots \times I_n \).

A first direct consequence of Mercer’s representation is summarized in the following lemma which gives a generalization of the Karhunen–Loève decomposition and is typically only stated for compact domains, see, e.g., [21, Theorem 2.5.5].

Lemma 3.4. Let \( \mathcal{G} \) be a hermitian, centered, strongly continuous second-order random field such that its covariance kernel \( K \) satisfies (3.1). Let \( I \subseteq \mathbb{N} \) and \( (e_i)_{i \in I} \) be as in Mercer’s representation (3.3) of \( K \). Then \( \mathcal{G} \in L^2(\rho) \) almost surely,

\[
\mathcal{G} = \sum_{i \in I} (\langle \mathcal{G}, e_i \rangle) e_i \quad \text{P-a.s. in } L^2(\rho),
\]

and \( \langle \mathcal{G}, e_i \rangle \), \( i \in I \), are mutually uncorrelated, centered, complex-valued random variables.

Proof. We know from Mercer’s representation (3.3) that \( (e_i)_{i \in I} \) is an orthonormal basis of Range \( T_K \). Thus, for the representation (3.4) to hold it remains to show that \( \mathcal{G} \) is almost surely contained in Range \( T_K \subseteq L^2(\rho) \). Tonelli’s theorem allows to deduce from (3.1)

\[
\mathbb{E}\left( \left\| \mathcal{G}_\rho \right\|_2 \right) = \mathbb{E}\left( \int_{\mathbb{R}^d} |\mathcal{G}(t)|^2 \rho(dt) \right) = \int_{\mathbb{R}^d} \mathbb{E}(|\mathcal{G}(t)|^2) \rho(dt) = \int_{\mathbb{R}^d} \mathbb{E}(K(t,t)) \rho(dt) < \infty,
\]

i.e., \( \mathcal{G} \in L^2(\rho) \). To show that \( \mathcal{G} \in \text{Range} \ T_K \), we choose \( u \in \ker \ T_K \). Applying Fubini’s theorem we find

\[
\mathbb{E}\left( \left\| \langle \mathcal{G}, u \rangle \right\|^2 \right) = \mathbb{E}\left( \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathcal{G}(s)u(s) \cdot \overline{\mathcal{G}(t)u(t)} \rho(ds) \rho(dt) \right)
\]

\[
= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathbb{E}\left( \mathcal{G}(s) \overline{\mathcal{G}(t)} \right) |u(t)\rho(dt)u(s)\rho(ds) = \langle T_K u, u \rangle = 0.
\]

Since \( u \in \ker \ T_K \) was arbitrary, this implies \( \mathcal{G} \in \text{Range} \ T_K \). Using that \( (e_i)_{i \in I} \) is an orthonormal basis of Range \( T_K \) the representation (3.4) follows. Finally, since \( \mathcal{G} \) is centered, \( \mathbb{E}(\langle \mathcal{G}, e_i \rangle) = 0 \), \( i \in I \). \[\Box\]

Note that in the above lemma no distributional assumption on the random field has been made. Adding Gaussianity allows to strengthen the statement of Lemma 3.4 in the sense that the random variables \( (\langle \mathcal{G}, e_i \rangle) \) are independent and complex normally distributed, see Corollary 3.8. In order to proceed, we recall the definition of the complex normal distribution.

Definition 3.5. A random vector \( Z \) with values in \( \mathbb{C}^n \) is complex normally distributed with expectation vector \( \mu := \mathbb{E}(Z) \), covariance matrix \( \Gamma := \mathbb{E}((Z-\mu)(Z-\mu)^*) \) and pseudo-covariance matrix \( C := \mathbb{E}((Z-\mu)(Z-\mu)^T) \) - in short \( Z \sim C \mathcal{N}_n(\mu, \Gamma, C) \) if

\[
\begin{pmatrix}
\text{Re} \ Z \\
\text{Im} \ Z
\end{pmatrix}
\sim
C\mathcal{N}_n
\begin{pmatrix}
\text{Re} \ \mu \\
\text{Im} \ \mu
\end{pmatrix}
\begin{pmatrix}
\frac{1}{2} \left( \text{Re}(\Gamma + C) & \text{Im}(\Gamma + C) \right) \\
\text{Im}(\Gamma + C) & \text{Re}(\Gamma + C)
\end{pmatrix}
\]
Remarks 3.6. 1. For the complex case the knowledge of both the covariance and pseudo-covariance is needed: starting from \( Z \sim CN_1(0, \gamma, c) \) with \( \gamma, c \in \mathbb{R}, c \neq 0 \), we find that \( \text{Re } Z \) and \( \text{Im } Z \) are independent random variables. Choosing \( \vartheta \in \mathbb{R} \) such that \( \sin 2\vartheta \neq 0 \), the new complex random variable \( Z' := e^{i\vartheta}Z \) has the same (co)variance \( \gamma \) as \( Z \) but

\[
\text{Cov}(\text{Re } Z', \text{Im } Z') = \frac{c}{2} \sin 2\vartheta \neq 0,
\]

i.e., \( Z' \) has dependent real and imaginary parts. In fact, \( Z' \sim CN_1(0, \gamma, e^{2i\vartheta}c) \).

2. Instead of using the three-parameter family \((\mu, \Gamma, C)\) one can also use the two-parameter family of the associated multivariate normal distribution in (3.5) to characterize complex normal distributions.

3. Beware that some authors (e.g., [23]) require the pseudo-covariance to vanish in the definition of the complex normal distribution and, similarly, complex Gaussian random fields are required to have pseudo-covariance kernel \( C \equiv 0 \) (e.g., [17]). Depending on the context such random fields are called proper [22] or circular [18].

However, in this article the general definition of complex normal distribution and complex Gaussian random field is employed.

Since the complex normal distribution is defined via multivariate normal distributions, the following properties of complex Gaussian random fields directly follow from the properties of real Gaussian fields, see Proposition 3.1.

Proposition 3.7. 1. A complex Gaussian random field \( G \) is uniquely determined by its mean function \( \mu \), covariance kernel \( K \) and pseudo-covariance kernel \( C \).

2. For a complex Gaussian vector \((X, Y)\) it holds that \( X \) and \( Y \) are independent if and only if \( X \) and \( Y \) are uncorrelated, i.e., if the covariance and the pseudo-covariance are zero.

3. Values of linear functionals of complex Gaussian random fields are (scalar) complex normally distributed random variables.

Since uncorrelatedness of (jointly) Gaussian random variables implies independence we can strengthen the statement of Lemma 3.4 under the assumption of Gaussianity.

Corollary 3.8. Let \( G \) be a hermitian, centered, strongly continuous complex Gaussian random field such that its covariance kernel \( K \) satisfies (3.1). Let \( I \subseteq \mathbb{N} \) and \((e_i)_{i \in I}\) be as in Mercer’s representation (3.3) of \( K \). Then \( G \in L^2(\rho) \) almost surely,

\[
G = \sum_{i \in I} \langle G, e_i \rangle e_i \quad \text{P-a.s. in } L^2(\rho), \tag{3.6}
\]

and \( \langle G, e_i \rangle \) are independent, centered, complex normally distributed random variables.

Proof. In Lemma 3.4 we already obtained the representation (3.6) and uncorrelatedness of \( \langle G, e_i \rangle, i \in I \). As values of linear functionals of a complex Gaussian random field, the \( \langle G, e_i \rangle \) are uncorrelated, jointly complex normally distributed random variables and, therefore, independent.

Although in the above representation (3.6) the random variables \( \langle G, e_i \rangle, i \in I \), are independent, we have – in general – no information on the (in)dependence of \( \text{Re } \langle G, e_i \rangle \) and \( \text{Im } \langle G, e_j \rangle, i, j \in I \), as the following observations show: for the covariance we find using Fubini’s theorem\(^3\)

\[
\text{Cov}(\langle G, e_i \rangle, \langle G, e_j \rangle) = E\left( \langle G, e_i \rangle \cdot \langle G, e_j \rangle \right) = E\left( \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} G(s)G(t) e_i(s) \cdot \overline{e_j(t)} \rho(ds)\rho(dt) \right)
\]

\[
= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} E\left( G(s)\overline{G(t)} \right) e_i(t) e_j(s) \rho(ds)\rho(dt)
\]

\[
= \langle T_K e_j, e_i \rangle = \alpha_j \delta_{i,j}, \quad \text{as } |G|^2 \infty.
\]

\(^3E\left( \int_{\mathbb{R}^d} |G(s)\overline{G(t)}| \rho(ds)\rho(dt) \right) \leq E\left( |G|^2 \right) < \infty
\]
where \( \delta_{i,j} \) denotes the Kronecker symbol. Analogously for the pseudo-covariance we obtain

\[
\mathbb{E}(\langle \mathcal{G}, e_i \rangle \cdot \langle \mathcal{G}, e_j \rangle) = \mathbb{E}\left( \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} G(s) \bar{G}(t) \rho(ds) \rho(dt) \right)
\]

\[
= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathbb{E}(G(s)G(t)) \bar{e}_j(t) \bar{e}_i(s) \rho(ds) \rho(dt)
\]

\[
= \int_{\mathbb{R}^d} K(s, t) \bar{e}_j(t) \bar{e}_i(s) \rho(ds) \rho(dt)
\]

\[
= \langle T_K e_j^*, e_i \rangle = \alpha_j \langle e_j^*, e_i \rangle, \quad (3.8)
\]

where \( e_j^*(t) = \bar{e}_j(-t) \). This implies

\[
\text{Cov}(\text{Re} \langle \mathcal{G}, e_i \rangle, \text{Im} \langle \mathcal{G}, e_i \rangle) = \frac{\alpha_i}{2} \text{Im} \langle e_i^*, e_i \rangle, \quad i \in I.
\]

Nevertheless the above representation (3.6) allows us to show our main result of this section, linking Gaussian random fields to Gaussian quadratic forms. Although the theorem can be deduced from results for Gaussian measures in infinite-dimensional spaces (see, e.g., [13 Comments on Section 1.2]) our proof is direct and relies on the already established Karhunen-Loève decomposition of the Gaussian random field given in Lemma 3.4.

**Theorem 3.9.** Let \( \mathcal{G} \) be a Hermitian, centered, strongly continuous complex Gaussian random field such that its covariance kernel \( K \) satisfies (3.1). Let \( I \subseteq \mathbb{N} \) and \((\alpha_i)_{i \in I}\) be as in Mercer’s representation (3.3) of \( K \). Then

\[
\|\mathcal{G}\|_p^2 = \sum_{i \in I} \alpha_i Z_i^2 \quad \text{P-a.s.,}
\]

where \((Z_i)_{i \in I}\) is a sequence of independent, standard normally distributed random variables.

**Proof.** Since \( T_K \) is compact, all eigenspaces to non-vanishing eigenvalues are finite-dimensional. Let \((\beta_i)_{i \in I'}\) be the mutually different positive eigenvalues of \( T_K \), i.e., \( \{\beta_i : i \in I'\} = \{\alpha_i : i \in I\} \) with \( \beta_i \neq \beta_j \) for \( i \neq j \) and \( I' \subseteq I \). Set \( J_i := \{k \in I : \alpha_k = \beta_i, i \in I'\} \). Thus the number of elements in \( J_i \) is the multiplicity of the eigenvalue \( \beta_i \) and the \( J_i \) are finite, mutually disjoint sets and from Corollary 3.8 we directly obtain the representation

\[
\|\mathcal{G}\|_p^2 = \sum_{i \in I} |\langle \mathcal{G}, e_i \rangle|^2 = \sum_{i \in I'} \sum_{k \in J_i} |\langle \mathcal{G}, e_k \rangle|^2 = \sum_{i \in I'} \sum_{k \in J_i} \left( |\langle \text{Re} \langle \mathcal{G}, e_k \rangle \rangle|^2 + |\langle \text{Im} \langle \mathcal{G}, e_k \rangle \rangle|^2 \right).
\]

Consider the \( \mathbb{R}^{|J_i|} \)-valued random vectors

\[
U_i = \frac{1}{\sqrt{|J_i|}} \langle \text{Re} \langle \mathcal{G}, e_k \rangle \rangle_{k \in J_i}, \quad V_i = \frac{1}{\sqrt{|J_i|}} \langle \text{Im} \langle \mathcal{G}, e_k \rangle \rangle_{k \in J_i}, \quad i \in I',
\]

collecting all \( e_k \) belonging to the eigenspace associated with \( \beta_i \). Since \( T_K \) is self-adjoint, all eigenspaces are mutually orthogonal. Therefore our considerations on the covariance (3.7) and on the pseudo-covariance (3.8) yield

\[
\text{Cov}(U_i, U_j) = \text{Cov}(U_i, V_j) = \text{Cov}(V_i, V_j) = 0, \quad i \neq j,
\]

and the covariance matrix \( \Sigma \) of the random vector \((U_i, V_i)^T\) has the symmetric block structure

\[
\Sigma = \frac{1}{2} \begin{pmatrix}
I_{|J_i|} + \langle \text{Re} \langle e_k^*, e_j \rangle \rangle_{j,k \in J_i} & \langle \text{Im} \langle e_k^*, e_j \rangle \rangle_{j,k \in J_i} \\
\langle \text{Im} \langle e_k^*, e_j \rangle \rangle_{j,k \in J_i} & I_{|J_i|} - \langle \text{Re} \langle e_k^*, e_j \rangle \rangle_{j,k \in J_i} - \langle \text{Im} \langle e_k^*, e_j \rangle \rangle_{j,k \in J_i}
\end{pmatrix}
\]

\[
=: \frac{1}{2} (I_{|J_i|} + B),
\]

where \( I_M \) denotes the identity matrix in \( \mathbb{R}^{M \times M} \) and

\[
B = \begin{pmatrix}
B_{\text{Re}} & B_{\text{Im}} \\
B_{\text{Im}} & -B_{\text{Re}}
\end{pmatrix}, \quad B_{\text{Re}} = \langle \text{Re} \langle e_k^*, e_j \rangle \rangle_{j,k \in J_i}, \quad B_{\text{Im}} = \langle \text{Im} \langle e_k^*, e_j \rangle \rangle_{j,k \in J_i}.
\]
We show that $B^2 = I_{2|J_i|}$, which yields $\Sigma^2 = \frac{1}{2}(I_{2|J_i|} + 2B + B^2) = \Sigma$. Using symmetry of $B$ we find

$$B^2 = \begin{pmatrix}
B_{\text{Re}}^2 + B_{\text{Im}}^2 & B_{\text{Re}}B_{\text{Im}} - B_{\text{Im}}B_{\text{Re}} \\
B_{\text{Im}}B_{\text{Re}} - B_{\text{Re}}B_{\text{Im}} & B_{\text{Re}}^2 + B_{\text{Im}}^2
\end{pmatrix} = B^2 = \begin{pmatrix}
B_{\text{Re}}^2 + B_{\text{Im}}^2 & 0 \\
0 & B_{\text{Re}}^2 + B_{\text{Im}}^2
\end{pmatrix}.$$  

Using the elementary equation $\text{Re} \ z \text{ Re} w + \text{Im} \ z \text{ Im} w = \text{Re} \ z \overline{w}$ we can compute for the block entries on the diagonal

$$(B_{\text{Re}}^2 + B_{\text{Im}}^2)_{j,k} = \sum_{m \in J_i} (\text{Re} <e_m^*, e_j> \text{ Re} <e_k^*, e_m> + \text{Im} <e_m^*, e_j> \text{ Im} <e_k^*, e_m>)$$

$$= \text{Re} \sum_{m \in J_i} <e_m^*, e_j>(e_m^*, e_k^*) = \text{Re} \left( \sum_{m \in J_i} (e_m^*, e_k^*)e_m^*, e_j) \right).$$

Symmetry of $\rho$ yields $<e_m^*, e_k^*> = <e_k^*, e_m^*>$ and since $(e_m^*)_{m \in J_i}$ is an orthonormal basis of the associated eigenspace we find

$$\sum_{m \in J_i} (e_k^*, e_m^*) e_m^* = e_k,$$

which implies

$$(B_{\text{Re}}^2 + B_{\text{Im}}^2)_{j,k} = \text{Re} <e_k^*, e_j> = \delta_{j,k}, \quad j, k \in J_i.$$  

As idempotent and positive semi-definite matrix, $\Sigma$ can have only the eigenvalues 0 and 1. Hence there exists an orthogonal matrix $R$ and a diagonal matrix $D = (d_{j,k})_{j,k=1,\ldots,2|J_i|} \in \{0, 1\}^{2|J_i| \times 2|J_i|}$ such that

$$D = R^T \Sigma R, \quad \text{trace } D = \sum_{\ell=1}^{2|J_i|} d_{\ell,\ell} = \text{trace } \Sigma = |J_i|.$$  

Setting

$$(W_\ell)_{\ell=1,\ldots,2|J_i|} = R^T \begin{pmatrix} U_i \\ V_i \end{pmatrix},$$

we find

$$\sum_{k \in J_i} \left[ (\text{Re} <G, e_k>)^2 + (\text{Im} <G, e_k>)^2 \right] = \beta_1 \|U_i\|^2 + \|V_i\|^2 = \beta_1 \sum_{\ell=1}^{2|J_i|} W_\ell^2$$  

(3.10)

and $W_1, \ldots, W_{2|J_i|}$ are mutually uncorrelated, centered random variables with variances $\mathbb{V}(W_\ell) = d_{\ell,\ell}$, $1 \leq \ell \leq 2|J_i|$, respectively. From the trace condition it is apparent that exactly $|J_i|$ of the variances are non-zero. By relabeling we can assume that $W_1, \ldots, W_{|J_i|}$ have unit variance. Using an enumeration $\{k_1, \ldots, k_{|J_i|}\}$ of $J_i$ and setting $Z_{k_\ell} := W_{k_\ell}, 1 \leq \ell \leq |J_i|$, we find by plugging (3.10) into (3.9) and rearranging the summation

$$\|G\|_\rho^2 = \sum_{i \in I'} \sum_{k \in J_i} \left[ (\text{Re} <G, e_k>)^2 + (\text{Im} <G, e_k>)^2 \right] = \sum_{i \in I'} \sum_{\ell=1}^{2|J_i|} \beta_1 W_\ell^2$$

$$= \sum_{i \in I'} \beta_1 \sum_{k \in J_i} Z_k^2 = \sum_{i \in I'} \sum_{k \in J_i} \alpha_k Z_k^2 = \sum_{i \in I} \alpha_i Z_i^2.$$  

Since the uncorrelated random variables $W_\ell$ – and thus $Z_i$ – arise as linear transformation of the Gaussian random vector $(U_i, V_i)^T$, they are (jointly) standard normally distributed, and hence independent. 

**Remark 3.10.** All positive Gaussian quadratic forms (with summable coefficients) arise as in Theorem 3.9, i.e., as squared norm of a Gaussian random field: in fact, let $Q = \sum_{i \in \mathbb{N}} \alpha_i Z_i^2$ be a Gaussian quadratic form with $\alpha_i \geq 0, \ i \in \mathbb{N}$, and $\sum_{i \in \mathbb{N}} \alpha_i < \infty$. Let $\rho$ be a nonnegative, symmetric, $\sigma$-finite
Borel measure on $\mathbb{R}^d$ and $(g_i)_{i \in \mathbb{N}}$ be an orthonormal sequence of continuous functions in $L^2(\rho)$ such that $g_i(-t) = g_i(t)$, $t \in \mathbb{R}^d$. Then

$$G(t) = \sum_{i \in \mathbb{N}} \sqrt{\alpha_i} g_i(t) Z_i, \quad t \in \mathbb{R}^d,$$

defines a centered, strongly continuous Gaussian random field $G$ and we find

$$\|G\|^2_\rho = \int_{\mathbb{R}} |G(t)|^2 \rho(dt) = \sum_{i,j \in \mathbb{N}} \sqrt{\alpha_i} \sqrt{\alpha_j} Z_i Z_j \langle g_i, g_j \rangle_\rho = \sum_{i \in \mathbb{N}} \alpha_i Z_i^2 = Q.$$

Note that in this construction, neither $\rho$ nor $(g_i)_{i \in \mathbb{N}}$ are uniquely determined.

The last result of this section gives a representation of the moments of the above Gaussian quadratic form (as studied in Lemma 2.3) in terms of the covariance kernel $K$ of the random field $G$. To this end, we denote for the sequence $(\alpha_i)_{i \in \mathbb{N}}$ from Mercer’s representation \((3.3)\) and $k \in \mathbb{N}$

$$\mu^{(k)} = \mu^{(k)}((\alpha_i)_{i \in \mathbb{N}}) := \sum_{i \in \mathbb{N}} \alpha_i^k. \quad (3.11)$$

Using standard operator theory it is obvious that $\alpha_i^k$, $i \in I$, are the (positive) eigenvalues of the operator $T_K^k$ and that $T_K^k$ is an integral operator with kernel given by iterated integration of $K$. In particular, we find the following representation:

**Lemma 3.11.** Let $K$ be the covariance kernel of a strongly continuous, second-order random field satisfying \((3.1)\). For $k \in \mathbb{N}$ and $u \in L^2(\rho)$

$$(T_K^k u)(s) = \int_{(\mathbb{R}^d)^k} K(s, t^{(k)}) \prod_{j=1}^{k-1} K(t^{(k+1-j)}, t^{(k-j)}) u(t^{(1)})\rho^{\otimes k}(dt^{(1)}, \ldots, dt^{(k)}), \quad s \in \mathbb{R}^d.$$

**Proof.** We proceed by induction on $k$. The statement for $k = 1$ reduces to the definition of $T_K$ and there is nothing to show. Assume the assertion is valid for some $k \in \mathbb{N}$. Then we find for $u \in L^2(\rho)$ and $s \in \mathbb{R}^d$

$$(T_K^{k+1} u)(s) = T_K (T_K^k u)(s) = \int_{(\mathbb{R}^d)^k} K(s, t^{(k+1)}) (T_K^k u)(t^{(k+1)}) \rho(dt^{(k+1)})$$

$$= \int_{\mathbb{R}^d} K(s, t^{(k+1)}) \int_{(\mathbb{R}^d)^k} K(t^{(k+1)}, t^{(k)}) \prod_{j=1}^{k-1} K(t^{(k+1-j)}, t^{(k-j)}) 
\cdot u(t^{(1)}) \rho^{\otimes k}(dt^{(1)}, \ldots, dt^{(k)})(dt^{(k+1)})$$

$$= \int_{(\mathbb{R}^d)^{k+1}} K(s, t^{(k+1)}) \prod_{j=1}^k K(t^{(k+2-j)}, t^{(k+1-j)}) u(t^{(1)}) \rho^{\otimes (k+1)}(dt^{(1)}, \ldots, dt^{(k+1)}),$$

where the induction assumption was used in step (*). Hence, the assertion for $k + 1$ is proven. \hfill $\square$

This representation allows us to connect the moments of the quadratic form $\|G\|^2_\rho$ with the covariance kernel $K$.

**Proposition 3.12.** Let $K$ be the covariance kernel of a hermitian, centered, strongly continuous second-order random field satisfying \((3.1)\). Let $I \subseteq \mathbb{N}$ and $(\alpha_i)_{i \in I}$ be as in Mercer’s representation \((3.3)\) of $K$. Then for $k \in \mathbb{N}$

$$\mu^{(k)} = \sum_{i \in I} \alpha_i^k = \int_{(\mathbb{R}^d)^k} \prod_{j=1}^{k-1} K(t^{(k-j+1)}, t^{(k-j)}) \cdot K(t^{(1)}, t^{(k)}) \rho^{\otimes k}(dt^{(1)}, \ldots, dt^{(k)}). \quad (3.12)$$
Remark 3.13. Since for the applications in Proof. Gaussian quadratic forms and sample distance multivariance
\[ \mu(t^{(1)}, t^{(1)}) = \int_{\mathbb{R}^d} K(t^{(1)}, t^{(1)}) \rho(dt^{(1)}). \]
Now assume \( k > 1 \). We obtain
\[ \mu^{(k)} = \sum_{i \in I} \alpha_i \int_{\mathbb{R}^d} K(t^{(k)}, t^{(k)}) \prod_{j=1}^{k-2} K(t^{(k-j)}, t^{(k-1-j)}) \cdot e_i(t^{(1)}) \cdot e_i(t^{(1)}) \rho^{\otimes(k-1)}(dt^{(1)}, \ldots, dt^{(k-1)}) \rho(dt^{(k)}) \]
where we have used Lemma 3.11 in step (\( * \)) and Mercer’s representation (3.3) in the penultimate line. \( \square \)

Remark 3.13. Since for the applications in (2.6) and in the upcoming Section 4 the representations of \( \mu^{(1)}, \ldots, \mu^{(4)} \) are of special interest, we rephrase \([3.12]\) in a more accessible form:
\[ \mu^{(1)} = \int K(t, t) \rho(dt), \]
\[ \mu^{(2)} = \int \int K(s, t) K(t, s) \rho(dt) \rho(ds), \]
\[ \mu^{(3)} = \int \int \int K(s, t) K(t, r) K(r, s) \rho(dt) \rho(ds) \rho(dr), \]
\[ \mu^{(4)} = \int \int \int \int K(s, t) K(t, r) K(r, u) K(u, s) \rho(dt) \rho(ds) \rho(dr) \rho(dr). \]

4 Sample distance multivariance

The basic setting for the detection of (in)dependence using distance multivariance is as follows, cf. \([4, 7]\).

Let \( X_i, 1 \leq i \leq n \), be random variables with values in \( \mathbb{R}^{d_i} \) and set \( X := (X_1, \ldots, X_n) \). Independent copies of \( X \) are denoted by \( X^{(i)} \) for \( 1 \leq i \leq N \). Samples of \( X \) are denoted by small \( x \), e.g., \( X^{(i)} = (x_1^{(i)}, \ldots, x_n^{(i)}) \) is a sample of \( X^{(i)} \).

Let \( \rho_i \) be symmetric measures on \( \mathbb{R}^{d_i} \) such that \( \int 1 \wedge |t_i|^2 \rho_i(dt_i) < \infty \) and \( \rho_S := \otimes_{i \in S} \rho_i \) for \( S \subseteq \{1, \ldots, n\} \). Moreover, \( \rho := \rho_{\{1, \ldots, n\}} \) and for \( t = (t_1, \ldots, t_n) \in \mathbb{R}^{\sum_{i=1}^n d_i} \) set \( t_S := (t_i)_{i \in S} \). The \( L^2 \)-norm with respect to \( \rho_S \) is denoted by \( \| \cdot \|_{\rho_S} \), e.g., \( \| g \|_{\rho_S} = \sqrt{\int |g(t_S)|^2 \rho(dt_S)} \). The characteristic function of \( X_i \) is denoted by \( f_i(t_i) := f_{X_i}(t_i) := \mathbb{E}(e^{itX_i}) \).

Then the distance multivariance \( M_{\rho_S} \) of \( X_1, \ldots, X_n \) is defined by
\[ M_{\rho_S}(X_1, \ldots, X_n) := \| Z_S \|_{\rho_S} \quad (4.1) \]
with \( Z_S(t_S) := Z_S(X_1, \ldots, X_n; t_S) := \mathbb{E} \left( \prod_{i \in S} (e^{iX_i t_i} - f_{X_i}(t_i)) \right) \quad (4.2) \)
and sample distance multivariance $^sM_{\rho_S}$ of $x^{(1)}, \ldots, x^{(N)}$ is defined by

$$^sM_{\rho_S}(x^{(1)}, \ldots, x^{(N)}) := \|^{s}Z_S\|_{\rho_S}$$  \hspace{1cm} (4.3)

with $^{s}Z_S(t_S) := ^sZ_S(x^{(1)}, \ldots, x^{(N)}; t_S) := \frac{1}{N} \sum_{t=1}^{N} \prod_{i \in S} \left( e^{ix_i(t_i)} - 1 - \frac{1}{N} \sum_{k=1}^{N} e^{ix_i^{(k)}(t_i)} \right)$.  \hspace{1cm} (4.4)

Note that the latter definition is different but equivalent to the definition given in [7] Eq. (4.1)], cf. [7] Eq. (4.2)]. Using (4.4) as definition makes it obvious that it is the natural choice of an empirical approximation to (4.2). For a proof of the convergence of this estimator see [7] Thm. 4.6]. Also note that the notation is slightly different to [7], since here we always write $(X_1, \ldots, X_n)$ although $S$ might be a proper subset of $\{1, \ldots, n\}$. This helps to keep the notation for total multivariance and $m$-multivariance and their estimators unified. Based on the above define

**total (distance) multivariance**: $\mathcal{M}_\rho(X_1, \ldots, X_n) := \sum_{2 \leq |S| \leq n \atop S \subseteq \{1, \ldots, n\}} M_{\rho_S}(X_1, \ldots, X_n)$,  \hspace{1cm} (4.5)

**$m$-(distance) multivariance**: $M_{m,\rho}(X_1, \ldots, X_n) := \sum_{|S| = m \atop S \subseteq \{1, \ldots, n\}} M_{\rho_S}(X_1, \ldots, X_n)$  \hspace{1cm} (4.6)

for $m \in \{2, \ldots, n\}$. The next result is fundamental to the theory of distance multivariance.

**Theorem 4.1** ([7] Theorem 3.4 and [4] Equation (5.2))). For random variables $X_1, \ldots, X_n$ the following characterizations of their (in)dependence hold

$$\mathcal{M}_\rho(X_1, \ldots, X_n) = 0 \iff X_i \text{ are independent},$$

$$M_{\rho}(X_1, \ldots, X_n) = 0 \text{ and } X_i \text{ are } (n-1)\text{-independent} \iff X_i \text{ are independent},$$

$$M_{m,\rho}(X_1, \ldots, X_n) = 0 \text{ and } X_i \text{ are } (m-1)\text{-independent} \iff X_i \text{ are } m\text{-independent},$$

where the random variables are called $k$-independent if any subfamily of $\{X_1, \ldots, X_n\}$ with $k$ elements is independent.

Thus distance multivariance can be used to characterize (in)dependence. Now, the beauty (practical utility) of this approach stems from the fact that for a sample $x^{(1)}, \ldots, x^{(N)}$ of $X$ the sample distance multivariance has the following computationally feasible representation

$$^sM_{\rho_S}^2(x^{(1)}, \ldots, x^{(N)}) = \frac{1}{N^2} \sum_{j,k=1}^{N} \prod_{i \in S} (A_i)_{j,k}$$

with $A_i := -CB_iC$, $C := I - \frac{1}{N}1_1$, $B_i := \left( \psi_i \left( x_i^{(j)} - x_i^{(k)} \right) \right)_{j,k=1, \ldots, N}$  \hspace{1cm} (4.7)

where $\psi_i(x_i) := \int_{\mathbb{R}^d} 1 - \cos(x_i \cdot t_i) \rho_i(dt_i)$, i.e., it is the sum of all entries of the Hadamard product of the $A_i$, which are the doubly centered distance matrices for the distances induced by the continuous negative definite functions corresponding to the measures $\rho_i$. For further details see [6]. Moreover also for sample total- and sample $m$-multivariance computationally feasible representations are available. They are much faster than just summing up the corresponding sample multivariance, as (4.5) and (4.6) would suggest.

**Remark 4.2** (Moment conditions). Note that for statistical tests based on distance multivariance (see [7] and Remark 2.3. of [4]) the following integrability conditions are required for all $1 \leq i \leq n$

$$E(\psi_i(X_i)) < \infty \text{ and } E((\log(1 + |X_i|^2))^{1+\epsilon}) < \infty \text{ for some } \epsilon > 0 \hspace{1cm} (4.8)$$
and the mixed moment condition
\[ \mathbb{E}(\prod_{i=1}^{n} \psi_{i}(X_{k_{i},i} - X'_{l_{i},i})) < \infty \text{ for all } k_{i}, l_{i} \in \{0,1\}, \ 1 \leq i \leq n, \] (4.9)

where \( X_{1,i} \) and \( X'_{1,i} \) are independent and distributed as \( X \), and \( X_{0,i} \) and \( X'_{0,i} \) are independent (of the previous and for all \( i \)) and distributed as \( X_{i} \).

A simple condition which implies (4.8) and (4.9) is
\[ \mathbb{E}(|X_{i}|^{2n}) < \infty \text{ for } 1 \leq i \leq n, \]

which is, for example, trivially satisfied if the random variables are bounded.

For testing independence the distribution of \( ^{N}\rho_{S}(X^{(1)}, \ldots, X^{(N)}) \) (or of a transformation of it) under the hypothesis of independence (i.e., \( X_{1}, \ldots, X_{n} \) are independent) has to be known or estimated, compare with [4, Sec. 4]. One approach is to use the conservative estimate (2.2) or our extension (2.1).

We summarize the methods in Section 4.5.

In some settings it is useful to normalize the estimators such that the limit has unit expectation, this is called **normalized sample distance multivariate**. It is denoted by \( M \) instead of \( N \) and it is obtained by replacing \( B_{i} \) in (4.7) by
\[ B_{i} := \frac{1}{\sqrt{n}} \sum_{j=1}^{N} \psi_{i}(x_{i}^{(j)} - x_{i}^{(k)}) \]

Furthermore, for **normalized total multivariate** and **normalized \( m \)-multivariate** the estimator is also scaled by \( (2^{n} - n - 1)^{-1} \) and \( \binom{n}{m}^{-1} \), respectively. For more details we refer to [4, Sec. 2].

Finally, note that distance multivariate and normalized distance multivariate are always translation invariant. Moreover, normalized distance multivariate is scale invariant if the measures \( \rho_{i} \) are such that the functions \( \psi_{i} \) given in (4.7) are of the form \( \psi_{i}(x_{i}) = |x_{i}| \), see [4, Prop. 2.1 and Eq. (3.2)].

### 4.1 Limit of the raw estimators – \( \sqrt{N} \cdot ^{N}Z_{S} \)

The following result simplifies the original representation obtained in [7, Eq. (4.20)] of the limit of the raw (i.e., without taking the norm) estimator \( \sqrt{N} \cdot ^{N}Z_{S} \). Based on it the moments of the limit distribution can be calculated directly, see Proposition [4.4].

**Theorem 4.3.** Let \( X_{1}, \ldots, X_{n} \) be independent satisfying (4.8), then \( ^{N}Z_{S}(t_{S}) = 0 \) for \( |S| = 1 \), and for \( |S| \geq 2 \)
\[ \sqrt{N} \cdot ^{N}Z_{S}(t_{S}) \xrightarrow{d} G_{S}(t_{S}) := \int_{S} \prod_{i \in S} \left( e^{i z_{i}} - f_{X_{i}}(t_{i}) \right) d\mathbb{W}(F_{X}(x)), \] (4.10)

where \( \mathbb{W} \) is a Brownian sheet indexed by \([0,1]^{n}\) and \( F_{X}(x) = (F_{X_{1}}(x_{1}), \ldots, F_{X_{n}}(x_{n})) \).

**Proof.** The proof is similar to the beginning of the proof of [7, Thm. 4.6]. Let \( X_{1}, \ldots, X_{n} \) be independent.

First recall a basic identity for products of differences
\[ \prod_{i \in S} (a_{i} - b_{i}) = \sum_{R \subseteq S} (-1)^{|S| - |R|} \left( \prod_{i \in R} a_{i} \cdot \prod_{j \in S \setminus R} b_{j} \right) \] (4.11)

Hence the independence of the \( X_{j} \), \( 1 \leq j \leq n \), implies
\[ \prod_{j \in S} (f_{j}(t_{j}) - ^{N}f_{j}(t_{j})) = \sum_{R \subseteq S} (-1)^{|S| - |R|} \left( f_{R}(t_{R}) \cdot \prod_{j \in S \setminus R} ^{N}f_{j}(t_{j}) \right). \]
and (4.4) becomes

\[ N Z_S(t_S) = \sum_{R \subseteq S} (-1)^{|S| - |R|} \left( f_R(t_R) \cdot \prod_{j \in S \setminus R} f_j(t_j) \right) \]

\[ = \sum_{R \subseteq S} (-1)^{|S| - |R|} \left( (N f_R(t_R) - f_R(t_R)) \cdot \prod_{j \in S \setminus R} f_j(t_j) \right) + \prod_{j \in S} (f_j(t_j) - N f_j(t_j)) \]

Recall that in general for a distribution function \( G \) on \( \mathbb{R}^n \) and a function \( g \) on \( \mathbb{R}^{|S|} \)

\[ \int_{\mathbb{R}^{|S|}} g(x_S) dG_S(x_S) = \int_{\mathbb{R}^n} g(x_S) dG(x). \]

Thus \( f_S(t_S) - f_S(t_S) = \int e^{ix \cdot t_S} d(N F_X(x) - F_X(x)) \) and by the central limit theorem

\[ \sqrt{N} (N F_X(x) - F_X(x)) \xrightarrow{d} N \] where \( Z \sim N(0, F_X(x)(1 - F_X(x)). \)

To avoid confusion, note that \( F_X \) is the common distribution function, and this is different to the vector of the marginal distribution functions \( F_X. \) Furthermore, the independence implies \( F_X = \prod_{i=1}^n F_X_i. \)

Extending the convergence to the sample paths (cf. [7, Equation (4.20)]) yields

\[ \sqrt{N} \cdot N Z_S(t_S) \xrightarrow{d} \sum_{R \subseteq S} (-1)^{|S| - |R|} \int e^{ix \cdot t_R} d\mathbb{B}(x) \prod_{j \in S \setminus R} f_X_j(t_j), \] where \( \mathbb{B} \) is a Gaussian random field indexed by \( \mathbb{R}^{d_1 + \cdots + d_n} \) with \( \mathbb{E}(\mathbb{B}(t)) = 0 \) and

\[ \mathbb{E}(\mathbb{B}(s) \mathbb{B}(t)) = \prod_{i=1}^n F_X_i(s_i \wedge t_i) - \prod_{i=1}^n F_X_i(s_i) F_X_i(t_i). \] Using (4.11) again in (4.12) yields

\[ \sqrt{N} \cdot N Z_S(t_S) \xrightarrow{d} \prod_{i \in S} \int e^{ix_i t_i} - f_X_i(t_i) \, d\mathbb{B}(x). \]

Note that for a Brownian bridge \( \tilde{B} \) from 0 to 0 with multi-dimensional index set \( [0, 1]^n \) one has \( \mathbb{E}(\tilde{B}(t)) = 0 \) and \( \mathbb{E}(\tilde{B}(s) \tilde{B}(t)) = \prod_{i=1}^n (s_i \wedge t_i) - \prod_{i=1}^n s_i t_i \) and thus

\[ \tilde{B}(\cdot) \overset{d}{=} \tilde{B}(F_X(\cdot)), \]

since both sides are centered Gaussian random fields with identical covariance structure, hereto note that \( F_X(s_i \wedge t_i) = F_X(s_i \wedge t_i). \)

For clarification, note that one might be tempted to consider the alternative \( \tilde{A}(F_X) \) where \( \tilde{A} \) is the classical Brownian bridge, i.e., it has the one-dimensional index set \( [0, 1] \) and \( \mathbb{E}(\tilde{A}(s) \tilde{A}(s')) = (s \wedge s') - ss'. \)

But note that in general \( \prod F_X(t_i) \neq \prod (F_X(t_i) \wedge F_X(t'_i)), \) and thus this would yield a different covariance than required by (4.13).

To continue the proof, recall that for a Brownian sheet \( \mathbb{W} \) indexed by \( [0, 1]^n \) also

\[ \left( \tilde{\mathbb{W}}(\tilde{t}) \right)_{\tilde{t} \in [0, 1]^n} \overset{d}{=} \mathbb{W}(\tilde{t}) - \mathbb{W}(1_n) \cdot \prod_{j=1}^n \tilde{t}_j \]
holds, where $1_n = (1, \ldots, 1) \in \mathbb{R}^n$. Thus
\[
\int \prod_{i \in S} (e^{i x_i t_i} - f_{X_i}(t_i)) \; d\mathbb{B}(x) = 
\int \prod_{i \in S} (e^{i x_i t_i} - f_{X_i}(t_i)) \; d\mathbb{W}(\mathbf{F}(x)) - \mathbb{W}(1_n) \int \prod_{i \in S} (e^{i x_i t_i} - f_{X_i}(t_i)) \; d\mathbf{F}(x)
\]
and
\[
\int \prod_{i \in S} (e^{i x_i t_i} - f_{X_i}(t_i)) \; d\mathbf{F}(x) = \prod_{i \in S} \int (e^{i x_i t_i} - f_{X_i}(t_i)) \; d\mathbf{F}(x_i) = 0
\]
implies the result, \((4.10)\).

As in \((4.10)\) we set for $S \subset \{1, \ldots, n\}$ with $|S| > 1$
\[
G_S(t_S) := \int \prod_{i \in S} (e^{i x_i t_i} - f_{X_i}(t_i)) \; d\mathbb{W}(\mathbf{F}(x)).
\]
The case $|S| = 1$ is excluded, since in this case the limit would be trivial and thus it differs from the function defined here.

Now we can calculate moments and properties of $G_S$ explicitly.

**Proposition 4.4.** Let $S, R \subset \{1, \ldots, n\}$ with $|S|, |R| > 1$. Then $G_S$ and $G_R$ are independent for $S \neq R$ and
\[
\begin{align*}
E(G_S(t_S)) &= 0, \quad \text{(4.14)} \\
E(G_S(t_S)G_S(t_S')) &= \prod_{i \in S} (f_i(t_i - t_i') - f_i(t_i)f_i(-t_i')), \quad \text{(4.15)} \\
E(G_S(t_S)G_S(t_S')) &= \prod_{i \in S} (f_i(t_i + t_i') - f_i(t_i)f_i(t_i')), \quad \text{(4.16)} \\
E(G_S(t_S)\overline{G_S}(t_S')) &= \prod_{i \in S} (1 - |f_i(t_i)|^2), \quad \text{(4.17)} \\
E(G_S(t_S)\overline{G_S}(t_S')G_S(t_S')\overline{G_S}(t_S')') &= \prod_{i \in S} (1 - |f_i(t_i)|^2) \cdot \prod_{i \in S} (1 - |f_i(t_i')|^2) \\
&\quad + \sum_{i \in S} |f_i(t_i + t_i') - f_i(t_i)f_i(t_i')|^2 \\
&\quad + \sum_{i \in S} |f_i(t_i - t_i') - f_i(t_i)f_i(-t_i')|^2. \quad \text{(4.18)}
\end{align*}
\]

**Proof.** Note that also the results of Section 3 yield such representations. Thus we sketch here only an alternative derivation of some of the statements using the explicit representation obtained in Theorem 3.3.

Recall the Itô isometry for a Brownian sheet $\mathbb{W}$ (e.g. \cite[Equation (1)]{22}) for two functions $f, g$ on $\mathbb{R}^n$:
\[
E \left( \int_{[0,1]^n} f(x) \; d\mathbb{W}(x) \cdot \int_{[0,1]^n} g(x) \; d\mathbb{W}(x) \right) = \int_{[0,1]^n} f(x)g(x) \; dx.
\]
Thus for two functions $f, g$ on $\mathbb{R}^n$ and independent $X_1, \ldots, X_n$:
\[
E \left( \int f(x) \; d\mathbb{W}(\mathbf{F}(x)) \cdot \int g(x) \; d\mathbb{W}(\mathbf{F}(x)) \right) = \int f(x)g(x) \; d\mathbf{F}(x),
\]
where \( d\mathbf{F}_\mathbf{X} = d\mathbf{F}_\mathbf{X} \) due to the independence. This implies

\[
\mathbb{E}(G_S(t_S)G_R(t'_R)) = \mathbb{E} \left[ \prod_{i \in S} (e^{ix_i \cdot t_i} - f_{X_i}(t_i)) \right] \mathbb{E} \left[ \prod_{i \in R} (e^{ix_i \cdot t'_i} - f_{X_i}(t'_i)) \right]
\]

\[
= \int \prod_{i \in S} (e^{ix_i \cdot t_i} - f_{X_i}(t_i)) \cdot \prod_{i \in R} (e^{-ix_i \cdot t'_i} - f_{X_i}(-t'_i)) \, d\mathbb{F}_\mathbf{S}(x_S)
\]

\[
= \begin{cases} 
0 & \text{for } S \neq R, \\
\prod_{i \in S} (f_i(t_i - t'_i) - f_i(t_i)f_i(-t'_i)) & \text{for } S = R.
\end{cases}
\]

Analogously, (4.16) is proved. Thus for \( S \neq R \) the random variables \( G_S \) and \( G_R \) are uncorrelated and they are jointly Gaussian. Therefore they are independent. \( \square \)

### 4.2 Limit of (scaled) sample distance multivariance \( - N \cdot \frac{\mathbb{M}_{2\rho_S}^2}{\mathbb{M}_{1\rho_S}^2} \)

Next we can derive a new representation of the \( L^2(\rho_S) \)-norm of the random field \( G_S \).

**Proposition 4.5.** Let \( G_S \) be the random field defined in (4.10). Then

\[
\|G_S\|_{\rho_S}^2 = \int \int \prod_{i \in S} \Psi_i(x_i, y_i) \, d\mathbb{W}(\mathbf{F}_\mathbf{X}(x)) \, d\mathbb{W}(\mathbf{F}_\mathbf{X}(y))
\]

with

\[
\Psi_i(x_i, y_i) = -\psi_i(x_i - y_i) + \mathbb{E}(\psi_i(X_i - y_i)) + \mathbb{E}(\psi_i(x_i - X'_i)) - \mathbb{E}(\psi_i(X_i - X'_i)),
\]

(4.19)

where \( (X'_1, \ldots, X'_n) \) is an independent copy of \( (X_1, \ldots, X_n) \) and the \( X_i \) are independent. Here \( \mathbb{W} \) and \( \mathbf{F}_\mathbf{X} \) are as in Theorem 4.3.

**Remark 4.6.** For the application of distance multivariance in independence testing it is fundamental to note that

\[
N \cdot \frac{\mathbb{M}_{2\rho_S}^2(X^{(1)}, \ldots, X^{(N)})}{\mathbb{M}_{1\rho_S}^2} \xrightarrow{d_{N \to \infty}} \|G_S\|_{\rho_S}^2
\]

for independent \( X_1, \ldots, X_n \). This statement is a non-trivial consequence (see [4, Theorem 4.6]) of the convergence noted in Theorem 4.3.

**Proof of Proposition 4.5** Note that due to the symmetry of \( \rho_i \)

\[
\int 1 - e^{ix_i \cdot t_i} \rho_i(dt_i) = \int 1 - e^{-ix_i \cdot t_i} \rho_i(dt_i) = \frac{1}{2} \int 2 - e^{ix_i \cdot t_i} - e^{-ix_i \cdot t_i} \rho_i(dt_i)
\]

\[
= \int 1 - \cos(x_i \cdot t_i) \rho_i(dt_i) = \psi_i(x_i),
\]

as well as,

\[
\int (e^{ix_i \cdot t_i} - f_{X_i}(t_i))(e^{-iy_i \cdot t_i} - f_{X_i}(-t_i)) \rho_i(dt_i) = \int (e^{-ix_i \cdot t_i} - f_{X_i}(-t_i))(e^{iy_i \cdot t_i} - f_{X_i}(t_i)) \rho_i(dt_i)
\]

\[
= \int (e^{ix_i \cdot t_i} - f_{X_i}(t_i))(e^{-iy_i \cdot t_i} - f_{X_i}(-t_i)) \rho_i(dt_i).
\]
Hence, we find
\[
\int \left( e^{ix \cdot t_i} - f_{X_i}(t_i) \right) \left( e^{-iy \cdot t_i} - f_{X_i}(-t_i) \right) \rho_i(dt_i) = \int \text{Re} \left[ \left( e^{ix \cdot t_i} - f_{X_i}(t_i) \right) \left( e^{-iy \cdot t_i} - f_{X_i}(-t_i) \right) \right] \rho_i(dt_i)
\]
\[
= \int \int \int \text{Re} \left[ \left( e^{ix \cdot t_i} - e^{iu \cdot t_i} \right) \left( e^{-iy \cdot t_i} - e^{-iv \cdot t_i} \right) \right] dF_{X_i}(u_i) dF_{X_i}(v_i) \rho_i(dt_i)
\]
\[
= \int \int \int \left[ \cos((x_i - y_i) \cdot t_i) - \cos((x_i - v_i) \cdot t_i)
\right.
\]
\[
\left. - \cos((u_i - y_i) \cdot t_i) + \cos((u_i - v_i) \cdot t_i) \right] dF_{X_i}(u_i) dF_{X_i}(v_i) \rho_i(dt_i)
\]
\[
= \int \int \int \left[ \cos((x_i - y_i) \cdot t_i) - 1 + 1 - \cos((x_i - v_i) \cdot t_i)
\right.
\]
\[
\left. - \cos((u_i - y_i) \cdot t_i) + 1 - 1 + \cos((u_i - v_i) \cdot t_i) \right] dF_{X_i}(u_i) dF_{X_i}(v_i) \rho_i(dt_i)
\]
\[
= -\psi_i(x_i - y_i) + \mathbb{E}(\psi_i(X_i - y_i)) + \mathbb{E}(\psi_i(x_i - X'_i)) - \mathbb{E}(\psi_i(X_i - X'_i)).
\]

The moment condition \((4.8)\) allows to apply Fubini’s theorem in the penultimate step \((\ast)\) since
\[
\int \int \int |\cos((x_i - y_i) \cdot t_i) - \cos((x_i - v_i) \cdot t_i) - \cos((u_i - y_i) \cdot t_i) + \cos((u_i - v_i) \cdot t_i)| \rho_i(dt_i) dF_{X_i}(u_i) dF_{X_i}(v_i)
\]
\[
\leq \int \int \int \left[ |\cos((x_i - y_i) \cdot t_i) - 1| + |1 - \cos((x_i - v_i) \cdot t_i)|
\right.
\]
\[
\left. + |1 - \cos((u_i - y_i) \cdot t_i)| + |\cos((u_i - v_i) \cdot t_i) - 1| \right] \rho_i(dt_i) dF_{X_i}(u_i) dF_{X_i}(v_i)
\]
\[
= \int \int \int \left[ 1 - \cos((x_i - y_i) \cdot t_i) + 1 - \cos((x_i - v_i) \cdot t_i)
\right.
\]
\[
\left. + 1 - \cos((u_i - y_i) \cdot t_i) + 1 - \cos((u_i - v_i) \cdot t_i) \right] \rho_i(dt_i) dF_{X_i}(u_i) dF_{X_i}(v_i)
\]
\[
= \psi_i(x_i - y_i) + \int \psi_i(x_i - v_i) dF_{X_i}(v_i) + \int \psi_i(u_i - y_i) dF_{X_i}(u_i)
\]
\[
+ \int \psi_i(u_i - v_i) dF_{X_i}(u_i) dF_{X_i}(v_i)
\]
\[
\leq \psi_i(x_i - y_i) + 2\psi_i(x_i) + 4 \int \psi_i(v_i) dF_{X_i}(v_i) + 2\psi_i(y_i) + 4 \int \psi_i(u_i) dF_{X_i}(u_i)
\]
\[
= \psi_i(x_i - y_i) + 2\psi_i(x_i) + 2\psi_i(y_i) + 8\mathbb{E}(\psi_i(X_i)) < \infty,
\]
where we used the inequality \(\psi_i(x + y) \leq 2\psi_i(x) + 2\psi_i(y)\) (a direct consequence of, e.g., [3, Prop. 4.3.3]).
for the negative definite function $\psi_i$ in the penultimate line. Thus,

$$\|G_S\|^2 = \left\| \prod_{i \in S} (e^{ix_i \cdot t_i} - f_{X_i}(t_i)) \right\|_d^2 \mathbb{W}(F_X(x)) \rho(dt)$$

$$= \int \left[ \prod_{i \in S} (e^{ix_i \cdot t_i} - f_{X_i}(t_i)) \right] \mathbb{W}(F_X(x)) \rho(dt)$$

$$= \int \prod_{i \in S} \mathbb{W}(F_X(x)) \rho(dt)$$

$$= \int \prod_{i \in S} \mathbb{W}(F_X(x)) \rho(dt)$$

$$= \prod_{i \in S} \mathbb{W}(F_X(x)) \rho(dt)$$

Furthermore, the moments can be calculated directly (which might become quite technical) or using the results of Section 4.

**Corollary 4.7.** The moments of the $L^2(\rho)$-norm of $G_S$ defined in (4.10) are given by

$$\mathbb{E}(\|G_S\|^2 \rho_S) = \mu_S^{(1)}$$

$$\text{Var}(\|G_S\|^2 \rho_S) = \mathbb{E}(\|G_S\|^2 \rho_S - \mu_S^{(1)})^2 = 2\mu_S^{(2)}$$

$$\mathbb{E}(\|G_S\|^2 \rho_S - \mu_S^{(1)})^4 = 8\mu_S^{(3)}$$

$$\text{skew}(\|G_S\|^2 \rho_S) = \frac{8\mu_S^{(3)}}{(2\mu_S^{(2)})^2} = \frac{4\mu_S^{(3)}}{\sqrt{2}(\mu_S^{(2)})^2}$$

$$\mathbb{E}(\|G_S\|^2 \rho_S - \mu_S^{(1)})^4 = 48\mu_S^{(4)} + 12(\mu_S^{(2)})^2$$

$$\text{exkurt}(\|G_S\|^2 \rho_S) = \frac{48\mu_S^{(4)} + 12(\mu_S^{(2)})^2}{(2\mu_S^{(2)})^2} - 3 = 12\frac{\mu_S^{(4)}}{(\mu_S^{(2)})^2},$$

with

$$\mu_S^{(k)} = \prod_{i \in S} \mu_i^{(k)}$$

and

$$\mu_i^{(k)} = \int \cdots \int \prod_{j=1}^{k-1} K_i(t_i^{(k-j+1)}, t_i^{(k-j)}) \cdot K_i(t_i^{(1)}, t_i^{(k)}) \rho_i(dt_i^{(1)}) \cdots \rho_i(dt_i^{(k)}) \quad (4.20)$$

and

$$K_i(s_i, t_i) := f_i(s_i - t_i) - f_i(s_i) f_i(-t_i) \text{ for } s_i, t_i \in \mathbb{R}^d \text{ and } 1 \leq i \leq n.$$
Remark 4.8. 1. Note that

\[ \mathbb{E}(\|G_S\|_{\rho_S}^2) = \prod_{i \in S} \mathbb{E}(\psi(X_i - X'_i)) \quad (4.21) \]
\[ \mathbb{E}(\|G_S\|_{\rho_S}^4) = \prod_{i \in S} \mathbb{E}(\psi(X_i - X'_i))^2 + 2 \prod_{i \in S} M_{\rho_i \otimes \rho_i}^2(X_i, X_i) \quad (4.22) \]
\[ \mathcal{V}(\|G_S\|_{\rho_S}^2) = 2 \prod_{i \in S} M_{\rho_i \otimes \rho_i}^2(X_i, X_i), \quad (4.23) \]

where

\[ M_{\rho_i \otimes \rho_i}^2(X_i, X_i) = \int \int [\mathbb{E}((e^{X_i t} - f_i X_i(s_i))(e^{X_i s_i} - f_i X_i(t_i)))^2] \rho_i(ds_i) \rho_i(dt_i) \]
\[ = \int [f_i(s_i + t_i) - f_i(s_i)f_i(t_i)]^2 \rho_i(ds_i) \rho_i(dt_i). \]

2. If \( \|G_S\|_{\rho_S}^2 \) is normalized by its expectation the skewness and excess-kurtosis are unaltered and

\[ \mathbb{E} \left( \frac{\|G_S\|_{\rho_S}^2}{\mu_S^{(1)}} \right) = 1 \quad \text{and} \quad \mathcal{V} \left( \frac{\|G_S\|_{\rho_S}^2}{\mu_S^{(1)}} \right) = 2 \frac{\mu_S^{(2)}}{(\mu_S^{(1)})^2}. \]

4.2.1 Moments of the limit distribution \(- \mu_i^{(k)}\)

In this section we consider the \( \mu_i^{(k)} \) defined in (4.20) for one fixed \( i \) and drop the subscript \( i \) for readability up to Corollary 4.12. Thus we have a random variable \( X \) and independent copies of it denoted by \( X', X''', X'''' \), a symmetric measure \( \rho \) satisfying \( \int 1 \land |t|^2 \rho(dt) < \infty \) and \( \psi(x) := \int 1 - \cos(x \cdot t) \rho(dt) \).

Lemma 4.9. The \( \mu_i^{(k)} \) given in (4.20) have the following representations

\[ \mu^{(1)} = \mathbb{E}(\psi(X - X')), \]
\[ \mu^{(2)} = \mathbb{E}(\psi(X - X')\psi(X' - X)) - 2\mathbb{E}(\psi(X - X')\psi(X' - X'')) + [\mathbb{E}(\psi(X' - X'))]^2, \]
\[ \mu^{(3)} = -3\mathbb{E}(\psi(X - X')\psi(X' - X'')\psi(X'' - X)) + 3\mathbb{E}(\psi(X - X')\psi(X' - X'')\psi(X'' - X'''')) \]
\[ -3\mathbb{E}(\psi(X - X')\psi(X' - X''))\mathbb{E}(\psi(X - X')) + [\mathbb{E}(\psi(X - X'))]^3, \]
\[ \mu^{(4)} = \mathbb{E}(\psi(X - X')\psi(X' - X'')\psi(X'' - X'''')\psi(X''' - X''')) \]
\[ -4\mathbb{E}(\psi(X - X')\psi(X' - X'')\psi(X'' - X'''')\psi(X''' - X'''))\mathbb{E}(\psi(X - X'')) \]
\[ + 2[\mathbb{E}(\psi(X - X')\psi(X' - X''))]^2 \]
\[ -4\mathbb{E}(\psi(X - X')\psi(X' - X''))[\mathbb{E}(\psi(X - X'))]^2 + [\mathbb{E}(\psi(X - X'))]^4. \]

Proof. The representation of \( \mu_i^{(1)} \) follows by (4.21).

Note that by (4.22) and [6, Equation (3.9)]

\[ \mu^{(2)} = M_{\rho \otimes \rho}^2(X, X) = \mathbb{E}(\psi(X - X')\psi(X' - X)) - 2\mathbb{E}(\psi(X - X')\psi(X' - X')) + [\mathbb{E}(\psi(X - X'))]^2. \]

By (3.12)

\[ \mu^{(3)} = \int K(s, t)K(t, r)K(r, s) \rho(ds) \rho(dt) \rho(dr) \]
\[ = \int \left[ f(s - t) - f(s)f(t) \right] \cdot \left[ f(t - r) - f(t)f(r) \right] \cdot \left[ f(r - s) - f(r)f(s) \right] \rho(ds) \rho(dt) \rho(dr). \]
Expanding the product and using the symmetry (i.e., that \( s, t, r \) can be interchanged) yields

\[
\mu^{(3)} = \int f(s-t)f(t-r)f(r-s) - 3f(s-t)f(t-r)f(r) \, ds \, dr \, dt
+ 3f(s-t)f(t-r)f(r) |f(s)|^2 - |f(s)f(t)f(r)|^2 \, \rho(ds)\rho(dt)\rho(dr).
\]

If \( X, X', X'', X''' \) are independent and identically distributed then the terms of the integrand can be rewritten as

\[
\begin{align*}
&f(s-t)f(t-r)f(r-s) = \mathbb{E} \left( e^{is(X-X')} e^{it(X'-X'')} e^{ir(X''-X)} \right) \\
&f(s-t)f(t-r)f(r) \, f(s) \, f(r) = \mathbb{E} \left( e^{is(X-X')} e^{it(X'-X'')} \right) \mathbb{E} \left( e^{ir(X''-X)} \right) \\
&|f(s)f(t)f(r)|^2 = \mathbb{E} \left( e^{is(X-X')} \right) \mathbb{E} \left( e^{ir(X-X')} \right)
\end{align*}
\]

Interchanging the order of integration, expanding the products and collecting the terms yields

\[
\mu^{(3)} = -\mathbb{E} (\psi(X-X')\psi(X'-X'')\psi(X''-X)) + 3\mathbb{E} (\psi(X-X')\psi(X'-X'')\psi(X''-X''')) - 3\mathbb{E} (\psi(X-X')\psi(X'-X'')) \mathbb{E} (\psi(X-X')) + [\mathbb{E} (\psi(X-X'))]^3.
\]

By an analogous (but longer) calculation one gets the representation of \( \mu^{(4)} \).

The estimation of these \( \mu^{(k)} \) is straightforward by the law of large numbers for V-statistics.

**Theorem 4.10.** Let \( x = (x^{(1)}, \ldots, x^{(N)}) \) be a sample of \( X \) and set \( B := (\psi(x^{(j)} - x^{(k)}))_{j,k=1,\ldots,N} \) then

\[
m := \frac{1}{N^2} |B| \xrightarrow{N \to \infty} \mu^{(1)},
\]

\[
\frac{1}{N^2} |B \circ B| - \frac{2}{N^3} |B|^2 + m^2 \xrightarrow{N \to \infty} \mu^{(2)},
\]

\[
\frac{1}{N^3} |B^2 \circ B| + \frac{3}{N^4} |B|^3 - \frac{3}{N^5} |B^2| m + m^3 \xrightarrow{N \to \infty} \mu^{(3)},
\]

\[
\frac{1}{N^4} |B^3 \circ B| - \frac{4}{N^5} |B|^4 + \frac{4}{N^6} |B^3| m^2 + 2 \left[ \frac{1}{N^5} |B^2|^2 \right]^2 - \frac{4}{N^7} |B^3|^2 m^2 + m^4 \xrightarrow{N \to \infty} \mu^{(4)},
\]

where \( \circ \) denotes the Hadamard product and for a matrix \( A \) the sum of the absolute values of its entries is denoted by \( |A| \). (But note that here all matrices have always non-negative values anyway.)

**Remark 4.11.** The estimator for \( \mu^{(2)} \) is nothing but the estimator of \( M(X, X) \), i.e.,

\[
\hat{M}(X, X) = \frac{1}{N^2} \left[ (I - \frac{1}{N} 1) B (I - \frac{1}{N} 1) \right] \circ \left[ (I - \frac{1}{N} 1) B (I - \frac{1}{N} 1) \right].
\]

**Proof of Theorem 4.10.** To estimate \( \mu^{(k)} \) note that by the strong law of large numbers for V-statistics

\[
\frac{1}{N^{p+1}} \sum_{k_1, \ldots, k_{p+1}=1}^{N} \prod_{j=1}^{p} \psi(X^{(k_j)} - X^{(k_{j+1})}) \xrightarrow{N \to \infty} \mathbb{E} \left( \prod_{j=1}^{p} \psi(X^{(j)} - X^{(j+1)}) \right)
\]

and for \( p > 1 \)

\[
\frac{1}{N^p} \sum_{k_1, \ldots, k_p=1}^{N} \psi(X^{(k_p)} - X^{(k_1)}) \prod_{j=1}^{p-1} \psi(X^{(k_j)} - X^{(k_{j+1})}) \xrightarrow{N \to \infty} \mathbb{E} \left( \psi(X^{(p)} - X^{(1)}) \prod_{j=1}^{p-1} \psi(X^{(j)} - X^{(j+1)}) \right).
\]
Moreover, the following estimators are unbiased by direct calculations

\[
\sum_{k_1, \ldots, k_p=1}^N \prod_{j=1}^p \psi(x^{(k_j)}) - x^{(k_{j+1})} = |B_p|,
\]

\[
\sum_{k_1, \ldots, k_p=1}^N \psi(x^{(k_p)}) - x^{(k_1)} \prod_{j=1}^{p-1} \psi(x^{(k_j)}) - x^{(k_{j+1})} = |B_{p-1} \circ B|.
\]

Now using these approximations for each of the summands in the representations given in Lemma 4.9 yield the estimators.

Putting Corollary 4.7 and Theorem 4.10 together yields the key result.

**Corollary 4.12.** Let \( (x^{(1)}, \ldots, x^{(N)}) \) be samples of \( (X_1, \ldots, X_n) \) (with possibly dependent components), \( S \subset \{1, \ldots, n\} \) with \( |S| \geq 2 \) and let \( \|G\|_{\rho_S}^2 \) be the distributional limit of the test statistic \( N \cdot \mathbb{M}_{\rho_S}^2 \) under the hypothesis of independence. Then

\[
\begin{align*}
\mathbb{S} \mu_S^{(1)} & \xrightarrow{N \to \infty} \mathbb{E}(\|G\|_{\rho_S}^2), \\
2 \cdot \mathbb{S} \mu_S^{(2)} & \xrightarrow{N \to \infty} \mathbb{V}(\|G\|_{\rho_S}^2), \\
8 \cdot \mathbb{S} \mu_S^{(3)} & \xrightarrow{N \to \infty} \mathbb{E} \left( (\|G\|_{\rho_S}^2 - \mathbb{E}(\|G\|_{\rho_S}^2))^4 \right), \\
48 \cdot \mathbb{S} \mu_S^{(4)} + 12 \cdot (\mathbb{S} \mu_S^{(2)})^2 & \xrightarrow{N \to \infty} \mathbb{E} \left( (\|G\|_{\rho_S}^2 - \mathbb{E}(\|G\|_{\rho_S}^2))^4 \right),
\end{align*}
\]

where \( \mathbb{S} \mu_S^{(k)} := \prod_{i \in S} \mathbb{S} \mu_i^{(k)}, \) and

\[
\begin{align*}
\mathbb{S} \mu_i^{(1)} & = \frac{1}{N^2} |B_i|, \\
\mathbb{S} \mu_i^{(2)} & = \frac{1}{N^2} |B_i \circ B_i| - 2 \frac{N}{N^3} |B_i^2| + \frac{1}{N^4} |B_i|^2, \\
\mathbb{S} \mu_i^{(3)} & = -\frac{1}{N^3} |B_i^2 \circ B_i| + \frac{3}{N^4} |B_i|^3 - 3 \frac{N}{N^3} |B_i^2| \frac{1}{N^2} |B_i| + \frac{1}{N^6} |B_i|^3, \\
\mathbb{S} \mu_i^{(4)} & = \frac{1}{N^2} |B_i^3 \circ B_i| - 4 \frac{N}{N^5} |B_i|^4 + \frac{4}{N^4} |B_i|^3 |B_i| + 2 \left( \frac{1}{N^3} |B_i^2| \right)^2 - 4 \frac{N}{N^3} |B_i^2| \frac{1}{N^4} |B_i|^2 + \frac{1}{N^8} |B_i|^4,
\end{align*}
\]

with \( B_i := (\psi(x^{(i)}_1 - x^{(k)})_{i=1,\ldots,N} \) and \( \psi_i \) is given in (4.7). As before \(|A| := \sum_{i,k=1}^N |a_{i,k}|.\)

**Remark 4.13.** Based on the given estimators the corresponding unbiased estimators can also be calculated, we require these for \( \mu_i^{(1)}, \mu_i^{(2)} \) and \( \mu_i^{(3)} \) (cf. Section 4.5). For \( \mu_i^{(1)} \) the unbiased estimator is

\[
\frac{1}{N(N-1)} |B_i| \xrightarrow{N \to \infty} \mu_i^{(1)}.
\]

Moreover, the following estimators are unbiased by direct calculations

\[
\begin{align*}
\mathbb{S} b_i & := \frac{1}{N(N-1)} |B_i \circ B_i| \xrightarrow{N \to \infty} b_i := \mathbb{E}(\psi_i(X_i - X_i')^2), \\
\mathbb{S} c_i & := \frac{1}{N(N-1)(N-2)} (|B_i^2| - |B_i \circ B_i|) \xrightarrow{N \to \infty} c_i := \mathbb{E}(\psi_i(X_i - X_i') \psi(X_i' - X_i'')), \\
\mathbb{S} d_i & := \frac{1}{N(N-1)(N-2)(N-3)} (|B_i|^2 + 2|B_i \circ B_i| - 4|B_i^2|) \xrightarrow{N \to \infty} d_i := [\mathbb{E}(\psi(X_i - X_i'))]^2.
\end{align*}
\]
Thus using the representation obtained in Lemma 4.9 the unbiased estimator for \( \mu_1^{(2)} \) is

\[ \frac{N}{N-1} \text{var} + \frac{N}{N-2} \text{cov} \rightarrow \mu_1^{(2)}. \]

Straightforward, but more tedious computations (see Section 6.2 in the Appendix), give unbiased estimators for the representation (4.24). Setting \( \epsilon_i := \mathbb{E}(\psi_i(X_i - X'_i)\psi_i(X'_i - X''_i)) \) and \( f_i := \mathbb{E}(\psi_i(X_i - X'_i)\psi_i(X'_i - X''_i)) \) one obtains

\[ \frac{N}{N-1} \frac{1}{N(N-1)(N-2)(N-3)} \left( \left| B_i^2 \right| - \left| B_i^2 \right| \right) \rightarrow \epsilon_i, \quad (4.36) \]

\[ \frac{N}{N-1} \frac{1}{N(N-1)(N-2)} \left( \left| B_i^2 \right| - \left| B_i^2 \right| \right) \rightarrow f_i, \quad (4.37) \]

\[ \frac{N}{N-1} \frac{1}{N(N-1)(N-2)} \left( \left| B_i^2 \right| + \left| B_i^2 \right| \right) \rightarrow m_i, \quad (4.38) \]

\[ \frac{N}{N-1} \frac{1}{N(N-1)(N-2)} \left( \left| B_i^2 \right| - \left| B_i^2 \right| \right) \rightarrow m_i, \quad (4.39) \]

where \( \text{cs}(A) \) denotes the vector of the column sums \( \sum_{k=1}^{N} A_{j,k}, 1 \leq j \leq N, \) of a matrix \( A. \)

Thus the unbiased estimator for \( \mu_1^{(3)} \) is

\[ -1 \cdot \frac{N}{N-1} \frac{1}{N(N-1)(N-2)(N-3)} \left( \left| B_i^2 \right| - \left| B_i^2 \right| \right) \rightarrow \mu_1^{(3)}. \]

4.3 Moments of the finite sample distribution

In practice one never has an infinite sample, thus in fact not the limiting distribution but the finite sample distribution is relevant. For sample distance multivaricace we show in the following that one can calculate (and estimate) the moments of the finite sample distribution. In general these moments can differ considerably from the limiting moments, cf. Example 5.3. Thus the use of these moments in the quadratic form estimates provides better (e.g., closer to the nominal size) tests than using the limit moments. But note that especially for very small sample sizes (the mythical \( N < 30 \)) the use of the central limit theorem is doubtful, i.e., the distribution of sample distance multivariateity might not yet be close to that of a Gaussian quadratic form (see Example 5.5).

In order to analyze the finite sample distribution we denote by \( ^{\text{n}}\Psi_i \) the empirical approximation to \( \Psi_i \) defined in (4.19), i.e.,

\[ ^{\text{n}}\Psi_i(x^{(j)}, x^{(k)}):= ^{\text{n}}\Psi_i(x^{(j)}, x^{(k)}; x^{(1)}, \ldots, x^{(N)}):= -\psi_i(x^{(j)} - x^{(k)}) + \frac{1}{N} \sum_{l=1}^{N} \psi_i(x^{(j)} - x^{(l)}) + \frac{1}{N} \sum_{m=1}^{N} \psi_i(x^{(m)} - x^{(k)}) - \frac{1}{N^2} \sum_{m,l=1}^{N} \psi_i(x^{(m)} - x^{(l)}). \]

(4.40)

Then by Eqs. (4.3), (4.4), or directly by noting that \( ^{\text{n}}\Psi_i(x^{(j)}, x^{(k)}) = (A_i)_{jk} \) with \( A_i \) given in (4.7), sample distance multivaricace has the expression

\[ ^{\text{n}}M^2(x^{(1)}, \ldots, x^{(N)}) = \frac{1}{N^2} \sum_{j,k=1}^{n} ^{\text{n}}\Psi_i(x^{(j)}, x^{(k)}). \]
Based on this one can calculate (under the hypothesis of independence) the expectation of the test statistic $N \cdot M^2$ and (with a lot of effort) also the variance.

**Theorem 4.14.** Let $X_1, \ldots, X_n$ be independent. Then

$$
\mathbb{E}(N \cdot M^2(X^{(1)}, \ldots, X^{(N)})) = \frac{(N-1) + (-1)^{n}(N-1)}{N^n} \prod_{i=1}^{n} \mathbb{E}(\psi_i(X_i - X'_i))
$$

(4.41)

$$
= \prod_{i=1}^{n} \left[\left(1 - \psi_i(X_i - X'_i)\right)^{\mu_i^{(1)}} + (N-1) \prod_{i=1}^{n} \left(\frac{1}{N} \mu_i^{(1)}\right)\right]
$$

(4.42)

$$
\mathbb{E}(N \cdot N^2(M^2(X^{(1)}, \ldots, X^{(N)}))) = \frac{1}{N^2} \sum_{k=1}^{n} C(N, k) \prod_{i=1}^{n} \left[b(N, k) b_i + c(N, k) c_i + d(N, k) d_i\right]
$$

(4.43)

where $b_i := \mathbb{E}(\psi_i(X_i - X'_i)^2)$, $c_i := \mathbb{E}(\psi_i(X_i - X'_i)\psi_i(X'_i - X''_i))$, and $d_i := [\mathbb{E}(\psi_i(X_i - X'_i))]^2$ and the coefficients $C(\cdot, \cdot), b(\cdot, \cdot), c(\cdot, \cdot), d(\cdot, \cdot)$ are given in Table 7 on page 56.

**Remark 4.15.** 1. Note that if $\mu_i^{(1)}$ is approximated by its unbiased estimator $\frac{1}{N(N-1)}[B_i]$ given in Remark 4.13 then $(1 - \frac{1}{N})$ times this estimator becomes the biased estimator of $\mu_i^{(1)}$ given in Theorem 4.10. Thus by (4.42) the unbiased estimate of the finite sample mean is close to the biased estimate of the limit mean. In fact for odd $n$ the biased limit mean estimate is larger, for even $n$ it is smaller.

2. Analyzing the limit behavior of the coefficients in (4.43) and of the whole moment recovers the limit result as derived in Corollary 4.7. This is indicated by the extra columns in Table 7 on page 56.

3. Note that the values $b_i, c_i, d_i$ in (4.43) can be directly estimated. Given a sample $x = (x^{(1)}, \ldots, x^{(N)})$ of $X$ and $B_i := (\psi_i(x_i^{(i)} - x_i^{(k)}))_{i,k=1,\ldots,N}$ then

$$
\frac{1}{N^2} |B_i B_i| \xrightarrow{N \to \infty} b_i,
$$

(4.44)

$$
\frac{1}{N^3} |B_i^2| \xrightarrow{N \to \infty} c_i,
$$

(4.45)

$$
\frac{1}{N^2} |B_i| \xrightarrow{N \to \infty} \sqrt{d_i} = \mathbb{E}(\psi_i(X_i - X'_i)).
$$

(4.46)

The corresponding unbiased estimators for $b_i, c_i, d_i$ are also available, see Remark 4.13. See also (4.26), which shows that these are also used for the estimation of the variance (or second moment) of the limit.

4. Note that for the case $k = 7$ (cf. Table 7 on page 56) the corresponding summand in (4.43) is roughly $N \sum_{i=1}^{n} (4c_i - 3d_i)$. Especially for large $n$ this summand (times $\frac{1}{N^2}$) vanishes very slowly as the sample size increases. In fact, the difference between the finite sample moment and the moment of the limit is mainly due to this summand.

*Proof of Theorem 4.14* The value of the expectation can be deduced from [7, Eqs. (4.11) and (4.16)]. We give here a shorter direct proof. The independence of the $X_i$ and the linearity of the expectation implies

$$
\mathbb{E}(N \cdot N^2(M^2(X^{(1)}, \ldots, X^{(N)}))) = \frac{1}{N} \sum_{j,k=1}^{n} \prod_{i=1}^{n} \mathbb{E}(\psi_i(X_i^{(j)}, X_i^{(k)})),
$$

(4.47)

and, using $\psi_i(0) = 0$ and (4.40), gives

$$
\mathbb{E}(\psi_i(X_i^{(j)}, X_i^{(k)})) = (\delta_{j,k} - 1)\mathbb{E}(\psi_i(X_i - X'_i)) + 2\frac{N - 1}{N}\mathbb{E}(\psi_i(X_i - X'_i)) - 2\frac{N^2 - N}{N^2}\mathbb{E}(\psi_i(X_i - X'_i))
$$

(4.48)
where $\delta_{j,k}$ denotes the Kronecker symbol, i.e., $\delta_{j,k} = 1$ for $j = k$ and $\delta_{j,k} = 0$ for $j \neq k$. The observation that in (4.47) are $N$ summands with $j = k$ and $N^2 - N$ summands with $j \neq k$ yields the formula for the expectation.

For the second moment we proceed analogously:

$$E(\frac{N}{N^2} \cdot M^2(X^{(1)}, \ldots, X^{(N)}))^2) = \frac{1}{N^2} \sum_{j,k,l,m=1}^{N} \prod_{i=1}^{n} E(\frac{N}{N^2} \cdot \Psi_i(X^{(j)}_i, X^{(k)}_i) \cdot \Psi_i(X^{(l)}_i, X^{(m)}_i)).$$

Now note that expanding the product in $E(\frac{N}{N^2} \cdot \Psi_i(X^{(j)}_i, X^{(k)}_i) \cdot \Psi_i(X^{(l)}_i, X^{(m)}_i))$ and using the linearity of the expectation yields summands of the form

$$E(\frac{N}{N^2} \cdot \Psi_i(X^{(j)}_i - X^{(k)}_i)) = \begin{cases} 0 & \text{if } j' = k' \text{ or } l' = m', \\ b_i & \text{if } |\{j',k'\} \cap \{l',m'\}| = 2, \\ c_i & \text{if } j' \neq k' \text{ and } l' \neq m' \text{ and } |\{j',k'\} \cap \{l',m'\}| = 1, \\ d_i & \text{if } |\{j',k',l',m'\}| = 4, \end{cases}$$

with $b_i := E(\frac{N}{N^2} \cdot \Psi_i(X^{(j)}_i - X^{(k)}_i))^2) = E(\frac{N}{N^2} \cdot \Psi_i(X^{(j)}_i - X^{(k)}_i))$, $c_i := E(\frac{N}{N^2} \cdot \Psi_i(X^{(j)}_i - X^{(k)}_i))$, $d_i := |E(\frac{N}{N^2} \cdot \Psi_i(X^{(j)}_i - X^{(k)}_i))|^2$. Moreover note that the value of $E(\frac{N}{N^2} \cdot \Psi_i(X^{(j)}_i, X^{(k)}_i) \cdot \Psi_i(X^{(l)}_i, X^{(m)}_i))$ also depends on the actual combination of $j, k, l, m$ (which is determined by the outer sum). A careful analysis shows that one has to distinguish 7 cases of the outer sum, the frequency of these cases is given by the coefficients $\gamma_i$ (which is determined by the outer sum). A careful analysis shows that one has to distinguish 7 cases of the outer sum, the frequency of these cases is given by the coefficients $\gamma_i$ (which is determined by the outer sum).

For the test of independence proposed in [7] (see also [26] for the classical case of distance covariance) it was necessary to normalize the test statistic by the expectation of the limit. In practice the normalization factor is estimated using

$$\gamma_i(X^{(1)}, \ldots, X^{(N)}) := \prod_{i=1}^{n} \gamma_i(X^{(1)}, \ldots, X^{(N)}) := \prod_{i=1}^{n} \gamma_i(X^{(1)}_i - X^{(k)}_i).$$

Thus for this case one has to analyze the distribution of the test statistic $\frac{N}{N^2} \cdot M^2$.

**Theorem 4.16.** Let $X_1, \ldots, X_n$ be independent. Then

$$E \left( N \cdot \frac{\gamma_i M^2(X^{(1)}, \ldots, X^{(N)})}{\gamma_i} \right) = 1 + (N - 1) \left( \frac{-1}{N - 1} \right)^n = 1 - \left( \frac{-1}{N - 1} \right)^{n-1},$$

$$E \left( N \cdot \frac{\gamma_i M^2(X^{(1)}, \ldots, X^{(N)})^2}{\gamma_i} \right) = \frac{1}{N^2} \sum_{k=1}^{7} C(N,k) \prod_{i=1}^{n} \left[ b(N,k) b_i + c(N,k) c_i + d(N,k) d_i \right].$$

where the coefficients $C(\ldots), b(\ldots), c(\ldots), d(\ldots)$ are as in the previous theorem (i.e., they are given in Table 1 on page 56). But the other terms have to be modified as follows:

$$b_i := E \left( \frac{\gamma_i(X^{(j)}_i - X^{(k)}_i)^2}{\gamma_i^2} \right), \quad c_i := E \left( \frac{\gamma_i(X^{(j)}_i - X^{(k)}_i)}{\gamma_i} \right), \quad d_i := E \left( \frac{\gamma_i(X^{(j)}_i - X^{(k)}_i)}{\gamma_i^2} \right).$$

**Remark 4.17.** 1. Note that $b_i, c_i, d_i$ in Theorem 4.16 are more difficult to estimate than those in Theorem 4.14. One approach is to estimate each expectation by the quotient of the expectations, i.e., $b_i, c_i, d_i$ of Theorem 4.14 divided by

$$E(\gamma_i^2(X^{(1)}, \ldots, X^{(N)})) = \frac{1}{N^2} (C(N,2) b_i + C(N,3) c_i + C(N,1) d_i).$$
where \( b_i, c_i \) and \( d_i \) can be approximated as in (4.44)-(4.46). An alternative idea (which did not prove useful in our simulations) is to use the estimators given in (4.44)-(4.46) but replace therein the \( B_i \) by the normalized distance matrices \( B_i := \frac{N}{|S|} B_i \).

2. Note that the normalizing factor \( \chi h \) given in (4.49) is the biased estimator of the limit expectation (cf. Corollary 4.12). One could also consider different normalization factors, e.g., the unbiased estimator given in Remark 4.13 or the finite sample estimator given in Theorem 4.14. These estimators are constant multiples of \( \chi h \) (where the constant depends on \( N \)). Thus in these cases the moments of the normalized sample multivariance are also just constant multiples of those derived in Theorem 4.16.

Proof of Theorem 4.16: The proof is analogous to the proof of Theorem 4.14 just note that the terms therein are now divided by \( \chi h(\mathbf{X}(1), \ldots, \mathbf{X}(N)) \), which yields that their expectations have a simple value. Here the fact that all summands of \( \chi h(\mathbf{X}(1), \ldots, \mathbf{X}(N)) \) are i.i.d., except those which vanish, implies

\[
\mathbb{E} \left( \psi_i(\mathbf{X}^{(j)} - \mathbf{X}^{(k)}) \right) = \begin{cases} 0 & \text{for } j = k, \\ \frac{N}{N-1} & \text{for } j \neq k. \end{cases}
\]  

(4.50)

For the second moment note that

\[
1 = \mathbb{E} \left( \frac{\chi h^2(\mathbf{X}(1), \ldots, \mathbf{X}(N))}{\chi h(\mathbf{X}(1), \ldots, \mathbf{X}(N))} \right) = C(N,2)b_{i,N} + C(N,3)c_{i,N} + C(N,1)d_{i,N}.
\]

But a further simplification seems not to hold, therefore the expected values in each case now depend on \( N \).

\[\square\]

4.4 Sample total multivarince and sample \( m \)-multivariance

Let \( C_m := \{ S \subset \{1, \ldots, n\} : |S| = m \} \) and \( C_{\text{total}} := \bigcup_{m=2}^n C_m \) then

\[
\chi M(\mathbf{X}(1), \ldots, \mathbf{X}(N)) := \sqrt{\sum_{S \in C_{\text{total}}} \chi M^2_S(\mathbf{X}(1), \ldots, \mathbf{X}(N))}
\]  

(4.51)

and

\[
\chi M_m(\mathbf{X}(1), \ldots, \mathbf{X}(N)) := \sqrt{\sum_{S \in C_m} \chi M^2_S(\mathbf{X}(1), \ldots, \mathbf{X}(N))}
\]  

(4.52)

are the estimators of total- and \( m \)-multivariance, respectively (for details see [4, Eq. (2.5) and (5.3)]). Since they are structurally identical we drop for the moment the subscript of \( C \).

Under the hypothesis of independence of the \( X_i \) we have, using the convergence of each summand (Remark 4.6),

\[
\sum_{S \in C} N \cdot \chi M^2_S(\mathbf{X}(1), \ldots, \mathbf{X}(N)) \xrightarrow{N \to \infty} \sum_{S \in C} \|G_S\|^2_{p_S}.
\]

(4.53)

Now the independence of \( G_S \) and \( G_R \) for \( S \neq R \) (cf. Proposition 4.4 and Corollary 4.7) imply that the moments of the limit are determined by quantities of the form

\[
g_C(\mu^{(k)}) := \sum_{S \in C \in S} \prod_{i \in S} \mu_i^{(k)}
\]  

(4.54)

which in turn can be estimated by the corresponding empirical versions \( g_C(\chi \mu^{(k)}) \). Note that the function
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g_C can be given for each case in a computationally more efficient form (compare with \cite{4} Eqs. (5.5) ff.):

\[
g_{C_{\text{total}}} (\mu) := \sum_{S \subseteq \{1, \ldots, n\} \atop |S| \geq 2} \prod_{i \in S} \mu_i = \prod_{i=1}^{n} (\mu_i + 1) - \sum_{i=1}^{n} \mu_i - 1,
\]

\[
g_{C_2} (\mu) := \sum_{S \subseteq \{1, \ldots, n\} \atop |S| = 2} \prod_{i \in S} \mu_i = \frac{1}{2} \left[ \left( \sum_{i=1}^{n} \mu_i \right)^2 - \sum_{i=1}^{n} \mu_i^2 \right],
\]

\[
g_{C_3} (\mu) := \sum_{S \subseteq \{1, \ldots, n\} \atop |S| = 3} \prod_{i \in S} \mu_i = \frac{1}{6} \left[ \left( \sum_{i=1}^{n} \mu_i \right)^3 - 3 \left( \sum_{i=1}^{n} \mu_i \right) \left( \sum_{i=1}^{n} \mu_i^2 \right) + 2 \sum_{i=1}^{n} \mu_i^3 \right].
\]

Thus we have proved the following extension of Corollary 4.12.

**Corollary 4.18.** Denote by \( H_C := \sum_{S \subseteq C} \|G_S\|_p^2 \) the distributional limit in (4.53) under the assumption of \( k \)-independence of the random variables, with \( k := \max\{|S| : S \subseteq C\} \). Then

\[
g_C(\gamma \mu^{(1)}) \xrightarrow{N \to \infty} \mathbb{E}(H_C),
\]

\[
2g_C(\gamma \mu^{(2)}) \xrightarrow{N \to \infty} \mathbb{V}(H_C),
\]

\[
8g_C(\gamma \mu^{(3)}) \xrightarrow{N \to \infty} \mathbb{E}(H_C - \mathbb{E}(H_C)^3),
\]

\[
48g_C(\gamma \mu^{(4)}) + 12g_C(\gamma \mu^{(2)}\gamma^2) \xrightarrow{N \to \infty} \mathbb{E}(H_C - \mathbb{E}(H_C)^4),
\]

where \( \gamma \mu^{(k)} = (\gamma \mu_1^{(k)}, \ldots, \gamma \mu_n^{(k)}) \) and \( \gamma \mu_i^{(k)} \) are the biased (Cor. 4.12) or unbiased (Rem. 4.13) estimators for \( \mu_i^{(k)} \). Here \( \mu^{(2)} \) denotes the Hardamard power of the vector, i.e., each component is squared.

**Remark 4.19.**

1. Proposition 4.13 yields also the representation

\[
\sum_{S \subseteq C} \|G_S\|_p^2 = \int \int g_C(\Psi(x,y)) \, d\mathcal{W}(F_X(x)) d\mathcal{W}(F_X(y))
\]

where \( \Psi = (\Psi_1, \ldots, \Psi_n) \) with \( \Psi_i \) defined in 4.19.

2. Sample total- and \( m \)-multivariance can be standardized by

\[
\frac{\sum_{S \subseteq C} N \cdot \gamma M^{(2)}_p - g_C(\gamma \mu^{(1)})}{\sqrt{2g_C(\gamma \mu^{(2)})}}.
\]

Note that by Proposition 4.14 the sums in (4.51) and (4.52) are (in the limit \( N \to \infty \)) a sum of independent random variables. Thus for the case of many summands (e.g., \( n \) large) one could also try to use the central limit theorem to determine its standardized distribution. At least in the case of \( m \)-multivariance with independent identically distributed marginals the limit is standard normally distributed (as \( n \to \infty \) and \( N \to \infty \)), since in this case all summands of the \( m \)-multivariance are independent and identically distributed. Naturally, this yields a test for \( m \)-independence based on the standard normal distribution. In fact this is related to the test of pairwise independence presented in [28]. But they use the square roots (with appropriated sign) of the unbiased distance covariance.

For the finite sample case we need analogous to (4.54) the following function defined for vectors \( u, v, w \in \mathbb{R}^n \)

\[
G_C(u, v, w) := \sum_{S \subseteq C} \sum_{S' \subseteq C} \left[ \prod_{i \in S \setminus S'} u_i \right] \cdot \left[ \prod_{i \in S \setminus S'} v_i \right] \cdot \left[ \prod_{i \in S \setminus S'} w_i \right].
\]
For the sets of interest $G_C$ has the following (numerically tractable) representations

$$G_{C_{total}}(u, v, w) := 1 + \sum_{k_1, k_2=1 \atop k_i \text{distinct}}^n u_{k_1}v_{k_2} + \sum_{k_1, k_2=1 \atop k_i \text{distinct}}^n (u_i + v_i) + \prod_{i=1}^n (u_i + v_i + w_i + 1)$$

$$G_{C_1}(u, v, w) := \frac{1}{2} \sum_{k_1, k_2=1 \atop k_i \text{distinct}}^n w_{k_1}w_{k_2} + \sum_{k_1, k_2, k_3=1 \atop k_i \text{distinct}}^n u_{k_1}v_{k_2}w_{k_3} + \frac{1}{4} \sum_{k_1, \ldots, k_4=1 \atop k_i \text{distinct}}^n u_{k_1}u_{k_2}v_{k_3}v_{k_4},$$

$$G_{C_2}(u, v, w) := \frac{1}{6} \sum_{k_1, k_2, k_3=1 \atop k_i \text{distinct}}^n u_{k_1}u_{k_2}w_{k_3}w_{k_4} + \frac{1}{2} \sum_{k_1, \ldots, k_4=1 \atop k_i \text{distinct}}^n u_{k_1}v_{k_2}u_{k_3}w_{k_4} + \frac{1}{36} \sum_{k_1, \ldots, k_5=1 \atop k_i \text{distinct}}^n u_{k_1}u_{k_2}u_{k_3}v_{k_4}v_{k_5}v_{k_6}.$$

Using $G_C$ we get the following extension of Theorem 4.14.

**Theorem 4.20.** Let $X_1, \ldots, X_n$ be $k$-independent with $k := \max\{|S| : S \in C\}$. Then

$$\mathbb{E} \left( \sum_{S \in C} N \cdot \mathcal{M}^2_{\rho_S} \right) = g_C \left( \left( 1 - \frac{1}{N} \right) \mu^{(1)} \right) + (N - 1) g_C \left( - \frac{1}{N} \right) \mu^{(1)}, \quad (4.57)$$

$$\mathbb{E} \left( \sum_{S \in C} N \cdot \mathcal{M}^2_{\rho_S} \right)^2 = \frac{1}{N^2} \sum_{k=1}^7 C(N, k) G_C \left( e_1(N, k) \mu^{(1)}, e_2(N, k) \mu^{(1)}, e_1(N, k) e_2(N, k) \right), \quad (4.58)$$

$$\mathbb{E} \left( \sum_{S \in C} N \cdot \mathcal{M}^2_{\rho_S} \right)^2 = \frac{1}{N^2} \sum_{k=1}^7 C(N, k) G_C \left( e_1(N, k) \mu^{(1)}, e_2(N, k) \mu^{(1)}, \frac{b(N, k) + c(N, k) e + d(N, k) d}{N^4} \right), \quad (4.59)$$

where the random variables are omitted in the notation on the left hand side. The coefficients $C(\ldots), b(\ldots), c(\ldots), d(\ldots)$ are as in Theorem 4.14 (i.e., they are given in Table 4 on page 30). Moreover, $b := (b_1, \ldots, b_n)$, the vectors $c, d$ are defined analogously and

$$e_1(N, k) := \begin{cases} - \frac{1}{N} & \text{for } k = 1, 2, 3 \\ 1 - \frac{1}{N} & \text{for } k = 4, 5, 6, 7 \\ \end{cases} \quad \text{and} \quad e_2(N, k) := \begin{cases} - \frac{1}{N} & \text{for } k = 1, 2, 3, 5, 6 \\ 1 - \frac{1}{N} & \text{for } k = 4, 7. \end{cases}$$

**Remark 4.21.** The three expectations in the above theorem are given in such a way, that plugging in unbiased estimators of the parameters $\mu^{(1)}, b, c, d$ the formula provides an unbiased estimate of the left hand side. This would not be the case if we just use the square of (4.57) for (4.58).

**Proof of Theorem 4.20.** Equation (4.57) is a direct consequence of (4.42) and (4.54). For (4.59) note that

$$\mathbb{E} \left( \sum_{S \in C} N \cdot \mathcal{M}^2_{\rho_S} \right)^2 = \sum_{S \in C} \sum_{S' \in C} \mathbb{E}(N \cdot \mathcal{M}^2_{\rho_S} \cdot N \cdot \mathcal{M}^2_{\rho_{S'}})$$
and
\[
\mathbb{E}(\kappa M_{ps}^2 \kappa M_{ps}^2) = \sum_{j,k=1}^{N} \sum_{l,m=1}^{N} \mathbb{E} \left[ \prod_{i \in S} \psi_i(x_i^{(j)}, x_i^{(k)}) \cdot \psi_i(x_i^{(l)}, x_i^{(m)}) \right]
\]
\[
= \sum_{j,k=1}^{N} \sum_{l,m=1}^{N} \left[ \prod_{i \in S} \mathbb{E} \left( \psi_i(x_i^{(j)}, x_i^{(k)}) \right) \right] \cdot \left[ \prod_{i \in S \setminus S'} \mathbb{E} \left( \psi_i(x_i^{(l)}, x_i^{(m)}) \right) \right]
\]
\[
\cdot \left[ \prod_{i \in S'} \mathbb{E} \left( \psi_i(x_i^{(j)}, x_i^{(k)}) \cdot \psi_i(x_i^{(l)}, x_i^{(m)}) \right) \right]
\]
The last factor is computed as in Theorem 4.14. The first and second factor can be simplified using (4.48) and considering the values of \(j, k, l, m\) according to the cases of Table 4. Here note that \(j = k\) and \(l = m\) for the cases 1, 2, 3, and \(j \neq k\) and \(l \neq m\) for the cases 4, 7.

In the cases 5, 6, half of the summands satisfy \(j = k\) and \(l \neq m\), for the other half is \(j \neq k\) and \(l = m\) thus it seems that one should consider these subcases, but due to symmetry of the sums \(\sum_{S \in C} \sum_{S' \in C}\) it simplifies to (4.59).

Equation (4.58) is proved analogously, just replacing the factors \(\mathbb{E} \left( \psi_i(x_i^{(j)}, x_i^{(k)}) \cdot \psi_i(x_i^{(l)}, x_i^{(m)}) \right)\) by \(\mathbb{E} \left( \psi_i(x_i^{(j)}, x_i^{(k)}) \right) \mathbb{E} \left( \psi_i(x_i^{(l)}, x_i^{(m)}) \right)\).

To formulate the analogous result for normalized multivariance define
\[
\kappa h_S(x^{(1)}, \ldots, x^{(N)}) := \prod_{i \in S} \kappa h_i(x_i^{(i)}), \quad \kappa h_i(x_i^{(i)}) := \prod_{k \neq i} \frac{1}{N^2} \sum_{j \neq k} \psi_i(x_i^{(j)} - x_i^{(k)}).
\]

**Theorem 4.22.** Let \(X_1, \ldots, X_n\) be \(k\)-independent with \(k := \max \{|S| : S \in C\}\). Then
\[
\mathbb{E} \left( \sum_{S \in C} N \frac{\kappa M_{ps}^2}{\kappa h_S} \right) = g_c(1_n) + (N-1)g_c \left( -\frac{1}{N-1} \right),
\]
\[
\mathbb{E} \left[ \left( \sum_{S \in C} N \frac{\kappa M_{ps}^2}{\kappa h_S} \right)^2 \right] = \frac{1}{N^2} \sum_{k=1}^{7} C(N, k) G_c \left( f_1(N, k) 1_n, f_2(N, k) 1_n, \frac{b(N, k) b_N + c(N, k) c_N + d(N, k) d_N}{N^4} \right),
\]
where the random variables are omitted in the notation on the left hand side. The coefficients \(C(\cdot, \cdot), b(\cdot, \cdot), c(\cdot, \cdot), d(\cdot, \cdot)\) are as in Theorem 4.16 (i.e., they are given in Table 4 on page 36). Moreover, \(1_n := (1, \ldots, 1) \in \mathbb{R}^n\), \(b_N := (b_1, \ldots, b_n, N)\), the vectors \(c_N, d_N\) are defined analogously and
\[
f_1(N, k) := \begin{cases} \frac{1}{N-1} & \text{for } k = 1, 2, 3 \\ \frac{1}{1} & \text{for } k = 4, 5, 6, 7 \end{cases}
\]
\[
f_2(N, k) := \begin{cases} \frac{1}{N-1} & \text{for } k = 1, 2, 3, 5, 6 \\ \frac{1}{1} & \text{for } k = 4, 7. \end{cases}
\]

**Proof.** Note that by (4.50)
\[
\mathbb{E} \left( \frac{\kappa h_i(x_i^{(j)}, x_i^{(k)})}{\kappa h_i(x^{(1)}, \ldots, x^{(N)})} \right) = \left( \delta_{j,k} - \frac{1}{N} \right) \frac{N}{N-1} = \begin{cases} \frac{1}{N-1} & \text{for } j = k, \\ \frac{1}{N-1} & \text{for } j \neq k. \end{cases}
\]

Now, the proof is analogous to the proof of Theorem 4.20. \qed
Remark 4.23. To avoid confusion, note that depending on the number of elements in \( C \), here denoted by \( |C| \), normalized sample multivariance is by definition
\[
\frac{1}{|C|} \sum_{S \in C} n_S M_2(x^{(1)}, \ldots, x^{(N)})
\]
Thus the values in Theorem 4.22 have to be scaled by \( \frac{1}{|C|} \) and \( \frac{1}{|C|^2} \), respectively.

4.5 Testing independence using distance multivariance

In order to use distance multivariance for independence tests of the random vectors \( X_1, \ldots, X_n \) the moment conditions given in Remark 4.2 have to hold. Depending on the type of multivariance the test statistic \( T \) and the corresponding additional assumptions are given in the following table.

| Multivariance | Test Statistic \( T \) | Assumption \( H_0 \) |
|---------------|------------------------|------------------|
| Multivariance | \( N \cdot \alpha M_2^2 \) | \( X_i \) are \((n - 1)\)-independent \( X_i \) are independent |
| Total Multivariance | \( N \cdot \alpha M_2^2 \) | - \( X_i \) are independent |
| \( m \)-Multivariance | \( N \cdot \alpha M_{m+2}^2 \) | \( X_i \) are \((m - 1)\)-independent \( X_i \) are \( m \)-independent |

Moreover one could also consider the corresponding normalized test statistics, i.e., replacing distance multivariance \( M \) by normalized distance multivariance \( \mathcal{M} \).

It is known by \cite[Thm. 4.6, 4.11, Cor. 4.17, 4.19]{4} that under these assumptions the test statistic \( T \) diverges to \( \infty \) for \( N \to \infty \) if and only if \( H_0 \) is violated. Thus it is standard to define the corresponding tests as follows, and due to the divergence property these tests are consistent against all alternatives for \( N \to \infty \) (under the stated assumptions).

**Test** (for a test statistic \( T \) which diverges to \( \infty \) if and only if \( H_0 \) is violated). Let \( x^{(i)} \), \( 1 \leq i \leq N \), be samples of \( X = (X_1, \ldots, X_n) \). Then a test of \( H_0 \) with significance level \( \lambda \) is given by rejecting \( H_0 \) if the \( p \)-value of the sample, i.e., \( \mathbb{P}(T(x^{(1)}_1, \ldots, x^{(N)}_N) \geq T(x^{(1)}_1, \ldots, x^{(N)}_N)) \), is less than \( \lambda \). Here for each \( i \) the vector \( x^{(i)}_{H_0} \) is distributed as \( X \) under \( H_0 \), i.e., with components satisfying \( H_0 \).

To actually perform such tests one has to compute or estimate the \( p \)-value for the given sample, each method constitutes a different test with its own empirical power and empirical size. There are various methods, which we collect here in some detail for the convenience of the reader and also in order to have a reference for the examples and comparisons in the next section.

1. **Quadratic form estimates:** By Theorem 4.3, Proposition 4.4, Remark 4.6 and Equation (4.53) the distributional limit of the test statistic can be written as the \( L^2(\rho) \)-norm of a centered, complex, hermitian Gaussian random field \( \mathcal{G} \) and hence as a Gaussian quadratic form \( Q = \sum_{i \in \mathbb{N}} \alpha_i Z_i^2 \), cf. Theorem 3.9. This also holds for \( m \)- and total multivariance, since their summands are independent (cf. Proposition 4.4).

1.a **Moment methods:** The \( p \)-value is estimated based on some of the moments of the quadratic form. In the following \( Y_r \) denotes a chi-squared distributed random variable with (possibly fractional) \( r \) degrees of freedom, for details see Remark 2.2.4.

- The classical estimate of Székely and Bakirov \cite{25} uses only the mean:
\[
\mathbb{P}(Q \geq x) \leq \Phi \left( \frac{Y_1 \geq x}{\mathbb{E}(Q)} \right).
\]
This method is only valid for \( \frac{x}{m} \geq 1.5365 \) or equivalently for \( p \)-values less than 0.215 (which is sufficient for any commonly used significance level). In this setting it is the simplest and most unrestricted approach, since the mean always exists under the basic assumptions (cf. Remark 4.2). In the case of univariate Bernoulli marginals it is sharp (Remark 4.25) but in general it is (very) conservative (e.g. Example 5.2).
The variance based estimate derived in Theorem 2.1 which uses the mean and variance:

\[ P(Q \geq x) \leq P \left( \alpha Y_1 \geq \frac{x}{\sqrt{V(Q)}} \right) \quad \text{with} \quad \alpha = \sqrt{\frac{V(Q)}{2E(Q)^2}}. \tag{4.63} \]

It is also only valid for p-values less than 0.215, see Remark 2.2.2.

Pearson's estimate, see, e.g., [11], uses mean, variance and skewness:

\[ P(Q \geq x) \approx P \left( \beta Y_1 - \frac{1}{\beta} \geq \sqrt{2} \cdot \frac{x - E(Q)}{\sqrt{V(Q)}} \right) \quad \text{with} \quad \beta = \frac{\text{skew}(Q)}{\sqrt{8}}. \tag{4.64} \]

Among the above moment methods this is the most powerful, see, e.g., Example 5.2.

LTZ's estimate (Liu et al. [15]) chooses under all (non-central) chi-squared distributions the one having the same first three moments as the quadratic form and minimizing the absolute error in the fourth moment. In our case, i.e., for central quadratic forms, their method reduces to Pearson's three-moment approach.

I.b Eigenvalue methods: The p-value is computed from the distribution function of a finite-dimensional quadratic form given by an approximation of (some of) the coefficients \( \alpha_i \) of the Gaussian quadratic form \( Q = \sum_{i \in \mathbb{N}} \alpha_i Z_i^2 \). The coefficients \( \alpha_i \) arise as eigenvalues of the integral operator \( T_K \) associated with the covariance kernel

\[ K(s, t) = \prod_{i=1}^{n} K_i(s_i, t_i) = \prod_{i=1}^{n} \left( f_i(s_i - t_i) - f_i(s_i) f_i(t_i) \right), \]

(see Theorem 3.9) which can be computed from the characteristic functions \( f_i \) of the marginals (if known) or estimated by the empirical characteristic functions \( \hat{f}_i \) based on the samples. Due to the product structure of \( K \) one can solve the eigenvalue problem for the kernels \( K_i \), separately (cf. Remark 3.3). A standard technique for integral operators is the Nyström method, cf. [2]: the integral is discretized using a suitable numerical quadrature scheme, i.e.,

\[ T_{K_i} u(s) = \int_{\mathbb{R}^{d_i}} K_i(s, t) u(t) \rho_i(dt) \approx \sum_{j=1}^{m} \langle \sqrt{w_j} K_i(t_j, t_k) \sqrt{w_k} \rangle_{j, k=1, \ldots, m}. \]

for some order \( m \in \mathbb{N} \), nodes \( t_1, \ldots, t_m \in \mathbb{R}^{d_i} \) and weights \( w_1, \ldots, w_m \geq 0 \) and the eigenvalues \( \alpha^{(i)}_j \) of \( T_{K_i} \) are approximated by computing the eigenvalues of the (symmetrized) matrix

\[ \left( \sqrt{w_j} K_i(t_j, t_k) \sqrt{w_k} \right)_{j, k=1, \ldots, m}. \]

The p-value is then computed, based on the estimated coefficients \( \alpha_i \), either by numerical approximation of series representations of the distribution function (e.g., [10, 27]) or numerical Fourier inversion of the distribution function (e.g., [3, 11]).

II. Central limit theorem: For identically distributed marginals the summands of \( m \)-multivariance are (in the limit under \( H_0 \)) independent and identically distributed random variables (see Remark 4.19), thus by the central limit theorem the quadratic form is (in the limit) normally distributed. This yields the approximation

\[ P(Q \geq x) \approx P \left( Z \geq \frac{x - E(Q)}{\sqrt{V(Q)}} \right), \tag{4.65} \]

where \( Z \) is a standard normally distributed random variable.
III. Sampling methods: The p-value is computed by evaluating an empirical distribution function which is obtained either using Monte Carlo simulations of the distribution under $H_0$ or by resampling from the sample with replacement (bootstrap) or without replacement (permutation), see [4] for details in the context of distance multivariance. In general these methods are slow, since for the estimate of the p-value of a given sample the test statistic has to be evaluated for many samples.

In the next section we will compare these methods using concrete examples. But before note that for most of these methods some parameters (in our case mostly moments) have to be known or estimated from the sample. In particular, this implies that these parameters have to exist, i.e., implicitly each method imposes these additional assumptions.

The previous sections provide many methods to estimate the required moments, and also each of these constitutes a different test with its own empirical power and empirical size. Here we briefly comment on the available options:

- Using the moments of the limit (Corollaries 4.12 and 4.18) or the finite sample versions (Section 4.3 Corollaries 4.20 and 4.22). The latter clearly provide a more precise description of the distribution of the test statistic. But note that only in the limit the test statistics are really Gaussian quadratic forms. Nevertheless, the examples of the next section indicate that the use of the finite sample versions is always recommended.

- Using unbiased or biased estimators (Remarks 4.13 and 4.15). In general unbiased estimators help to prevent systematic errors, thus their use is (if available) recommended. But keep in mind that a functional transformation of an unbiased estimator is usually not unbiased anymore, thus the method as a whole might be still biased.

- Using standard distance multivariance or normalized distance multivariance (Remark 4.8.2 Theorems 4.16 and 4.22). For multivariance the tests with and without normalization can differ since without normalization different marginals might have (depending on their scale) different influence on the value. For $m$- and total multivariance the normalization matters also in a second way: With normalization each summand of $m$- and total multivariance has (under $H_0$) the same expected value, but without normalization this is not necessarily the case. Thus for $m$- and total multivariance with not identically distributed marginals it is certainly recommended to use the normalized version. Also for the other cases it seems reasonable to use normalized multivariance since this appears to be more robust (Ex. 5.9) and for $\psi_i = | \cdot |$ it is scale invariant (cf. the end of the introduction to Section 4).

Remark 4.24 (Bias vs. conservative). For the moment methods given above an overestimation (i.e., a value larger than the true value) of the mean $m$ and of the variance $v$ results in a larger (thus more conservative) p-value. In this sense a positive bias (in contrast to a negative bias) is preferred for the parameter estimation.

The behavior of (4.64) for a biased skewness is not obvious.

Remark 4.25 (The classical estimate is sharp for univariate Bernoulli marginals). In the case that $X_j, j \in S$, are independent and identically Bernoulli distributed with parameter $\frac{1}{2}$ one finds from the characteristic function $f_j(t_j) = \frac{1}{2}(e^{it_j} + 1)$ and Proposition 4.4 that the limiting random field $G_S$ has covariance kernel

$$K_S(t_S, t'_S) = \mathbb{E}(G_S(t_S)\overline{G}_S(t'_S)) = \prod_{j \in S} (f_j(t_j - t'_j) - f_j(t_j)f_j(-t'_j)) = \prod_{j \in S} \frac{1}{4}(e^{it_j} - 1)(e^{-it'_j} - 1) =: g_S(t_s)\cdot \overline{g}_S(t'_s).$$

Therefore, the associated operator $T_{K_S}$, see (3.2), has rank one and $\|g_S\|_{p_S}^2$ is its only non-vanishing eigenvalue. Thus,

$$G_S(t_s) = \|g_S\|_{p_S}^2 g_S(t_s) \cdot Z,$$
for some standard normally distributed random variable $Z$ and the associated Gaussian quadratic form follows a scaled chi-squared distribution,

$$\|G_S\|_{\rho_S}^2 = \|g_S\|_{\rho_S}^2 Y_1,$$

cf. Corollary 3.8 and Theorem 3.9. In particular, for the limiting distribution in the normalized case, the bound (4.62) is sharp.
Table 1: The coefficients for the representation of the variance of the finite sample estimator (Theorem 4.14) and the overall limit behavior. The coefficient \( a \) corresponds to the 0 terms, thus it does not show in the actual representation formula.
5 Examples, simulations and discussions

In this section we collect examples which illustrate various aspects of our results. Of major interest is certainly a comparison of the empirical power and empirical size of the tests introduced in Section 4.5 for a basic example which distinguishes the methods see Example 5.1 and for a comprehensive study see Example 5.10. The first step to the estimation of the p-values is the estimation of the parameters corresponding to the marginal distributions, the estimation is either based on the samples (Ex. 5.6) or done a priori for known marginals (Ex. 5.8). Thereafter the joint moments (i.e., the actually required parameters) can be estimated (Ex. 5.7) and finally the tests can be performed.

For the sake of clarity, let us summarize and recall the framework. We consider random variables $X_i$ with values in $\mathbb{R}^d_i$ and symmetric measures $\rho_i$ on $\mathbb{R}^d_i$ such that $\int 1 \wedge |t_i|^2 \rho_i(dt_i) < \infty$, $1 \leq i \leq n$. Based on $N$ samples $x^{(1)}, \ldots, x^{(N)}$ of $X = (X_1, \ldots, X_n)$, we are interested in the test statistics discussed in Section 4.5 e.g., $N \cdot \hat{M}_p^2(X^{(1)}, \ldots, X^{(N)})$ with $p = \otimes_{i=1}^n \rho_i$.

In this setting the key parameters are $\rho_i^{(k)}$ as defined in Corollary 4.7 and $b_i, c_i, d_i$ defined in Remark 4.13. To estimate these and to use them in further computations we refer to the options summarized in Section 4.5 (the key terms which we use here are mostly printed in bold in that section).

There is an infinite choice of possible examples, we try to concentrate on some key aspects. Thus as sample distributions we mostly consider the Bernoulli distribution (an extremal distribution for our setting in the sense of Remark 4.25), the uniform distribution (in some sense this is the other extremal, see [3] Example 7.9, case $n = 5$]) and the normal distribution (which is a standard assumption for samples). For the tests, there are two types of examples:

- $H_0$ examples: The marginals satisfy $H_0$ and the empirical size of the test is of major interest. It should be close to or smaller (i.e., conservative tests) than the significance level.

- dependence examples: The marginals violate $H_0$ and the empirical power of the test is of major interest. It should be large – but not larger than one could expect based on the true distribution of the test statistic under $H_0$ (cf. robustness discussed in Ex. 5.9).

If not mentioned otherwise we use in the examples the following conventions: Simulations are based on 10000 samples, the tests are performed with significance level 0.05, the benchmark (true) p-value is computed by the empirical distribution function of a Monte Carlo (re)sample of the test statistic under $H_0$. Where it is called ‘(re)sample’ since we resample without replacement each of the 10000 samples once, which provides (almost) $H_0$ data also for dependent data. The measures $\rho_i$ are such that the functions $\psi_i(x_i) := \int_{\mathbb{R}^d_i} 1 - \cos(x_i \cdot t_i) \rho_i(dt_i)$, cf. (4.7), are the Euclidean distance on $\mathbb{R}^d$, i.e., $\psi_i(y) = |y|$ for $y \in \mathbb{R}^d$. For general examples with other distances (but without the moment based tests) see [7] and [4].

For the construction of examples with higher order dependence we briefly recall the classical example of a dice in the shape of a tetrahedron (e.g., [3] Example 7.1) with sides colored $r, g, b$ and the forth side has all three colors on it. For each color define a Bernoulli random variable $Y_i$ which is 1 if and only if the corresponding color shows (at the bottom of the tetrahedron) after a throw of this dice. The three random variables $(Y_1, Y_2, Y_3)$ are dependent but pairwise independent.

**Example 5.1** (Comparison of the moment methods – normal tetrahedron). Let $(Y_1, Y_2, Y_3)$ be the random variables corresponding to the tetrahedron mentioned above, $Z_1, Z_2, Z_3$ be independent standard normal random variables and define $(X_1, X_2, X_3) := (Y_1, Y_2, Y_3) + r \cdot (Z_1, Z_2, Z_3)$. Figure 7 shows the empirical power for the three moment methods depending on the sample size for the case $r = 0.5$. Pearson’s approximation matches the benchmark, the variance based estimate is slightly less powerful and the classical method is clearly outperformed. Nevertheless, since the test is consistent against all alternatives in the limit $N \to \infty$ each method has power 1.
Example 5.2 (Multivariate Bernoulli marginals). Let $Y_i$ be independent Bernoulli distributed random variables and define $X_1 := (Y_1, \ldots, Y_5)$ and $X_2 := (Y_6, \ldots, Y_{10})$. Now consider the sample distance multivariance corresponding to $M(X_1, X_2)$. We computed 10000 samples of this for $N = 100$, and estimated (from these samples directly, i.e., not with our methods which would only require one sample) the empirical distribution and its mean, variance and skewness. The distribution function and the estimates are plotted in Figure 2. This illustrates several important aspects: 1. For multivariate Bernoulli marginals the classical estimate is not sharp, in contrast to the univariate case (cf. Remark 4.25). 2. The classical and our variance based estimate are only tail estimates, and they can be very conservative. 3. Pearson’s approximation (which uses only one parameter more than the variance based estimate) works astonishingly well.
Example 5.3 (Variants of the classical estimate). Let $X_i$ be independent Bernoulli random variables. The classical estimate is (in the limit) sharp for this case, see Remark 4.25. But for the finite sample case there are at least four ways to estimate the mean which is required for the tail estimate: the biased or unbiased estimator for the limit or for the finite sample mean. In Figure 3 the empirical size of the corresponding tests is depicted for (very) small sample sizes. The unbiased finite sample estimator is closest to the true value. As expected (Remarks 4.15.1 and 4.24) the biased limit estimator is very close to it but it is slightly less conservative. The biased finite sample estimator yields a (too) liberal behavior, the unbiased limit estimator yields a (too) conservative behavior. The latter becomes even more obvious for $n > 2$, see Figure 4.
Example 5.4 (Moment estimation is faster than resampling). We compare the time for computation of all moment estimates for one sample with the time of one evaluation of multivariance for one resampling. In Figure 5 their ratio is depicted, i.e., the number of evaluations of multivariance (with resampling the data) which can be performed in the time it takes to compute all moment estimates. We use normally distributed marginals and take in the ratio the median of the computation time of 100 repetitions.

Note that [26] suggest the use of \( \left\lfloor 200 + \frac{5000}{N} \right\rfloor \) resampling samples, thus – by the numbers in Figure 5 – the moment approach is clearly faster than the resampling approach even for small samples.
Figure 5: The number of evaluations of multivariance (with resampling the data) which can be performed in the time of the computation of all moment estimates (Ex. 5.4).

Example 5.5 (Estimation of the parameters $\mu_i, b_i, c_i, d_i$ of the marginals). There are four settings for the estimation of the moments corresponding to the marginal distribution: with or without bias for multivariance with or without normalization.

Figures 6, 7 and 8 show the estimation of $\mu^{(1)}, \mu^{(2)}, \mu^{(3)}$ and $b, c, d$. Of these the biased estimators clearly show the bias for small sample sizes. In the case of unbiased estimators without normalization the estimators are really unbiased. But note that in the case of using unbiased estimators for normalized multivariance there is a bias, since the transformation of the estimator creates a bias (see also the comment on biased and unbiased estimators in Section 4.3).
Figure 6: Convergence of the estimates of the parameters of the marginal distribution for Bernoulli variates (Ex. 5.5). The shaded regions describe the 5% to 95% quantile of the estimates and the labeled line is the mean.

Figure 7: Convergence of the estimates of the parameters of the marginal distribution for uniformly distributed variates (Ex. 5.5).
Example 5.6 (A priori parameter estimation for known marginals). In the case of known marginal distributions one can also use precomputed values for the parameters $\mu^{(1)}_i, \mu^{(2)}_i, \mu^{(3)}_i$. To compare different numerical approaches based on the derived representations we give theoretical values (obtained from straightforward but tedious computations assisted by MAPLE) against the following three numerical schemes (implemented in MATLAB):

1. use Nyström’s method to estimate (some of) the coefficients $\alpha_i$, $i \in I$, and use \( (3.11) \);
2. use numerical quadrature to compute the iterated integrals of the kernels $K$ in \( (3.12) \);
3. use numerical quadrature to compute the expectations in Lemma 4.9.

We compare the results against values of the estimators $\bar{\mu}^{(k)}$ based on generated samples using

4. the biased estimators for the summands given in Corollary 4.12 or
5. the unbiased estimators for the summands given in Remark 4.13.

Results for four univariate marginal distributions (Bernoulli with $p = \frac{1}{2}$, uniform distribution on $[0, 1]$, standard normal distribution, exponential distribution with $\lambda = 1$) are summarized in Table 2 on page 50 where we used 100 nodes for the quadratures and the estimators are based on sample size $N = 1000$.

Example 5.7 (Estimation of the (joint) moments). For the case of normal marginals Figure 9 shows the estimates of the moments of the test statistic depending on $n$ for fixed $N = 100$. In particular for larger $n$ this shows that the limit variance underestimates the finite sample variance by far. In Figure 8 the estimates depending on $N$ for fixed $n = 5$ are shown. These show that for small $N$ the limit mean overestimates the finite sample mean, and for large $N$ the finite sample variance decreases (very) slowly to the limit variance.
**Example 5.8** (Distribution of the finite sample estimator). Most methods of Section 4.5 use the finite sample estimators as if the test statistic is distributed as a Gaussian quadratic form. Although the other examples show that this works very well, one should be aware of the fact that in general the distribution is not that of a Gaussian quadratic form. As extrem example consider the case of Bernoulli marginals. In this case the distribution of $N \cdot ^{N} M^{2}(X^{(1)}, \ldots, X^{(N)})$ is a discrete distribution taking only finitely many values, e.g., for $N = 10$ there are only 35 different values (realized in 10000 samples). See Figure 11 for the empirical counting density, which is very irregular.
Figure 11: Counting density (based on 10000 samples) of sample distance multivariance with Bernoulli marginals for small samples $N = 10$ (Ex. 5.8).

**Example 5.9 (Robustness).** Here we consider a case where the assumptions of the tests, i.e., the moment condition given in Remark 4.2 and the implicit assumptions on the existence of the parameters by each method, are violated.

Let $X_i$ be random variables with Student’s t-distribution with 1 degree of freedom, thus their expectation does not exist. Figure 12 shows that therefore the moment estimates are problematic. In Figure 13 the empirical size (for independent $X_i$) is shown, which looks reasonable – but shows already strange behavior for $n = 3$. Moreover, we also consider a dependent sample, similarly to [26, Example 1(b)]. Let $(Y_1, \ldots, Y_{10})$ be multivariate t-distributed with 1 degree of freedom and the scale matrix being the identity plus a block matrix with $5 \times 5$ blocks being 0, 0.1, 0.1, 0. In Figure 14 the power of the tests is depicted. Note that the methods appear to be much more powerful than the benchmark. In Figure 15 the same example is computed for normalized multivariance, here only Pearson’s method is liberal.
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1. Nest estimates

2. unbiased

3. biased

4. normalized

5. not normalized

Figure 12: Estimation of the marginal moments for Student-t distributed variates, which violate the basic assumptions (Ex. 5.9).

Figure 13: Empirical size of the moment methods for Student-t distributed variates, which violate the basic assumptions (Ex. 5.9).
Example 5.10 (All methods, all examples). To give recommendations for applications of our methods we performed a (huge) study. Here we try a brief description:

We considered examples of this paper and many other examples discussed in [4, 26, 28] (see Section 6.3 in the Appendix for more details). For each (that is also for each specific parameter choices in the examples, e.g., sample sizes, dimensions, correlations parameters) we computed (for 10000 samples) the benchmark p-values (using normalized distance multivariance) and our estimates. Hereto we used various combinations of the moment estimations and p-value estimation as discussed in Section 4.5.
Then the relative mean squared error of the estimates in comparison to the benchmark was computed (considering only the relevant tail). Moreover, also for each case it was noted if the p-value was conservative in comparison to the benchmark (plus some margin of error). The results are summarized in Figure 16 and details are given in Section 6.3 in the Appendix.

For the methods described in Section 4.5 we use the abbreviations: classical estimate (c1), variance based estimate (cv), Pearson’s approximation (pe) and the central limit theorem method (clt). For the moment estimators we append to the methods name: limit (l) or finite sample (N), biased (b) or unbiased (u). Finally we appended (.no) if the normalized multivariance was used. Recall that we did not derive a finite sample estimator for the skewness, thus it is always estimated by its limit estimator.

Before deriving any conclusions note that by definition the results of this comparison depend on the choice of the utility function (i.e., here we prefer methods which ‘are not liberal and have small relative mean squared error’) and on the choice of examples. Nevertheless also with other utility functions and for other subsets of the data (see Section 6.3 in the Appendix for more details) the following observations appear:

- Pearson’s estimate used with the unbiased finite sample estimators for normalized multivariance performs very good. It has the lowest relative mean squared error for the estimates, thus it is closest to the benchmark power/empirical size.

In the case of dependent multivariate marginals it appears for small samples to be (too) liberal, i.e., more powerful than the benchmark - this requires further investigation.

- The variance estimate (in particular, used with the unbiased finite sample estimators for normalized multivariance) and the classical estimate are conservative. Theoretically the classical estimate is more conservative and this also shows in the dependence examples, see also Example 5.1. If the variance is large then both methods coincide.

- For \( m \)-multivariate with identically distributed marginals and \( n \) not too small (e.g., \( n > 10 \)) also the central limit theorem method shows good performance.

- There are some deviations which are notable:
  - In some examples the relative mean squared error increases with decreasing sample size (e.g., for \( N < 30 \)) – which seems somehow natural given the greater variability of estimates based on less data. Anyway, in this setting the resampling method could be considered as an alternative, in particular, since for small \( N \) the speed advantage of the moment methods is less pronounced (Example 5.4).
  - With increasing dimension (\( n \) large, e.g., \( n > 30 \)) also p-values of Pearson’s estimate become conservative for standard multivariance and total multivariance.
  - Due to its erratic behavior we excluded the example already discussed in Example 5.9, i.e., dependent Student distributed random variables with 1 degree of freedom which do not satisfy the moment conditions given in Remark 4.2 which are a prerequisite for the application of distance multivariance.
In the first plot are Gaussian quadratic forms and sample distance multivariance examples in the second are dependence examples, for details see Section 6.3 in the Appendix. The relative mean squared error to the benchmark (with cutoff at 1) is colored green to blue, and the heatmap is overlayed with red for cases where the p-value estimates were not conservative. The columns are ordered with decreasing error from left to right (treating ‘not conservative’ as error of size 2).
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**Table 2:** Comparison of numerical approximation schemes for the sums of coefficients for four univariate marginals (Ex. 5.6).

| $k$ | 1   | 2   | 3   |
|-----|-----|-----|-----|
| Bernoulli marginal |     |     |     |
| theoretical value | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{3}$ |
| 1. Nyström method | 0.475400 | 0.226005 | 0.107443 |
| 2. quadrature (kernels) | 0.475400 | 0.226005 | 0.107443 |
| 3. quadrature (expectations) | 0.500000 | 0.250000 | 0.125000 |
| 4. estimator (biased) | 0.499712 | 0.249712 | 0.124784 |
| 5. estimator (unbiased) | 0.500212 | 0.250212 | 0.125159 |
| uniform marginal |     |     |     |
| theoretical value | $\frac{1}{3}$ | $\frac{2}{15}$ | $\frac{8}{21}$ |
| 1. Nyström method | 0.287288 | 0.044055 | 0.008424 |
| 2. quadrature (kernels) | 0.287288 | 0.044055 | 0.008424 |
| 3. quadrature (expectations) | 0.333306 | 0.044459 | 0.008468 |
| 4. estimator (biased) | 0.336099 | 0.045536 | 0.008784 |
| 5. estimator (unbiased) | 0.336436 | 0.045538 | 0.008777 |
| normal marginal |     |     |     |
| theoretical value | $\frac{2}{\sqrt{\pi}}$ | $\frac{4\pi+12(1-\sqrt{3})}{3\sqrt{\pi}}$ | $\frac{8-8\pi+12\sqrt{3}-12\sqrt{3}+18\arctan 2\sqrt{3}}{\pi\sqrt{\pi}}$ |
| 1. Nyström method | 1.082144 | 0.401209 | 0.217387 |
| 2. quadrature (kernels) | 1.082144 | 0.401209 | 0.217387 |
| 3. quadrature (expectations) | 1.123745 | 0.408878 | 0.221314 |
| 4. estimator (biased) | 1.099665 | 0.385760 | 0.205712 |
| 5. estimator (unbiased) | 1.100766 | 0.385105 | 0.205009 |
| exponential marginal |     |     |     |
| theoretical value | $\frac{1}{\sqrt{\pi}}$ | $\frac{1}{\sqrt{\pi}}$ | $\frac{1}{\sqrt{\pi}}$ |
| 1. Nyström method | 0.953846 | 0.333081 | 0.166583 |
| 2. quadrature (kernels) | 0.953846 | 0.333081 | 0.166583 |
| 3. quadrature (expectations) | 0.995893 | 0.339694 | 0.169711 |
| 4. estimator (biased) | 0.964818 | 0.314795 | 0.152974 |
| 5. estimator (unbiased) | 0.965784 | 0.313787 | 0.151984 |
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6 Appendix

6.1 Notes on $x_0$ in the quadratic form estimate

We are interested in an explicit upper bound for $x_0$ in Theorem 2.1. Here we recall the setting in the final steps of its proof: Let $\alpha \in (0, 1]$ and $x_0(\alpha)$ be such that

$$0 < P \left( \frac{1}{1/\alpha} Y_{\lfloor 1/\alpha \rfloor} \leq x_0(\alpha) \right) = P \left( \frac{1}{1/\alpha + 1} Y_{\lfloor 1/\alpha \rfloor + 1} \leq x_0(\alpha) \right) < 1.$$ 

By [25, Prop. 1] the value of $x_0(\alpha)$ is unique, the function $\alpha \mapsto x_0(\alpha)$ is increasing on $(0, 1]$ and bounded by $x_0(1) \approx 1.536404$ (see Figure 17 for a plot of $x_0(\alpha)$). Furthermore, by [25, Prop. 1', p. 189],

$$P \left( \frac{1}{1/\beta} Y_{\lfloor 1/\beta \rfloor} \leq x \right) = \inf_{n \in \mathbb{N}, \frac{1}{n} \leq \beta} P \left( \frac{1}{n} Y_n \leq x \right)$$

for all $x \geq x_0(\beta)$. By this the statement of Theorem 2.1 was reduced in the proof to the inequality

$$\min \left\{ P \left( \frac{1}{1/\beta} Y_{\lfloor 1/\beta \rfloor} \leq x \right), P(Y_{\lfloor 1/\beta \rfloor} + (1 - \beta \lfloor 1/\beta \rfloor) Y_{\lfloor 2/\beta \rfloor} \leq x) \right\} \geq P(\alpha Y_{\frac{1}{\alpha}} \leq x) \quad (6.1)$$

for all $x \geq x_0(\beta)$ and all $\beta \leq \alpha$. By direct implementation $x_0(\alpha, \beta)$ – the smallest $x$ for which (6.1) holds – can be computed and it is less than $x_0(\alpha)$, see Figure 17.

To illustrate the difficulty of an analytic approach note that we have to prove the two inequalities

$$P \left( \frac{1}{1/\beta} Y_{\lfloor 1/\beta \rfloor} \leq x \right) \geq P(\alpha Y_{\frac{1}{\alpha}} \leq x), \quad (6.2)$$

$$P(Y_{\lfloor 1/\beta \rfloor} + (1 - \beta \lfloor 1/\beta \rfloor) Y_{\lfloor 2/\beta \rfloor} \leq x) \geq P(\alpha Y_{\frac{1}{\alpha}} \leq x). \quad (6.3)$$

The first inequality holds since (using results of numerical computations) for $x \geq x_0(\alpha)$ the function $r \mapsto P(\frac{1}{r} Y_r \leq x)$ is either increasing or convex with dominant value on the integers (i.e., it reaches on an interval $[i, i+1]$ the maximum on the right end point). Thus an analytic proof for (6.2) would ‘just’ amount to a calculation of the extreme values of this function – although the density is known explicitly it seems to be intangible (or at least very technical). For the second inequality it becomes even more difficult.

Figure 17: $x_0(\alpha)$ and $x_0(\alpha, \beta)$ (Sec. 6.1).
Gaussian quadratic forms and sample distance multivariance

Figure 18: The value of \( \alpha \mapsto 1 - \mathbb{P}(\alpha Y \geq x_0(\alpha)) \) with level 0.21 as horizontal line (Sec. 6.1, see also Remark 2.2.2).

6.2 Derivation of the unbiased estimator for \( \mu_i^{(3)} \)

In this section we give a more detailed exposition on the derivation of unbiased estimators for the summands in the representation (4.24) of \( \mu_i^{(3)} \), cf. Remark 4.13. For the sake of simplicity, we omit the dependence on the marginal and define

\[
\begin{align*}
    b &:= \mathbb{E}(\psi(X - X')^2), \\
    c &:= \mathbb{E}(\psi(X - X')\psi(X' - X'')) , \\
    g &:= \mathbb{E}(\psi(X - X')^3), \\
    u &:= m^3, \\
    w &:= b \cdot m, \\
    y &:= c \cdot m.
\end{align*}
\]

Then (4.24) reads \( \mu_i^{(3)} = -c + 3f - 3y + u \). Given a sample \( x = (x^{(1)}, \ldots, x^{(N)}) \) of \( X \) and \( B := (\psi(x^{(j)} - x^{(k)}))_{j,k = 1, \ldots, N} \) it is straightforward to find the following unbiased estimators for \( m, e, g \) and \( h \):

\[
\begin{align*}
    \frac{1}{N(N-1)}|B| &\xrightarrow{N \to \infty} m, \\
    \frac{1}{N(N-1)(N-2)}|B^2 \circ B| &\xrightarrow{N \to \infty} e, \\
    \frac{1}{N(N-1)}|B \circ B| &\xrightarrow{N \to \infty} g, \\
    \frac{1}{N(N-1)(N-2)}(|(B \circ B) \cdot B| - |B \circ B|) &\xrightarrow{N \to \infty} h.
\end{align*}
\]

In order to estimate \( f \) we start from the obvious (biased) estimator

\[
\hat{f} = \frac{1}{N^4} \sum_{j,k,l,m=1}^N \psi(x^{(j)} - x^{(k)})\psi(x^{(k)} - x^{(l)})\psi(x^{(l)} - x^{(m)}) = \frac{1}{N^4}|B^3|
\]
and obtain (for independent copies $X^{(\ell)}$, $1 \leq \ell \leq N$, of $X$)

$$
N^4 \mathbb{E}(\hat{f}) = \sum_{j=1}^{N} \sum_{k \neq j} \mathbb{E} \left( \psi(X^{(j)} - X^{(k)})^3 \right) \\
+ \sum_{m \neq j,k} \mathbb{E} \left( \psi(X^{(j)} - X^{(k)})^2 \psi(X^{(j)} - X^{(m)}) \right) \\
+ \sum_{\ell \neq j,k} \mathbb{E} \left( \psi(X^{(j)} - X^{(k)}) \psi(X^{(k)} - X^{(\ell)}) \psi(X^{(\ell)} - X^{(j)}) \right) \\
+ \mathbb{E} \left( \psi(X^{(j)} - X^{(k)}) \psi(X^{(k)} - X^{(\ell)})^2 \right) \\
+ \sum_{m \neq j,k,\ell} \mathbb{E} \left( \psi(X^{(j)} - X^{(k)}) \psi(X^{(k)} - X^{(\ell)}) \psi(X^{(\ell)} - X^{(m)}) \right) 
$$

$$
= N(N - 1)g + 2N(N - 1)(N - 2)h + N(N - 1)(N - 2)e \\
+ N(N - 1)(N - 2)(N - 3)f.
$$

Inserting the previously determined unbiased estimators for $e, g$ and $h$ we arrive at (4.37), i.e.,

$$
\frac{1}{N(N - 1)(N - 2)(N - 3)} \left( |B^3| - |B^2 \circ B| - 2|B \circ B| \cdot B| + |B \circ B \circ B| \right) \xrightarrow{N \to \infty} f.
$$

Similarly the estimators for the auxiliary variables $v$ and $w$ are obtained

$$
\frac{1}{N(N - 1)(N - 2)(N - 3)} \left( \text{cs}(B) \circ \text{cs}(B) \circ \text{cs}(B) \right) + 2 |B \circ B \circ B| \\
- 3 |(B \circ B) \cdot B| \xrightarrow{N \to \infty} v,
$$

$$
\frac{1}{N(N - 1)(N - 2)(N - 3)} \left( |B \circ B| \cdot |B| - 4 |(B \circ B) \cdot B| + 2 |B \circ B \circ B| \right) \xrightarrow{N \to \infty} w,
$$

where $\text{cs}(B)$ denotes the vector of the column sums of $B$.

To find an unbiased estimator for $y = c \cdot m$ we start from

$$
\hat{y} = \frac{1}{N^5} \sum_{j,k,\ell,m,n=1}^{N} \psi(x^{(j)} - x^{(k)}) \psi(x^{(k)} - x^{(\ell)}) \psi(x^{(m)} - x^{(n)}) = \frac{1}{N^5} |B^2| \cdot |B|
$$
and obtain

\[ N^5 \mathcal{E}(\hat{g}) = \sum_{j} \sum_{k \neq j} 2 \mathbb{E} \left( \psi(X^{(j)} - X^{(k)})^3 \right) + 4 \sum_{n \neq j, k} \mathbb{E} \left( \psi(X^{(j)} - X^{(k)})^2 \psi(X^{(n)} - X^{(j)}) \right) \]

\[ + \sum_{m \neq j, k} \sum_{n \neq j, k, m} \mathbb{E} \left( \psi(X^{(j)} - X^{(k)})^2 \psi(X^{(m)} - X^{(n)}) \right) \]

\[ + \sum_{\ell \neq k, j} \left[ 2 \mathbb{E} \left( \psi(X^{(j)} - X^{(k)})^2 \psi(X^{(k)} - X^{(\ell)}) \right) \right. \]

\[ \left. + 2 \mathbb{E} \left( \psi(X^{(j)} - X^{(k)}) \psi(X^{(k)} - X^{(\ell)}) \right) \right] \]

\[ = 2N(N - 1)^g + 4N(N - 1)(N - 2)h + N(N - 1)(N - 2)(N - 3)w + 4N(N - 1)(N - 2)h \]

\[ 2N(N - 1)(N - 2)e + 2N(N - 1)(N - 2)(N - 3)v + 4N(N - 1)(N - 2)(N - 3)f \]

\[ + N(N - 1)(N - 2)(N - 3)(N - 4)g. \]

Thus, inserting all previously determined unbiased estimators we arrive at (4.38), i.e.,

\[ \frac{(N - 5)!}{N!} \left( |B|^2 \cdot |B| - |B \circ B| \cdot |B| - 2| \circ \circ \circ \circ \circ \circ \circ \circ \circ | \right) \]

\[ - 4|B \circ B| - 4|B^3| + 2|B^2 \circ B| + 10(|B \circ B \cdot B|) \xrightarrow{N \to \infty} y = m \cdot c. \]

Finally, for \( u = m^3 \) we start from

\[ \hat{u} = \frac{1}{N^6} \sum_{j, k, \ell, m, n, o = 1} N \psi(x^{(j)} - x^{(k)}) \psi(x^{(\ell)} - x^{(m)}) \psi(x^{(n)} - x^{(o)}) = \frac{1}{N^6} |B|^3 \]
to obtain

\[ N \theta \mathbb{E}(\bar{u}) = \sum_{j=1}^{N} \sum_{k \neq j} \left[ 4 \mathbb{E}(\psi(X^{(j)} - X^{(k)})^3) \right] \\
+ 2 \sum_{n \neq j, k} \left[ 4 \mathbb{E}(\psi(X^{(j)} - X^{(k)})^2 \psi(X^{(n)} - X^{(j)}) \right] \\
+ \sum_{o \neq j, k, n} \mathbb{E}(\psi(X^{(j)} - X^{(k)})^2 \psi(X^{(n)} - X^{(o)})) \right] \\
+ 2 \sum_{m \neq j, k} \left[ 4 \mathbb{E}(\psi(X^{(j)} - X^{(k)})^2 \psi(X^{(j)} - X^{(m)}) \right] \\
+ 2 \mathbb{E}(\psi(X^{(j)} - X^{(k)}) \psi(X^{(j)} - X^{(m)}) \psi(X^{(m)} - X^{(k)})) \right] \\
+ 2 \sum_{o \neq j, k, m} \mathbb{E}(\psi(X^{(j)} - X^{(k)}) \psi(X^{(j)} - X^{(m)}) \psi(X^{(m)} - X^{(o)})) \right] \\
+ \sum_{n \neq j, k, m, o} \sum_{o \neq j, k, m, n} \mathbb{E}(\psi(X^{(j)} - X^{(k)}) \psi(X^{(j)} - X^{(m)}) \psi(X^{(n)} - X^{(o)})) \right] \\
= N(N - 1)(4g + 2(N - 2)(4h + (N - 3)w) \\
+ 4(N - 2)(4h + 2e + 4(N - 3)f + 2(N - 3)v + (N - 3)(N - 4)y) \\
+ (N - 2)(N - 3)(4w + 8f + 8(N - 4)y + (N - 4)(N - 5)u) \\
+ 4N(N - 1)g + 4N(N - 1)(N - 2)(6h + 2e) + N(N - 1)(N - 2)(N - 3)(6w + 24f + 8v) \\
+ 12N(N - 1)(N - 2)(N - 3)(N - 4)g + N(N - 1)(N - 2)(N - 3)(N - 4)(N - 5)u. \]
Inserting all previously determined unbiased estimators we arrive at (4.39), i.e.,
\[
\frac{(N-6)!}{N!} ([B]^3 + 16|B \circ B \circ B| - 48(B \circ B) \cdot B| - 8|B^2 \circ B| \\
+ 6|B| \cdot |B \circ B| + 24|B^3| + 16|\text{cs}(B) \circ \text{cs}(B) \circ \text{cs}(B)| - 12|B^2| \cdot |B|) \xrightarrow{N \to \infty} u = m^3.
\]

6.3 Details of the comparative study (Example 5.10)

To complement the brief description in Example 5.10 we provide here some more details. First the examples are explained, thereafter some aspects are discussed.

We consider the following examples (using the labels also used in the figures, e.g., Figure 16):

### multivariate:

- **H₀ examples:**
  - `mv_bern, mv_unif, mv_normal:` Bivariate multivariate with independent multivariate marginals of dimension 5 (with independent components). `bern` denotes the Bernoulli distribution with success probability \( \frac{1}{2} \), `unif` denotes the uniform distribution on \([0, 1]\) and `normal` denotes the standard normal distribution. If not stated otherwise, these abbreviations have the same meaning also in the other examples.
  - `SRB2H₀, SRB3H₀:` The \( H₀ \) examples corresponding to `SRB2` and `SRB3` (see below).
  - `student, bernoulli, uniform, normal:` With the named marginals for \( N = 10, 20, \ldots, 100 \) and \( n = 2, 3 \)
  - `bernoulli_n, uniform_n, normal_n:` With the named marginals for \( N = 100 \) and \( n = 3, 4, \ldots, 9, 10, 15, 20, 25, 30, 40, 50, 75, 100 \).
  - `mixed:` \( n = 6 \) with marginals of the exponential (with parameter 1), normal, Bernoulli, uniform, Poisson (with parameter 1) and binomial distribution (with parameters 10 and \( \frac{1}{2} \)).

- **dependence examples:**
  - `mvnormal:` Bivariate standard normal distribution with scale matrix \( \Sigma = \begin{pmatrix} 1 & 0.1 \\ 0.1 & 1 \end{pmatrix} \).
  - `SRB1a:` Example 1.(a) of [26]. The same as `mvnormal` but with multidimensional marginals with dimension 5, the covariance matrix then coincides with the matrix described in Example 5.9
  - `SRB2:` Example 2 of [26] (multiplicative dependence): \( Y₁, \ldots, Y₅, Z₁, \ldots, Z₅ \sim N(0,1) \) independent and \( X¹ := (Y₁, \ldots, Y₅) \), \( X₂ := (Y₁Z₁, \ldots, Y₅Z₅) \).
  - `SRB3:` Example 3 of [26] (non-linear functional dependence): \( Y₁, \ldots, Y₅ \sim N(0,1) \) independent and \( X¹ := (Y₁, \ldots, Y₅) \), \( X₂ := (\log(Y₁)^2, \ldots, \log(Y₅)^2) \).
  - `normal_tetrahedron, uniform_tetrahedron, tetrahedron:` The normal tetrahedron is defined in Example 5.1. Replacing therein \( Zₗ \) with uniform random variables or with constant 0 variables yields the other two.

### m-multivariate: Here the suffix `m2` indicates that 2-multivariate is considered, analogously for `m3`.

- **H₀ examples:**
  - `normal_tetrahedron_m2, uniform_tetrahedron_m2, tetrahedron_m2, mixed_m3, mixed_m2, bernoulli_n_m3, bernoulli_n_m2, normal_n_m3, normal_n_m2, uniform_n_m3, uniform_n_m2:` Same as the examples having the same name without the suffix.
  - `dep_struct_several_m2:` This is an example with higher order dependence structure (dependence structure with several clusters) discussed in [4] Example 7.5. There are 25 Bernoulli random variables, which are pairwise independent but have dependences of higher order, and
an independent standard normal random variable.

dep\_struct\_several\_H0\_m3: This is the $H_0$ example to the above for 3-multivariance, i.e.,
here the random variables have the same marginal distributions as above and they are inde-
pendent.

yao\_H0\_m2, yao\_coins\_H0\_m3: These are the $H_0$ examples to those with the corresponding
names below.

dependence examples:

yao\_AR\_m2, yao\_block\_m2, yao\_band\_m2, yao\_coins\_m3: These are examples of \cite{28} which are
also discussed in \cite{4} Example 7.15. For the first three $N = 60$ and $n = 50, 100, 200, 400, 800$
where the random variables are jointly multivariate normally distributed and their dependence
is auto-regressive (AR), given by a block structure (block) or a band structure (band). In the
coins example the random variables are pairwise independent Bernoulli random variables,
but (some) triples are dependent. For this the parameters $n = 18, 36, 72$ and $N = 60, 100, 200$
are used.

dep\_struct\_several\_m3: See dep\_struct\_several\_H0\_m3.

total multivariance: Here the suffix \_mt indicates that total multivariance is considered. All these
examples are already described above, we list them here just for convenience.

$H_0$ examples:

bernoulli\_n\_mt, normal\_n\_mt, uniform\_n\_mt, dep\_struct\_several\_H0\_mt, mixed\_mt.

dependence examples:

uniform\_tetrahedron\_mt, normal\_tetrahedron\_mt, tetrahedron\_mt,

dep\_struct\_several\_mt.

From these examples samples were generated (10000 samples for each parameter setting). Then the
methods described in Section 4.5 were used to estimate the p-value of each sample.

Thereafter the relative mean squared error of these p-values to the benchmark was computed. Here the
benchmark is the p-value computed by the empirical distribution of normalized (total, $m$-)multivariance
of 10000 samples obtained from the given 10000 samples by resampling each only once (hence we say
that it is obtained by 'Monte Carlo (re)sampling').

Since the classical estimate (4.62) and the variance based estimate (4.63) are only tail estimates we
skipped those samples where the p-value and the benchmark were above 0.21 (cf. Remark 2.2.2). If both,
the estimate and the benchmark p-value, were below 0.001 the error was set to 0, since below this the
value of the benchmark (based on a sample of size 10000) would rely on less than 10 samples. This
seems also reasonable since in applications usually significance levels between 0.1 and 0.001 are used.
For values below, the exact size is of less (or no) interest.

Moreover, for each parameter setting we noted for how many of the 10000 samples the estimated
p-value was larger than the benchmark plus a margin of error. Where this margin was taken to be the
minimum of 0.05 and 50% of the benchmark. The method was then marked to be too liberal (for the
given parameter setting) if more then 30% of the samples were overestimated.

Based on the above the heatmaps in Figure 16 were computed.

Certainly some of the above is disputable. We are aware of this, and we hope that our choices reflect
the interests of the readers. To complement it we discuss briefly some further aspects:

• One could argue that only tests with a fixed significance level $\lambda$ are performed. Thus one would
only compare the power/empirical size for a fixed significance level and not compare the p-values
directly. This yields with $\lambda = 0.05$ the results summarized in Figure 19. In contrast our above
method does, roughly speaking, a comparison uniformly over all possible $\lambda$, which allows the
detection of differences which are otherwise lost due to averaging.

• Instead of our huge comparison one could (and for special situations should) concentrate on a
subset: For example, see Figure 20 for a comparison of $m$-multivariance for cases with $n > 10$, it
shows that the central limit theorem method works well in this setting. It actually works also for the partly mixed case of **dep_struct_several**. Figure 27 shows the performance for cases with \( n > 30 \), note that Pearson’s estimate only becomes conservative for standard multivariate and total multivariate. For \( m \)-multivariate it works well since in a sense only \( m = 2, 3 \) variables are considered, thus it is actually a lower dimensional case.

Figure 19: Heatmaps of the same examples in the same order as in Figure 16, but here the differences of the empirical size/power of the method and the benchmark is depicted (without overlay). The scale is from -1 (blue, conservative) by 0 (green, zero difference) to 1 (red, liberal).
Figure 20: Heatmap of the performance of the methods (columns) for various examples (rows). Here: all examples with $m$-multivariance and $n > 10$. The relative mean squared error to the benchmark (with cutoff at 1) is colored green to blue, and the heat map is overlayed with red for cases where the p-value estimates were not conservative. The columns are ordered with decreasing error from left to right (treating 'not conservative' as error of size 2).

Figure 21: Heatmap of the performance of the methods (columns) for various examples (rows). Here: all examples with $n > 30$. The relative mean squared error to the benchmark (with cutoff at 1) is colored green to blue, and the heat map is overlayed with red for cases where the p-value estimates were not conservative. The columns are ordered with decreasing error from left to right (treating 'not conservative' as error of size 2).