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Author(s): Dümbgen, Lutz; Nordhausen, Klaus

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Approximating Symmetrized Estimators of Scatter via Balanced Incomplete U-Statistics

Lutz Dümbgen^{*} and Klaus Nordhausen University of Bern and University of Jyväskylä

Abstract

We derive limiting distributions of symmetrized estimators of scatter, where instead of all $n(n -$ 1)/2 pairs of the *n* observations we only consider *nd* suitably chosen pairs, $1 \le d \le \lfloor n/2 \rfloor$. It turns out that the resulting estimators are asymptotically equivalent to the original one whenever $d = d(n) \rightarrow \infty$ at arbitrarily slow speed. We also investigate the asymptotic properties for arbitrary fixed d. These considerations and numerical examples indicate that for practical purposes, moderate fixed values of d between 10 and 20 yield already estimators which are computationally feasible and rather close to the original ones.

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Corresponding author: Lutz Dümbgen, e-mail: duembgen@stat.unibe.ch

1 Introduction

Robust estimation of multivariate scatter for a distribution P on \mathbb{R}^q , $q \geq 1$, is a recurring topic in statistics. For instance, different estimators of multivariate scatter are an important ingredient for independent component analysis (ICA) or invariant coordinate selection (ICS), see [Nordhausen](#page-23-0) [et al.](#page-23-0) [\(2008\)](#page-23-0), [Tyler et al.](#page-24-0) [\(2009\)](#page-24-0) and the references therein. Other potential applications are classification methods and multivariate regression, see for instance [Nordhausen and Tyler](#page-23-1) [\(2015\)](#page-23-1). Of particular interest are symmetrized estimators of scatter which are defined in Section [2.](#page-3-0) Throughout this paper we consider independent random vectors X_1, X_2, \ldots, X_n with distribution P. The symmetrized estimators are just standard functionals of scatter (with given center $0 \in \mathbb{R}^q$) applied to the empirical distribution

$$
\hat{Q}_n := \binom{n}{2}^{-1} \sum_{1 \leq i < j \leq n} \delta_{X_j - X_i}^s,
$$

where $\delta_z^s := 2^{-1}(\delta_z + \delta_{-z})$, and δ_z denotes Dirac measure at $z \in \mathbb{R}^q$. Thus, \hat{Q}_n is the empirical distribution of all $n(n - 1)$ differences of two different observations, and it may be viewed as a measure-valued version of a U-statistic as introduced by [Hoeffding](#page-23-2) [\(1948\)](#page-23-2). It is an unbiased estimator of the symmetrized distribution

$$
Q = Q(P) := \mathcal{L}(X_1 - X_2). \tag{1}
$$

Here and throughout, $\mathcal{L}(\cdot)$ stands for 'distribution of'. The computation of symmetrized Mestimators of scatter is rather time-consuming, whence some people refrain from using them. However, the symmetrized estimators have two desirable properties: one avoids the estimation of a location nuisance parameter, and the underlying scatter functional has the so-called block independence property as explained in Section [2;](#page-3-0) see also Dümbgen [\(1998\)](#page-22-0) and Sirkiä et al. [\(2007\)](#page-23-3).

To diminish the computational burden, one could replace the empirical distribution \hat{Q}_n with the empirical distribution

$$
\hat{Q}_{n,d} := (nd)^{-1} \sum_{i=1}^{n} \sum_{j=i+1}^{i+d} \delta_{X_j - X_i}^s
$$

for some integer $1 \le d \le (n-1)/2$, where $X_{n+s} := X_s$ for $1 \le s \le n$. This is a measure-valued version of a reduced U-statistic as introduced by [Blom](#page-22-1) [\(1976\)](#page-22-1) and [Brown and Kildea](#page-22-2) [\(1978\)](#page-22-2). Other authors, e.g. [Lee](#page-23-4) [\(1990\)](#page-23-4), call this a balanced incomplete U-statistic. In the context of estimation of scatter, [Miettinen et al.](#page-23-5) [\(2016\)](#page-23-5) illustrate the potential benefits of $\hat{Q}_{n,d}$ compared to \hat{Q}_n in simulations. As a preliminary proof of concept, they present the asymptotic properties of the estimator $2^{-1} \int_{\mathbb{R}^q} y y^\top \hat{Q}_{n,d}(dy)$ in comparison to the usual sample covariance matrix $2^{-1} \int_{\mathbb{R}^q} y y^\top \hat{Q}_n(dy)$. Their findings are encouraging, but the latter estimator can be computed rather easily in $O(n)$ steps and is non-robust of course.

The purpose of the present paper is to provide an in-depth analysis of robust and smooth symmetrized scatter estimators based on \hat{Q}_n and $\hat{Q}_{n,d}$, where the computation time with \hat{Q}_n can

definitely become a limiting factor. It turns out that these two scatter estimators are asymptotically equivalent whenever $d = d(n) \rightarrow \infty$. Here and throughout the sequel, asymptotic statements are meant as $n \to \infty$. More precisely, if $\Sigma(\cdot)$ is our functional of scatter, then it will be shown that the following statements are true: There exist two stochastically independent and centered Gaussian random matrices G_1, G_2 whose distribution depends only on P and $\Sigma(\cdot)$ such that

$$
\sqrt{n} \big(\mathbf{\Sigma}(\hat{Q}_{n,d(n)}) - \mathbf{\Sigma}(Q) \big) = \sqrt{n} \big(\mathbf{\Sigma}(\hat{Q}_n) - \mathbf{\Sigma}(Q) \big) + o_p(1) \rightarrow_{\mathcal{L}} \mathbf{G}_1
$$

provided that $d(n) \to \infty$. Here ' $o_p(1)$ ' denotes a random term converging to zero in probability, and ' \rightarrow _{*C*}' denotes convergence in distribution. For any fixed integer $d \ge 1$,

$$
\sqrt{n} \big(\mathbf{\Sigma}(\hat{Q}_{n,d}) - \mathbf{\Sigma}(Q) \big) \rightarrow_{\mathcal{L}} \mathbf{G}_1 + d^{-1/2} \mathbf{G}_2.
$$

This explains why for sufficiently large but fixed d, the estimator $\Sigma(\hat{Q}_{n,d})$ is a good surrogate for ${\boldsymbol \Sigma}(\hat{Q}_n).$

An easy way to compute $\Sigma(\hat{Q}_{n,d})$ is to generate a data matrix containing the nd differences $X_j - X_i$, where $i \in \{1, ..., n\}$ and $j \in \{i+1, ..., i+d\}$, and to apply $\Sigma(\cdot)$ to the empirical distribution $(nd)^{-1} \sum_{k=1}^{nd} \delta_{Y_k}^s$ of these nd vectors Y_k . But for large values of nd, this may be too cumbersome. A possible alternative is to compute the average $d^{-1} \sum_{\ell=1}^d \Sigma(\hat{Q}_{n,1}^{(\ell)})$ $\binom{k}{n,1}$ with the same $d \geq 1$, where $\hat{Q}_{n,1}^{(1)}$ $\hat{Q}_{n,1}^{(1)},\ldots,\hat{Q}_{n,1}^{(d)}$ $n_1^{(d)}$ are defined as $\hat{Q}_{n,1}$, but with d random permutations of the observations X_1, X_2, \ldots, X_n . It turns out that for fixed d, this average has the same asymptotic distribution as $\mathbf{\Sigma}(\hat{Q}_{n,d})$.

The remainder of this paper is organized as follows: In Section [2,](#page-3-0) we recall some basic facts about scatter functionals and symmetrized scatter functionals as presented by Dümbgen et al. [\(2015\)](#page-23-6). In Section [3,](#page-7-0) the asymptotic results mentioned before are stated in detail. The theory is illustrated with numerical examples in Section [4.](#page-8-0) All proofs are deferred to Section [5](#page-11-0) and Appendix A. The starting point is standard theory for complete and incomplete U -statistics as presented, for instance, by [Serfling](#page-23-7) [\(1980\)](#page-23-7) and [Lee](#page-23-4) [\(1990\)](#page-23-4). Suitable modifications of these results, combined with linear expansions for functionals of scatter yield the asymptotic distributions of $\Sigma(\hat{Q}_n)$ and $\Sigma(\hat{Q}_{n,d})$. For the averaging estimator $d^{-1}\sum_{\ell=1}^d \Sigma(\hat{Q}_{n,d}^{(\ell)})$ $\binom{(\ell)}{n,1}$, we derive and use a variation of the combinatorial central limit theorem of [Hoeffding](#page-23-8) [\(1951\)](#page-23-8). This result is potentially of independent interest, for instance, in the context of kernel mean embeddings as used in machine learning [\(Muandet et al., 2017\)](#page-23-9).

2 Functionals of Scatter

The material in this section is adapted from the survey of Dümbgen et al. (2015) , where the latter builds on previous work of [Tyler](#page-24-1) [\(1987\)](#page-24-1), [Kent and Tyler](#page-23-10) [\(1991\)](#page-23-10) and [Dudley et al.](#page-22-3) [\(2009\)](#page-22-3).

The space of symmetric matrices in $\mathbb{R}^{q \times q}$ is denoted by $\mathbb{R}^{q \times q}_{sym}$, and $\mathbb{R}^{q \times q}_{sym,+}$ stands for its subset of positive definite matrices. The identity matrix in $\mathbb{R}^{q \times q}$ is written as I_q . The Euclidean norm of a vector $v \in \mathbb{R}^q$ is denoted by $||v|| = \sqrt{v^{\top}v}$. For matrices M, N with identical dimensions we write

$$
\langle M, N \rangle \; := \; \operatorname{tr}(M^\top N) \quad \text{and} \quad \|M\| \; := \; \sqrt{\langle M, M \rangle},
$$

so $||M||$ is the Frobenius norm of M.

2.1 Functionals of scatter for centered distributions

Let Q be a given family of probability distributions on \mathbb{R}^q which are viewed as centered around 0. In our specific applications, this is plausible, because Q consists of symmetrized distributions. We consider a function $\Sigma: \mathcal{Q} \to \mathbb{R}^{q \times q}_{sym,+}$, called a functional of scatter, and $\Sigma(Q)$ is the scatter matrix of $Q \in \mathcal{Q}$. For the general theory presented in the next section, we assume that \mathcal{Q} and Σ have two important properties.

Linear equivariance. We assume that for any nonsingular matrix $B \in \mathbb{R}^{q \times q}$ and any distribution $Q \in \mathcal{Q}$, the distribution $Q^B := \mathcal{L}(BY)$ with $Y \sim Q$ belongs to $\mathcal Q$ too, and that

$$
\Sigma(Q^B) = B\Sigma(Q)B^{\top}.
$$
 (2)

Linear equivariance has some interesting implications. For instance, if $Q \in \mathcal{Q}$ is spherically symmetric in the sense that $Q^B = Q$ for all orthogonal matrices $B \in \mathbb{R}^{q \times q}$, then $\Sigma = cI_q$ for some $c > 0$. Furthermore, if $Q^B = Q$ for some matrix $B = \text{diag}(\xi_1, \dots, \xi_q)$ with $\xi \in \{-1, 1\}^q$, then for arbitrary different indices $i, j \in \{1, \ldots, q\}$, the (i, j) -th component of $\Sigma(Q)$ satisfies

$$
\Sigma(Q)_{ij} = 0 \quad \text{whenever } \xi_i \neq \xi_j. \tag{3}
$$

Differentiability. We assume that Q is an open subset of the family of all probability distributions on \mathbb{R}^q in the topology of weak convergence. Moreover, for any distribution $Q \in \mathcal{Q}$, there exists a bounded, measurable and even function $J = J_Q : \mathbb{R}^q \to \mathbb{R}^{q \times q}_{sym}$ such that $\int_{\mathbb{R}^q} J dQ = 0$, and for other distributions $\check{Q} \in \mathcal{Q}$,

$$
\Sigma(\check{Q}) = \Sigma(Q) + \int_{\mathbb{R}^q} J d\check{Q} + o\left(\left\|\int_{\mathbb{R}^q} J d\check{Q}\right\|\right)
$$

as $\check{Q} \to Q$ weakly. Note that this differentiability property of $\Sigma(\cdot)$ implies its robustness in the sense that $\Sigma(\check Q)\to\Sigma(Q)$ as $\check Q\to Q$ weakly, because then $\int_{\R^q} J\,d\check Q\to \int_{\R^q} J\,dQ=0.$

M-functionals of scatter. An important example for Σ are M-functionals of scatter, driven by a function $\rho : [0, \infty) \to \mathbb{R}$ with the following properties: ρ is twice continuously differentiable such that $\psi(s) := s\rho'(s)$ satisfies the inequalities $\psi'(s) > 0$ for $s > 0$ and $q < \psi(\infty)$:= $\lim_{s\to\infty}\psi(s)<\infty$. For any distribution Q on \mathbb{R}^q and $\Sigma\in\mathbb{R}^{q\times q}_{\text{sym},+}$, let

$$
L_{\rho}(\Sigma, Q) := \int_{\mathbb{R}^q} \left[\rho(y^\top \Sigma^{-1} y) - \rho(y^\top y) \right] Q(dy) + \log \det(\Sigma). \tag{4}
$$

The function $L_{\rho}(\cdot, Q)$ has a unique minimizer $\Sigma(Q)$ on $\mathbb{R}_{{\rm sym},+}^{q \times q}$ if and only if

$$
Q(\mathbb{W}) \ < \ \frac{\psi(\infty) - q + \dim(\mathbb{W})}{\psi(\infty)}
$$

for any linear subspace W of \mathbb{R}^q with $0 \le \dim(W) < q$. The set Q of distributions which satisfy the latter constraints is open with respect to weak convergence.

A particular example for a function ρ with the stated properties is given by $\rho(s) = \rho_{\nu}(s)$: $(\nu + q) \log(s + \nu)$, where $\nu > 0$.

The function $J = J_Q$ is rather complicated in general. But in case of a spherically symmetric distribution Q with $\Sigma(Q) = I_q$,

$$
J(y) = \frac{q+2}{q+2+2\kappa} \rho'(\|y\|^2) \left(yy^\top - \frac{\|y\|^2}{q} I_q \right) + \frac{1}{1+\kappa} \left(\rho'(\|y\|^2) \frac{\|y\|^2}{q} - 1 \right) I_q
$$

for $y \in \mathbb{R}^q$, where $\kappa := q^{-1} \int_{\mathbb{R}^q} \rho''(||y||^2) ||y||^4 Q(dy) \in (-1, \infty)$.

2.2 Tyler's (1987) functional of scatter

For any distribution Q on \mathbb{R}^q such that $Q({0}) = 0$ and $\Sigma \in \mathbb{R}^{q \times q}_{sym,+}$, let

$$
L_0(\Sigma, Q) := q \int_{\mathbb{R}^q} \log \left(\frac{y^\top \Sigma^{-1} y}{y^\top y} \right) Q(dy) + \log \det(\Sigma).
$$

Note that $L_0(t\Sigma, Q) = L_0(\Sigma, Q)$ for all $t > 0$. The function $L_0(\cdot, Q)$ has a unique minimizer $\Sigma_0(Q)$ on the set $\left\{ \Sigma \in \mathbb{R}^{q \times q}_{sym,+} : \det(\Sigma) = 1 \right\}$ if and only if

$$
Q(\mathbb{W}) \; < \; \frac{\dim(\mathbb{W})}{q}
$$

for any linear subspace W of \mathbb{R}^q with $1 \leq \dim(\mathbb{W}) < q$. The set of all distributions Q which satisfy the latter constraints and $Q({0}) = 0$ is denoted by Q_0 .

The functional Σ_0 satisfies a restricted equivariance property: For any $Q \in \mathcal{Q}_0$ and any nonsingular matrix $B \in \mathbb{R}^{q \times q}$ with $|\det(B)| = 1$, equation [\(2\)](#page-4-0) holds true with Σ_0 in place of Σ. This implies that $\Sigma_0(Q) = I_q$ if Q is spherically symmetric. Moreover, if $Q^B = Q$ with $B = diag(\xi_1, \dots, \xi_q)$ and $\xi \in \{-1, 1\}^q$, then [\(3\)](#page-4-1) is satisfied with Σ_0 in place of Σ .

The functional Σ_0 is also differentiable in the following sense: For any distribution $Q \in \mathcal{Q}_0$ there exists a bounded, continuous and even function $J:\mathbb{R}^q\setminus\{0\}\to\mathbb{R}^{q\times q}_{\text{sym}}$ such that $\int_{\mathbb{R}^q}J\,dQ=0$, trace $\left(\mathbf{\Sigma}_{0}(Q)^{-1}J\right)\equiv0,$ and for any distribution $\check{Q}\in\mathcal{Q},$

$$
\Sigma_0(\check{Q}) = \Sigma_0(Q) + \int_{\mathbb{R}^q} J d\check{Q} + o\left(\left\|\int_{\mathbb{R}^q} J d\check{Q}\right\|\right)
$$

as $\check{Q} \to Q$ weakly. Again, the function $J = J_Q$ is rather complicated in general. But in case of a spherically symmetric distribution $Q \in \mathcal{Q}_0$,

$$
J(y) = (q+2)(\|y\|^{-2}yy^{\top} - q^{-1}I_q), \quad y \in \mathbb{R}^q \setminus \{0\}.
$$

2.3 Symmetrized M-functionals of scatter

Now we consider a general distribution P on \mathbb{R}^q and want to define its scatter matrix without having to specify a center of P. To this end we consider the symmetrized distribution $Q = Q(P)$ as defined in [\(1\)](#page-2-0). Then the symmetrized version of the functional of scatter Σ is given by

$$
\Sigma^{\rm s}(P) := \Sigma(Q(P)).
$$

Here we assume that P belongs to the family P of all probability distributions on \mathbb{R}^q such that $Q(P) \in \mathcal{Q}$. In case of an M-functional Σ with underlying function ρ , a sufficient condition for $P \in \mathcal{P}$ is that

$$
P(H) = 0 \quad \text{for any hyperplane } H \subset \mathbb{R}^q. \tag{5}
$$

Analogously, one may define the symmetrized version of Tyler's functional Σ_0 via $\Sigma_0^s(P)$:= $\Sigma_0(Q(P))$, where we assume that P belongs to the family P_0 of all probability distributions on \mathbb{R}^p such that $Q(P) \in \mathcal{Q}_0$. Again, condition [\(5\)](#page-6-0) is sufficient for that.

As to the benefits of symmetrization, suppose that P is elliptically symmetric with unknown center $\mu_* \in \mathbb{R}^q$ and unknown scatter matrix $\Sigma_* \in \mathbb{R}^{q \times q}_{sym,+}$. That means, the distribution of $\sum_{k=1}^{\infty} (X_1 - \mu_k)$ is spherically symmetric. Then $Q(P)$ is elliptically symmetric with center 0 and the same scatter matrix Σ_* . Note that Σ_* is defined only up to positive multiples. This is no problem as long as one is mainly interested in the shape matrix shape(Σ_*), where

$$
\operatorname{shape}(\Sigma) \; := \; \det(\Sigma)^{-1/q} \, \Sigma
$$

for $\Sigma \in \mathbb{R}^{q \times q}_{sym,+}$, that is, shape (Σ) is a positive multiple of Σ with determinant one. For instance, in connection with principal components, regression coefficients and correlation measures, multiplying Σ_* with a positive scalar has no impact. Our specific choice of shape(Σ) is justified by [Paindaveine](#page-23-11) [\(2008\)](#page-23-11).

Symmetrization has a second, even more important advantage: Consider an arbitrary distribution P, not necessarily symmetric in any sense. Suppose that a random vector $X \sim P$ may be written as $X = [X_a^{\top}, X_b^{\top}]^{\top}$ with independent subvectors $X_a \in \mathbb{R}^{q(a)}$ and $X_b \in \mathbb{R}^{q(b)}$. Then $\Sigma^{\rm s}(P)$ is block-diagonal in the sense that

$$
\mathbf{\Sigma}^{\rm s}(P) \;=\; \begin{bmatrix} \mathbf{\Sigma}_{\rm a}(P) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Sigma}_{\rm b}(P) \end{bmatrix}
$$

with certain matrices $\Sigma_a(P) \in \mathbb{R}^{q(a) \times q(a)}_{sym,+}$ and $\Sigma_b(P) \in \mathbb{R}^{q(b) \times q(b)}_{sym,+}$.

At this point, it is not clear whether \hat{Q}_n or $\hat{Q}_{n,d}$ belongs to \mathcal{Q} . As explained in Section [5,](#page-11-0) \hat{Q}_n and $\hat{Q}_{n,d}$ converge weakly in probability to Q, uniformly in $1 \leq d \leq (n-1)/2$. Thus, $\mathbb{P}(\hat{Q}_n \in \mathcal{Q})$ and $\min_{1 \leq d \leq (n-1)/2} \mathbb{P}(\hat{Q}_{n,d} \in \mathcal{Q})$ converge to 1. The same conclusion is true for $(\Sigma_0, \mathcal{Q}_0)$ in place of (Σ, \mathcal{Q}) , if we assume that P has no atoms, that is, if $P({x}) = 0$ for any $x \in \mathbb{R}^q$. Here is also a non-asymptotic result for M -estimators of scatter in case of smooth distributions P :

Proposition 1. Suppose that P satisfies [\(5\)](#page-6-0). With probability one, $\hat{Q}_n({0}) = \hat{Q}_{n,d}({0}) = 0$, and in the case of $n > q$,

$$
\hat{Q}_n(\mathbb{W}), \hat{Q}_{n,d}(\mathbb{W}) \ < \ \frac{\dim(\mathbb{W})}{q}
$$

for arbitrary linear subspaces W of \mathbb{R}^q with $1 \leq \dim(W) < q$ and $1 \leq d \leq (n-1)/2$.

This theorem implies that for the M-functional $\Sigma(\cdot)$, the symmetrized M-estimators $\Sigma(\hat{Q}_n)$ and $\sum(\hat{Q}_{n,d})$ are well-defined almost surely for $1 \leq d \leq (n-1)/2$, provided that $n > q$ and F satisfies [\(5\)](#page-6-0). The same conclusion is true for Tyler's M-functional $\Sigma_0(\cdot)$ in place of $\Sigma(\cdot)$.

3 Asymptotic Expansions and Distributions

In what follows, $\Sigma(\cdot)$ denotes either a linear equivariant and differentiable scatter functional or Tyler's functional $\Sigma_0(\cdot)$. In addition to \hat{Q}_n and $\hat{Q}_{n,d}$, we consider the usual empirical distribution of the observations X_i ,

$$
\hat{P}_n \; := \; n^{-1} \sum_{i=1}^n \delta_{X_i}.
$$

Theorem 2. Suppose that $\Sigma(Q)$ is well-defined for $Q = Q(P)$. With $J = J_Q$, define

$$
H_1(x) := \mathbb{E} J(x - X_1) \quad \text{and} \quad H_2(x, y) := J(x - y) - H_1(x) - H_1(y)
$$

for $x, y \in \mathbb{R}^q$, where $J(0) := 0$ in connection with Tyler's functional. Let G_1 and G_2 be two stochastically independent Gaussian random matrices in $\mathbb{R}_\text{sym}^{q \times q}$ such that $\mathbb{E} G_1 = \mathbb{E} G_2 = 0$, and

$$
\mathbb{E}(\langle A, G_1 \rangle^2) = \mathbb{E}(\langle A, H_1(X_1) \rangle^2), \n\mathbb{E}(\langle A, G_2 \rangle^2) = \mathbb{E}(\langle A, H_2(X_1, X_2) \rangle^2)
$$

for all matrices $A \in \mathbb{R}^{q \times q}_{sym}$. If $(n-1)/2 \ge d(n) \to \infty$, then

$$
\left\{\Sigma(\hat{Q}_n)\right\}_{\Sigma(\hat{Q}_{n,d(n)})} = \Sigma(Q) + 2\int_{\mathbb{R}^q} H_1 d\hat{P}_n + o_p(n^{-1/2}).
$$

For fixed integers $d \geq 1$,

$$
\Sigma(\hat{Q}_{n,d}) = \Sigma(\hat{Q}_n) + \mathbf{M}_{n,d} + o_p(n^{-1/2}),
$$

where

$$
\mathbf{M}_{n,d} := (nd)^{-1} \sum_{i=1}^{n} \sum_{j=i+1}^{i+d} H_2(X_i, X_j).
$$

Moreover,

$$
\left(\sqrt{n}\int_{\mathbb{R}^q}H_1\,d\hat{P}_n,\sqrt{nd}\,\mathbf{M}_{n,d}\right)\,\rightarrow_{\mathcal{L}}\,(\mathbf{G}_1,\mathbf{G}_2).
$$

In particular, as $d(n) \rightarrow \infty$,

$$
\frac{\sqrt{n}(\mathbf{\Sigma}(\hat{Q}_n)-\mathbf{\Sigma}(Q))}{\sqrt{n}(\mathbf{\Sigma}(\hat{Q}_{n,d(n)})-\mathbf{\Sigma}(Q))}\Bigg\}\rightarrow_{\mathcal{L}}2G_1,
$$

whereas for fixed integers $d \geq 1$,

$$
\sqrt{n} \big(\mathbf{\Sigma}(\hat{Q}_{n,d}) - \mathbf{\Sigma}(Q) \big) \rightarrow_{\mathcal{L}} 2G_1 + d^{-1/2}G_2.
$$

It remains to explain the asymptotic properties of the alternative estimator $d^{-1}\sum_{\ell=1}^d\mathbf{\Sigma}(\hat{Q}_{n,1}^{(\ell)})$ $\binom{k}{n,1}$ where $\hat{Q}_{n,1}^{(\ell)}$ $\prod_{i=1}^{(\ell)}$ is defined as $\hat{Q}_{n,1}$ with $(X_{\Pi^{(\ell)}(i)})_{i=1}^n$ in place of $(X_i)_{i=1}^n$. Here $\Pi^{(1)}, \ldots, \Pi^{(d)}$ are independent random permutations of $\{1, 2, ..., n\}$, and independent from the data $(X_i)_{i=1}^n$.

Theorem 3. For fixed $d \ge 1$ and $1 \le \ell \le d$,

$$
\Sigma(\hat{Q}_{n,1}^{(\ell)}) = \Sigma(Q) + 2 \int_{\mathbb{R}^q} H_1 d\hat{P}_n + M_{n,1}^{(\ell)} + o_p(n^{-1/2}),
$$

where

$$
M_{n,1}^{(\ell)} \;:=\; n^{-1}\sum_{i=1}^n H_2(X_{\Pi^{(\ell)}(i)},X_{\Pi^{(\ell)}(i+1)})
$$

with $\Pi^{(\ell)}(n+1) := \Pi^{(\ell)}(1)$. Moreover,

$$
\sqrt{n}\Big(\int_{\mathbb{R}^q} H_1 d\hat{P}_n, M_{n,1}^{(1)}, \ldots, M_{n,1}^{(d)}\Big) \to_{\mathcal{L}} (\mathbf{G}_1, \mathbf{G}_2^{(1)}, \ldots, \mathbf{G}_2^{(d)})
$$

with independent random matrices G_1 and $G_2^{(1)}$ $\mathbf{G}_2^{(1)},\ldots,\mathbf{G}_2^{(d)}$ $_2^{(d)}$, where G_1 and $G_2^{(\ell)}$ $\frac{1}{2}$ have the same distribution as G_1 and G_2 , respectively, in Theorem [2.](#page-7-1) In particular,

$$
\sqrt{n}\Big(d^{-1}\sum_{\ell=1}^d{\bm{\Sigma}}(\hat{Q}_{n,1}^{(\ell)})-{\bm{\Sigma}}(Q)\Big)\ \to_{\mathcal{L}}\ 2{\bm{G}}_1+d^{-1/2}{\bm{G}}_2.
$$

This theorem shows that averaging $\mathbf{\Sigma}(\hat{Q}_{n,1}^{(\ell)})$ $n_{n,1}^{(\ell)}$) over $\ell = 1, \ldots, d$ is asymptotically equivalent to computing $\mathbf{\Sigma}(\hat{Q}_{n,d})$. One could guess that averaging over $d(n)$ random permutations with $d(n) \to \infty$ leads to an estimator with the same asymptotic distributions as $\Sigma(\hat{Q}_n)$. But this is not obvious, because the average of $d(n)$ random variables which are uniformly of order $o_p(1)$ need not be of order $o_p(1)$ too.

4 Numerical Illustration

The computations are based on Partial Newton algorithms proposed by Dümbgen et al. [\(2016\)](#page-23-12). They are implemented in the R package *fastM* by Dümbgen et al. [\(2014\)](#page-22-4) which is publicly available on CRAN.

As explained in Section [2.3,](#page-6-1) in numerous applications one is mainly interested in the scatter matrix up to positive scalars. Thus we illustrate the previous results with the shape matrix $H :=$ shape($\Sigma(Q)$) and its estimators

$$
\hat{H}_n := \operatorname{shape}(\Sigma(\hat{Q}_n)),
$$

\n
$$
\hat{H}_{n,d} := \operatorname{shape}(\Sigma(\hat{Q}_{n,d})),
$$

\n
$$
\hat{H}_{n,d}^{\text{rand}} := \operatorname{shape} \Big(d^{-1} \sum_{\ell=1}^d \Sigma(\hat{Q}_{n,1}^{(\ell)}) \Big).
$$

Figure 1: $(q, n) = (10, 100)$: Relative approximation errors $D(\hat{\boldsymbol{H}}_{n,d}, \hat{\boldsymbol{H}}_n)/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$.

On the one hand, we look at the approximation errors, that is, the distances between $\hat{H}_{n,d}$, $\hat{H}_{n,d}^{\text{rand}}$ n,d and the full estimator \hat{H}_n . The distance between two matrices $\Sigma_1, \Sigma_2 \in \mathbb{R}^{q \times q}_{sym,+}$ is measured by the so-called geodesic distance

$$
D(\Sigma_1, \Sigma_2) := \Bigl(\sum_{j=1}^q \log[\lambda_j(\Sigma_1^{-1} \Sigma_2)]^2\Bigr),
$$

where $\lambda_1(\cdot) \geq \cdots \geq \lambda_q(\cdot)$ are the ordered real eigenvalues of a matrix $A \in \mathbb{R}^{q \times q}$. On the other hand, we look at the estimation errors, that is, the distances between the estimators \hat{H}_n , $\hat{H}_{n,d}$, $\hat{\boldsymbol{H}}_{n,d}^{\text{rand}}$ and the true shape matrix \boldsymbol{H} .

We simulated 2000 times a data set of size $n = 100$ in dimension $q = 10$, where each observation X_i had independent components with standard exponential distribution. The scatter functional was the M-functional with $\rho(s) = \rho_1(s) = (q+1) \log(s+1)$ for $s \ge 0$. In this particular example, $\Sigma(P)$ is not a multiple of I_q , but the symmetrized distributions $Q = Q(P)$ yields $H = I_q$. Figures [1](#page-9-0) and [2](#page-10-0) show box-and-whiskers plots of the resulting relative approximation errors

$$
D(\hat{\boldsymbol{H}}_{n,d}, \hat{\boldsymbol{H}}_n)/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})
$$
 and $D(\hat{\boldsymbol{H}}_{n,d}^{\text{rand}}, \hat{\boldsymbol{H}}_n)/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H}),$

respectively, for $1 \le d \le 49$. Figure [3](#page-10-1) shows these ratios in one plot for $1 \le d \le 15$.

Figures [4,](#page-11-1) [5](#page-12-0) and [6](#page-12-1) are analogous, this time with the relative estimation errors

$$
D(\hat{\boldsymbol{H}}_{n,d}, \boldsymbol{H})/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})
$$
 and $D(\hat{\boldsymbol{H}}_{n,d}^{\text{rand}}, \boldsymbol{H})/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H}).$

Figure 2: $(q, n) = (10, 100)$: Relative approximation errors $D(\hat{\boldsymbol{H}}_{n,d}^{\text{rand}}, \hat{\boldsymbol{H}}_n)/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$.

Figure 3: $(q, n) = (10, 100)$: Relative approximation errors $D(\hat{\boldsymbol{H}}_{n,d}, \hat{\boldsymbol{H}}_n)/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$ (blue) and $D(\hat{\boldsymbol{H}}_{n,d}^{\mathrm{rand}}, \hat{\boldsymbol{H}}_n)/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$ (green).

Figure 4: $(q, n) = (10, 100)$: Relative estimation errors $D(\hat{\boldsymbol{H}}_{n,d}, \boldsymbol{H})/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$.

The median of the estimation error $D(\hat{H}_n, H)$ in the simulations was equal to 1.1643. Interestingly, the relative estimation errors approach 1 more quickly than the relative approximation arrors approach 0. With respect to relative estimation error, a value $d = 10$, say, seems to be sufficient, although the approximation errors for this value are still substantial.

We did the same simulations and calculations for sample size $n = 400$ instead of $n = 100$. Figures [7](#page-13-0) and [8](#page-13-1) show the resulting relative approximation errors and relative estimation errors. This time, the median of $D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$ was only 0.5662. But note that the relative errors are similarly distributed for both sample sizes. The main difference seems to be that with increasing sample size the differences between $\hat{H}_{n,d}$ and $\hat{H}_{n,d}^{\text{rand}}$ become smaller.

The simulation results are coherent with the asymptotic theory and confirm our claim that moderately large values of d yield already estimators with similar precision as the full symmetrized M-estimators. Therefore for larger sample sizes, computational costs are no longer a hindrance to apply symmetrized scatter matrices in practice.

5 Proofs

Proof of Proposition [1.](#page-7-2) Some of our arguments are similar to parts of Section 8.2 of Dümbgen [et al.](#page-23-6) [\(2015\)](#page-23-6), but for the reader's convenience, we present a complete and self-contained proof here.

Figure 5: $(q, n) = (10, 100)$: Relative estimation errors $D(\hat{\boldsymbol{H}}_{n,d}^{\text{rand}}, \boldsymbol{H})/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$.

Figure 6: $(q, n) = (10, 100)$: Relative estimation errors $D(\hat{\boldsymbol{H}}_{n,d}, \boldsymbol{H})$ (blue) and $D(\hat{\boldsymbol{H}}_{n,d}^{\text{rand}}, \boldsymbol{H})$ (green).

Figure 7: $(q, n) = (10, 400)$: Relative approximation errors $D(\hat{\boldsymbol{H}}_{n,d}, \hat{\boldsymbol{H}}_n)/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$ (blue) and $D(\hat{\boldsymbol{H}}_{n,d}^{\mathrm{rand}}, \hat{\boldsymbol{H}}_n)/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$ (green).

Figure 8: $(q, n) = (10, 400)$: Relative estimation errors $D(\hat{\boldsymbol{H}}_{n,d}, \boldsymbol{H})/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$ (blue) and $D(\hat{\boldsymbol{H}}_{n,d}^{\mathrm{rand}}, \boldsymbol{H})/D(\hat{\boldsymbol{H}}_n, \boldsymbol{H})$ (green).

Step 0. For arbitrary different indices $i, j \in \{1, \ldots, n\}$, the vector $X_j - X_i \neq 0$ almost surely, because $\mathbb{P}(X_j - X_i = 0) = \mathbb{E} \mathbb{P}(X_j \in \{X_i\} | X_i) = 0$. Hence, $\hat{Q}_n(\{0\}) = \hat{Q}_{n,d}(\{0\}) = 0$ for $1 \leq d \leq (n-1)/2.$

Step 1. Let S be the set of all index sets $\{i, j\}$, $1 \le i < j \le n$. Let $\mathcal{E}_o \subset \mathcal{S}$, and set $V_o :=$ $\bigcup_{E \in \mathcal{E}_o} E$. Suppose that the graph (V_o, \mathcal{E}_o) is connected. That means, for arbitrary $\{i, j\} \in \mathcal{E}$, there exist $T \in \mathbb{N}$ and indices i_0, i_1, \ldots, i_T in V_o such that $i_0 = i$, $i_T = j$, and $\{i_{t-1}, i_t\} \in \mathcal{E}_o$ for $1 \le t \le T$. Then for any index $i_0 \in V_0$, the following three linear spaces are identical:

$$
\mathbb{W}_1 := \text{span}(X_i - X_{i_o} : i \in V_o),
$$

$$
\mathbb{W}_2 := \text{span}(X_j - X_i : \{i, j\} \in \mathcal{E}_o),
$$

$$
\mathbb{W}_3 := \text{span}(X_j - X_i : i, j \in V_o).
$$

The inclusions $\mathbb{W}_1, \mathbb{W}_2 \subset \mathbb{W}_3$ are obvious. On the other hand, for $i, j \in V_o$, the vector $X_i - X_i =$ $(X_j - X_{i_0}) - (X_i - X_{i_0}) \in \mathbb{W}_1$, whence $\mathbb{W}_3 \subset \mathbb{W}_1$. Finally, by connectednes of (V_o, \mathcal{E}_o) , for arbitrary different indices $i, j \in V_o$, there exist $T \in \mathbb{N}$ and indices $i_0, i_1, \ldots, i_T \in V_o$ such that $i_0 = i, i_T = j$, and $\{i_{t-1}, i_t\} \in \mathcal{E}_o$ for $1 \le t \le T$. Hence, $X_j - X_i = \sum_{t=1}^T (X_{i_t} - X_{i_{t-1}}) \in \mathbb{W}_2$, and this shows that $\mathbb{W}_3 \subset \mathbb{W}_2$.

Step 2. Let \mathcal{E} be an arbitrary subset of \mathcal{S} , and let $V := \bigcup_{E \in \mathcal{E}} E$. Let V_1, \ldots, V_M be the $M \geq 1$ maximal connected components of the graph (V, \mathcal{E}) . That means, $\mathcal{E} = \bigcup_{m=1}^{M} \mathcal{E}_m$ with sets $\mathcal{E}_m \subset \mathcal{S}$ such that the sets $V_m := \bigcup_{E \in \mathcal{E}_m} E$ are disjoint, and each subgraph (V_m, \mathcal{E}_m) is connected. Then, the linear space

$$
\mathbb{W} := \text{span}(X_i - X_j : \{i, j\} \in \mathcal{E})
$$

has almost surely dimension

$$
\dim(\mathbb{W}) \ = \ \min(S, q) \quad \text{with} \quad S \ := \ \sum_{m=1}^{M} (\#V_m - 1).
$$

To verify this, fix an arbitrary point $i_m \in V_m$ for $1 \le m \le M$. Then Step 1 shows that

$$
\mathbb{W} = \sum_{m=1}^{M} \text{span}(X_j - X_{i_m} : j \in V_m \setminus \{i_m\}),
$$

and it suffices to show that in case of $S \leq q$, the vectors $X_j - X_{i_m}$, $j \in V_m \setminus \{i_m\}, 1 \leq m \leq j_m$ M, are almost surely linearly independent. But this can be shown by induction: Let $\{\{i_m, j\}$: $1 \leq m \leq M, j \in V_m \setminus \{i_m\}\} = \{(k_1, \ell_1), \ldots, (k_S, \ell_S)\}$ with $k_1, \ldots, k_S \in \{i_1, \ldots, i_M\}$ and $\ell_s \in \bigcup_{m=1}^M V_m \setminus \{i_m\}.$ Then, by Step 0, $X_{\ell_1} - X_{k_1} \neq 0$ almost surely, and for $1 \le s < S$ and $W_s := \text{span}(X_{\ell_r} - X_{k_r} : 1 \leq r \leq s),$

$$
\mathbb{P}(X_{\ell_{s+1}} - X_{k_{s+1}} \notin \mathbb{W}_s)
$$

= $\mathbb{E} \mathbb{P}(X_{\ell_{s+1}} \notin X_{k_{s+1}} + \mathbb{W}_s | X_i : i \in \{i_1, ..., i_M\} \cup \{\ell_1, ..., \ell_s\}) = 0.$

Step 3. With (V, \mathcal{E}) and its subgraphs (V_m, \mathcal{E}_m) , $1 \le m \le M$, as in Step 2,

$$
\#\mathcal{E} \ \leq \ \sum_{m=1}^M \binom{\#V_m}{2} \ \leq \ \binom{S+1}{2}.
$$

The first inequality is a consequence of $\#\mathcal{E}_m \leq {\#V_m \choose 2}$ for $1 \leq m \leq M$. The second inequality follows from the fact that the mapping

$$
\mathcal{E} \ni \{i, j\} \mapsto \begin{cases} \{i, j\} & \text{for } i, j \in V_m \setminus \{i_m\}, 1 \le m \le M, \\ \{0, j\} & \text{for } i = i_m, j \in V_m \setminus \{i_m\}, 1 \le m \le M, \end{cases}
$$

is injective, and the images are subsets of $\{0\} \cup \bigcup_{m=1}^{M} V_m \setminus \{i_m\}$ with two elements.

For a fixed integer $d \ge 1$ with $d \le (n-1)/2$, let S_d be the subset of all $\{i, j\} \in S$ such that $0 < j - i \le d$ or $j - i \ge n - d$. That means, for any $i \in \{1, ..., n\}$ there are exactly 2d indices $j \in \{1, \ldots, n\}$ such that $\{i, j\} \in S_d$. Then

$$
\#(\mathcal{E}\cap\mathcal{S}_d)\leq Sd \quad \text{unless } M=1 \text{ and } V=\{1,2,\ldots,n\}.
$$

To see this, note that in case of $M > 1$ or $V \neq \{1, 2, \ldots, n\}$, all sets V_m are different from $\{1,\ldots,n\}$. For a given $m \in \{1,\ldots,M\}$, let $k \in \{1,\ldots,n\} \setminus V_m$. To get an upper bound for $\#(\mathcal{E}_m \cap \mathcal{S}_d)$, we may assume without loss of generality that $k = n$. Otherwise, we could transform $\{1, 2, \ldots, n\}$ with the permutation $i \mapsto T(i) := 1_{[i \leq k]}(i+n-k)+1_{i > k}(i-k)$, because $\{i, j\} \in S_d$ if and only if $\{T(i), T(j)\}\in \mathcal{S}_d$. Now, if $i_0 < i_1 < \cdots < i_{q_m} < n$ are the elements of V_m , then

$$
\#(\mathcal{E}_m \cap \mathcal{S}_d) = \# \{ \{i_a, i_b\} : 0 \le a < b \le q_m, i_b - i_a \le d \text{ or } i_b - i_a \ge n - d \}
$$

\n
$$
\le \# \{ \{a, b\} : 0 \le a < b \le q_m, b - a \le d \}
$$

\n
$$
+ \# \{ \{i, j\} : 1 \le i < j < n, j - i \ge n - d \}
$$

\n
$$
= \# \{ \{a, a + c\} : 1 \le c \le d, 0 \le a \le q_m - c \}
$$

\n
$$
+ \# \{ \{i, j\} : 1 \le i < d, n - d + i \le j < n \}
$$

\n
$$
\le \sum_{c=1}^d (q_m + 1 - c) + \sum_{i=1}^{d-1} (d - i)
$$

\n
$$
= q_m d - \sum_{c'=0}^{d-1} c' + \sum_{i'=1}^{d-1} i' = q_m d = (\# V_m - 1)d.
$$

Step 4. Since there are only finitely many nonempty subsets \mathcal{E} of \mathcal{S} , we may conclude from Step 2 that for any nonempty set $\mathcal{E} \subset \mathcal{S}$, the dimension of span $(X_j - X_i : \{i, j\} \in \mathcal{E})$ is given by $S = S(\mathcal{E})$ as defined in Step 2. Now we consider an arbitrary linear subspace W of \mathbb{R}^q with dimension $q' < q$ such that $\mathcal{E} = \mathcal{E}(\mathbb{W}) := \{ \{i, j\} \in \mathcal{S} : X_j - X_i \in \mathbb{W} \}$ is nonempty. Then Step 3 implies that

$$
\hat{Q}_n(\mathbb{W}) \leq {n \choose 2}^{-1} {q'+1 \choose 2}
$$
 and $\hat{Q}_{n,d}(\mathbb{W}) \leq \frac{q'}{n}$.

But

$$
{n \choose 2}^{-1} {q'+1 \choose 2} = \frac{q'}{q} \frac{q(q'+1)}{n(n-1)} \le \frac{q'}{q} \frac{q^2}{n(n-1)} \text{ and } \frac{q'}{n} = \frac{q'}{q} \frac{q}{n}.
$$

Both factors $q^2/(n(n-1))$ and q/n are strictly smaller than 1 if and only if $n > q$. This proves our claim about \hat{Q}_n and $\hat{Q}_{n,d}$. \Box

Some facts about complete and balanced incomplete U-statistics. Let us first recollect some well-known facts about U-statistics of order two [\(Serfling, 1980;](#page-23-7) [Lee, 1990\)](#page-23-4), with obvious adaptations to vector-valued kernels and the particular distributions \hat{Q}_n and $\hat{Q}_{n,d}$. For some integer $r \geq 1$, let $f : \mathbb{R}^q \to \mathbb{R}^r$ be measurable such that $\mathbb{E}(\|f(X_1 - X_2)\|^2) < \infty$. With the symmetrized function $f^{s}(x) := 2^{-1}(f(x) + f(-x))$, define $f_0 := \mathbb{E} f(X_1 - X_2) = \mathbb{E} f^{s}(X_1 - X_2)$ and

$$
f_1(x) := \mathbb{E} f^s(x - X_1) - f_0, \quad f_2(x, y) := f^s(x - y) - f_0 - f_1(x) - f_1(y)
$$

for $x, y \in \mathbb{R}^q$. Then the covariance matrices $\Gamma := \text{Var}(f(X_1 - X_2)), \Gamma^s := \text{Var}(f^s(X_1 - X_2)),$ $\Gamma_1 := \text{Var}(f_1(X_1))$ and $\Gamma_2 := \text{Var}(f_2(X_1, X_2))$ satisfy the (in)equalities

$$
\Gamma \geq \Gamma^s = 2\Gamma_1 + \Gamma_2.
$$

Here and subsequently, inequalities between symmetric matrices refer to the Loewner partial order on $\mathbb{R}^{q \times q}_{sym}$. The random vectors $f_1(X_i)$, $1 \leq i \leq n$, and $f_2(X_i, X_j)$, $1 \leq i \leq j \leq n$, are centered and uncorrelated, and

$$
U_n := \int_{\mathbb{R}^q} f \, d\hat{Q}_n = f_0 + 2 \int_{\mathbb{R}^q} f_1 \, d\hat{P}_n + M_n,
$$

$$
U_{n,d} := \int_{\mathbb{R}^q} f \, d\hat{Q}_{n,d} = f_0 + 2 \int_{\mathbb{R}^q} f_1 \, d\hat{P}_n + M_{n,d},
$$

where

$$
M_n := \binom{n}{2}^{-1} \sum_{1 \le i < j \le n} f_2(X_i, X_j), \quad M_{n,d} := (nd)^{-1} \sum_{i=1}^n \sum_{j=i+1}^{i+d} f_2(X_i, X_j).
$$

Moreover, $\mathbb{E}(U_n) = \mathbb{E}(U_{n,d}) = f_0$, and

$$
n\operatorname{Var}(U_n) = 4\Gamma_1 + n\operatorname{Var}(M_n) = 4\Gamma_1 + 2(n-1)^{-1}\Gamma_2
$$

\n
$$
n\operatorname{Var}(U_{n,d}) = 4\Gamma_1 + n\operatorname{Var}(M_{n,d}) = 4\Gamma_1 + d^{-1}\Gamma_2
$$
 (6)

The final ingredient for the proof of Theorem [2](#page-7-1) is a result about the asymptotic joint distribution of $\int_{\mathbb{R}^q} f_1 d\hat{P}_n$ and $M_{n,d}$.

Proposition 4. For any fixed $d \ge 1$, the random pair $(\sqrt{n} \int_{\mathbb{R}^q} f_1 d\hat{P}_n)$, √ \overline{nd} $M_{n,d}$ converges in distribution to $\mathcal{N}_r(0, \Gamma_1) \otimes \mathcal{N}_r(0, \Gamma_2)$.

Proof of Proposition [4.](#page-16-0) The proof of this result uses a standard trick for sequences of m -dependent random variables, in our case, $m = d + 1$. For a fixed number $k \geq d$, let

$$
S_n := n^{-1/2} \sum_{i=1}^n f_1(X_i) = \sqrt{n} \int_{\mathbb{R}^q} f_1 d\hat{P}_n,
$$

\n
$$
S_n^k := n^{-1/2} \sum_{\ell=1}^{\lfloor n/k \rfloor} Y_\ell^k \text{ with } Y_\ell^k := \sum_{i=\ell k-k+1}^{\ell k} f_1(X_i),
$$

\n
$$
T_n := (nd)^{-1/2} \sum_{i=1}^n \sum_{j=i+1}^{i+d} f_2(X_i, X_j) = \sqrt{n} dM_{n,d},
$$

\n
$$
T_n^k := (nd)^{-1/2} \sum_{\ell=1}^{\lfloor n/k \rfloor} Z_\ell^k \text{ with } Z_\ell^k := \sum_{i=\ell k-k+1}^{\ell k} \sum_{j=i+1}^{\min(i+d,\ell k)} f_2(X_i, X_j).
$$

The random pairs $(Y_{\ell}^k, Z_{\ell}^k), \ell \geq 1$, are independent and identically distributed with $\mathbb{E}(Y_{\ell}^k) =$ $\mathbb{E}(Z_{\ell}^k) = 0$ and

$$
\text{Var}(Y_{\ell}^k) = k \Gamma_1, \quad \text{Var}(Z_{\ell}^k) = \left(k - \frac{d-1}{2}\right) d \Gamma_2, \quad \text{Cov}(Y_{\ell}^k, Z_{\ell}^k) = 0.
$$

Consequently, it follows from the multivariate central limit theorem and Slutzky's lemma that

$$
(S_n^k, T_n^k) \to_{\mathcal{L}} \mathcal{N}_r(0, \Gamma_1) \otimes \mathcal{N}_r\Big(0, \Big(1-\frac{d-1}{2k}\Big)\Gamma_2\Big),
$$

and the distribution on the right hand side converges weakly to $\mathcal{N}_r(0, \Gamma_1) \otimes \mathcal{N}_r(0, \Gamma_2)$ as $k \to \infty$. Moreover,

$$
\mathbb{E}(\|S_n - S_n^k\|^2) \le \frac{k-1}{n} \operatorname{trace}(\Gamma_1) \to 0,
$$

$$
\mathbb{E}(\|T_n - T_n^k\|^2) \le \left(\frac{d-1}{2k} + \frac{k-1}{nd}\right) \operatorname{trace}(\Gamma_2) \to \frac{d-1}{2k} \operatorname{trace}(\Gamma_2),
$$

and the right hand side converges to 0 as $k \to \infty$. This implies that (S_n, T_n) converges in distribution to $\mathcal{N}_r(0, \Gamma_1) \otimes \mathcal{N}_r(0, \Gamma_2)$. \Box

Proof of Theorem [2.](#page-7-1) Let \check{Q}_n stand for \hat{Q}_n , $\hat{Q}_{n,d(n)}$ with $(n-1)/2 \geq d(n) \to \infty$, or $\hat{Q}_{n,d}$ with fixed $d \geq 1$. For any bounded, continuous function $f : \mathbb{R}^q \to \mathbb{R}$,

$$
\mathbb{E}\Big|\int_{\mathbb{R}^q} f\,d\check{Q}_n - \int_{\mathbb{R}^q} f\,dQ\Big| \ \leq \ (2/n)^{1/2} \|f\|_{\infty}.
$$

This follows from inequality [\(6\)](#page-16-1) applied to real-valued functions. This implies that $d_{\mathcal{L}}(\check{Q}_n, Q) \to_p$ 0. In particular,

$$
\Sigma(\check{Q}_n) = \Sigma(Q) + \int_{\mathbb{R}^q} J d\check{Q}_n + o\Big(\Big\|\int_{\mathbb{R}^q} J d\check{Q}_n\Big\|\Big).
$$

We may identify $\mathbb{R}^{q \times q}_{sym}$ with \mathbb{R}^r , where $r = q(q+1)/2$. Then $\int_{\mathbb{R}^q} J d\check{Q}_n$ is a (complete or balanced incomplete) U -statistic with vector-valued kernel function, and it follows from boundedness of $J(\cdot)$ with $\int_{\mathbb{R}^q} J dQ = 0$ and the general considerations about U-statistics that $\int_{\mathbb{R}^q} J d\phi_n =$ $O_p(n^{-1/2})$. Consequently,

$$
\Sigma(\check{Q}_n) = \Sigma(Q) + \int_{\mathbb{R}^q} J d\check{Q}_n + o_p(n^{-1/2}),
$$

so we may replace $\Sigma(\check{Q}_n) - \Sigma(Q)$ with the matrix-valued U-statistic $\int_{\mathbb{R}^q} J d\check{Q}_n$. But then the assertions of Theorem [2](#page-7-1) are direct consequences of the general considerations about U-statistics and Proposition [4.](#page-16-0) \Box

For the proof of Theorem [3](#page-8-1) we need a variation of Proposition [4](#page-16-0) for the random vectors

$$
\tilde{M}_{n,1} := n^{-1} \sum_{i=1}^{n} f_2(X_{\Pi(i)}, X_{\Pi(i+1)}),
$$

where Π is uniformly distributed on the set of all permutations of $\{1, 2, \ldots, n\}$, independent from $(X_i)_{i=1}^n$, and $\Pi(n+1) := \Pi(1)$.

Proposition 5. Let $d_{\mathcal{L}}(\cdot, \cdot)$ be a metric on the space of probability distributions on \mathbb{R}^r which metrizes weak convergence. Then,

$$
d_{\mathcal{L}}\Big(\mathcal{L}\big(\sqrt{n}\,\tilde{M}_{n,1}\,\big|\,(X_i)_{i=1}^n\big),\mathcal{N}_r(0,\Gamma_2)\Big) \to_p 0.
$$

Proof of Proposition [5.](#page-18-0) By means of the Cramér–Wold device, it suffices to consider the case $r = 1$. Then the random variable $\sqrt{n} \tilde{M}_{n,1}$ can be written as $\sum_{i=1}^{n} A_{\Pi(i),\Pi(i+1)}$ with the random matrix

$$
A = A(X_1, \ldots, X_n) := (n^{-1/2} 1_{[i \neq j]} f_2(X_i, X_j))_{i,j=1}^n \in \mathbb{R}_{sym}^{n \times n}.
$$

As explained in the appendix, there exist permutations $B = B(\cdot | \Pi)$ and $B^* = B^*(\cdot | \Pi)$ such that

$$
\sum_{i=1}^{n} A_{\Pi(i),\Pi(i+1)} = \sum_{i=1}^{n} A_{i,B^*(i)},
$$

while B is uniformly distributed on the set of all permutations of $\{1, \ldots, n\}$, and

$$
\mathop{\mathrm{I\!E}}\nolimits \bigl(\# \bigl\{ i \in \{ 1, \ldots, n \} : B(i) \neq B^*(i) \bigr\} \bigr) \ \leq \ 1 + \log(n).
$$

Consequently,

$$
\sqrt{n}\tilde{M}_{n,1} = \sum_{i=1}^{n} A_{i,B(i)} + R_n,
$$

where $R_n := \sum_{i=1}^n (A_{i,B^*(i)} - A_{i,B(i)})$ satisfies

$$
\mathbb{E}|R_n| \leq 2(1 + \log(n))n^{-1/2}\mathbb{E}|f_2(X_1, X_2)| \to 0.
$$

Hence, it suffices to show that the conditional distribution of $\sum_{i=1}^{n} A_{i,B(i)}$, given $(X_i)_{i=1}^n$, converges weakly in probability to $\mathcal{N}(0, \Gamma_2)$. Distributions of this type have been investigated by [Hoeffding](#page-23-8) [\(1951\)](#page-23-8). It follows from Hoeffding's results and elementary inequalities presented in Section [A.2](#page-21-0) that it suffices to verify the following three properties of the random symmetric matrices $A = A(X_1, \ldots, X_n)$:

$$
\mathbb{E}\Big|n^{-1}\sum_{i,j=1}^n A_{i,j}^2 - \Gamma_2\Big| \to 0,\tag{7}
$$

$$
\mathbb{E}\Big(\sum_{i=1}^{n} \bar{A}_i^2\Big) \to 0,\tag{8}
$$

$$
\mathbb{E}\Big(n^{-1}\sum_{i,j=1}^n A_{i,j}^2 \min(|A_{i,j}|,1)\Big) \to 0,
$$
\n(9)

where $\bar{A}_i := n^{-1} \sum_{j=1}^n A_{i,j}$.

For an arbitrary threshold $c > 0$, we split $f_2(x, y)^2$ into the bounded function $g_c(x, y) :=$ $f_2(x,y)^21_{[f_2(x,y)^2\leq c]}$ and the remainder $h_c(x,y) := f_2(x,y)^21_{[f_2(x,y)^2>c]}$. Then the left-hand side of [\(7\)](#page-19-0) equals

$$
\mathbb{E}\Big|n^{-2}\sum_{i,j=1}^{n}1_{[i\neq j]}f_2(X_i,X_j)^2-\Gamma_2\Big|
$$
\n
$$
\leq n^{-1}\Gamma_2+2\mathbb{E} h_c(X_1,X_2)+n^{-2}\mathbb{E}\Big|\sum_{i,j=1}^{n}\big(g_c(X_i,X_j)-\mathbb{E} g_c(X_1,X_2)\big)\Big|
$$
\n
$$
\leq n^{-1}\Gamma_2+2\mathbb{E} h_c(X_1,X_2)+n^{-2}\operatorname{Var}\Big(\sum_{i,j=1}^{n}g_c(X_i,X_j)\Big)^{1/2}
$$
\n
$$
\leq n^{-1}\Gamma_2+2\mathbb{E} h_c(X_1,X_2)+cn^{-1/2}
$$
\n
$$
\to 2\mathbb{E} h_c(X_1,X_2).
$$

The last inequality follows from the facts that

$$
Cov(g_c(X_i, X_j), g_c(X_k, X_\ell)) \begin{cases} = 0 & \text{if } \{i, j\} \cap \{k, \ell\} = \emptyset, \\ \leq c^2/4 & \text{else,} \end{cases}
$$

and that the number of quadruples (i, j, k, ℓ) with $\{i, j\} \cap \{k, \ell\} \neq \emptyset$ is smaller than $4n^3$. Since by dominated convergence, $\mathbb{E} h_c(X_1, X_2) \to 0$ as $c \to \infty$, Condition [\(7\)](#page-19-0) is satisfied.

The left-hand side of [\(8\)](#page-19-1) equals $n \mathbb{E}(\bar{A}_1^2)$, and \bar{A}_1 is the sum of the uncorrelated, centered random variables $f_2(X_1, X_j)$, $2 \le j \le n$, times $n^{-3/2}$. Consequently,

$$
n \mathop{\mathrm{I\!E}}\nolimits(\bar{A}_1^2) \ \leq \ n^{-1} \mathop{\mathrm{I\!E}}\nolimits \bigl(f_2(X_1, X_2)^2 \bigr) \ \to \ 0.
$$

Finally, the left-hand side of [\(9\)](#page-19-2) is not larger than

$$
\mathbb{E}(f_2(X_1,X_2)^2 \min\{n^{-1/2}|f_2(X_1,X_2)|,1\}) \to 0
$$

by dominated convergence.

 \Box

Proof of Theorem [3.](#page-8-1) Since $(\hat{P}_n, \hat{Q}_{n,1}^{(\ell)})$ (n, n, n, n) has the same distribution as $(\hat{P}_n, \hat{Q}_{n,1}, M_{n,1})$, the first assertion is a direct consequence of Theorem [2](#page-7-1) with $d = 1$. The second part is a consequence of the central limit theorem, applied to $\int_{\mathbb{R}^q} H_1 d\hat{P}_n$, and Proposition [5,](#page-18-0) applied to $\sqrt{n} M_{n,1}^{(\ell)}$. The final statement is a consequence of the first and second part and the continuous mapping theorem. \Box

A Auxiliary results

A.1 A particular coupling of random permutations

Preparations. For an integer $n \geq 1$, let S_n be the set of all permutations of $\langle n \rangle := \{1, 2, ..., n\}$. A cycle in S_n is a permutation $\sigma \in S_n$ such that for $m \geq 1$ pairwise different points $a_1, \ldots, a_m \in S_n$ $\langle n \rangle$,

$$
a_1 \ \mapsto \ a_2 \mapsto \ \cdots \ \mapsto \ a_m \ \mapsto \ a_1,
$$

while $\sigma(i) = i$ for $i \in \langle n \rangle \setminus \{a_1, \ldots, a_m\}$. (In case of $m = 1, \sigma(i) = i$ for all $i \in \langle n \rangle$.) We write

$$
\sigma \ = \ (a_1,\ldots,a_m)_{\rm c}
$$

for this mapping and note that it has m equivalent representations

$$
\sigma = (a_1, \ldots, a_m)_c = (a_2, \ldots, a_m, a_1)_c = \cdots = (a_m, a_1, \ldots, a_{m-1})_c.
$$

Any permutation $\sigma \in S_n$ can be written as

$$
\sigma = (a_{11}, \ldots, a_{1m(1)})_c \circ \cdots \circ (a_{k1}, \ldots, a_{km(k)})_c,
$$

where the sets $\{a_{j1}, \ldots, a_{jm(j)}\}, 1 \leq j \leq k$, form a partition of $\langle n \rangle$. Note that the cycles $(a_{j1},...,a_{jm(j)})_c, 1 \le j \le m$, commute. This representation of σ as a combination of cycles is unique if we require, for instance, that

$$
a_{jm(j)} = \min\{a_{j1}, \dots, a_{jm(j)}\} \quad \text{for } 1 \le j \le k
$$

and

$$
a_{1m(1)} < \cdots < a_{km(k)}.
$$

In what follows, let S_n^* be the set of all permutations $\sigma \in S_n$ consisting of just one cycle, i.e.

$$
\sigma = (a_1, a_2, \ldots, a_n)_c
$$

with pairwise different numbers $a_1, a_2, \ldots, a_n \in \langle n \rangle$.

The coupling. The standardized cycle representation of $\sigma \in S_n$ gives rise to a particular mapping $S_n \ni \pi \mapsto (\sigma, \sigma^*) \in S_n \times S_n^*$ such that $\pi \mapsto \sigma$ is bijective. For fixed $\pi \in S_n$ and any index $i \in \langle n \rangle$ let

$$
M_i := \langle n \rangle \setminus \{ \pi(s) : 1 \le s < i \},
$$

i.e. $\langle n \rangle = M_1 \supset M_2 \supset \cdots \supset M_n = \{\pi(n)\}\$, and $\# M(i) = n + 1 - i$. Let $1 \le t_1 < t_2 < \cdots <$ $t_k = n$ be those indices i such that $\pi(i) = \min(M_i)$. Then

$$
\sigma := (\pi(1), ..., \pi(t_1))_c \circ (\pi(t_1 + 1), ..., \pi(t_2))_c \circ \cdots \circ (\pi(t_{k-1} + 1), ..., \pi(t_k))_c
$$

defines a permutation of $\langle n \rangle$ with standardized cycle representation. This is essentially the construction used by [Feller](#page-23-13) [\(1945\)](#page-23-13) to investigate the number of cycles of a random permuation. Moreover,

$$
\sigma^* := (\pi(1), \pi(2), \ldots, \pi(n))_c
$$

defines a permutation in S_n^* such that

$$
\{i \in \langle n \rangle : \sigma(i) \neq \sigma^*(i)\} = \begin{cases} \emptyset & \text{if } k = 1, \\ \{t_1, \ldots, t_k\} & \text{if } k \ge 2. \end{cases}
$$

Suppose that π is a random permutation with uniform distribution on S_n . Then σ is a random permutation with uniform distribution on S_n too, because $\pi \mapsto \sigma$ is a bijection. Since the conditional distribution of $\pi(i)$, given $(\pi(s))_{1 \leq s < i}$, is the uniform distribution on M_i , the random variables

$$
Y_i := 1_{[\pi(i) = \min(M_i)]}, \quad i \in \langle n \rangle,
$$

are stochastically independent Bernoulli random variables with $\mathbb{P}(Y_i = 1) = (n + 1 - i)^{-1} =$ $1 - \mathbb{P}(Y_i = 0)$. Consequently,

$$
\mathbb{E}\left(\#\left\{i \in \langle n\rangle : \sigma(i) \neq \sigma^*(i)\right\}\right) \leq \sum_{i=1}^n (n+1-i)^{-1} = 1 + \sum_{j=2}^n j^{-1} \leq 1 + \log(n),
$$

because $j^{-1} \le \int_{j-1}^{j} x^{-1} dx = \log(j) - \log(j-1)$ for $2 \le j \le n$.

A.2 Some inequalities related to Lindeberg type conditions

In connection with Gaussian approximations and Stein's method, see [Stein](#page-23-14) [\(1986\)](#page-23-14) or [Barbour and](#page-22-5) [Chen](#page-22-5) [\(2005\)](#page-22-5), the quantity

$$
L(X) := \mathbb{E}(X^2 \min(|X|, 1))
$$

for a square-integrable random variable X plays an important role. Elementary considerations show that $\overline{3}$

$$
h(x) \ \leq \ x^2 \min(|x|, 1) \ \leq \ \sqrt{2} \ h(x) \quad \text{with} \quad h(x) \ := \ \frac{|x|^3}{\sqrt{1 + x^2}}
$$

for arbitrary $x \in \mathbb{R}$. Moreover, $h : \mathbb{R} \to [0, \infty)$ is an even, convex function such that $h(2x) \leq$ 8h(x). Consequently, for arbitrary $x, y \in \mathbb{R}$, Jensen's inequality implies that

$$
(x + y)^2 \min(|x + y|, 1) \le \sqrt{2} \mathbb{E} h(x + y)
$$

\n
$$
\le 2^{-1/2} (h(2x) + h(2y))
$$

\n
$$
\le \sqrt{32} \mathbb{E} h(x) + \sqrt{32} \mathbb{E} h(y)
$$

\n
$$
\le 6x^2 \min(|x|, 1) + 6y^2 \min(|y|, 1) \le 6x^2 \min(|x|, 1) + 6y^2.
$$

For a symmetric matrix $A \in \mathbb{R}^{n \times n}$, we define its row means $\overline{A}_i := n^{-1} \sum_{j=1}^n A_{ij}$ and its overall mean $\bar{A} := n^{-2} \sum_{i,j=1}^n A_{ij}$. Let $\tilde{A} := (A_{ij} - \bar{A}_i - \bar{A}_j + \bar{A})_{i,j=1}^n$. Then elementary calculations and the previous inequalities reveal that

$$
0 \ \leq \ n^{-1} \sum_{i,j=1}^{n} A_{ij}^2 - n^{-1} \sum_{i,j=1}^{n} \tilde{A}_{ij}^2 \ \leq \ 2 \sum_{i=1}^{n} \bar{A}_i^2
$$

and

$$
n^{-1} \sum_{i,j=1}^{n} \tilde{A}_{ij}^{2} \min(|\tilde{A}_{ij}|, 1) \leq 6n^{-1} \sum_{i,j=1}^{n} A_{ij}^{2} \min(|A_{ij}|, 1) + 12 \sum_{i=1}^{n} \bar{A}_{i}^{2}.
$$

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