EXACT FIRST MOMENTS OF THE RV COEFFICIENT BY INVARIANT ORTHOGONAL INTEGRATION

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October 4, 2022

ABSTRACT

The RV coefficient measures the similarity between two multivariate configurations, and its significance testing has attracted various proposals in the last decades. We present a new approach, the invariant orthogonal integration, permitting to obtain the exact first four moments of the RV coefficient under the null hypothesis. It consists in averaging along the Haar measure the respective orientations of the two configurations, and can be applied to any multivariate setting endowed with Euclidean distances between the observations. Our proposal also covers the weighted setting of observations of unequal importance, where the exchangeability assumption, justifying the usual permutation tests, breaks down.

The proposed RV moments express as simple functions of the kernel eigenvalues occurring in the weighted multidimensional scaling of the two configurations. The expressions for the third and fourth moments seem original. The first three moments can be obtained by elementary means, but computing the fourth moment requires a more sophisticated apparatus, the Weingarten calculus for orthogonal groups. The central role of standard kernels and their spectral moments is emphasized.

Keywords RV coefficient · weighted multidimensional scaling · spectral moments · invariant orthogonal integration · Weingarten calculus

1 Introduction

The RV coefficient is a well-known measure of similarity between two datasets, each consisting of multivariate profiles measured on the same \( n \) observations or objects. This contribution proposes a new approach, the invariant orthogonal integration, permitting to obtain the exact first four moments of the RV coefficient under the null hypothesis of absence of relation between the two datasets. The main results, theorem [1] and corollary [1] are exposed in section 3.1. The approach is fully nonparametric, and allows the handling of weighted objects, typically made of aggregates such as regions, documents or species, which abound in multivariate analysis.

In the present distance-based data-analytic approach, data sets are constituted by weighted configurations specified by the object weights together with their pair dissimilarities, assumed to be squared Euclidean. Factorial coordinates, reproducing the dissimilarities, and permitting a maximum compression of the configuration inertia, obtain by weighted multidimensional scaling. The latter, seldom exposed in the literature and hence briefly recalled in section [2.1] is a direct generalization of classical scaling. The central step is provided by the spectral decomposition of the matrix of weighted centered scalar products or kernel. It permits to decompose the spectral eigenspace into a trivial one-dimensional part, determined by the object weights, common to both configurations, and a non-trivial part of dimension \( n - 1 \), orthogonal to the square root of the weights. The weighted RV coefficient obtains as the normalized scalar product between the kernels of the two configurations (section 2.2), and turns out to be equivalent to its original definition expressed by cross-covariances [Escoufier, 1973] [Robert and Escoufier, 1976].
After recalling the above preliminaries, somewhat lengthy but necessary, the heart of this contribution can be uncovered: invariant orthogonal integration consists in computing the expected null moments of the RV coefficient by averaging, along the invariant Haar orthogonal measure in the non-trivial eigenspace, the orientations of one configuration with respect to the other, by orthogonal transformation of, say, the first eigenspace (section 3.2). It constitutes a distinct alternative, with different outcomes, to the traditional permutation approach, whose exchangeability assumption breaks down for weighted objects: typically, the profile dispersion is expected to be larger for lighter objects (Bavaud, 2013) and the $n$ object scores cannot follow the same distribution. The present approach also yields a novel significance test for the RV coefficient (equation 16), taking into account skewness and kurtosis corrections to the usual normal approximation.

Computing the moments of the RV coefficient requires to evaluate the orthogonal coefficients $\hat{K}_{ij}$ constituted by Haar expectations of orthogonal monomials. Low-order moments can be computed, with increasing difficulty, by elementary means (section 3.3), but the fourth-order moment requires a more systematic approach (section 3.6), provided by the Weingarten calculus developed by workers in random matrix theory and free probability. Both procedures yield the same results for low-order moments (section 3.7), which is both expected and reassuring.

The first RV moment (11) coincides with all known proposals. The second centered RV moment (12) is particularly enlightening: the RV skewness is simply proportional to the product of the effective dimensionality of both configurations, thus elucidating the often noticed positive skewness of the RV coefficient. The third centered RV moment (13) is particularly enlightening: the RV skewness is simply proportional to the product of the skewness of both configurations, thus elucidating the often noticed positive skewness of the RV coefficient. The fourth moment (14) is also simple to express and to compute, yet more difficult to interpret.

### 2 Euclidean configurations in a weighted setting: a concise remainder

#### 2.1 Weighted multidimensional scaling and standard kernels

Consider $n$ objects endowed with positive weights $f_i > 0$ with $\sum_{i=1}^{n} f_i = 1$, as well with pairwise dissimilarities $D = (D_{ij})$ between pairs of objects. The $n \times n$ matrix $D$ is assumed to be squared Euclidean, that is of the order $D_{ij} = \|x_i - x_j\|^2$ for $x_i, x_j \in \mathbb{R}^r$, with $r \leq n - 1$. The pair $(f, D)$ constitutes a weighted configuration, with $f_i = 1/n$ for unweighted configurations.

Weighted multidimensional scaling aims at determining object coordinates $X = (x_{i\alpha}) \in \mathbb{R}^{n \times r}$ reproducing the dissimilarities $D$ while expressing a maximum amount of dispersion or inertia $\Delta$ (3) in low dimensions. It is performed by the following weighted generalization of the well-known Torgerson–Gower scaling procedure (see e.g. Borg and Groenen, 2005): first, define $\Pi = \text{diag}(f)$, as well as the weighted centering matrix $H = I_n - 1_n f^\top$, which obeys $H^2 = H$. However, $H^\top \neq H$, unless $f$ is uniform.

Second, compute the matrix $B$ of scalar products by double centering: $B = -\frac{1}{2} H D H^\top$. Third, define the $n \times n$ kernel $K$ as the matrix of weighted scalar products:

$$K = \sqrt{\Pi} B \sqrt{\Pi}, \quad \text{that is} \quad K_{ij} = \sqrt{f_i f_j} B_{ij}.$$

Fourth, perform the spectral decomposition with $\hat{U}$ orthogonal and $\hat{\Lambda}$ diagonal

$$K = \hat{U} \hat{\Lambda} \hat{U}^\top \quad \hat{U}^\top \hat{U} = \hat{U}^\top \hat{U} = I_n \quad \hat{\Lambda} = \text{diag}(\lambda).$$

By construction, $K$ possesses one trivial eigenvalue $\lambda_0 = 0$ associated to the eigenvector $\sqrt{T}$ and $n - 1$ non-negative eigenvalues decreasingly ordered as $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{n-1} \geq 0$, among which $r = \text{rg}(K)$ are strictly positive.

From now on the trivial eigenspace will be discarded: set $\tilde{U} = (\sqrt{T} | U)$, where $U \in \mathbb{R}^{n \times (n-1)}$ and $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_{n-1})$. Direct substitution from (1) yields

$$K = \tilde{U} \Lambda \tilde{U}^\top \quad \tilde{U}^\top \tilde{U} = I_{n-1} - \sqrt{T} T_{\tilde{U}}^\top \quad T_{\tilde{U}}^\top U = I_{n-1} \quad U^\top \sqrt{T} U = 0_n. \quad (2)$$

Finally, the searched for coordinates obtain as $X = \Pi^{-\frac{1}{2}} U \Lambda^{\frac{1}{2}}$, that is $x_{i\alpha} = u_{i\alpha} \sqrt{\lambda_\alpha} / \sqrt{f_i}$. One verifies easily that

$$D_{ij} = \sum_{\alpha=1}^{n-1} (x_{i\alpha} - x_{j\alpha})^2 \quad \Delta = \frac{1}{2} \sum_{i,j=1}^{n} f_i f_j D_{ij} = \text{Tr}(K) = \sum_{\alpha=1}^{n-1} \lambda_\alpha. \quad (3)$$
Exact first moments of the RV coefficient by invariant orthogonal integration

Figure 1: Two weighted configurations \((f, D_X)\) (left) and \((f, D_Y)\) (right) embedded in \(\mathbb{R}^{n-1}\)

The kernels considered here are positive semi-definite and obey in addition \(K\sqrt{f} = 0\). We call them standard kernels. They can be related to the weighted version of centered kernels of Machine Learning (see e.g. [Cortes et al., 2012]). To each weighted configuration \((f, D)\) corresponds a unique standard kernel \(K\), and conversely.

The matrix \(K_0 = I_n - \sqrt{f} \sqrt{f}^\top\) appearing in (2) constitutes a standard kernel, referred to as the neutral kernel in view of property \(K_0 K = K_0 K = K\) for any standard kernel \(K\). The corresponding dissimilarities are the weighted discrete distances

\[
D_{ij}^0 = \begin{cases} 
\frac{1}{f_i} + \frac{1}{f_j} & \text{for } i \neq j \\
0 & \text{otherwise.}
\end{cases}
\]

2.2 The RV coefficient

Consider two weighted configurations \((f, D_X)\) and \((f, D_Y)\) endowed with the same weights \(f\), or equivalently two standard kernels \(K_X\) and \(K_Y\) (Figure 1). Their similarity can be measured by the weighted RV coefficient defined as

\[
RV = RV_{XY} = \frac{\text{Tr}(K_X K_Y)}{\sqrt{\text{Tr}(K_X^2) \text{Tr}(K_Y^2)}}
\]

which constitutes the cosine similarity between the vectorized matrices \(K_X\) and \(K_Y\). As a consequence, \(RV_{XY} \geq 0\) (since \(K_X\) and \(K_Y\) are positive semi-definite), \(RV_{XY} \leq 1\) (by the Cauchy-Schwarz inequality) and \(RV_{XX} = 1\).

Quantity (4) is a straightforward weighted generalization of the RV coefficient (Escoufier, 1973; Robert and Escoufier, 1976), consider multivariate features \(X \in \mathbb{R}^{n \times p}\) and \(Y \in \mathbb{R}^{n \times q}\), directly entering into the definition of \(D_X\) and \(D_Y\) as coordinates, or equivalently as \(K_X = \sqrt{\Pi X_c \Pi X_c^\top} \sqrt{\Pi}\) and \(K_Y = \sqrt{\Pi Y_c \Pi Y_c^\top} \sqrt{\Pi}\), where \(X_c = H X\) and \(Y_c = H Y\) are the centered scores.

The weighted covariances are \(\Sigma_{XX} = X_c^\top \Pi X_c\) and \(\Sigma_{YY} = Y_c^\top \Pi Y_c\). The cross-covariances are \(\Sigma_{XY} = X_c^\top \Pi Y_c\) and \(\Sigma_{YX} = Y_c^\top \Pi X_c\) = \(\Sigma_{XY}^\top\). The original RV coefficient is defined in the feature space as

\[
RV_{XY} = \frac{\text{Tr}(\Sigma_{XY} \Sigma_{YX})}{\sqrt{\text{Tr}(\Sigma_{XX}^2) \text{Tr}(\Sigma_{YY})}}
\]

Proving the identity of (4) and (5) is easy.

3 Computing the moments of the RV coefficient by invariant orthogonal integration

3.1 Main result and significance testing

Define the CV coefficient by the quantity \(CV = \text{Tr}(K_X K_Y)\).
Theorem 1 (Main result). Under invariant orthogonal integration (section 2.1), in which case

$$E(CV) = (n - 1) \lambda \overline{\lambda}$$

(6)

$$E(CV^2) = \frac{2(n - 1)^2}{(n - 2)(n + 1)} \lambda^2 \mu^2$$

(7)

$$E(CV^3) = \frac{8(n - 1)^3}{(n - 3)(n - 2)(n + 1)(n + 3)} \lambda^3 \mu^3$$

(8)

$$E(CV^4) = \frac{12(n - 1)^3}{(n - 4)(n - 3)(n - 2)n(n + 1)(n + 3)(n + 5)} \left\{ 4(n^2 - n + 2) \lambda^4 \mu^2 + (n^4 + n^3 - 15n^2 - 13n + 98) \lambda^2 \lambda^2 \mu^2 - 4(2n^2 - n - 7) (\lambda^2 \lambda^2 \mu^2 + \lambda^2 \lambda^2 \mu^2) \right\}$$

(9)

where $$CV_c = CV - E(CV)$$. Spectral moments and centered spectral moments read

$$\lambda_v = \frac{1}{n - 1} \sum_{a=1}^{n} \lambda^a = \frac{1}{n - 1} \sum_{a=1}^{n} \text{Tr}(K^a) = \text{tr}(K^a)$$

$$\lambda^2 = \frac{1}{n - 1} \sum_{a=1}^{n} (\lambda^a)^2$$

(10)

where $$\lambda^a = \lambda_a - \overline{\lambda}$$ and $$\text{tr}(A) = \text{tr}(A)/(n - 1)$$ denotes the normalized trace. Centered spectral moments can be transformed into normalized traces, and conversely. For instance, $$\lambda^2 = \text{tr}(K^3) - 3 \text{tr}(K^2) \text{tr}(K) + 2 \text{tr}^3(K)$$. Identity $$RV = CV / \sqrt{\text{Tr}(K^2) / \text{Tr}(K^2_v)} = CV / \sqrt{(n - 1) \lambda^2 \mu^2}$$ directly yields:

**Corollary 1** (First cumulants of the RV coefficient). Under invariant orthogonal integration, the first cumulants of the RV coefficient, that is its expectation, variance, skewness and excess kurtosis are, in order,

$$E(RV) = \frac{1}{n - 1} \text{Tr}(K^a) \text{Tr}(K^b) = \frac{\lambda \mu}{\sqrt{\lambda^2 \mu^2}} = \frac{\sqrt{\nu(\lambda)} \nu(\mu)}{n - 1}$$

(11)

$$\text{Var}(RV) = E(RV^2) - E(RV)^2 = \frac{2(n - 1 - \nu(\lambda))(n - 1 - \nu(\mu))}{(n - 2)(n - 1)^2(n + 1)}$$

(12)

$$\lambda(\lambda) = \frac{E(RV^3)}{E^2(RV^2)} = \frac{\sqrt{8(n - 2)(n + 1)}}{(n - 3)(n + 3)} a(\lambda) a(\mu)$$

(13)

$$\Gamma(RV) = \frac{E(RV^4)}{E^2(RV^2)} - 3 = \frac{E(CV^4)}{E^2(CV^2)} - 3$$

(see (9) and (7))

(14)

where $$RV_c = RV - E(RV)$$, and $$a(\lambda) = \lambda^3 / (\overline{\lambda^2})^2$$ is the spectral skewness. The quantity

$$\nu(\lambda) = \text{Tr}^2(K^a) / \text{Tr}(K^2_v) = \left( \sum_{a \geq 1} \lambda^a \right)^2 / \left( \sum_{a \geq 1} (\lambda^a)^2 \right) = (n - 1) \lambda^2 / \lambda^2$$

(15)

has appeared at times as an adjusted degrees of freedom in multivariate tests of the general linear model (see e.g. Geisser and Greenhouse [1958], Worsley and Friston [1995], Schlich [1996], Abdi [2010]). It provides a measure of sphericity or effective dimensionality of configuration ($F$, $D_X$). Its minimum $$\nu(\lambda) = 1$$ is attained for univariate configurations. Its maximum $$\nu(\lambda) = n - 1$$ is attained for uniform dilatations of the discrete distances $D_X$ (section 2.1), in which case $$\text{Var}(RV) = 0$$ since RV is then concentrated on $$\sqrt{\nu(\mu)/(n - 1)}$$.

The second-order Cornish-Fisher cumulant expansion permits to approximatively redress the normal quantiles by taking into account the skewness and the “taillleness” of a non-normal distribution (see e.g. Kendall and Stuart [1977], Amédée-Manesme et al. [2019]). The observed RV is statistically significant at level $$\alpha$$ if (one-tailed test)

$$\frac{RV - E(RV)}{\sqrt{\text{Var}(RV)}} > Z_{1-\alpha}$$

$$= \frac{6}{(u_{1-\alpha} - 1) + \frac{\Lambda(RV)}{24} (u_{1-\alpha}^3 - 3u_{1-\alpha}) - \frac{\Lambda^2(RV)}{36} (2u_{1-\alpha}^3 - 5u_{1-\alpha})}$$

(16)

$$= \text{correct to the normal distribution}$$

correction to the normal distribution
3.2 Invariant orthogonal integration

The rest of the paper is devoted to presenting invariant orthogonal integration and proving Theorem 1.

Consider two standard kernels \( K_X = UAU^\top \) and \( K_Y = VMV^\top \) with \( M = \text{diag}(\mu) \), where \( U, V \in \mathbb{R}^{n \times (n-1)} \). The numerator \( CV \) of RV in (4) reads

\[
CV = \text{Tr}(K_X K_Y) = \text{Tr}(UAU^\top VMV^\top) = \sum_{\alpha=1}^{n-1} \sum_{\beta=1}^{n-1} \lambda_{\alpha \beta} P_{\alpha \beta}
\]

(17)

where

\[
P_{\alpha \beta} = \sum_{i,j=1}^{n} u_{i\alpha} u_{j\beta} v_{i\beta} v_{j\beta} = \left( \sum_{i=1}^{n} u_{i\alpha} v_{i\beta} \right)^2 .
\]

Identities \( UU^\top = I_n - \sqrt{t} \sqrt{t}^\top, \sqrt{t}^\top \sqrt{t} = 0_n \) and \( V^\top UU^\top V = I_{n-1} \) from (2) imply the joint orthogonality property \( V^\top UU^\top V = I_{n-1} \), yielding

\[
P_{\beta \beta} = \sum_{\alpha=1}^{n-1} P_{\alpha \beta} = \sum_{i,j=1}^{n} (u_{ij} - \sqrt{t} f_i f_j) v_{i\beta} v_{j\beta} = \sum_{i=1}^{n} v_{i\beta}^2 = 1
\]

(18)

and, similarly, \( P_{\alpha \bullet} = 1 \). Hence, the matrix \( P = (P_{\alpha \beta}) \in \mathbb{R}^{(n-1) \times (n-1)} \) is non-negative, and doubly stochastic: it expresses as a mixture of permutations of \( S_{n-1} \) (Birkhoff–von Neumann theorem). In particular, one gets the crude estimate

\[
\sum_{\alpha \geq 1} \lambda_{\alpha n-\alpha} \leq CV \leq \sum_{\alpha \geq 1} \lambda_{\alpha \mu_\alpha} .
\]

The null hypothesis \( H_0 \) states that the two configurations \( (f, D_X) \) and \( (f, D_Y) \) are unrelated. Under \( H_0 \), any relative orientation of a configuration with respect to the other is equally likely. Hence, the first configuration will be rotated by replacing \( U = (u_{\alpha i}) \) by \( UT \), where \( T = (t_{\alpha i}) \in O_{n-1} \), the orthogonal group of dimension \( n - 1 \). This rotation acts in the non-trivial eigenspace only, leaving the weights \( f \) unchanged. The term \( \text{Tr}(K_X^2) \) remains the same, and the \( CV \) coefficient becomes

\[
CV(T) = \text{Tr}(UTAT^\top U^\top VMV^\top) = \sum_{\alpha=1}^{n-1} \sum_{\beta=1}^{n-1} \lambda_{\alpha \beta} P_{\alpha \beta}(T)
\]

(19)

where

\[
P_{\alpha \beta}(T) = \sum_{\alpha, \beta=1}^{n-1} t_{\alpha \alpha} t_{\beta \beta} \sum_{i,j=1}^{n} u_{i\alpha} u_{j\beta} v_{i\beta} v_{j\beta} .
\]

(20)

The idea of invariant orthogonal integration is to compute the expectation of the moments

\[
E(CV^q) := \int_{O_{n-1}} CV^q(T) \, d\mu(T) \quad q = 1, 2, \ldots
\]

(21)

by averaging over all possible rotations \( T \in O_{n-1} \) distributed by the invariant Haar measure \( d\mu(T) \) normalized to \( \int_{O_{n-1}} d\mu(T) = 1 \). The moment generating function reads

\[
E(\exp(t CV)) = \int_{O_{n-1}} \exp(t \text{Tr}(TAT^\top A)) \, d\mu(T) \quad \text{with} \quad A = U^\top VMV^\top U .
\]

(22)

Define \( [n] = \{1, 2, \ldots, n\} \). Computing (21) involves the orthogonal coefficients, defined in whole generality as

\[
I_\alpha^\omega = \int_{O_{n-1}} d\mu(T) \, t_{a_1 \omega_1} t_{a_2 \omega_2} \ldots t_{a_q \omega_q}
\]

(23)

where the multi-indices \( \alpha = (a_1 a_2 \ldots a_q) \) and \( \omega = (\omega_1 \omega_2 \ldots \omega_q) \) are elements of \( [n-1]^{2q} \) that is, \( \alpha \) and \( \omega \) are words of length \( 2q \) on the alphabet \([n-1]\).
To ease the notations, define \( A_q = [n-1]^q \) and, for \( \alpha = (\alpha_1 \ldots \alpha_q) \in A_q \), define \( \alpha \alpha = (\alpha_1 \alpha_2 \alpha_2 \ldots \alpha_q \alpha_q) \in A_{2q} \). Identities (19), (20), (21) and (23) yield
\[
\mathbb{E}(CV^\alpha) = \sum_{\alpha_1 \ldots \alpha_q = 1}^{n-1} \lambda_{\alpha_1} \cdots \lambda_{\alpha_q} \sum_{\beta_1 \ldots \beta_q = 1}^{n-1} \mu_{\beta_1} \cdots \mu_{\beta_q} \sum_{i_1 \ldots i_{2q} = 1}^n v_{i_1} \beta_1 v_{i_2} \beta_2 v_{i_3} \beta_2 \ldots v_{i_{2q}} \beta_{4q} v_{i_{2q}+1} \beta_{4q} v_{i_{2q}+2} \beta_{4q} \cdots v_{i_{2q}} \beta_{4q} v_{i_{2q}} \beta_{4q}.
\]

The knowledge of \( T^\alpha_a \) together with joint orthogonality properties will yield exact expressions for \( \mathbb{E}(CV^\alpha) \) in terms of spectral moments of \( \lambda \) and \( \mu \), or equivalently in terms of traces of integer powers of \( K_X \) and \( K_Y \), as demonstrated in the next sections for \( q = 1, 2, 3, 4 \).

### 3.3 Computing low-order orthogonal coefficients

Evaluating the orthogonal coefficients (23) is a major topic in random matrix theory and free probability, and its systematic handling is presented in section 3.6. Yet, as observed by some authors (see e.g. Aubert and Lam, 2005; Braun, 2006; Yamamoto and Kudo, 2017), well-inspired invariance considerations (Lemmas 1 and 2 below) suffice in determining more directly the values of the orthogonal coefficients of low order.

Since \( d\mu(T) = d\mu(T) \), coefficients (23) are zero unless each index in \( \alpha \) and in \( \omega \) occurs an even number of times, with a total of \( 2q \) occurrences, where \( q \) defines the order of the orthogonal coefficient. Also, applying the same permutation on the two multi-indexes, or exchanging the multi-indexes leaves the coefficients unchanged. Furthermore, the particular value taken by an index is irrelevant: only matters its multiplicity. For instance:

\[
T^\alpha_{abcd} = T^\alpha_{abdc} = T^\alpha_{dabc} \neq T^\alpha_{adcb} \quad \text{in general} ; \quad T^\alpha_{abc} = T^\alpha_{ac} = 0 \quad \text{if } a \neq b.
\]

Also, for \( \alpha \neq \gamma \) and \( a \neq b \),

\[
T^\alpha_{aabb} = T^\alpha_{bb} = T^\alpha_{bba} = T^\alpha_{1212} = T^\alpha_{1122} \quad \text{.}
\]

**Lemma 1** (proved in the Appendix). *Let \( \alpha \neq \gamma \) and let \( \epsilon \) be a multi-index not containing \( \alpha, \gamma \). For any indices \( a, b, c, d \) and multi-index \( \epsilon \) of the same size as \( \epsilon \)*

\[
T^\alpha_{abcd} \epsilon = T^\alpha_{ab} \epsilon + T^\alpha_{bc} \epsilon + T^\alpha_{cd} \epsilon = T^\alpha_{abc} \epsilon + T^\alpha_{ad} \epsilon + T^\alpha_{b} \epsilon.
\]

*In particular,*

\[
T^\alpha_{abcd} \epsilon = T^\alpha_{ab} \epsilon = T^\alpha_{bc} \epsilon = T^\alpha_{cd} \epsilon.
\]

*and*

\[
T^\alpha_{a} \epsilon = T^\alpha_{b} \epsilon = T^\alpha_{c} \epsilon = T^\alpha_{d} \epsilon.
\]

**Lemma 2.** *For any multi-index \( \epsilon \) not containing \( a \), and for any unrestricted multi-index \( \epsilon \) of the same size,*

\[
\sum_{a=1}^{n-1} T^\alpha_{a} \epsilon = \delta_{\alpha \beta} T^\epsilon_{\epsilon}.
\]

**Proof.** (26) follows directly from \( TT^T = I_{n-1} \), that is \( \sum_{a=1}^{n-1} t_{aa} t_{a\beta} = \delta_{\alpha \beta} \).

### 3.4 The first and second moments

The computation of the first moment, which has been derived in the literature under various strategies, is straightforward: \( T^\alpha_{ab} = \delta_{ab} T^\alpha_{aa} \), where \( T^\alpha_{aa} \) is independent of \( a \) and \( \alpha \). By (17), (24), (26) and joint orthogonality

\[
T^\alpha_{aa} = \frac{1}{n-1} \quad \text{E}(P_{a\beta}) = \frac{1}{n-1} \quad \text{E}(CV) = \frac{1}{n-1} \sum_{\alpha, \beta = 1}^{n-1} \lambda_{a} \mu_{\beta}.
\]

The computation of the second moment involves four orthogonal coefficients, namely (all super- and sub-indices in (28) are distinct)

\[ E := T^\alpha_{aaaa} \quad F := T^\alpha_{aacc} = T^\alpha_{aaaa} \quad G := T^\alpha_{aaacc} \quad H := T^\alpha_{aaacc} \quad (28) \]
They satisfy

\[ F + G + 2H = E + 3F \]

\[ (n - 2)G + F \]

\[ \frac{1}{n - 1} \]

\[ (n - 2)H + F \]

with solution

\[ E = 3(n - 2)k , \quad F = (n - 2)k , \quad G = nk , \quad H = -k , \quad k = \frac{1}{(n - 2)(n - 1)(n + 1)} \]

Hence (the expression is also valid for four possibly coinciding sub-indices, since \( E = 3F \))

\[ T^{\alpha\gamma\alpha\alpha}_{\alpha\beta\gamma\delta \cdots} = (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\delta} \delta_{\gamma\beta} + \delta_{\alpha\gamma} \delta_{\beta\delta}) F \]

and (for \( \alpha \neq \gamma \))

\[ T^{\alpha\gamma\gamma\gamma}_{\alpha\beta\gamma\delta \cdots} = \delta_{\alpha\beta} \delta_{\gamma\delta} G + (\delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\gamma\beta}) H \]

As a result, performing \( \delta_{\alpha\gamma} \times \) \( \delta_{\beta\delta} \times (1 - \delta_{\alpha\gamma}) \times \delta_{\gamma\delta} \) yields the general formula, where the super- and the sub-indices may be distinct or not

\[ T^{\alpha\gamma\gamma\gamma}_{\alpha\beta\gamma\delta \cdots} = k [n\delta_{\alpha\beta} \delta_{\gamma\delta} - (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\delta} \delta_{\gamma\beta}) - 2\delta_{\alpha\gamma} \delta_{\beta\delta} \delta_{\gamma\delta} + (n - 1)\delta_{\alpha\gamma}(\delta_{\beta\delta} + \delta_{\gamma\beta})] \]

which finally implies, in view of \[ (24) \] and joint orthogonality,

\[ E(P_{\alpha\beta} P_{\gamma\delta} P_{\epsilon\zeta}) = k [n - 2\delta_{\alpha\gamma} - 2\delta_{\beta\delta} + 2(n - 1)\delta_{\alpha\gamma} \delta_{\beta\delta}] \]

Hence, by \[ (24) \] and \[ (10) \]

\[ E(CV^2) = \kappa(n - 1)^3 [n(n - 1)]^2 \mu^2 - 2n^2 \mu^2 - 2n^2 \mu^2 + 2n^2 \mu^2 \]

Subtracting \( E^2(CV) \) obtained in \[ (27) \], substituting the value of \( k \) in \[ (29) \] and rearranging terms yields \[ (7) \]. Expressions for the second centered moments \[ (7) \] and \[ (12) \] are simpler than the corresponding quantities obtained, in the unweighted setting, by averaging over all permutations of the \( n \) objects: the latter contain additional correction terms, as derived in \[ Kazi-Aoual et al. (1995) \]. See also \[ Heo and Ruben Gabriel (1998), Josse et al. (2008) and Abd (2010) \].

### 3.5 The third moment

The third moment reads

\[ E(CV^3) = \sum_{\alpha, \beta, \gamma, \delta, \epsilon, \zeta = 1}^{n - 1} \lambda_{\alpha} \lambda_{\beta} \lambda_{\gamma} \lambda_{\epsilon} \lambda_{\delta} \lambda_{\zeta} \ E(P_{\alpha\beta} P_{\gamma\delta} P_{\epsilon\zeta}) \]

where

\[ E(P_{\alpha\beta} P_{\gamma\delta} P_{\epsilon\zeta}) = \sum_{i,j,k,l,s,t = 1}^{n} v_{ij} \beta_1 v_{j} \beta_2 v_{k1} \delta_1 v_{s1} \epsilon_1 v_{l1} \zeta_1 \sum_{b,c,d,e,f = 1}^{n} T^{\alpha\gamma\gamma\gamma}_{\alpha\beta\gamma\delta \cdots} u_{ia} u_{jb} u_{kc} u_{ld} u_{se} u_{tf} \]

and involves eleven third-order orthogonal coefficients, namely (all super- and sub-indices in \[ (36) \] are distinct)

\[ L := T^{\alpha\alpha\alpha\alpha\alpha\alpha} \quad M := T^{\alpha\alpha\alpha\alpha\alpha\alpha} \quad N := T^{\alpha\alpha\alpha\alpha\alpha\alpha} \quad P := T^{\alpha\alpha\alpha\alpha\alpha\alpha} \]

\[ Q := T^{\alpha\alpha\alpha\alpha\alpha\alpha} \quad R := T^{\alpha\alpha\alpha\alpha\alpha\alpha} \quad S := T^{\alpha\alpha\alpha\alpha\alpha\alpha} \quad T := T^{\alpha\alpha\alpha\alpha\alpha\alpha} \]

Handcrafted computations are a bit awkward, yet feasible, with the result

**Lemma 3** (proved in the Appendix),

\[ \frac{1}{\hat{k}} E(P_{\alpha\beta} P_{\gamma\delta} P_{\epsilon\zeta}) = (n^2 + n - 4) - 2(n + 1)(\sigma + \tau) + 16(\varphi + \psi) + 8\sigma \]

\[ - 8(n - 1)(\sigma \varphi + \tau \varphi) + 8(n - 1)^2 \varphi \psi + 2(n - 3)(n + 3) \omega \]

where

\[ \hat{k} = \frac{k}{(n - 3)(n + 3)} = \frac{1}{(n - 3)(n - 2)(n - 1)(n + 1)(n + 3)} \]

and

\[ \sigma = \delta_{\alpha\gamma} + \delta_{\alpha\epsilon} + \delta_{\gamma\epsilon} \quad \tau = \delta_{\beta\delta} + \delta_{\beta\zeta} + \delta_{\delta\zeta} \quad \omega = \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\epsilon} \delta_{\beta\zeta} + \delta_{\gamma\epsilon} \delta_{\delta\zeta} \]

\[ \varphi = \delta_{\alpha\gamma} \delta_{\alpha\epsilon} \delta_{\gamma\epsilon} = \delta_{\alpha\gamma} \delta_{\alpha\epsilon} = \delta_{\alpha\gamma} \delta_{\gamma\epsilon} = \delta_{\alpha\epsilon} \delta_{\gamma\epsilon} \quad \psi = \delta_{\beta\delta} \delta_{\beta\zeta} \delta_{\delta\zeta} = \delta_{\beta\delta} \delta_{\beta\zeta} = \delta_{\beta\delta} \delta_{\delta\zeta} = \delta_{\beta\delta} \delta_{\delta\zeta} \]
Exact first moments of the RV coefficient by invariant orthogonal integration

One can check with (32) that
\[ \sum_{\varepsilon=1}^{n-1} E(P_{\alpha\beta}P_{\gamma\delta} \varepsilon \zeta) = \sum_{\varepsilon=1}^{\eta-1} E(P_{\alpha\beta}P_{\gamma\delta} \varepsilon \zeta) = E(P_{\alpha\beta}P_{\gamma\delta}) \]
as it must. Inserting (37) in (34) and using (10) yields
\[
E(\text{CV}^3) = (n^2 + n - 4)(n-1)^2 \lambda^3 - 6(n+1)(n-1)\lambda \mu - 24(\lambda \mu^2 + \lambda \mu^2) + 8\lambda \mu^2 .
\]
(40)
The centered third moment
\[
E(\text{CV}^3) = E((\text{CV} - E(\text{CV}))^3) = E(\text{CV}^3) - 3 E(\text{CV}^2) E(\text{CV}) + 2 E^3(\text{CV})
\]
finally reads, by (27), (33) and (38)
\[
\frac{E(\text{CV}^3)}{8(n-1)^4} = 4\lambda^3 - 6(\lambda \mu^2 + \lambda \mu^2) + 9 \lambda \mu^2 - 3(\lambda^2 \mu + \lambda^2 \mu) + \lambda \mu^2 = (\lambda^3 - 3\lambda \mu^2 + 2\lambda \mu^2 - 3\lambda \mu^2 + 2\mu^2) = \lambda^3 \mu^2
\]
thus proving (8). This exact expression for the third moment seems original, and is considerably simpler than the corresponding expression derived by averaging on the n! object permutations (Kazi-Aoual et al. 1995). It depends directly on n, but only indirectly on f through the eigenvalue spectra. Expression (13) for the RV skewness is particularly transparent, and elucidates the cause of the marked positive asymmetry of the RV coefficient, often reported in the literature (see e.g. Mielke 1984, [Heo and Ruben Gabriel] 1998, [Josse et al.] 2008, Zhang et al. 2009): plainly, a(\lambda) > 0 and a(\mu) > 0 for typical scree plots.

3.6 The fourth moment

Computing E(RV^4), or equivalently E(CV^4) is clearly untractable with the former pedestrian approach, and a more systematic strategy is needed. The latter is provided by the work around the orthogonal Weingarten functions (see Collins and Śniady 2006, Collins and Matsumoto 2009, Matsumoto 2012, Collins et al. 2013, Mingo and Speicher 2013, [Mingo and Speicher] 2017).

Consider \( P_{2q} \), the set of all partitions of \{1, 2, \ldots, 2q\} whose all blocks are of length two, also called pairings. There are \((2q-1)!! = (2q-1)(2q-3) \cdots 5 \cdot 3 - 3 \cdot 2 \cdot 1\) distinct pairings. For instance, for \( q = 4 \)
\[ \sigma = (13|25|46|78) \quad \text{and} \quad \tau = (15|26|34|78) \]
constitute such pairings. Their join \( \sigma \vee \tau \) (the finest partition coarser than both \( \sigma \) and \( \tau \)) is \( \sigma \vee \tau = (12345678) \).

In general, the join \( \sigma \vee \tau \) of two pairings \( \sigma, \tau \in P_{2q} \) is a partition made of \( N(\sigma \vee \tau) \) blocks of even sizes \( 2l_1, 2l_2, 2l_3, \ldots \), with \( l_1 \geq l_2 \geq l_3 \ldots \) and \( \sum_{c=1}^{N(\sigma \vee \tau)} c = q \). The multi-index \( \ell = (l_1, l_2, l_3 \ldots) \) constitutes an integer partition of \( q \) (noted \( \ell \vdash q \)), and defines the type \( \ell(\sigma \vee \tau) \) of \( \sigma \vee \tau \).

For \( q = 4 \), five integer partitions or types are possible, namely
\[ \ell = (1, 1, 1, 1) \equiv (1^4) \quad \ell = (2, 1, 1) \quad \ell = (2, 2) \quad \ell = (3, 1) \quad \ell = (4) .
\]
The orthogonal coefficients (23) turn out to express (Collins and Śniady 2006) as
\[
I_n^\omega = \sum_{\sigma \in P_{2q}} \sum_{\tau \in P_{2q}} \delta_\sigma(\omega) \delta_\tau(\alpha) Wg(\ell(\sigma \vee \tau))
\]
(42)
where (considering now \( \sigma \) and \( \tau \) as permutations exchanging the indices belonging to the same block of two), the multi-Kronecker symbols select the pairings \( \sigma \) and \( \tau \) compatible with the multi-indices, in the sense
\[
\delta_\sigma(\omega) = \prod_{r=1}^{q} \delta_{\omega_r(2r-1), \omega_r(2r)} \quad \delta_\tau(\alpha) = \prod_{r=1}^{q} \delta_{\alpha_r(2r-1), \alpha_r(2r)}
\]
(43)
In other words, \( \delta_\sigma(\omega) = 1 \) if \( \omega_a = \omega_i \) for each pair \((s,t)\) in \(\sigma\) (which implies that all indices in \(\omega\) must occur an even number of times), and \( \delta_\sigma(\omega) = 0 \) otherwise.

The quantities \( W_g(\ell(\sigma \vee \tau)) \) appearing in (42) are the orthogonal Weingarten functions, and depend upon the dimension \( d = n - 1 \) as well. They have been computed up to order \( q = 6 \) \citep{CollinsMatsumoto2009}. For \( q = 4 \):

\[
\begin{align*}
W_g(1^4) &= \phi(n - 3)(n + 2)(n^2 + 4n - 4) \\
W_g(2, 1, 1) &= \phi(-n^3 - 3n^2 + 6n + 4) \\
W_g(2, 2) &= \phi(n^2 + 3n + 14) \\
W_g(3, 1) &= \phi(n - 1)(2n + 6) \\
W_g(4) &= -\phi(5n + 1)
\end{align*}
\]

where \( \phi = \frac{1}{(n - 4)(n - 3)(n - 2)(n - 1)n(n + 1)(n + 3)(n + 5)} \).

Substituting (42) in (24) yields

\[
\mathbb{E}(\mathcal{CV}^2) = \sum_{\sigma \in \mathcal{P}_{2q}} \sum_{\tau \in \mathcal{P}_{2q}} W_g(\ell(\sigma \vee \tau)) \sum_{\alpha \in A_q} \delta_\sigma(\alpha \alpha) \lambda_\alpha \sum_{\beta \in A_q} \delta_\tau(\beta \beta) \mu_\beta
\]

\[
= \sum_{\sigma \in \mathcal{P}_{2q}} \sum_{\tau \in \mathcal{P}_{2q}} W_g(\ell(\sigma \vee \tau)) \text{Tr}_\sigma(K_X) \text{Tr}_\tau(K_Y)
\]

\[
= \sum_{\sigma \in \mathcal{P}_{2q}} \sum_{\tau \in \mathcal{P}_{2q}} (n - 1)^{N(\sigma \vee \sigma_0) + N(\tau \vee \sigma_0)} W_g(\ell(\sigma \vee \tau)) \prod_{c=1}^{N(\sigma \vee \sigma_0)} \frac{X_c}{\mu_c} \prod_{c=1}^{N(\tau \vee \sigma_0)} \frac{Y_c}{\mu_c}
\]

where the following lemmas and definitions have been used:

**Lemma 4** (another variant of joint orthogonality, proved in the Appendix).

\[\sum_{a \in A_q} \sum_{b \in A_q} \delta_\sigma(a) \mu_b = \delta_\omega(\sigma)\]

**Lemma 5.** Consider the reference pairing \( \sigma_0 = (12\ldots[q]q) \in \mathcal{P}_{2q} \), and consider the type \( \ell(\sigma \vee \sigma_0) \), also called coset-type of \( \sigma \) \rlcite{Matsumoto2012, CollinsEtal2013}. Define

\[
\text{Tr}_\sigma(K) = \prod_{c=1}^{N(\sigma \vee \sigma_0)} \text{Tr}(K^c) \\
\text{tr}_\sigma(K) = \prod_{c=1}^{N(\sigma \vee \sigma_0)} \text{tr}(K^c)
\]

Then \( \sum_{\alpha \in A_q} \delta_\sigma(\alpha \alpha) \lambda_\alpha = \text{Tr}_\sigma(K_X) \), which also reads

\[
\text{Tr}_\sigma(K_X) = (n - 1)^{N(\sigma \vee \sigma_0)} \text{tr}_\sigma(K_X) = (n - 1)^{N(\sigma \vee \sigma_0)} \prod_{c=1}^{N(\sigma \vee \sigma_0)} X^c
\]

**Proof.** Consider \( \omega = \alpha \alpha \in A_{2q} \). By construction, \( \omega_{(2q-1)} = \omega_{2q} \), that is \( \delta_{\sigma_0}(\omega) = 1 \). On the other hand, the term \( \delta_\sigma(\alpha \alpha) \) imposes \( \omega_{(2q-1)} = \omega_{2q} \). Hence all indices of \( \omega \) in the blocks of \( \sigma \vee \sigma_0 \) (of sizes \( 2l_1, 2l_2, 2l_3, \ldots, 2l_{N(\sigma \vee \sigma_0)} \)) are identical, that is the sum on \( \alpha \) involves \( N(\sigma \vee \sigma_0) \) unconstrained indices respectively repeated exactly \( (l_1, l_2, l_3, \ldots, l_{N(\sigma \vee \sigma_0)}) \) times.

Transforming expression (46) into an effective formula requires to determine, among the \( ((2q - 1)!!)^2 \) pairings \( (\sigma, \tau) \) entering into the sum, how many are jointly of type \( \ell(\sigma \vee \tau), \ell(\sigma \vee \sigma_0) \) and \( \ell(\tau \vee \sigma_0) \).

For \( q = 4 \), Table II gives the distribution of joint counts of the 105\(^2 = 11025 \) pairings \( (\sigma, \tau) \), among the \( 5^3 = 125 \) possible trivariate types. Those counts have, for lack of foreseeable analytical approach, been mechanically computed with the help of the R package igraph \citep{CsardiEtal2006}, by the functions union() (determining the join of two pairings coded as binary graphs) and components() (determining the join type).

Working with centered quantities notably simplifies the computations:
Table 1: Trivariate type counts for \( q = 4 \): each table refers to the type of \( \sigma \lor \tau \), namely \((1^4), (2,1,1), (2,2), (3,1), (4)\) from left to right and top to bottom. Rows refer to the type of \( \sigma \lor \sigma_0 \), and columns to the type of \( \tau \lor \sigma_0 \).

| \( (1^4) \) | \( (2,1,1) \) | \( (2,2) \) | \( (3,1) \) | \( (4) \) |
|----------|----------------|-------------|-------------|--------|
| \((1^4)\) | 1              | 12          | 12          | 32     |
| \((2,1,1)\) | 12             | 24          | 96          | 48     |
| \((2,2)\) | 24             | 96          | 96          | 48     |
| \((3,1)\) | 96             | 192         | 192         | 288    |
| \((4)\) | 48             | 288         | 240         | 768    | 960    |

Lemma 6.

\[
\text{CV}_c = \text{CV} - \mathbb{E}(\text{CV}) = \sum_{\alpha=1}^{n-1} \sum_{\beta=1}^{n-1} \lambda_{\alpha}^{c} \mu_{\beta}^{c} P_{\alpha \beta} .
\]

Proof. By (6), (17) and \( P_{\bullet \bullet} = P_{\bullet \beta} = 1 \),

\[
\begin{align*}
&\sum_{\alpha=1}^{n-1} \sum_{\beta=1}^{n-1} \lambda_{\alpha}^{c} \mu_{\beta}^{c} P_{\alpha \beta} = \sum_{\alpha \beta} (\lambda_{\alpha} - X)(\mu_{\beta} - \mu) P_{\alpha \beta} = \sum_{\alpha \beta} \lambda_{\alpha} \mu_{\beta} P_{\alpha \beta} - (n-1)X\mu \\
&- (n-1)X\mu + (n-1)X\mu = \sum_{\alpha \beta} \lambda_{\alpha} \mu_{\beta} P_{\alpha \beta} - (n-1)X\mu = \text{CV} - \mathbb{E}(\text{CV}) = \text{CV}_c .
\end{align*}
\]

Consequently, (49) entails

\[
\mathbb{E}(\text{CV}_c^2) = \sum_{\sigma \in \mathcal{P}_{2q}} \sum_{\tau \in \mathcal{P}_{2q}} (n-1)^{N(\sigma \lor \sigma_0) + N(\tau \lor \sigma_0)} \text{Wg}(\ell(\sigma \lor \tau)) \prod_{c=1}^{N(\sigma \lor \sigma_0)} \lambda_{\alpha}^{c}^{2} \prod_{c=1}^{N(\tau \lor \sigma_0)} \mu_{\beta}^{c}^{2} (49)
\]

in which, for \( q = 4 \), the contributions of \( \sigma \) and \( \tau \) coset types \((1^4), (2,1,1), (2,2), (3,1), (4)\), associated to \( X_{c} = 0 \) or \( \mu_{c} = 0 \), are zeroed: only \((2,2)\) and \((4)\) survive, with contributions indicated by the boxed counts in Table 1.

Explicitly, the coefficient of \( \lambda_{\alpha}^{c}^{2} X_{c}^{2} \mu_{\beta}^{c}^{2} \mu_{\beta}^{c} \) in (49) is

\[
(n-1)^{4}[12 \text{Wg}(1^4) + 24 \text{Wg}(2,1,1) + 60 \text{Wg}(2,2) + 48 \text{Wg}(4)]
\]

\[
= 12 \phi (n-1)^{4} (n^4 + n^3 - 15n^2 - 13n + 98),
\]

the coefficient of \( \lambda_{\alpha}^{c}^{2} \mu_{\beta}^{c}^{2} \mu_{\beta}^{c}^{2} \) is

\[
(n-1)^{2}[48 \text{Wg}(1^4) + 288 \text{Wg}(2,1,1) + 240 \text{Wg}(2,2) + 768 \text{Wg}(3,1) + 960 \text{Wg}(4)]
\]

\[
= 48 \phi (n-1)^{4} (n^2 - n + 2),
\]

and the coefficient of \( \lambda_{\alpha}^{c}^{2} \mu_{\beta}^{c}^{2} \) and \( \lambda_{\alpha}^{c}^{2} X_{c}^{2} \mu_{\beta}^{c}^{2} \) is

\[
(n-1)^{3}[96 \text{Wg}(2,1,1) + 48 \text{Wg}(2,2) + 192 \text{Wg}(3,1) + 240 \text{Wg}(4)]
\]

\[
= -48 \phi (n-1)^{4} (2n^2 - n - 7).
\]

The final expressions in the above follow from (44) and, together with (45), prove (49). They have been further checked with the software Mathematica. Expression (49) for the fourth moment is relatively simple, but it lacks elegance and direct interpretation.
3.7 The third moment, revisited

Applying the steps of previous section for \( q = 3 \) reveals that the contribution of coset-types \((1, 1, 1)\) and \((2, 1)\) for \( \sigma \) or \( \tau \) is zero by consequence of centration. Hence, only the coset-types \((3)\) contribute to (49), which is therefore simply proportional to \( \lambda^3 \mu^3 \). The conciseness of expressions (8) and (13) is thus elucidated. The proportionality coefficient is determined by the boxed components of Table 2 as

\[
(n - 1)^2 [8 Wg(1^3) + 24 Wg(2, 1) + 32 Wg(3)] = \frac{8(n - 1)^3}{(n - 3)(n - 2)(n + 1)(n + 3)}
\]

which is exactly expression (8), obtained much more indirectly in section 3.5. The values of the Weingarten coefficients in (50) were obtained from Collins and Śniady (2006). They read with the present notations \((d = n - 1)\) and (38) as

\[
Wg(1^3) = \hat{\kappa} (n^2 + n - 4) \quad Wg(2, 1) = -\hat{\kappa} (n + 1) \quad Wg(3) = 2\hat{\kappa}
\]

Those coefficients coincide, in order, with the values \(U\), \(V\) and \(W\) defined in (36) and determined in (51), as they must in view of (42).

In conclusion, the pedestrian approach of sections 3.3, 3.4 and 3.5 exactly matches the systematic approach of sections 3.6 and 3.7: a circumstance both expected and relieving, apt to boost confidence in the soundness of the invariant orthogonal integration approach.

4 Discussion and conclusion

The weighted RV coefficient measures the similarity between two weighted Euclidean configurations, and this contribution proposes exact expressions for the first four moments of the RV. Considering weighted objects extends the traditional uniform framework. It also provides precious guidance for separating the trivial and non-trivial eigenspaces resulting form the spectral decomposition of the standard kernels occurring in the weighted multidimensional scaling of both configurations.

Our approach, invariant orthogonal integration, is nonparametric, and consists in averaging the relative orientation of both configurations by performing Haar integration on orthogonal matrices \( T \in O_{n-1} \) acting in the non-trivial eigenspace only. The resulting expressions are simpler and easier to interpret than their traditional counterparts obtained by averaging on permutation matrices \( S \) between \( n \) objects. In view of \( SS^\top = I_n \), permutations also do constitute rotations, but in \( O_n \), and their indiscriminate use is furthermore questionable in the weighted setting. Comparing the present approach to the parametric approach, postulating multivariate normal distribution for the object features, is left open for future investigations.

Also, our approach is object-oriented, as in traditional Data Analysis and Machine Learning, rather than variable-oriented as in Mathematical Statistics. Its use requires to dispose of squared Euclidean dissimilarities between objects, possibly weighted, and some of its numerous applications (including spatial autocorrelation and network clustering) will be illustrated in forthcoming publications. This contribution underlines in particular the key role played by the standard kernel, central to weighted multidimensional scaling, and whose spectrum governs the values of the RV moments. Correlatively, it appears that the humble scree plot should deserve more consideration, beyond its limited role in selecting the number of spectral dimensions: mentioning and interpreting its effective dimensionality, skewness and fourth spectral moment could arguably become systematic in practice.

Computing the fourth RV moment did require to recourse to the Weingarten calculus, whose apparatus, arguably demanding for the neophyte, turned out decisive for the pursuit of our objective. One may reasonably hope that future developments along that line will enrich the present results, replacing in particular the mechanical
computation of Tables 1 and 2 by true mathematical arguments. However, determining the analytical, exact null distribution of RV, may reveal itself out of reach: as a matter of fact, the moment generating function (22) is an orthogonal analog of the celebrated Harish-Chandra trace integral for the unitary group, whose analytical expression has been determined ever since the fifties (Harish-Chandra 1957) (see also e.g. Tao 2013 and McSwiggen 2021). Yet, discovering a corresponding expression for the orthogonal case, precisely, has not been achieved so far.

Proofs

Proof of Lemma 1. Let \( \alpha \neq \gamma \) and consider the matrix \( \hat{T} \) with components

\[
\hat{t}_{aa} = \cos \xi t_{aa} - \sin \xi t_{a\gamma} \quad \hat{t}_{a\gamma} = \sin \xi t_{aa} + \cos \xi t_{a\gamma} \quad \hat{t}_{a\beta} = t_{a\beta} \quad \text{for } \beta \neq \alpha, \gamma
\]

for any \( a \), where \( \xi \) is an arbitrary, fixed angle. Then \( \hat{T} \) is an orthogonal matrix, as likely as \( T \), that is \( d\mu(T) = d\mu(\hat{T}) \). To ease the notations, take \( \varepsilon \) and \( e \) in Lemmas 1 and 2 playing no active role in what follows, as empty. Then

\[
I_{<a>\langle b\rangle c\langle d\rangle e\alpha\beta} = \mathbb{E}(\cos \xi t_{aa} - \sin \xi t_{a\gamma})[\cos \xi t_{bb} - \sin \xi t_{b\gamma}][\sin \xi t_{cc} + \cos \xi t_{c\gamma}][\sin \xi t_{dd} + \cos \xi t_{d\gamma}]
\]

\[
= 2 \cos^2 \xi \sin^2 \xi I_{<a>\langle b\rangle c\langle d\rangle e\alpha\beta} + (\cos^4 \xi + \sin^4 \xi)I_{<a>\langle b\rangle c\langle d\rangle e\gamma\beta} - 2 \cos^2 \xi \sin^2 \xi I_{<a>\langle b\rangle c\langle d\rangle e\gamma\beta} - 2 \cos^2 \xi \sin^2 \xi I_{<a>\langle b\rangle c\langle d\rangle e\gamma\alpha}
\]

Multiplying the l.h.s. by \( \cos^4 \xi + \sin^4 \xi + 2 \cos^2 \xi \sin^2 \xi = 1 \) and simplifying yields

\[
I_{<a>\langle b\rangle c\langle d\rangle e\alpha\beta} = I_{<a>\langle b\rangle c\langle d\rangle e\gamma\beta} + I_{<a>\langle b\rangle c\langle d\rangle e\gamma\alpha}.
\]

Proof of Lemma 2. Lemmas 1 and 2 entail the following relations between orthogonal coefficients (26)

\[
S^{254} U + 2V \quad T^{254} V + 2W \quad M^{254} 3N \quad P^{254} 3S
\]

\[
R^{254} 3T \quad E^{26} (n - 2)M + L \quad E^{26} (n - 2)P + M \quad F^{26} (n - 3)N + 2M
\]

\[
F^{26} (n - 3)S + 2Q \quad F^{26} (n - 2)Q + M \quad G^{26} (n - 3)U + 2S \quad H^{26} (n - 3)V + 2T
\]

\[
0^{26} (n - 2)R + M \quad 0^{26} (n - 2)T + N \quad 0^{26} (n - 3)W + 2T
\]

with solution (recall that \( E, F, G, H \) in (29) are already known)

\[
L = \frac{15(n - 2)}{n + 3} \kappa \quad M = \frac{3(n - 2)}{n + 3} \kappa \quad N = \frac{n - 2}{n + 3} \kappa \quad P = \frac{3(n + 2)}{n + 3} \kappa
\]

\[
Q = \frac{n}{n + 3} \kappa \quad R = -\frac{3}{n + 3} \kappa \quad S = \frac{n + 2}{n + 3} \kappa \quad T = -\frac{1}{n + 3} \kappa
\]

(51)

Consider first \( \alpha = \gamma = \varepsilon \), and assume the sub-indices of the orthogonal coefficients to be matched into three distinct pairs. There are 5 \( \times \) 3 = 15 such pairings, namely

\[
T_{abedf}^{\alpha\alpha\alpha\alpha\alpha} = N\left\{ \delta_{ab} \delta_{cd} \delta_{ef} + \delta_{ac} \delta_{bd} \delta_{ef} + \delta_{ad} \delta_{bc} \delta_{ef} + \delta_{ae} \delta_{bd} \delta_{ef} + \delta_{af} \delta_{bc} \delta_{ef} + \delta_{ad} \delta_{ce} \delta_{ef} + \delta_{ae} \delta_{ce} \delta_{ef} + \delta_{af} \delta_{ce} \delta_{ef} + \delta_{ad} \delta_{de} \delta_{ef} + \delta_{ae} \delta_{de} \delta_{ef} + \delta_{af} \delta_{de} \delta_{ef} \right\}.
\]

(52)

In (52), the first term preserves the three pairs in the reference partition \((ab|cd|ef)\), the next six terms preserve one pair only, and the eight remaining terms mix all pairs. It turns out that (52) also holds for coinciding pairs in view of \( M = 3N \) and \( L = 5M \). By joint orthogonality, the sum in (51) reads

\[
\mathbb{E}(P_{a\beta} P_{a\gamma} P_{a\varepsilon}) = (1 + 2\delta_{\beta\delta} + 2\delta_{\delta\varepsilon} + 2\delta_{\varepsilon\beta} + 8\delta_{\beta\delta} + 8\delta_{\delta\varepsilon} + 8\delta_{\varepsilon\beta})N.
\]

(53)

Consider now \( \alpha = \gamma \neq \varepsilon \). Distinguishing between cases preserving or not the pair \((ef)\) yields

\[
T_{abedef}^{\alpha\alpha\alpha\alpha\alpha} = S\left\{ \delta_{ab} \delta_{cd} \delta_{ef} + \delta_{ac} \delta_{bd} \delta_{ef} + \delta_{ad} \delta_{bc} \delta_{ef} + \delta_{ae} \delta_{bd} \delta_{ef} + \delta_{af} \delta_{bc} \delta_{ef} + \delta_{ad} \delta_{ce} \delta_{ef} + \delta_{ae} \delta_{ce} \delta_{ef} + \delta_{af} \delta_{ce} \delta_{ef} + \delta_{ad} \delta_{de} \delta_{ef} + \delta_{ae} \delta_{de} \delta_{ef} + \delta_{af} \delta_{de} \delta_{ef} \right\} + T\left\{ \delta_{ab} \delta_{cd} \delta_{ef} + \delta_{ac} \delta_{bd} \delta_{ef} + \delta_{ad} \delta_{bc} \delta_{ef} + \delta_{ae} \delta_{bd} \delta_{ef} + \delta_{af} \delta_{bc} \delta_{ef} + \delta_{ad} \delta_{ce} \delta_{ef} + \delta_{ae} \delta_{ce} \delta_{ef} + \delta_{af} \delta_{ce} \delta_{ef} + \delta_{ad} \delta_{de} \delta_{ef} + \delta_{ae} \delta_{de} \delta_{ef} + \delta_{af} \delta_{de} \delta_{ef} \right\}
\]

(54)
which also holds for three preserved pairs since $3S + 12T = M$. By joint orthogonality, (55) reads

$$
\begin{align*}
\text{for } \alpha = \gamma &\neq \varepsilon & \mathbb{E}(P_{\alpha\beta}P_{\gamma\delta}P_{\epsilon\zeta}) &= (1 + 2\delta_{\beta\delta})S + (2\delta_{\beta\zeta} + 2\delta_{\epsilon\zeta} + 8\delta_{\beta\delta}\delta_{\epsilon\zeta})T, \\
\text{for } \alpha = \varepsilon &\neq \gamma & \mathbb{E}(P_{\alpha\beta}P_{\delta\epsilon}P_{\gamma\zeta}) &= (1 + 2\delta_{\epsilon\zeta})S + (2\delta_{\beta\delta} + 2\delta_{\epsilon\zeta} + 8\delta_{\beta\delta}\delta_{\epsilon\zeta})T, \\
\text{for } \gamma = \epsilon &\neq \alpha & \mathbb{E}(P_{\alpha\beta}P_{\gamma\delta}P_{\zeta\epsilon}) &= (1 + 2\delta_{\epsilon\zeta})S + (2\delta_{\beta\delta} + 2\delta_{\epsilon\zeta} + 8\delta_{\beta\delta}\delta_{\epsilon\zeta})T.
\end{align*}
$$

(55)

In the remaining case $\alpha \neq \gamma \neq \varepsilon$, the same reasoning yields

$$
\mathbb{I}_{abcd}\mathbb{I}_{ef} = U\{a_{ab}a_{cd}a_{ef}\} + V\{a_{ac}a_{bd}a_{ef} + a_{ad}a_{bc}a_{ef} + a_{ae}a_{bd}a_{ef} + a_{af}a_{bc}a_{ef} + a_{bc}a_{de}a_{ef} + a_{bd}a_{ce}a_{ef} + a_{bf}a_{cd}a_{ef} + a_{bf}a_{cd}a_{ef} + a_{bf}a_{cd}a_{ef} + a_{bf}a_{cd}a_{ef} + a_{bf}a_{cd}a_{ef} + a_{bf}a_{cd}a_{ef}\}
$$

(58)

Also valid for three preserved pairs since $U + 6V + 8W = N$, and finally

$$
\begin{align*}
\text{for } \alpha \neq \gamma &\neq \varepsilon & \mathbb{E}(P_{\alpha\beta}P_{\gamma\delta}P_{\epsilon\zeta}) &= U + (2\delta_{\beta\delta} + 2\delta_{\epsilon\zeta} + 8\delta_{\beta\delta}\delta_{\epsilon\zeta})V + 8\delta_{\beta\delta}\delta_{\epsilon\zeta}W.
\end{align*}
$$

(59)

To ease notations, use definitions (39) multiply both sides of (53) by $\varphi$, of (55) by $\delta_{\alpha\gamma}(1 - \delta_{\alpha\varepsilon})(1 - \delta_{\gamma\varepsilon}) = \delta_{\alpha\gamma} - \varphi$, of (56) by $\delta_{\alpha\varepsilon} - \varphi$, of (57) by $\delta_{\gamma\varepsilon} - \varphi$, of (59) by $(1 - \delta_{\alpha\gamma})(1 - \delta_{\alpha\varepsilon})(1 - \delta_{\gamma\varepsilon}) = 1 - \sigma + 2\varphi$, and add the whole to obtain the unrestricted expression (37).

Proof of Lemma 2

$$
\begin{align*}
\sum_{n \in \mathcal{A}_{2g}} \delta_n(a) u_{ia} &= \sum_{n \in \mathcal{A}_{2g}} \delta_n(a) u_{ia} \sum_{n \in \mathcal{A}_{2g}} \prod_{r=1}^{q} \delta_{a_n(2r-1),a_n(2r)} u_{ia} \\
&= \prod_{r=1}^{q} \sum_{a_n(2r-1)=1}^{n-1} u_{a_n(2r-1),a_n(2r-1)} u_{a_n(2r-1),a_n(2r)} \\
&= \prod_{r=1}^{q} [\delta_{a_n(2r-1),a_n(2r)} - \sqrt{f_{a_n(2r-1)} f_{a_n(2r)}}].
\end{align*}
$$

Summing the latter on $\prod_{r=1}^{q} \sum_{n \in \mathcal{A}_{2g}} u_{i_n(2r-1),i_n(2r)} v_{i_n(2r-1),i_n(2r)}$ yields, by the joint orthogonality property of section 3.2

$$
\prod_{r=1}^{q} \sum_{i_n(2r-1)=1}^{n} u_{i_n(2r-1),i_n(2r-1)} v_{i_n(2r-1),i_n(2r-1)} w_{i_n(2r-1),i_n(2r)} = \prod_{r=1}^{q} \delta_{a_n(2r-1),a_n(2r)} w_{i_n(2r-1),i_n(2r)} = \delta_{i}(\omega).
$$

References

Abdi, H. (2010). Congruence: Congruence coefficient, RV coefficient, and Mantel coefficient. Encyclopedia of research design, 3:222–229.

Amédée-Manesme, C.-O., Barthélémy, F., and Maillard, D. (2019). Computation of the corrected Cornish–Fisher expansion using the response surface methodology: application to var and cvar. Annals of Operations Research, 281(1):423–453.

Aubert, S. and Lam, C. (2003). Invariant integration over the unitary group. Journal of Mathematical Physics, 44(12):6112–6131.

Bavaud, F. (2013). Testing spatial autocorrelation in weighted networks: the modes permutation test. Journal of Geographical Systems, 15(3):233–247.

Borg, I. and Groenen, P. J. (2005). Modern multidimensional scaling: Theory and applications. Springer Science & Business Media.

Braun, D. (2006). Invariant integration over the orthogonal group. Journal of Physics A: Mathematical and General, 39(47):14581.

Collins, B. and Matsumoto, S. (2009). On some properties of orthogonal Weingarten functions. Journal of Mathematical Physics, 50(11):113516.

Collins, B., McDonald, D., and Saad, N. (2013). Compound Wishart matrices and noisy covariance matrices: Risk underestimation. arXiv preprint arXiv:1306.5510.
Collins, B. and Śniady, P. (2006). Integration with respect to the Haar measure on unitary, orthogonal and symplectic group. *Communications in Mathematical Physics*, 264(3):773–795.

Cortes, C., Mohri, M., and Rostamizadeh, A. (2012). Algorithms for learning kernels based on centered alignment. *The Journal of Machine Learning Research*, 13:795–828.

Csardi, G., Nepusz, T., et al. (2006). The igraph software package for complex network research. *InterJournal, Complex Systems*, 1695(5):1–9.

Escoufier, Y. (1973). Le traitement des variables vectorielles. *Biometrics*, 29(4):751–760.

Geisser, S. and Greenhouse, S. W. (1958). An extension of Box’s results on the use of the $f$ distribution in multivariate analysis. *The Annals of Mathematical Statistics*, 29(3):885–891.

Harish-Chandra (1957). Differential operators on a semisimple Lie algebra. *American Journal of Mathematics*, pages 87–120.

Heo, M. and Ruben Gabriel, K. (1998). A permutation test of association between configurations by means of the RV coefficient. *Communications in Statistics-Simulation and Computation*, 27(3):843–856.

Josse, J., Pagès, J., and Husson, F. (2008). Testing the significance of the RV coefficient. *Computational Statistics & Data Analysis*, 53(1):82–91.

Kazi-Aoual, F., Hitier, S., Sabatier, R., and Lebreton, J.-D. (1995). Refined approximations to permutation tests for multivariate inference. *Computational statistics & data analysis*, 20(6):643–656.

Kendall, M. and Stuart, A. (1977). The advanced theory of statistics. vol. 1: Distribution theory. *London: Griffin*.

Matsumoto, S. (2012). General moments of the inverse real Wishart distribution and orthogonal Weingarten functions. *Journal of Theoretical Probability*, 25(3):798–822.

McSwiggen, C. (2021). The Harish-Chandra integral: An introduction with examples. *L'Enseignement Mathématique*, 67(3):229–299.

Robert, P. and Escoufier, Y. (1976). A unifying tool for linear multivariate statistical methods: the RV-coefficient. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 25(3):257–265.

Schlich, P. (1996). Defining and validating assessor compromises about product distances and attribute correlations. In *Data handling in science and technology*, volume 16, pages 259–306. Elsevier.

Tao, T. (2013). The Harish-Chandra-Itzykson-Zuber integral formula. What’s new (blog) [https://terrytao.wordpress.com/2013/02/08/the-harish-chandra-itzykson-zuber-integral-formula](https://terrytao.wordpress.com/2013/02/08/the-harish-chandra-itzykson-zuber-integral-formula).

Worsley, K. J. and Friston, K. J. (1995). Analysis of fmri time-series revisited—again. *Neuroimage*, 2(3):173–181.

Yamamoto, Y. and Kudo, S. (2017). Probabilistic analysis of an estimator for the Frobenius norm of a matrix product. *SIAM Letters*, 9:9–12.

Zhang, H., Tian, J., Li, J., and Zhao, J. (2009). RV-coefficient and its significance test in mapping brain functional connectivity. In *Medical Imaging 2009: Biomedical Applications in Molecular, Structural, and Functional Imaging*, volume 7262, pages 627–635. SPIE.