

The delta method for analytic functions of random operators with application to functional data

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In this paper, the asymptotic distributions of estimators for the regularized functional canonical correlation and variates of the population are derived. The method is based on the possibility of expressing these regularized quantities as the maximum eigenvalue and the corresponding eigenfunctions of an associated pair of regularized operators, similar to the Euclidean case. The known weak convergence of the sample covariance operator, coupled with a delta-method for analytic functions of covariance operators, yields the weak convergence of the pair of associated operators. From the latter weak convergence, the limiting distributions of the canonical quantities of interest can be derived with the help of some further perturbation theory.

Keywords: delta-method for analytic functions of covariance operators; perturbation theory; regularization of operators; regularized functional canonical correlation and variates; weak convergence

1. Introduction

This paper deals with the asymptotic distribution theory of functional canonical correlations and their variates. Although tailored to these particular problems, the methodology is of a generic character and may also apply to questions regarding the asymptotic distribution of other statistics used in functional data analysis. The problem will be formulated in a general Hilbert space setting where the Hilbert space is tacitly assumed to be infinite-dimensional and separable.

In this infinite-dimensional case, some difficulties regarding the definition of the sample canonical correlation have already been observed in Leurgans *et al.* (1993). The authors of that paper argue that some kind of smoothing or regularization is indispensable when dealing with the sample canonical correlation. These difficulties are essentially due to the fact that the sample covariance operator has a so-called finite-dimensional kernel (Riesz and Sz.-Nagy (1990)), while acting on an infinite-dimensional space. Leurgans *et al.* (1993) realize smoothing by introducing a roughness penalty term. Although there is a connection between Tikhonov regularization of inverse operators (employed in this paper) and the use of penalty terms, the relation with the roughness penalty cannot be established within the present context of our paper. He *et al.* (2004) apply dimension reduction/augmentation at the level of the actual data and base the empirical canonical correlation on these modified data. This approach differs considerably from ours, which is based on regularization of the canonical correlation itself. The results in He *et al.*

(2004) are for fixed sample size and the asymptotics in Leurgans *et al.* (1993) remain restricted to consistency.

In Cupidon *et al.* (2006) it has been observed that the population canonical correlation, although well defined in principle, is, in general, a supremum of a certain functional, rather than a maximum, so that a maximizer (i.e., a pair of canonical variates) may not always exist in the ambient Hilbert space. Another deficiency is that, even if the canonical correlation corresponds to a maximum and canonical variates do exist, these quantities cannot be interpreted as the maximum eigenvalue and corresponding eigenvector of a pair of associated operators, as is true in the Euclidean setting. The development in Cupidon *et al.* (2006) shows that all of these deficiencies of the population canonical correlation can be remedied if a modification is employed, based on regularization of the inverses of the operators involved. Also, some relations between the actual population quantities and their regularized versions are established in that paper.

The present approach to finding the asymptotic distribution of the regularized sample canonical correlation and its variates hinges to a great extent on the interpretation of both the regularized sample and the regularized population quantities as spectral characteristics of associated pairs of operators. In Section 4 of this paper, the asymptotic distribution of a regularized version of the sample canonical correlation and its variates will be derived. In the Euclidean case, where regularization is not needed, this approach has been pursued in Ruymgaart and Yang (1997), exploiting certain results in Watson (1983).

One of the main tools needed to derive the desired asymptotics is a delta-method for analytic functions of certain random operators (more specifically, sample covariance operators). This delta-method might be of independent interest and is considered in Section 3. It is based on the existence of a Fréchet derivative of an analytic function of a compact, strictly positive Hermitian operator, tangentially to the space of all compact Hermitian operators. Because we cannot make the simplifying assumption that the increments commute with the operator at which the function is evaluated, the expression for the Fréchet derivative requires an extra correction term. The delta-method yields the asymptotic distribution of the associated operators, from which the asymptotics of their eigenvalues and eigenvectors can be derived in a similar manner as in Dauxois *et al.* (1982).

As has been observed above, without regularization, the population canonical variates do not, in general, exist and, consequently, it seems appropriate to maintain a fixed level of regularization for suitable asymptotics. Mathematically, a fixed level of regularization leads to root-sample-size asymptotics. When the regularization parameter tends to zero, however, this rate will depend on the (typically unknown) eigenvalues of the covariance operator.

In Section 2, some basic notation and definitions are introduced. For practical implementation of the results of Section 4, the estimation of unknown parameters will be needed, an issue addressed in Section 5. An example and some further comments are given in Section 6. The mathematical results for perturbation of compact, positive Hermitian operators that, in particular, yield the Fréchet derivative are reviewed without proof in the Appendix.

2. Basic notation, definitions and assumptions

Let $(\Omega, \mathcal{F}, \mathbb{P})$ denote a probability space, \mathbb{H} an infinite dimensional, separable Hilbert space with inner product $\langle \cdot, \cdot \rangle$, norm $\| \cdot \|$ and σ -field of Borel sets $\mathcal{B}_{\mathbb{H}}$, and let $X : \Omega \rightarrow \mathbb{H}$ be a random

element in \mathbb{H} , that is, an $(\mathcal{F}, \mathcal{B}_{\mathbb{H}})$ -measurable mapping. Throughout, it will be required that

$$\mathbb{E}\|X\|^4 < \infty. \tag{2.1}$$

Under this condition, the mean $\mathbb{E}X = \mu \in \mathbb{H}$ exists, meaning that (Laha and Rohatgi (1979))

$$\mathbb{E}\langle f, X \rangle = \langle f, \mu \rangle \quad \forall f \in \mathbb{H}. \tag{2.2}$$

Under assumption (2.1), the covariance operator Σ of X also exists. It is known to be uniquely determined by the relation

$$\mathbb{E}\langle f, X - \mu \rangle \langle X - \mu, g \rangle = \mathbb{E}\langle f, ((X - \mu) \otimes (X - \mu))g \rangle = \langle f, \Sigma g \rangle \quad \forall f, g \in \mathbb{H}, \tag{2.3}$$

where “ \otimes ” denotes the tensor product in \mathbb{H} . We will also write

$$\Sigma = \mathbb{E}(X - \mu) \otimes (X - \mu). \tag{2.4}$$

Such a covariance operator is nonnegative Hermitian and has finite trace $\mathbb{E}\|X\|^2$, so it is also compact. We will therefore assume, without real loss of generality, that

$$\Sigma \text{ is strictly positive, that is, } \langle f, \Sigma f \rangle > 0 \quad \forall f \neq 0 \tag{2.5}$$

and hence that Σ is injective. It is well known that Σ has spectral representation

$$\Sigma = \sum_{k=1}^{\infty} \lambda_k P_k, \tag{2.6}$$

where $\lambda_1 > \lambda_2 > \dots \downarrow 0$ are the eigenvalues of Σ and P_1, P_2, \dots the projections onto the corresponding finite-dimensional eigenspaces.

Let \mathcal{L} denote the Banach space of all bounded linear operators that map \mathbb{H} into itself. The ordinary operator norm in \mathcal{L} will be denoted by $\|\cdot\|$ without confusion. Of particular importance in this paper, however, is the subspace $\mathcal{L}(\text{HS})$ of all Hilbert–Schmidt operators. This space becomes a separable Hilbert space when it is endowed with the inner product

$$\langle U, V \rangle_{\text{HS}} = \sum_{k=1}^{\infty} \langle U e_k, V e_k \rangle, \quad U, V \in \mathcal{L}(\text{HS}), \tag{2.7}$$

where e_1, e_2, \dots is an orthonormal basis of \mathbb{H} . This inner product does not depend on the choice of basis; see Lax (2000). The norm and tensor product in $\mathcal{L}(\text{HS})$ will be denoted by $\|\cdot\|_{\text{HS}}$ and \otimes_{HS} , respectively.

The space $\mathcal{L}(\text{HS})$ is important for the study of weak convergence of the sample covariance operator. At this point, let us simply note that $\Sigma \in \mathcal{L}(\text{HS})$ and that $(X - \mu) \otimes (X - \mu)$ is a random element in $\mathcal{L}(\text{HS})$. As a random element in this Hilbert space, it has its own covariance

operator; this operator exists due to condition (2.1) and can easily be seen to equal (cf. (2.3) and (2.4))

$$\begin{aligned} &\mathbb{E}\{(X - \mu) \otimes (X - \mu) - \Sigma\} \otimes_{\text{HS}} \{(X - \mu) \otimes (X - \mu) - \Sigma\} \\ &= \mathbb{E}\{(X - \mu) \otimes (X - \mu)\} \otimes_{\text{HS}} \{(X - \mu) \otimes (X - \mu)\} - \Sigma \otimes_{\text{HS}} \Sigma \\ &= \Sigma_{\text{HS}}. \end{aligned} \tag{2.8}$$

Next, let us suppose that \mathbb{H}_1 and \mathbb{H}_2 are two closed subspaces of \mathbb{H} such that

$$\mathbb{H} = \mathbb{H}_1 \oplus \mathbb{H}_2, \quad \mathbb{H}_1 \perp \mathbb{H}_2. \tag{2.9}$$

Denote the orthogonal projection of \mathbb{H} onto \mathbb{H}_j by Π_j , let $X_j = \Pi_j X$, $\mu_j = \Pi_j \mu$ and let Σ_{jk} denote the restriction of Σ to \mathbb{H}_k and \mathbb{H}_j , that is,

$$\Sigma_{jk} = \Pi_j \Sigma \Pi_k, \quad j, k = 1, 2. \tag{2.10}$$

Because the Π_j are bounded and Σ is Hilbert–Schmidt (and hence compact), each operator Σ_{jk} is still Hilbert–Schmidt (and hence compact). In addition, the Σ_{jj} are strictly positive Hermitian. Let us also note that

$$\Sigma_{12}^* = (\Pi_1 \Sigma \Pi_2)^* = \Pi_2 \Sigma \Pi_1 = \Sigma_{21}. \tag{2.11}$$

Similarly to (2.6), Σ_{jj} has a spectral representation of the form

$$\Sigma_{jj} = \sum_{k=1}^{\infty} \lambda_{jk} P_{jk}, \quad j = 1, 2, \tag{2.12}$$

where $\lambda_{j1} > \lambda_{j2} > \dots \downarrow 0$ are the eigenvalues of Σ_{jj} and P_{j1}, P_{j2}, \dots the projections onto the corresponding finite dimensional eigenspaces.

Suppose, now, that we are given a random sample X_1, X_2, \dots, X_n of independent copies of X . The usual estimators of μ and Σ are

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i, \quad \widehat{\Sigma} = \frac{1}{n} \sum_{i=1}^n (X_i - \bar{X}) \otimes (X_i - \bar{X}), \tag{2.13}$$

respectively. This operator $\widehat{\Sigma}$ has all of the properties of Σ , including its being of Hilbert–Schmidt type, except that it has a so-called finite-dimensional kernel (Riesz and Sz. Nagy (1990)) with a range of dimension at most n . Hence, this operator can never be injective, not even when Σ is (as we assume). The fact that $\widehat{\Sigma}$ is not injective is the source of difficulties associated with defining the sample principal canonical correlation that turns out to always be 1, as has been pointed out by Leurgans *et al.* (1993). These authors state that regularization is indispensable in the sample case.

The canonical correlation concept considered here can also be viewed from the perspective of Hilbert-space-indexed processes (e.g., Parzen (1970)) corresponding to \mathbb{H} inner products involving the random elements $X_j = \Pi_j X$, $j = 1, 2$. Thus, it has direct ties to (functional) analysis of

variance and discriminant analysis that parallel the relationship between these methods for classical multivariate analysis (e.g., Kshirsagar (1972), Eubank and Hsing (2006) and Shin (2006)). The necessity of regularization in this context follows from results in Bickel and Levina (2004), while the use of regularized discriminant analysis methods with functional data has been explored by Hastie *et al.* (1995).

Cupidon *et al.* (2006) argue that regularization is expedient, even when the population canonical correlation is considered, because, without it, canonical variates may not exist and the relation with the spectral characteristics of an associated pair of operators is lost. Hence, in this paper, both the sample and the population canonical correlation will be regularized and compared at the same fixed, but arbitrary, level of the regularization parameter.

In order to specify the regularization that will be employed here, let us replace Σ with $\alpha I + \Sigma$ and $\widehat{\Sigma}$ with $\alpha I + \widehat{\Sigma}$, where I is the identity operator and $\alpha > 0$. Let us also replace Σ_{jk} and $\widehat{\Sigma}_{jk}$ with

$$\Pi_j(\alpha I + \Sigma)\Pi_k = \begin{cases} (\alpha I_j + \Sigma_{jj}), & j = k, \\ \Sigma_{jk}, & j \neq k, \end{cases} \tag{2.14}$$

$$\Pi_j(\alpha I + \widehat{\Sigma})\Pi_k = \begin{cases} (\alpha I_j + \widehat{\Sigma}_{jj}), & j = k, \\ \widehat{\Sigma}_{jk}, & j \neq k, \end{cases} \tag{2.15}$$

respectively, where $I_j = \Pi_j$ is essentially the identity operator restricted to \mathbb{H}_j . Let us write $\mathbb{H}_1^0 = \mathbb{H}_1 \setminus \{0\}$, $\mathbb{H}_2^0 = \mathbb{H}_2 \setminus \{0\}$ for brevity.

Definition 2.1. Fix $\alpha > 0$. The regularized squared principal canonical correlation (RSPCC) for the population is defined as

$$\rho^2 = \rho^2(\alpha) = \max_{\substack{f_1 \in \mathbb{H}_1^0 \\ f_2 \in \mathbb{H}_2^0}} \frac{\langle f_1, \Sigma_{12} f_2 \rangle^2}{\langle f_1, (\alpha I_1 + \Sigma_{11}) f_1 \rangle \langle f_2, (\alpha I_2 + \Sigma_{22}) f_2 \rangle}. \tag{2.16}$$

Its sample analogue is $\widehat{\rho}^2 = \widehat{\rho}^2(\alpha)$, obtained from (2.16) by replacing Σ_{jk} with $\widehat{\Sigma}_{jk}$. Pairs of maximizers will be respectively denoted by $f_1^* = f_{1\alpha}^*$, $f_2^* = f_{2\alpha}^*$ for the population and by $\widehat{f}_1 = \widehat{f}_{1\alpha}$, $\widehat{f}_2 = \widehat{f}_{2\alpha}$ for the sample. The corresponding canonical variates are

$$\langle X, f_j^* \rangle, \langle X, \widehat{f}_j^* \rangle, \quad j = 1, 2. \tag{2.17}$$

Warning. Since, throughout the sequel, $\alpha > 0$ will be arbitrary, but fixed, the dependence on α is henceforth suppressed in the notation.

Several properties have been shown in Cupidon *et al.* (2006), in particular, that, for $\alpha > 0$, a maximizer always exists. This can, in fact, be seen as an implication of the following result of that paper. Define the operators ($\alpha > 0$)

$$R_1 = (\alpha I_1 + \Sigma_{11})^{-1/2} \Sigma_{12} (\alpha I_2 + \Sigma_{22})^{-1} \Sigma_{21} (\alpha I_1 + \Sigma_{11})^{-1/2}, \tag{2.18}$$

$$R_2 = (\alpha I_2 + \Sigma_{22})^{-1/2} \Sigma_{21} (\alpha I_1 + \Sigma_{11})^{-1} \Sigma_{12} (\alpha I_2 + \Sigma_{22})^{-1/2} \tag{2.19}$$

and their sample analogues \widehat{R}_1 and \widehat{R}_2 . Since all factors defining these operators are bounded, with Σ_{12} and Σ_{21} or their sample analogues even Hilbert–Schmidt (and hence compact) it follows that these operators are also Hilbert–Schmidt (and hence compact). It will be assumed that

$$\begin{cases} R_1 \text{ and } R_2 \text{ have a largest eigenvalue with one-dimensional eigenspace} \\ \text{generated by } f_1^* \text{ and } f_2^*, \text{ respectively, where } \|f_1^*\| = \|f_2^*\| = 1. \end{cases} \tag{2.20}$$

Theorem 2.1. *For $\alpha > 0$, we have*

$$\rho^2 = \text{largest eigenvalue of } R_j = \langle f_j^*, R_j f_j^* \rangle \tag{2.21}$$

for $j = 1, 2$. A similar result holds true for $\widehat{\rho}^2$.

The maximizers or canonical variates are essentially unique if the eigenspaces corresponding to this maximal eigenvalue are one-dimensional. The same properties hold true for the sample analogue.

3. A delta-method for analytic functions of the sample covariance operator

Assuming (2.1), Dauxois *et al.* (1982) have shown the fundamental result

$$\sqrt{n}(\widehat{\Sigma} - \Sigma) \xrightarrow{d} \mathcal{G}, \quad \text{as } n \rightarrow \infty, \text{ in } \mathcal{L}(\text{HS}), \tag{3.1}$$

where \mathcal{G} is a zero-mean Gaussian random element in the Hilbert space $\mathcal{L}(\text{HS})$ with covariance operator

$$\mathbb{E} \mathcal{G} \otimes_{\text{HS}} \mathcal{G} = \Sigma_{\text{HS}}, \tag{3.2}$$

as defined in (2.8). The continuous mapping theorem immediately yields that

$$\sqrt{n}(\widehat{\Sigma}_{jk} - \Sigma_{jk}) \xrightarrow{d} \Pi_j \mathcal{G} \Pi_k = \mathcal{G}_{jk}, \quad \text{as } n \rightarrow \infty, \text{ in } \mathcal{L}(\text{HS}). \tag{3.3}$$

Let $D \subset \mathbb{C}$ be the open domain in the complex plane defined by

$$D = \left\{ z \in \mathbb{C} : \min_{0 \leq x \leq \|\Sigma\|} |z - x| < \frac{1}{2}\alpha \right\}, \tag{3.4}$$

where $\alpha > 0$ is the regularization parameter. This domain can be used for all the specific functions we need to consider. It seems worthwhile, however, to first consider an arbitrary function

$$\varphi : D \rightarrow \mathbb{C}, \quad \text{analytic on } D. \tag{3.5}$$

As in the Appendix, let \mathcal{C}_H denote the class of all compact Hermitian operators on \mathbb{H} and \mathcal{L}_H the class of all bounded Hermitian operators. Let us consider the operator $\varphi(\Sigma + \mathcal{P})$ in \mathcal{L}_H , for \mathcal{P}

in \mathcal{C}_H with $\|\mathcal{P}\| < \frac{1}{3}\alpha$. This operator-valued function has a Fréchet derivative at Σ , tangentially to \mathcal{C}_H , denoted by φ'_Σ and given by (A.6). This operator $\varphi'_\Sigma: \mathcal{C}_H \rightarrow \mathcal{L}_H$ is bounded in the usual operator norm.

If $\mathcal{L}_H(\text{HS}) \subset \mathcal{C}_H$ is the subspace of all Hermitian Hilbert–Schmidt operators, we even have

$$\varphi'_\Sigma: \mathcal{L}_H(\text{HS}) \rightarrow \mathcal{L}_H(\text{HS}), \quad \text{bounded in } \|\cdot\|_{\text{HS}}. \tag{3.6}$$

To see this, take $\mathcal{P} \in \mathcal{L}_H(\text{HS})$ and observe that

$$\|\varphi'_\Sigma \mathcal{P}\|_{\text{HS}}^2 = \sum_{k=1}^{\infty} \|\varphi'_\Sigma \mathcal{P}e_k\|^2 \leq \|\varphi'_\Sigma\|^2 \sum_{k=1}^{\infty} \|\mathcal{P}e_k\|^2 = \|\varphi'_\Sigma\|^2 \|\mathcal{P}\|_{\text{HS}}^2 < \infty, \tag{3.7}$$

exploiting the boundedness of φ'_Σ in the usual operator norm. It is well known (Lax (2000)) that

$$\|T\| \leq \|T\|_{\text{HS}}, \quad T \in \mathcal{L}(\text{HS}). \tag{3.8}$$

We are now ready to establish a “delta-method” for random operators. For random matrices, the result follows from Watson (1983) and can be found in Ruymgaart and Yang (1997).

Theorem 3.1. *If (2.1) is satisfied, it then follows that*

$$\sqrt{n}\{\varphi(\widehat{\Sigma}) - \varphi(\Sigma)\} \xrightarrow{d} \mathcal{H}, \quad \text{as } n \rightarrow \infty, \text{ in } \mathcal{L}(\text{HS}), \tag{3.9}$$

where \mathcal{H} is the zero-mean Gaussian random element of $\mathcal{L}(\text{HS})$ given by

$$\mathcal{H} = \varphi'_\Sigma \mathcal{G} = \sum_{j \geq 1} \varphi'(\lambda_j) P_j \mathcal{G} P_j + \sum_{j \neq k} \frac{\varphi(\lambda_k) - \varphi(\lambda_j)}{\lambda_k - \lambda_j} P_j \mathcal{G} P_k, \tag{3.10}$$

with \mathcal{G} given in (3.1).

Proof. Let us consider $\widehat{\mathcal{P}} = \widehat{\Sigma} - \Sigma$ as a random perturbation (cf. Dauxois *et al.* (1982), Watson (1983)) and note that, by (3.1) and (3.8), we have $\|\widehat{\mathcal{P}}\| \leq \|\widehat{\mathcal{P}}\|_{\text{HS}} = \mathcal{O}_p(n^{-1/2})$ as $n \rightarrow \infty$. This implies that, for numbers $n^{-1/2} \ll \epsilon_n \ll n^{-1/4}$ we have

$$\mathbb{P}(\Omega_n) = \mathbb{P}\{\omega \in \Omega : \|\widehat{\mathcal{P}}(\omega)\| < \epsilon_n\} \rightarrow 1 \quad \text{as } n \rightarrow \infty. \tag{3.11}$$

According to Theorem A.1 and (3.12), we have, for n sufficiently large,

$$\begin{aligned} \sqrt{n}\{\varphi(\widehat{\Sigma}) - \varphi(\Sigma)\} &= \sqrt{n}\{\varphi(\widehat{\Sigma}) - \varphi(\Sigma)\} \mathbf{1}_{\Omega_n} + \sqrt{n}\{\varphi(\widehat{\Sigma}) - \varphi(\Sigma)\} \mathbf{1}_{\Omega_n^c} \\ &= \sqrt{n}\{\varphi'_\Sigma \widehat{\mathcal{P}} + \mathcal{O}(\|\widehat{\mathcal{P}}\|^2)\} \mathbf{1}_{\Omega_n} + \sigma_p(1) \\ &= \varphi'_\Sigma (\sqrt{n}(\widehat{\Sigma} - \Sigma)) + \sigma_p(1). \end{aligned} \tag{3.12}$$

The results in the theorem follow from (3.12) by applying (3.1) once more, in conjunction with (3.6) and the continuous mapping theorem. □

Remark 3.1. The double sum in (3.1) is, in fact, a correction term that is needed because we may not assume that the “increments” $\widehat{P} = \widehat{\Sigma} - \Sigma$ and Σ commute; see also Remark A.1.

In order to obtain asymptotic distributions for functional canonical correlations and variates, Theorem 3.1 will be employed for the specific functions

$$\varphi_p(z) = (\alpha + z)^{-p/2}, \quad z \in D, \quad p = 1, 2. \tag{3.13}$$

These functions are indeed analytic on D . For brevity, let us simply write $\varphi'_{p,j}$ for the Fréchet derivative evaluated at Σ_{jj} . It is immediate from (2.9) that $\|\Sigma_{jj}\| \leq \|\Sigma\|$ and therefore the domain D can still be used for Σ_{jj} . The following corollary is immediate from these remarks, (3.3) and Theorem 3.1.

Corollary 3.1. *With φ_p as in (3.13), we have, for $j = 1, 2$,*

$$\sqrt{n}\{\varphi_p(\widehat{\Sigma}_{jj}) - \varphi_p(\Sigma_{jj})\} \xrightarrow{d} \varphi'_{p,j} \mathcal{G}_{jj}, \tag{3.14}$$

where the limit is a zero-mean Gaussian random element in $\mathcal{L}(\text{HS})$ and, more explicitly,

$$\begin{aligned} \varphi'_{p,j} \mathcal{G}_{jj} = & -\frac{p}{2} \sum_{k \geq 1} \frac{1}{(\alpha + \lambda_{jk})^{(p+2)/2}} P_{jk} \mathcal{G}_{jj} P_{jk} \\ & + \sum_{m \neq n} \frac{(\alpha + \lambda_{jm})^{p/2} - (\alpha + \lambda_{jn})^{p/2}}{(\lambda_{jn} - \lambda_{jm})(\alpha + \lambda_{jm})^{p/2}(\alpha + \lambda_{jn})^{p/2}} P_{jm} \mathcal{G}_{jj} P_{jn}. \end{aligned} \tag{3.15}$$

4. Asymptotics for the sample RSPCC and variates

The basic ingredients for the asymptotic distribution of the sample RSPCC and its variates are the weak limits of the associated operators \widehat{R}_1 and \widehat{R}_2 (cf. (2.17) and (2.18)) from which these quantities are derived. These limits follow rather routinely with the help of Corollary 3.1. It has already been observed that $R_j, \widehat{R}_j \in \mathcal{L}(\text{HS})$ for $j = 1, 2$.

Let us introduce the following zero-mean Gaussian elements of $\mathcal{L}(\text{HS})$:

$$\mathcal{R}_{11} = (\varphi'_{1,1} \mathcal{G}_{11}) \Sigma_{12} \varphi_2(\Sigma_{22}) \Sigma_{21} \varphi_1(\Sigma_{11}), \tag{4.1}$$

$$\mathcal{R}_{12} = \varphi_1(\Sigma_{11}) \mathcal{G}_{12} \varphi_2(\Sigma_{22}) \Sigma_{21} \varphi_1(\Sigma_{11}), \tag{4.2}$$

$$\mathcal{R}_{13} = \varphi_1(\Sigma_{11}) \Sigma_{12} (\varphi'_{2,2} \mathcal{G}_{22}) \Sigma_{21} \varphi_1(\Sigma_{11}), \tag{4.3}$$

$$\mathcal{R}_{14} = \varphi_1(\Sigma_{11}) \Sigma_{12} \varphi_2(\Sigma_{22}) \mathcal{G}_{21} \varphi_1(\Sigma_{11}), \tag{4.4}$$

$$\mathcal{R}_{15} = \varphi_1(\Sigma_{11}) \Sigma_{12} \varphi_2(\Sigma_{22}) \Sigma_{21} \varphi'_{1,1}(\mathcal{G}_{11}), \tag{4.5}$$

$$\mathcal{R}_1 = \sum_{j=1}^5 \mathcal{R}_{1j} \tag{4.6}$$

and, similarly,

$$\mathcal{R}_{21} = (\varphi'_{1,2}\mathcal{G}_{22})\Sigma_{21}\varphi_2(\Sigma_{11})\Sigma_{12}\varphi_1(\Sigma_{22}), \tag{4.7}$$

$$\mathcal{R}_{22} = \varphi_1(\Sigma_{22})\mathcal{G}_{21}\varphi_2(\Sigma_{11})\Sigma_{12}\varphi_1(\Sigma_{22}), \tag{4.8}$$

$$\mathcal{R}_{23} = \varphi_1(\Sigma_{22})\Sigma_{21}(\varphi'_{2,1}\mathcal{G}_{11})\Sigma_{12}\varphi_1(\Sigma_{22}), \tag{4.9}$$

$$\mathcal{R}_{24} = \varphi_1(\Sigma_{22})\Sigma_{21}\varphi_2(\Sigma_{11})\mathcal{G}_{12}\varphi_1(\Sigma_{22}), \tag{4.10}$$

$$\mathcal{R}_{25} = \varphi_1(\Sigma_{22})\Sigma_{21}\varphi_2(\Sigma_{11})\Sigma_{12}\varphi'_{1,2}(\mathcal{G}_{22}), \tag{4.11}$$

$$\mathcal{R}_2 = \sum_{j=1}^5 \mathcal{R}_{2j}. \tag{4.12}$$

Theorem 4.1. *Let (2.1) be satisfied. We have*

$$\sqrt{n}(\widehat{R}_j - R_j) \xrightarrow{d} \mathcal{R}_j, \quad \text{as } n \rightarrow \infty, \text{ in } \mathcal{L}(\text{HS}) \text{ for } j = 1, 2. \tag{4.13}$$

Proof. It suffices to prove (4.13) for $j = 1$. The left-hand side of (4.13) can be decomposed as $\sum_{j=1}^5 \widehat{\mathcal{R}}_{1j}$, where, for instance,

$$\widehat{\mathcal{R}}_{11} = \sqrt{n}\{\varphi_1(\widehat{\Sigma}_{11}) - \varphi_1(\Sigma_{11})\}\widehat{\Sigma}_{12}\varphi_2(\widehat{\Sigma}_{22})\widehat{\Sigma}_{21}\varphi_1(\widehat{\Sigma}_{11}). \tag{4.14}$$

It follows from (3.14) that the first factor in (4.14) equals $\varphi'_{1,2}\mathcal{G}_{22} + \sigma_p(1)$. Relation (3.3) and the continuity of the functions in (3.14) imply that the product of the remaining four factors equals $\Sigma_{21}\varphi_2(\Sigma_{11})\Sigma_{12}\varphi_1(\Sigma_{22}) + \mathcal{O}_p(1)$. In combination, these results yield that $\widehat{\mathcal{R}}_{11} = \mathcal{R}_{11} + \mathcal{O}_p(1)$. In a similar manner, one can deal with $\widehat{\mathcal{R}}_{12}, \dots, \widehat{\mathcal{R}}_{15}$. Eventually, this produces $\sqrt{n}(\widehat{R}_1 - R_1) = \sum_{j=1}^5 \widehat{\mathcal{R}}_{1j} + \sigma_p(1)$ and we are done. \square

To establish (4.13), we have exploited the delta-method of (3.14), based on the Fréchet derivative, in order to deal with the factors in the product defining \widehat{R}_j . Once the limiting distributions of the random operators have been established, we may proceed as in Dauxois *et al.* (1982) to find the asymptotic distributions of eigenvalues and eigenvectors. For completeness, the required perturbation results in the infinite-dimensional situation are briefly summarized in the [Appendix](#) and proofs of the two main theorems below are included.

First, some more notation will be needed. The compact operators R_j and \widehat{R}_j are nonnegative Hermitian and have spectral representations

$$R_j = \sum_{k=1}^{\infty} \rho_{jk} Q_{jk}, \quad \widehat{R}_j = \sum_{k=1}^{\infty} \widehat{\rho}_{jk} \widehat{Q}_{jk}, \quad j = 1, 2, \tag{4.15}$$

where $\rho_{j1} > \rho_{j2} > \dots \downarrow 0$ and $\widehat{\rho}_{j1} > \widehat{\rho}_{j2} > \dots \downarrow 0$ are the distinct eigenvalues and Q_{jk}, \widehat{Q}_{jk} the orthogonal projections onto the corresponding finite dimensional eigenspaces. Assumption (2.20) implies that

$$\rho_{j1} = \rho_j^2, \quad Q_{j1} = f_j^* \otimes f_j^*, \quad j = 1, 2. \tag{4.16}$$

We also have, by Definition 2.1 and Theorem 2.1, that

$$\widehat{\rho}_{j1} = \widehat{\rho}^2, \quad j = 1, 2. \tag{4.17}$$

The operators

$$A_j = \sum_{k=2}^{\infty} \frac{\rho_{j1}}{\rho_{j1} - \rho_{jk}} Q_{jk}, \quad j = 1, 2, \tag{4.18}$$

will also be needed.

Theorem 4.2. *Let (2.1) and (2.19) be satisfied. The sample RSPCC then has a normal distribution in the limit:*

$$\sqrt{n}(\widehat{\rho}^2 - \rho^2) \xrightarrow{d} N(0, \sigma^2) \quad \text{as } n \rightarrow \infty, \tag{4.19}$$

where

$$\sigma^2 = \mathbb{E} \langle \mathcal{R}_j f_j^*, f_j^* \rangle^2, \quad j = 1, 2. \tag{4.20}$$

Proof. The proof is in the same vein as that of Theorem 3.1. However, let us now consider the random perturbation $\widehat{\mathcal{P}} = \widehat{R}_j - R_j$ and define Ω_n for the same ϵ_n , but with $\widehat{\mathcal{P}}$ as above. In the present situation, it is (4.13) that guarantees that $\mathbb{P}(\Omega_n) \rightarrow 1$ as $n \rightarrow \infty$.

It follows from Theorem A.2 that

$$\widehat{Q}_{j1} \mathbf{1}_{\Omega_n} = \widehat{f}_j^* \otimes \widehat{f}_j^* \mathbf{1}_{\Omega_n} \tag{4.21}$$

for n sufficiently large. Application of Theorem A.3 yields

$$\begin{aligned} \sqrt{n}(\widehat{\rho}_{j1} - \rho_{j1}) &= \sqrt{n}(\widehat{\rho}_{j1} - \rho_{j1}) \mathbf{1}_{\Omega_n} + \sqrt{n}(\widehat{\rho} - \rho) \mathbf{1}_{\Omega_n^c} \\ &= \sqrt{n} \langle \widehat{\mathcal{P}} f_j^*, f_j^* \rangle \mathbf{1}_{\Omega_n} + \mathcal{O}(\|\widehat{\mathcal{P}}\|^2 \mathbf{1}_{\Omega_n}) + \sigma_p(1) \\ &= \langle \sqrt{n}(\widehat{R}_j - R_j) f_j^*, f_j^* \rangle + \sigma_p(1) \\ &\xrightarrow{d} \langle \mathcal{R}_j f_j^*, f_j^* \rangle, \quad \text{as } n \rightarrow \infty. \end{aligned} \tag{4.22}$$

Because of (4.16) and (4.17), the expression on the left in (4.22) equals the one on the left in (4.19), so the theorem follows. □

Theorem 4.3. *Assuming the validity of (2.1) and (2.19), we have*

$$\sqrt{n}(\widehat{f}_j^* - f_j^*) \xrightarrow{d} A_j \mathcal{R}_j f_j^*, \quad \text{as } n \rightarrow \infty, \text{ in } \mathbb{H} \text{ for } j = 1, 2. \tag{4.23}$$

Proof. Let us consider the same random perturbation $\widehat{\mathcal{P}} = \widehat{R}_j - R_j$ and the same sets Ω_n as in the proof of Theorem 4.2. Let us also recall (4.21). It follows from Theorem A.2 that

$$\widehat{f}_j^* \mathbf{1}_{\Omega_n} = (f_j^* + A_j \mathcal{P} f_j^*) \mathbf{1}_{\Omega_n} + \mathcal{O}(\mathcal{P}^2 \mathbf{1}_{\Omega_n}). \tag{4.24}$$

In the same manner as (4.22), we now obtain

$$\sqrt{n}(\widehat{f}_j^* - f_j^*) = A_j \sqrt{n}(\widehat{R}_j - R_j) f_j^* + \sigma_p(1) \xrightarrow{d} A_j \mathcal{R}_j f_j^* \quad \text{as } n \rightarrow \infty, \quad (4.25)$$

which proves the theorem. □

5. Further specification of limiting distributions

The distributions on the right in (4.19) and (4.23) contain unknown parameters that must be estimated for practical implementation. Let us first consider the variance in (4.20). Substituting (4.6) or (4.7) yields

$$\sigma^2 = \sum_{k=1}^5 \sum_{m=1}^5 \mathbb{E} \langle \mathcal{R}_{jk} f_j^*, f_j^* \rangle \langle \mathcal{R}_{jm} f_j^*, f_j^* \rangle. \quad (5.1)$$

Subsequent substitution of the expressions for the \mathcal{R}_{jk} shows, after reworking the inner products, that the expression for σ^2 in (5.1) is a sum of terms of the type

$$\mathbb{E} \langle \mathcal{G} f, g \rangle \langle \mathcal{G} p, q \rangle, \quad (5.2)$$

where $f, g, p, q \in \mathbb{H}$ depend on Σ and where \mathcal{G} is given in (3.1).

Lemma 5.1. *If $f, g, p, q \in \mathbb{H}$ are known, we can express (5.2) as*

$$\mathbb{E} \langle \mathcal{G} f, g \rangle \langle \mathcal{G} p, q \rangle = \langle q \otimes p, \Sigma_{\text{HS}} g \otimes f \rangle_{\text{HS}}, \quad (5.3)$$

where Σ_{HS} is the covariance operator of \mathcal{G} in (3.2).

Proof. Let us assume that $f, g, p, q \neq 0$ because, otherwise, (5.3) is trivial. Hence, we can construct two orthonormal bases of \mathbb{H} , viz. e_1, e_2, \dots and d_1, d_2, \dots , with

$$e_1 = \frac{f}{\|f\|}, \quad d_1 = \frac{p}{\|p\|}. \quad (5.4)$$

Rewriting and evaluating the right-hand side of (5.3), we obtain

$$\begin{aligned} \langle q \otimes p, \Sigma_{\text{HS}} g \otimes f \rangle_{\text{HS}} &= \mathbb{E} \langle q \otimes p, (\mathcal{G} \otimes_{\text{HS}} \mathcal{G}) g \otimes f \rangle_{\text{HS}} \\ &= \mathbb{E} \langle \mathcal{G} g, g \otimes f \rangle_{\text{HS}} \langle \mathcal{G} p, q \otimes p \rangle_{\text{HS}} \\ &= \mathbb{E} \left\{ \sum_{k=1}^{\infty} \langle f, e_k \rangle \langle \mathcal{G} e_k, g \rangle \right\} \left\{ \sum_{m=1}^{\infty} \langle p, d_m \rangle \langle \mathcal{G} d_m, q \rangle \right\} \\ &= \mathbb{E} \langle \mathcal{G} f, g \rangle \langle \mathcal{G} p, q \rangle, \end{aligned} \quad (5.5)$$

as was to be shown. □

Since the f, g, p, q depend on Σ , we can replace them on the right in (5.3) with estimators obtained by substituting $\widehat{\Sigma}$ for Σ . Also, Σ_{HS} is unknown and we may replace this operator with the estimator

$$\widehat{\Sigma}_{\text{HS}} = \frac{1}{n} \sum_{i=1}^n [\{(X_i - \bar{X}) \otimes (X_i - \bar{X}) - \widehat{\Sigma}\} \otimes_{\text{HS}} \{(X_i - \bar{X}) \otimes (X_i - \bar{X}) - \widehat{\Sigma}\}]. \tag{5.6}$$

Let us next turn to the Gaussian random element in \mathbb{H} , on the right in (4.23). Substitution of (4.6) or (4.7) shows that the covariance operator of this random element is determined by covariances of the type

$$\sigma^2(f, g) = \sum_{k=1}^5 \sum_{m=1}^5 \mathbb{E} \langle f, \mathcal{R}_{jk} f_j^* \rangle \langle \mathcal{R}_{jm} f_j^*, g \rangle \tag{5.7}$$

and this can be seen to be a sum of terms of type

$$\mathbb{E} \langle p, \mathcal{G} f_j^* \rangle \langle \mathcal{G} f_j^*, q \rangle, \tag{5.8}$$

in the same way as above. In this case, explicit expressions for p and q involve the operator A_j and hence the unknown ρ_{jk} and \underline{Q}_{jk} (see (4.18) and (4.15)). These quantities can be estimated by the corresponding quantities for $\widehat{\mathcal{R}}_j$ and $\widehat{\Sigma}_{\text{HS}}$ can again be estimated by (5.6) so that, in principle, an estimator of (5.7) is available. An alternative to this estimation scheme could perhaps be formulated using resampling and bootstrap methods. We will not explore this idea further here.

6. Example and some remarks

The purpose of this paper is to establish some fundamental results regarding functional canonical correlations and their variates, at a fixed, but arbitrary, level of the regularization parameter $\alpha > 0$. Although the question of how to choose this parameter in practice is certainly of great interest and relevance, it is not the main concern of this paper and would require a lengthy discussion of further theory and numerical simulations beyond the scope and purpose of this work.

As a compromise, in this section, we present an explicit example that seems suitable for such simulations. It concerns two dependent standard Brownian motion processes that allow for canonical correlations in the entire range from 0 to 1. To construct these processes, let

$$e_m(t) = \sqrt{2} \sin\left(\left(m - \frac{1}{2}\right)\pi t\right), \quad t \in \mathbb{R}, \quad m \in \mathbb{N}, \tag{6.1}$$

$$\lambda_m = \left\{ \frac{1}{(m - 1/2)\pi} \right\}^2, \quad m \in \mathbb{N}. \tag{6.2}$$

Let ξ_{jm} be i.i.d. $N(0, 1)$ -random variables for $m \in \mathbb{N}$ and $j = 1, 2$. Choose $a_m, b_m \in \mathbb{R}$ such that

$$a_m^2 + b_m^2 = 1, \quad m \in \mathbb{N}, \tag{6.3}$$

and define ($j = 1, 2$)

$$e_{jm} = e_m(t - (j - 1))\mathbf{1}_{[j-1, j]}(t), \quad 0 \leq t, \tag{6.4}$$

$$\begin{cases} U_{1m} = \sqrt{\lambda_m}\xi_{1m}, & m \in \mathbb{N}, \\ U_{2m} = \sqrt{\lambda_m}(a_m\xi_{1m} + b_m\xi_{2m}), & m \in \mathbb{N}. \end{cases} \tag{6.5}$$

For both values of j , the

$$U_{jm} \text{ are independent } N(0, \lambda_m), \quad m \in \mathbb{N}. \tag{6.6}$$

Obviously,

$$X_j(t) = \sum_{m=1}^{\infty} U_{jm}e_{jm}(t), \quad 0 \leq t \leq 2, \tag{6.7}$$

is the Karhunen–Loève expansion of a standard Brownian motion, starting at $t = 0$ for $j = 1$ and at $t = 1$ for $j = 2$. If we define

$$X(t) = X_1(t) + X_2(t), \quad 0 \leq t \leq 2, \tag{6.8}$$

then this process is a random function in $\mathbb{H} = L^2(0, 2)$ and X_j can be considered as its projection onto $\mathbb{H}_j = L^2(j - 1, j)$.

Because

$$\gamma_{km} = \mathbb{E}U_{1k}U_{2m} = \sqrt{\lambda_k\lambda_m} a_m\delta_{km}, \tag{6.9}$$

a straightforward, but tedious, calculation (see Cupidon *et al.* (2006)) shows that ρ^2 is the largest eigenvalue of the diagonal matrix \mathcal{R} with elements

$$\mathcal{R}(k, j) = \begin{cases} \frac{a_k^2\lambda_k^2}{(\alpha + \lambda_k)^2}, & k = j, \\ 0, & k \neq j. \end{cases} \tag{6.10}$$

If we assume that

$$1 \geq a_1^2 \geq a_2^2 \geq \dots, \tag{6.11}$$

then the largest eigenvalue of this matrix equals

$$\rho^2 = \frac{a_1^2\lambda_1^2}{(\alpha + \lambda_1)^2}. \tag{6.12}$$

Choosing $a_1^2 = 0$ yields $X_1 \perp\!\!\!\perp X_2$ and $\rho^2 = 0$, and choosing a_1^2 close to 1 and α close to 0 yields a ρ^2 close to 1.

A sample of size n of processes can be obtained by generating n independent, suitably truncated sets of i.i.d. $N(0, 1)$ -random variables and \widehat{R}_1 can, in principle, be numerically approximated, by first approximating \overline{X} and $\widehat{\Sigma}$ in (2.13). Finally, this should yield a specific value of

$\widehat{\rho}^2$ and hence of $\sqrt{n}(\widehat{\rho}^2 - \rho^2)$. This sampling process may be repeated N times. Each of the N runs yields a value of the standardized empirical canonical correlation and these values could be summarized in a histogram. All of this might be repeated for several values of the regularization parameter $\alpha > 0$. Numerical procedures are available, but their implementation is rather involved. Apart from these simulations, some criterion should be formulated that yields an optimal value of α in theory, like the mean integrated square error for curve estimation. The entire issue of gaining insight into the choice of regularization parameter seems a topic of independent interest.

Appendix: Some perturbation theory

In this appendix, we briefly summarize some results from perturbation theory. A more general version of these results can be found in a technical report by Gilliam *et al.* (2006). In slightly different form, Theorem A.2 and Theorem A.3 can be found in Dauxois *et al.* (1982). Some monographs on perturbation theory for operators are Kato (1966), Rellich (1969) and Chatelin (1983). For matrices, Theorem A.1 can be found in Bhatia (2007). It has already been observed that the delta-method for functions of matrices can be found in Ruymgaart and Yang (1997).

All operators considered here map the infinite dimensional, separable Hilbert space \mathbb{H} into itself. As in the main body of the paper, the inner product and norm in \mathbb{H} will be denoted by $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$, respectively, and we will use \mathcal{L}_H to denote all bounded Hermitian operators on \mathbb{H} , with \mathcal{C}_H denoting the subspace of all compact Hermitian operators and \mathcal{C}_H^+ the subset of all strictly positive Hermitian operators. Without confusion, the operator norm will also be denoted by $\| \cdot \|$.

Let $T \in \mathcal{C}_H^+$ be arbitrary, but fixed. Such an operator has a spectral representation of the form

$$T = \sum_{j=1}^{\infty} \lambda_j P_j, \tag{A.1}$$

where $\lambda_1 > \lambda_2 > \dots \downarrow 0$ are the distinct eigenvalues in decreasing order and P_1, P_2, \dots are the projections onto the corresponding finite-dimensional eigenspaces.

The operator T will be perturbed with a compact Hermitian operator $\mathcal{P} \in \mathcal{C}_H$. For $r > 0$, we will write

$$\mathcal{O}(\|\mathcal{P}\|^r) \tag{A.2}$$

to indicate any quantity (operator, vector, number) whose norm or absolute value is of the indicated order as $\|\mathcal{P}\| \rightarrow 0$.

The perturbed operator $\widetilde{T} = T + \mathcal{P}$ is no longer strictly positive, but still $\widetilde{T} \in \mathcal{C}_H$. This operator has spectral representation

$$T = \sum_{j=1}^{\infty} \widetilde{\lambda}_j \widetilde{P}_j, \tag{A.3}$$

where $\widetilde{\lambda}_1, \widetilde{\lambda}_2, \dots$ are distinct nonzero eigenvalues such that $|\widetilde{\lambda}_1| \geq |\widetilde{\lambda}_2| \geq \dots \downarrow 0$, and $\widetilde{P}_1, \widetilde{P}_2, \dots$ are the projections onto the corresponding finite-dimensional eigenspaces.

Furthermore, let $\varphi : D \rightarrow \mathbb{C}$ be analytic on the open domain $D \subset \mathbb{C}$, where

$$D \supset [-\epsilon, \|T\| + \epsilon] \quad \text{for some } \epsilon > 0. \tag{A.4}$$

Theorem A.1. *We have*

$$\varphi(\tilde{T}) = \varphi(T) + \varphi'_T \mathcal{P} + \mathcal{O}(\|\mathcal{P}\|^2), \tag{A.5}$$

where $\varphi'_T : \mathcal{C}_H \rightarrow \mathcal{L}_H$ is bounded and given by

$$\varphi'_T \mathcal{P} = \sum_{j \geq 1} \varphi'(\lambda_j) P_j \mathcal{P} P_j + \sum_{j \neq k} \sum \frac{\varphi(\lambda_k) - \varphi(\lambda_j)}{\lambda_k - \lambda_j} P_j \mathcal{P} P_k. \tag{A.6}$$

Remark A.1. The double sum in (A.6) is a correction term that is needed because the increment $\Pi \in \mathcal{C}_H$ is arbitrary and therefore does not, in general, commute with T . This generality is needed for statistical application, as in Theorem 3.1; see also Remark 3.1. If T and Π do commute, however, then the double sum would disappear and we would obtain the much simpler expression

$$\varphi'_T \mathcal{P} = \sum_{j \geq 1} \varphi'(\lambda_j) P_j \mathcal{P} = (\varphi'(T)) \mathcal{P}. \tag{A.7}$$

In other words, in this case, the Fréchet derivative φ'_T equals the operator $\varphi'(T)$, obtained by applying the usual functional calculus with the derivative φ' of φ ; see also Dunford and Schwartz (1957), Theorem VII.6.10 for commuting operators.

Theorem A.2. *If the range of P_1 is one-dimensional so that $P_1 = p_1 \otimes p_1$ for some unit vector $p_1 \in \mathbb{H}$, then there exists a unit vector $\tilde{p}_1 \in \mathbb{H}$ such that $\tilde{P}_1 = \tilde{p}_1 \otimes \tilde{p}_1$ for \mathcal{P} sufficiently small. We have, moreover, that*

$$\tilde{p}_1 = p_1 + A \mathcal{P} p_1 + \mathcal{O}(\|\mathcal{P}\|^2), \tag{A.8}$$

where $A : \mathbb{H} \rightarrow \mathbb{H}$ is the bounded operator

$$A = \sum_{j=2}^{\infty} \frac{\varphi(\lambda_1)}{\lambda_1 - \lambda_j} P_j. \tag{A.9}$$

Theorem A.3. *If the range of P_1 is one-dimensional and hence $P_1 = p_1 \otimes p_1$ for some unit vector $p_1 \in \mathbb{H}$, then we have*

$$\tilde{\lambda}_1 = \lambda_1 + \langle \mathcal{P} p_1, p_1 \rangle + \mathcal{O}(\|\mathcal{P}\|^2). \tag{A.10}$$

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