The multirank likelihood and cyclically monotone Monte Carlo: a semiparametric approach to CCA

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Abstract

Many analyses of multivariate data are focused on evaluating the dependence between two sets of variables, rather than the dependence among individual variables within each set. Canonical correlation analysis (CCA) is a classical data analysis technique that estimates parameters describing the dependence between such sets. However, inference procedures based on traditional CCA rely on the assumption that all variables are jointly normally distributed. We present a semiparametric approach to CCA in which the multivariate margins of each variable set may be arbitrary, but the dependence between variable sets is described by a parametric model that provides a low-dimensional summary of dependence. While maximum likelihood estimation in the proposed model is intractable, we develop a novel MCMC algorithm called cyclically monotone Monte Carlo (CMMC) that provides estimates and confidence regions for the between-set dependence parameters. This algorithm is based on a multirank likelihood function, which uses only part of the information in the observed data in exchange for being free of assumptions about the multivariate margins. We illustrate the proposed inference procedure on nutrient data from the USDA.

Keywords: marginal likelihood, optimal transport, Gaussian copula

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1 Introduction

Scientific studies often involve the collection of multivariate data with complex interdependencies. In some cases, a study will be concerned with the pairwise dependence between individual variables. In other cases, however, the dependence of interest is between non-overlapping sets of variables. For instance, in a dietary study, it may be of interest to characterize the association between the proportions of macronutrients and the proportions of micronutrients in a variety of foods without regards to the dependence within nutrient sets. Other examples are encountered in biological studies concerning the relationship between diet and the human microbiome (Chen et al., 2013), psychological studies comparing attachment types to personality disorders (Sherry and Henson, 2005), and neuroscience studies comparing brain imaging results to non-imaging measurements (see e.g. Winkler et al. (2020) for a survey).

One approach to characterizing the association between sets of variables is to conduct hypothesis tests for independence. Classical methods using Wilks’ Λ statistic (Mardia et al., 1979), as well as modern methods using the distance covariance (Bakirov et al., 2006), and the Ball covariance (Pan et al., 2020) are available for this purpose. While each of these tests relies on some assumptions about the multivariate marginal distributions of the variable sets, recently Shi et al. (2020), Deb and Sen (2021), and Ghosal and Sen (2021) have proposed tests for independence that allow the marginal distributions of the variable sets to be arbitrary. In analogy to tests for independence based on univariate ranks, these tests are based on the multivariate ranks introduced by Chernozhukov et al. (2017).

The multivariate ranks described by these authors are appealing because test statistics based on these ranks yield approximate or exact null distributions that do not assume anything about the multivariate distributions of the variable sets. However, model-based
approaches to the analysis of multivariate data have some advantages compared to such non-parametric approaches. For example, some models have parameters that provide low-dimensional summaries of the association between the variable sets, which may be scientifically interpretable. Canonical correlation analysis (CCA) is a classical data analysis technique that estimates such parameters. First described by [Hotelling (1936)], CCA can be motivated from several perspectives, including invariance with respect to transformations under the general linear group [Eaton (1983)], estimation in a latent factor model [Bach and Jordan (2005)], and statistical whitening [Jendoubi and Strimmer (2019)]. Given random vectors $\mathbf{y}_1, \mathbf{y}_2$ taking values in $\mathbb{R}^{p_1}, \mathbb{R}^{p_2}$, CCA identifies a pair of linear transformations $\mathbf{B}_1, \mathbf{B}_2$ such that the canonical variables $\mathbf{z}_1 = \mathbf{B}_1^\top \mathbf{y}_1$ and $\mathbf{z}_2 = \mathbf{B}_2^\top \mathbf{y}_2$ satisfy

$$\text{Var}(\mathbf{z}_1) = \mathbf{I}_{p_1}$$
$$\text{Var}(\mathbf{z}_2) = \mathbf{I}_{p_2}$$
$$\text{Cov}(\mathbf{z}_1, \mathbf{z}_2) = \mathbf{\Lambda}$$

where $\mathbf{\Lambda}$ is a diagonal matrix with ordered diagonal entries $1 > \lambda_1 \geq \cdots \geq \lambda_d \geq 0$, which are known as the canonical correlations. The ordering of the canonical correlations implies, for example, that the correlation of the first element of $\mathbf{z}_1$ with that of $\mathbf{z}_2$ is the largest among correlations between linear combinations of $\mathbf{y}_1$ with those of $\mathbf{y}_2$. Because they are a function of the original variables, the canonical variables may be useful in exploratory analyses where the goal is to understand which of the original variables is contributing to the association between variable sets. Additionally, the canonical correlations might be helpful in determining the effective dimensionality of the between-set association. However, estimation and uncertainty quantification for the parameters of CCA is challenging without the restrictive assumption that the variables from each set are jointly normally distributed.

In this article, we develop a semiparametric approach to CCA, which preserves the
parametric model for between-set dependence, but allows the multivariate margins of each variable set to be arbitrary. Our model extends existing proposals for semiparametric CCA (Zoh et al., 2016; Agniel and Cai, 2017; Yoon et al., 2020), which assume that the multivariate marginal distributions of the variable sets can be described by a Gaussian copula. In fact, our model may be seen as a generalization of the Gaussian copula model to vector-valued margins, much like the vector copula introduced by Fan and Henry (2020). Unlike these authors, however, we present an inference strategy that allows for estimation of and uncertainty quantification for parameters describing the association between variable sets, even when the transformations parameterizing the multivariate margins are unknown. Our inference strategy is based on a multirank likelihood, which uses only part of the information in the observed data in exchange for being free of assumptions about the multivariate margins. While maximum likelihood estimation with the multirank likelihood is intractable, we show that Bayesian estimation of the between-set dependence parameters can be achieved with a novel Metropolis-Hastings algorithm called cyclically monotone Monte Carlo (CMMC).

In the first part of Section 2 of this article, we describe a CCA parameterization of the multivariate normal model for variable sets, which separates the parameters describing between-set dependence from those determining the multivariate marginal distributions of the variable sets. We then introduce our model for semiparametric CCA, a Gaussian transformation model whose multivariate margins are parameterized by cyclically monotone functions. In Section 3, we define the multirank likelihood and use it to develop a Bayesian inference strategy for obtaining estimates and confidence regions for the CCA parameters. We then discuss the details of the CMMC algorithm, which allows us to simulate values subject to the constraint imposed by the multirank likelihood. In Section 4 we illustrate the
use of our model for semiparametric CCA on simulated datasets and apply it to studying the relationship between macronutrients and micronutrients in a sample from the USDA’s food database. We conclude with a discussion of possible extensions to this work in Section 5. Proofs of the propositions in this article are in the Appendix. By default, roman characters referring to mathematical objects in this article are italicized. However, where necessary, we use italicized and un-italicized roman characters to distinguish between random variables and elements of their sample spaces.

2 Semiparametric CCA

Let $Y$ be a random mean-zero $n \times (p_1 + p_2)$ data matrix with independent rows, with the first $p_1$ columns given by the $n \times p_1$ matrix $Y_1$ and the last $p_2$ columns given by the $n \times p_2$ matrix $Y_2$. The columns of $Y_1$ and of $Y_2$ represent two separate variable sets, the association between which we are interested in quantifying. One model to evaluate the dependence between the variable sets is the multivariate normal model,

$$Y = [Y_1 \ Y_2] \sim N_{n \times (p_1 + p_2)} (0, \Sigma \otimes I_n),$$

where $\Sigma$ is an unknown positive definite matrix and “$\otimes$” is the Kronecker product. One way to evaluate the association between variable sets $Y_1$ and $Y_2$ is to parameterize $\Sigma$ as

$$\Sigma = \begin{bmatrix} \Sigma_1 & \Omega \\ \Omega^T & \Sigma_2 \end{bmatrix}$$

where $\Sigma_1$ and $\Sigma_2$ are the marginal covariance matrices of $Y_1$ and $Y_2$, respectively. This parameterization of the multivariate normal model is written so that the covariance matrix is partitioned into $p_1$- and $p_2$-dimensional blocks, and the cross-covariance is denoted by a $p_1 \times p_2$ matrix parameter $\Omega$. Note that $\Omega$ characterizes the dependence between variable
sets, but it is also implicitly a function of $\Sigma_1$ and $\Sigma_2$ because the joint covariance matrix $\Sigma$ must be positive definite. Our objective is to evaluate the dependence between two sets of variables without respect to the dependence within variable sets, so we work instead with the CCA parameterization of the multivariate normal distribution, which we express as

$$Z = [Z_1 \ Z_2] \sim N_{n \times (p_1+p_2)} \left( 0, \begin{bmatrix} I_{p_1} & Q_1\Lambda Q_2^\top \\ Q_2\Lambda Q_1^\top & I_{p_2} \end{bmatrix} \otimes I_n \right),$$

(3)

$$y_i = \begin{bmatrix} y_{i,1} \\ y_{i,2} \end{bmatrix} = \begin{bmatrix} \Sigma_1^{1/2} z_{i,1} \\ \Sigma_2^{1/2} z_{i,2} \end{bmatrix}$$

where $y_{i,j}$ and $z_{i,j}$ are the $i^{th}$ rows of $Y_j$ and $Z_j$, $j \in \{1, 2\}$. Here, $Q_1 \in \mathbb{R}^{p_1 \times d}$, $Q_2 \in \mathbb{R}^{p_2 \times d}$ are orthogonal matrices, $\Lambda \in \mathbb{R}^{d \times d}$ is a diagonal matrix with decreasing entries in $[0, 1)$, and $d = \min(p_1, p_2)$. Going forward, we refer to $(Q_1, Q_2, \Lambda)$ as the CCA parameters, as they neither determine nor depend on $\Sigma_1$ and $\Sigma_2$, the marginal covariances of $Y_1$ and $Y_2$. Conversely, the $p_1$-variate marginal distribution of $Y_1$ and the $p_2$-variate marginal distribution of $Y_2$ are completely determined by $\Sigma_1$ and $\Sigma_2$, respectively, and do not depend on the CCA parameters.

The distribution theory of traditional CCA (Mardia et al., 1979; Anderson, 1999) is based on the multivariate normal model for $[Y_1 \ Y_2]$, in which the CCA parameters are the estimands. As the CCA parameterization of the multivariate normal model makes clear, there are two aspects to this model: a multivariate normal model for between-set dependence and a pair of linear transformations parameterizing the multivariate margins of the variable sets. While the normal dependence model is appealing because of the availability of straightforward inferential methods, the assumption that the transformations are linear is restrictive. In particular, this assumption is inappropriate for the analysis of many multivariate datasets, such as those containing data with restricted range, data
of mixed type, or other data whose joint distribution is not approximately multivariate normal. Our proposal for semiparametric CCA is therefore to expand the class of marginal transformations to a larger set of functions, large enough to accommodate any pair of marginal distributions on $\mathbb{R}^{p_1}$ and $\mathbb{R}^{p_2}$. Specifically, our semiparametric CCA model is

$$Z = [Z_1 \ Z_2] \sim N_{n \times (p_1 + p_2)} \begin{pmatrix} I_{p_1} & Q_1 \Lambda Q_2^\top \\ Q_2 \Lambda Q_1^\top & I_{p_2} \end{pmatrix} \otimes I_n,$$

(4)

$$y_i = \begin{bmatrix} y_{i,1} \\ y_{i,2} \end{bmatrix} = \begin{bmatrix} G_1(z_{i,1}) \\ G_2(z_{i,2}) \end{bmatrix},$$

with the model parameters being the CCA parameters $(Q_1, Q_2, \Lambda)$ and the unknown transformations $G_1 \in \mathcal{G}^{p_1}$ and $G_2 \in \mathcal{G}^{p_2}$ that determine the marginal distributions of $y_{i,1}$ and $y_{i,2}$, respectively.

The sets $\mathcal{G}^{p_1}$ and $\mathcal{G}^{p_2}$ of possible values of $G_1$ and $G_2$ should be large enough to allow the marginal distributions of $y_{i,1}$ and $y_{i,2}$ to be arbitrary, but not so large that non-identifiability prohibits inference on the CCA parameters. For this reason, we parameterize our model so that $\mathcal{G}^{p_j}$ is the class of \textit{cyclically monotone} functions on $\mathbb{R}^{p_j}$. The following two propositions show that the resulting model for semiparametric CCA achieves the desired balance of flexibility and identifiability. We postpone the definition of cyclical monotonicity until the following section and state the propositions below.

**Proposition 2.1.** Let $P$ be a probability distribution on $\mathbb{R}^p$ and let $z \sim N(0, I_p)$. Further, let

$$\mathcal{G}^p = \{G \mid G : \mathbb{R}^p \to \mathbb{R}^p \text{ is cyclically monotone} \}.$$

Then there exists a unique $G \in \mathcal{G}^p$ such that

$$y = G(z) \sim P.$$
This proposition shows that there exist unique cyclically monotone transformation pairs \(G_1, G_2\) that yield arbitrary marginal distributions \(P_1, P_2\) for the rows of our data matrices \(Y_1, Y_2\). Additionally, in the submodel for which the multivariate margins \(P_1\) and \(P_2\) are absolutely continuous with respect to Lebesgue measure, our model for semiparametric CCA is essentially identifiable, as described in the following proposition.

**Proposition 2.2.** Let \(\theta = (G_1, G_2, Q_1, Q_2, \Lambda)\) and let \(P_\theta\) denote the joint probability distribution of an observation \((y_{i,1}, y_{i,2})\) from the model (4) with absolutely continuous \(p_1\)- and \(p_2\)-dimensional marginal distributions \(P_1, P_2\). Then the model (4) is identifiable up to simultaneous permutation and sign change of the columns of \(Q_1, Q_2\). Specifically, if \(P_\theta = P_\theta'\), then

1. \(G_1 = G_1', \ G_2 = G_2'\);
2. \(\Lambda = \Lambda'\);
3. \(Q_1 = Q_1'PS, \ Q_2 = Q_2'PS\), where \(S \in \mathbb{R}^{d \times d}\) is any diagonal matrix with diagonal entries in \([-1, 1]\) and \(P\) is any permutation matrix with \(P_k = e_k\) if \(\lambda_k \neq \lambda_l\ \forall l \neq k\).

Note that the ambiguity in the columns of \(Q_1, Q_2\) is a feature of the matrix SVD, and is not unique to our model. The preceding two propositions show that our model for semiparametric CCA using cyclically monotone transformations is not only an extension of traditional CCA, but also an extension of existing methods for semiparametric CCA (Zoh et al., 2016; Agniel and Cai, 2017; Yoon et al., 2020). These methods infer the CCA parameters indirectly through inference of a \((p_1 + p_2) \times (p_1 + p_2)\) correlation matrix, which parameterizes a \((p_1 + p_2)\)-dimensional Gaussian copula model. While the Gaussian copula model is semiparametric in the sense that the univariate margins of the variable sets may be arbitrary, it still assumes that the multivariate marginal distributions of the
variable sets (and any subsets of those variables) are distributed according to a Gaussian copula model. By contrast, our model for semiparametric CCA using cyclically monotone transformations allows for arbitrary multivariate marginal distributions, even those that cannot be described by a Gaussian copula.

2.1 Cyclical monotonicity

Before discussing our estimation and inference strategy for semiparametric CCA, we define cyclical monotonicity and provide some intuition for its attendant properties. Cyclical monotonicity is a geometric condition on subsets of \( \mathbb{R}^p \times \mathbb{R}^p \) that generalizes one-dimensional monotonicity to \( p \geq 2 \). It is defined as follows:

**Definition 2.1** (Cyclical monotonicity). A subset \( S \) of \( \mathbb{R}^p \times \mathbb{R}^p \) is said to be *cyclically monotone* if, for any finite collection of points \( \{(z_1, y_1), \ldots, (z_n, y_n)\} \subseteq S \),

\[
\langle y_1, z_2 - z_1 \rangle + \langle y_2, z_3 - z_2 \rangle + \cdots + \langle y_n, z_1 - z_n \rangle \leq 0
\]

(5)

where \( \langle \rangle \) is the Euclidean inner product. Equivalently,

\[
\langle y_1, z_1 \rangle + \langle y_2, z_2 \rangle + \cdots + \langle y_k, z_k \rangle \geq \langle y_1, z_{\sigma(1)} \rangle + \langle y_2, z_{\sigma(2)} \rangle + \cdots + \langle y_n, z_{\sigma(n)} \rangle
\]

(6)

for any permutation \( \sigma \).

Stating that a function \( G : \mathbb{R}^p \to \mathbb{R}^p \) is cyclically monotone means that its graph—the set of all pairs \( (z, G(z)) \)—is cyclically monotone. Cyclically monotone functions are “curl-free” in the sense that they coincide exactly with the set of gradients of convex functions (Rockafellar [1966]), so they possess a regularity that is similar to that of positive definite, symmetric linear operators. In fact, the linear function \( z \to \Sigma^{1/2} z \) is cyclically monotone for \( \Sigma \) symmetric and positive definite, so the semiparametric CCA model \([4]\) generalizes
the Gaussian CCA model \[3\]. Cyclically monotone functions also correspond to *optimal transport maps* between measures with finite second moments \[\text{Ambrosio and Gigli, 2013}\] when such maps exist. As we show in the following section, the geometry of cyclical monotonicity plays a critical role in our strategy for estimating the CCA parameters.

### 3 Inference for the CCA parameters

For the moment, consider the submodel in which \(G_1\) and \(G_2\) are restricted so that the marginal distributions they induce have densities with respect to Lebesgue measure. Let \(Y \in \mathbb{R}^{n \times (p_1 + p_2)}\) be the observed value of \(Y\) and denote the corresponding likelihood as

\[
L(G_1, G_2, Q_1, Q_2, \Lambda; Y) = p(Y|G_1, G_2, Q_1, Q_2, \Lambda).
\]

Inference for semiparametric CCA is challenging because the likelihood depends on the infinite dimensional parameters \(G_1, G_2\). If \(G_1, G_2\) were known, inference for the CCA parameters could proceed by maximizing a multivariate Gaussian likelihood in \(Q_1, Q_2, \Lambda\) using \(z_{i,j} = G_j^{-1}(y_{i,j})\) as the data. However, in practice the \(G_j\)’s are unknown. Faced with similar problems in semiparametric copula estimation—for which the marginal transformations are univariate monotone functions \(g_j\)—previous authors have used pseudolikelihood methods \[\text{Oakes, 1994}\]. One pseudolikelihood method is to first construct an estimator for each univariate transformation function \(\hat{g}_j\) using the corresponding empirical CDF, and then to maximize the parametric copula likelihood using \(\hat{z}_{i,j} = \hat{g}_j^{-1}(y_{i,j})\) as a plug-in estimate for the data. Under certain conditions, this procedure has been shown to produce consistent and asymptotically normal estimators \[\text{Genest et al., 1995}\].

Conceivably, such an approach could be implemented for estimation of the CCA parameters, whereby the multivariate ranks of \[\text{Hallin, 2017}\] or \[\text{Ghosal and Sen, 2021}\] are used.
as plug-in estimates for the latent \( z_{i,j} \)'s in (4). In the case that \( G_1, G_2 \) are continuous, the consistency of such estimators for the CCA parameters would follow from Proposition 5.1 of Hallin (2017) or Theorem 4.1 of Ghosal and Sen (2021) combined with an application of the continuous mapping theorem. However, inference for such an approach is currently limited to point estimation. Additionally, even for copula models generated by univariate transformations, plug-in pseudolikelihood estimators have been shown to be inconsistent when the distribution of the data has discrete support (Genest and Nešlehová, 2007).

3.1 The multirank likelihood

An alternative to using plug-in methods for semiparametric copula inference is to use a type of marginal likelihood based on the univariate ranks of each variable, called the rank likelihood (Hoff, 2007; Hoff et al., 2014). The rank likelihood is a function of the copula parameters only, and provides inferences that are invariant to strictly monotonic transformations of each variable. Here we generalize this approach for the semiparametric CCA model, by constructing what we call a multirank likelihood, which can be interpreted as a likelihood for the CCA parameters based on information from the data that does not depend on the infinite-dimensional parameters \( G_1 \) and \( G_2 \). This information can be characterized as follows: because each \( y_{i,j} \) is a cyclically monotone transformation of the latent variable \( z_{i,j} \), \( Z_j \) and \( Y_j \) must be in cyclically monotone correspondence, meaning \( Z_j \) has to lie in the set

\[
\{ Z_j \in \mathbb{R}^{n \times p_j} : \{(z_{i,j}, y_{i,j})\}_{i=1}^{n} \text{ is cyclically monotone} \}. \tag{8}
\]

Let \( Z \stackrel{\text{cm}}{\sim} Y \) denote that both \( Z_1, Y_1 \) and \( Z_2, Y_2 \) are in cyclically monotone correspondence, and note that under our model, \( Z \stackrel{\text{cm}}{\sim} Y \) with probability 1. Now suppose it is observed that \( Y = Y \) for some \( Y \in \mathbb{R}^{n \times (p_1+p_2)} \). Then part of the information from the data is that
We define the multirank likelihood $L_M$ to be the probability of this event, as a function of the model parameters:

$$
\Pr(Z \overset{cm}\sim Y | Q_1, Q_2, \Lambda, G_1, G_2) = \Pr(Z \overset{cm}\sim Y | Q_1, Q_2, \Lambda) \\
\equiv L_M(Q_1, Q_2, \Lambda : Y).
$$

The multirank likelihood depends on the CCA parameters only and not on the infinite-dimensional parameters $G_1$ and $G_2$, because the distribution of $Z$ does not depend on $G_1, G_2$. The multirank likelihood can also be interpreted as a type of marginal likelihood, as follows: for convenience, consider the case where the margins of $Y$ are discrete. Having observed $Y = Y$ for some $Y \in \mathbb{R}^{n \times (p_1 + p_2)}$, the full likelihood can be decomposed as follows:

$$
L(Q_1, Q_2, \Lambda, G_1, G_2 : Y) = \Pr(Y = Y | Q_1, Q_2, \Lambda, G_1, G_2) \\
= \Pr(Z \overset{cm}\sim Y, Y = Y | Q_1, Q_2, \Lambda, G_1, G_2) \\
= \Pr(Z \overset{cm}\sim Y, Y = Y | Q_1, Q_2, \Lambda, G_1, G_2) \\
= \Pr(Z \overset{cm}\sim Y | Q_1, Q_2, \Lambda) \times \Pr(Y = Y | Z \overset{cm}\sim Y, Q_1, Q_2, \Lambda, G_1, G_2) \\
\equiv L_M(Q_1, Q_2, \Lambda : Y) \times \Pr(Y = Y | Z \overset{cm}\sim Y, Q_1, Q_2, \Lambda, G_1, G_2),
$$

where the second line holds because $Z \overset{cm}\sim Y$ happens with probability one. Thus the multirank likelihood can be viewed as a type of marginal likelihood [Severini 2000, Section 8.3], derived from the marginal probability of the event $Z \overset{cm}\sim Y$.

### 3.2 Posterior simulation

In principle, the multirank likelihood could be used directly to derive estimators for the CCA parameters and to quantify the uncertainty in those estimators. For example, it could be maximized as a function of the CCA parameters and confidence regions for these maximum likelihood estimators could be derived by integrating against it. However, maximizing
the multirank likelihood as a function of the CCA parameters requires evaluation of the integral

\[ \int_{\mathbb{C}^n} \Gamma_{CCA}(Z; Q_1, Q_2, \Lambda) dZ \]

where \( \Gamma_{CCA} \) denotes the \( n \times (p_1 + p_2) \) matrix normal density function with the CCA parameterization. As this expression makes clear, simply calculating the multirank likelihood for a particular value of the CCA parameters involves computing an integral over a complicated domain, which makes many classical inferential methods intractable.

By contrast, Bayesian inference for the CCA parameters admits a conceptually straightforward procedure. Below, we show how to construct a Markov Chain having stationary distribution equal to

\[ p(Q_1, Q_2, \Lambda | Z \sim Y) \propto L_M(Q_1, Q_2, \Lambda : Y) \times p(Q_1, Q_2, \Lambda) \]

from which we generate a sequence of parameter values whose distribution approximates the posterior distribution of the CCA parameters using the multirank likelihood. These simulated values can be used to obtain posterior estimates and confidence regions for the CCA parameters. Since the multirank likelihood is difficult to evaluate, we proceed by a data augmentation scheme (Dempster et al., 1977; Gelfand and Smith, 1990), in which we iterate a Markov Chain for the CCA parameters as well as for the latent variables \( Z_1, Z_2 \).

The supports of the CCA parameters are, respectively, the Stiefel manifolds \( \mathcal{Y}_{p_1,d}, \mathcal{Y}_{p_2,d} \), and the subset of \([0,1]^d\) on which \( \lambda_1 \geq \cdots \geq \lambda_d \). Since each of these is a compact set, we can set uniform priors on the CCA parameter spaces while still ensuring these are proper. Given these uniform priors, the full conditional distributions of \( Z_1, Q_1, \Lambda \) using the multirank
likelihood are

\[
Z_1 \mid - \sim N_{n \times p_1}^{cm}(B_1(I_{p_1} + A_1)^{-1}, (I_{p_1} + A_1)^{-1} \otimes I_n) \\
A_1 = Q_1(\Lambda^{-2} - I)^{-1}Q_1^T, B_1 = Z_2Q_2(\Lambda - \Lambda^{-1})^{-1}Q_1^T,
\]

\[
Q_1 \mid - \sim \text{BMF}(A_1, B_1, C_1)
\]

\[
A_1 = -Z_1^TZ_1/2, B_1 = (\Lambda^{-2} - I)^{-1}, C_1 = Z_1^TZ_2Q_2(\Lambda^{-1} - \Lambda)^{-1},
\]

\[
\Lambda \mid - \sim P_\Lambda(a, b, c) \propto \prod_{k=1}^d (1 - \lambda_k^2)^{-n/2} e^{-\frac{(a_k + b_k)/2 + c_k}{2(1 + \lambda_k)}} e^{-\frac{(a_k + b_k)/2 - c_k}{2(1 - \lambda_k)}}
\]

\[
a = \text{diag}(Q_1^TZ_1Z_1Q_1), b = \text{diag}(Q_2^TZ_2Z_2Q_2), c = \text{diag}(Q_1^TZ_1Z_2Q_2).
\]

The full conditional distributions of \(Z_2, Q_2\) are analogous to those of \(Z_1, Q_1\) with the variable set subscripts interchanged. Here, the notation \(N_{n \times p_1}^{cm}Y_1\) refers to the matrix normal distribution truncated to the set of matrices in cyclically monotone correspondence with \(Y_1\), while the BMF distribution is the Bingham-von Mises-Fisher distribution parameterized as in Hoff (2009).

If we could directly simulate from all of the full conditional distributions above, then iteratively simulating from each full conditional in a Gibbs sampler would produce a sequence of parameter values with approximately the desired distribution. However, it is more practical to simulate the CCA parameters using other MCMC methods that yield the same stationary distribution. For simulation of \(Q_1, Q_2\), we combine elliptical slice sampling based on matrix-normal priors (Murray et al., 2010) with the polar expansion strategy of Jauch et al. (2021). To simulate each \(\lambda_k\), we use an independent proposal density informed by the mode of the full conditional density for \(\lambda_k\) and accept the new value with a Metropolis-adjusted probability. More details on simulation of the CCA parameters are provided in the Appendix. In the next section, we introduce the CMMC algorithm, which we use to simulate new values of the latent \(z\)'s subject to the truncation imposed by
3.3 Cyclically monotone Monte Carlo

Cyclically monotone Monte Carlo (CMMC) is an algorithm for simulating values from a desired probability density subject to a cyclically monotone constraint. Specifically, if \( Z \) has distribution with density \( f(Z) \), CMMC iterates a Markov Chain whose stationary distribution has density

\[
p(Z|Z \overset{\text{cm}}{\sim} Y) \propto f(Z) I[Z \overset{\text{cm}}{\sim} Y].
\]

In this section, the symbols \( Z, Y \) refer to just one of the variable sets \( Z_j, Y_j \), and \( Z \overset{\text{cm}}{\sim} Y \) denotes that the matrices \( Z \in \mathbb{R}^{n \times p} \) and \( Y \in \mathbb{R}^{n \times p} \) are in cyclically monotone correspondence. Rearranging Definition 2.1 shows that \( Z \overset{\text{cm}}{\sim} Y \) is equivalent to the condition that

\[
\sum_{i=1}^{n} \|z_i - y_i\|_2^2 = \min_{\sigma = (\sigma(1), ..., \sigma(n)) \in S_n} \sum_{i=1}^{n} \|z_i - y_{\sigma(i)}\|_2^2.
\]

(12)

where \( z_i \) and \( y_i \) are the \( i \)th rows of \( Z \) and \( Y \). In other words, \( \{(z_i, y_i)\}_{i=1}^{n} \) is cyclically monotone if and only if the identity pairing \( \sigma_0 \) solves an optimal assignment problem between point sets \( \{z_1, ..., z_n\} \) and \( \{y_1, ..., y_n\} \). Therefore, the following naive algorithm constitutes one iterate of a Markov Chain with the desired stationary distribution:

1. Simulate a new \( Z^* \) using a proposal distribution with full support on \( \mathbb{R}^{n \times p} \).

2. Obtain \( \sigma^* \), the optimal assignment between \( \{z_i^*\}_{i=1}^{n} \) and \( \{y_i\}_{i=1}^{n} \).

3. If \( \sigma^* = \sigma_0 \), then accept \( Z^* \) with a Metropolis-adjusted probability. Otherwise, reject \( Z^* \).

Unfortunately, this type of scheme quickly becomes infeasible as \( n \) grows even to modest sizes because algorithms for solving the assignment problem have a worst-case complexity
of $O(n^3)$ \cite{PeyreCuturi2018} and the probability of naively simulating a $Z^*$ that is optimally paired with $Y$ shrinks at a factorial rate. However, it is possible to use the dual to the assignment problem to more efficiently produce simulated values for which cyclical monotonicity is preserved.

Specifically, let $Z^{(t)}$ be the $t^{th}$ iterate of a Markov chain for $Z$ and denote the cost of assigning $z_i^{(t)}$ to $y_j$ as $c_{ij}^{(t)} = \|z_i^{(t)} - y_j\|_2^2$. The complementary slackness conditions of the assignment problem imply that $\sigma_0$ is an optimal pairing for $(Z^{(t)}, Y)$ if and only if there exist real vectors $u^{(t)}, v^{(t)} \in \mathbb{R}^n$, sometimes called dual variables, such that

$$ u_i^{(t)} + v_i^{(t)} = c_{ii}^{(t)}, \ i = 1, \ldots, n $$

$$ u_i^{(t)} + v_j^{(t)} \leq c_{ij}^{(t)}, \ i \neq j. $$

Assuming that such vectors exist at iteration $t$, the inequalities above imply that the slack

$$ s_{ij}^{(t)} = c_{ij}^{(t)} - u_i^{(t)} - v_j^{(t)} $$

is greater than or equal to zero for all $(i, j)$, with $s_{ij}^{(t)} = 0$ at $i = j$. These conditions show that for every update of $Z^{(t)}$, there are corresponding updates to $u^{(t)}, v^{(t)}$ that preserve cyclical monotonicity, and vice versa. While there are potentially many choices of such updates, we describe a coordinate-wise scheme that leads to closed-form intervals for which cyclical monotonicity is preserved.

Let a proposal for the next iterate in the Markov chain be $Z^*$, for which only entry $ik$ has been updated as $z_{ik}^* = z_{ik}^{(t)} + \epsilon$. Then the updated costs are

$$ c_{ij}^* = \epsilon^2 + 2\epsilon(z_{ik}^{(t)} - y_{jk}) + c_{ij}^{(t)}, \ j = 1, \ldots, n. $$

Consider now the dual update $u_i^* = u_i^{(t)} + \epsilon^2 + 2\epsilon(z_{ik}^{(t)} - y_{ik})$ while keeping all other dual variables fixed. Substituting $v_i^{(t)} = c_{ii}^{(t)} - u_i^{(t)}$ into (14) results in the set of inequalities

$$ 2\epsilon(y_{ik} - y_{jk}) + s_{ij}^{(t)} \geq 0, \ j = 1, \ldots, n, $$

(16)
which leads to upper and lower bounds on \( \epsilon \)

\[
[\epsilon_-, \epsilon_+] = \left[ \max_{l: y_{ik} > y_{ik}} \left\{ -\frac{s_{il}^{(t)}}{2(y_{ik} - y_{lk})} \right\}, \min_{l: y_{ik} < y_{ik}} \left\{ \frac{s_{il}^{(t)}}{2(y_{ik} - y_{lk})} \right\} \right].
\] (17)

This is a closed interval containing zero, except when \( y_{ik} = \max_l y_{ik} \) or \( y_{ik} = \min_l y_{ik} \), in which case the interval is unbounded, and either \( \epsilon_- = -\infty \) or \( \epsilon_+ = \infty \). By construction, simulating a new value of \( z_{ik}^* \) in the interval \([z_{ik}^{(t)} + \epsilon_-, z_{ik}^{(t)} + \epsilon_+]\) preserves cyclical monotonicity across iterates of the Markov Chain. Alternatively, we can set \( v_i^* = v_i^{(t)} + \epsilon^2 + 2\epsilon(z_{ik}^{(t)} - y_{ik}) \) and keep all other dual variables fixed. Performing a similar substitution as before yields the following constraints on \( \epsilon \):

\[
\epsilon^2 + 2\epsilon(z_{ik}^{(t)} - y_{jk}) + s_{ij}^{(t)} \geq 0, \quad j = 1, \ldots, n
\]

\[
-\epsilon^2 - 2\epsilon(z_{ik}^{(t)} - y_{ik}) + s_{li}^{(t)} \geq 0, \quad l = 1, \ldots, n.
\] (18)

Note that the original optimality conditions in (13) guarantee that the above inequalities hold at \( \epsilon = 0 \). Further, one can check that the region described by the intersection of these quadratic inequalities is either a closed interval around the origin or the origin itself. The expression for this safe interval is more involved than the previous one, but it can still be written in closed form and computed in \( O(n) \) time. The bounds for this interval are

\[
\epsilon_- = \max \left\{ \max_l \left\{ (y_{ik} - z_{ik}^{(t)}) - \sqrt{(y_{ik} - z_{ik}^{(t)})^2 + s_{li}} \right\}, \right. \\
\left. \max_{j: y_{jk} < z_{ik}^{(t)}} \left\{ (y_{jk} - z_{ik}^{(t)}) + \sqrt{(y_{jk} - z_{ik}^{(t)})^2 - s_{ij}} \right\} \right\}
\]

\[
\epsilon_+ = \min \left\{ \min_l \left\{ (y_{ik} - z_{ik}^{(t)}) + \sqrt{(y_{ik} - z_{ik}^{(t)})^2 + s_{li}} \right\}, \right. \\
\left. \min_{j: y_{jk} > z_{ik}^{(t)}} \left\{ (y_{jk} - z_{ik}^{(t)}) - \sqrt{(y_{jk} - z_{ik}^{(t)})^2 - s_{ij}} \right\} \right\}.
\] (19)

Again, by construction, simulating from the interval \([\epsilon_-, \epsilon_+]\) preserves cyclical monotonicity.

To ensure that the iterates of the Markov Chain have the right stationary distribution, all that remains is to choose a proposal density for the \( z_{ik} \)'s, and to accept new values with
a Metropolis-adjusted probability. Following the logic above, the $O(n^2p)$ algorithm below details a CMMC scheme constituting one iteration of the Markov Chain for $Z$:

- For each of $i = 1, \ldots, n$, $k = 1, \ldots, p$,
  - Simulate $\delta \sim \text{Bernoulli}(1/2)$.
  - If $\delta = 1$, find safe interval $[z_{ik}^{(t)} + \epsilon_-, z_{ik}^{(t)} + \epsilon_+]$ using (17). If $\delta = 0$, use (19).
  - Propose $z_{ik}^* \sim N(0,1)$ truncated to $[z_{ik}^{(t)} + \epsilon_-, z_{ik}^{(t)} + \epsilon_+]$.
  - Calculate acceptance ratio $r := \frac{f(z_{ik}^{*})\phi(z_{ik}^{*})}{f(z_{ik}^{(t)})\phi(z_{ik}^{(t)})}$ where $\phi$ is the standard normal density truncated to $[z_{ik}^{(t)} + \epsilon_-, z_{ik}^{(t)} + \epsilon_+]$.
  - With probability $r$:
    * Set $z_{ik}^{(t+1)} := z_{ik}^*$.
    * If $\delta = 1$, set $s_{ij}^{(t+1)} := s_{ij}^{(t)} + 2(z_{ik}^* - z_{ik}^{(t)})(y_{ik} - y_{jk})$, $j \neq i$.
    * If $\delta = 0$, set
      
      $$
      s_{ij}^{(t+1)} := s_{ij}^{(t)} + (z_{ik}^* - z_{ik}^{(t)})^2 + 2(z_{ik}^* - z_{ik}^{(t)})(z_{ik}^{(t)} - y_{jk}), \quad j \neq i
      $$
      
      $$
      s_{li}^{(t+1)} := s_{li}^{(t)} - (z_{ik}^* - z_{ik}^{(t)})^2 - 2(z_{ik}^* - z_{ik}^{(t)})(z_{ik}^{(t)} - y_{ik}), \quad l \neq i.
      $$

Note that to initialize the Markov Chain, one can simulate a $Z^{(0)}$ with standard normal entries, solve an optimal assignment problem between $Z^{(0)}$ and $Y$ to find the initial slacks, and then reorder the rows of $Z^{(0)}$ in accordance with the optimal assignment.

### 3.4 Missing data and mixed data

The algorithm for estimation of the CCA parameters can be modified to accommodate data missing at random (MAR). For instance, if $y_{i,1}$ is missing, then the multirank likelihood does not impose a cyclically monotone constraint on $z_{i,1}$. The CMMC algorithm can
therefore be initialized by solving an assignment problem between $Y_{-i,1}$ and $Z_{-i,1}^{(0)}$. Then, at each iteration, a new value for $z_{i,1}$ can be simulated from the full conditional distribution

$$z_{i,1} \sim N_{p_1}(Q_1 \Lambda Q_2^T z_{i,2}, I_{p_1} - Q_1 \Lambda^2 Q_1^T).$$

(20)

When simulating values in a CMMC step for the other latent variables, the constraints in (17) can be computed over $Y_{-i,1}$. The case of multiple missing rows in either $Y_1$ or $Y_2$ may be treated analogously. The situation of individual entries missing, however, is more complicated and requires imputation under the MAR assumption. We reserve this case for future work on sampling with cyclically monotone constraints.

In contrast to methods based on the multivariate ranks of Chernozhukov et al. (2017), in principle the multirank likelihood can be used in a Bayesian inference procedure with data of mixed type, including binary, count-based, or proportion data. However, it is not yet clear how much information about the CCA parameters is lost when the margins are discrete. Further work is needed to establish results on identifiability in the case of multivariate marginals that are not absolutely continuous.

4 Examples

4.1 Simulations

To illustrate how our model for semiparametric CCA extends existing models, we compare estimators derived from our method for semiparametric CCA to those of standard CCA and Gaussian copula-based CCA, where the latter corresponds to the family of models proposed by Zoh et al. (2016), Agniel and Cai (2017), and Yoon et al. (2020). Specifically, we evaluate the estimators of each method on data simulated from the semiparametric CCA model (4) using three different choices of cyclically monotone transformations. In
each simulation, \( p_1 = p_2 = 2 \). For the first simulation, we choose the positive definite, symmetric matrices
\[
\Sigma_1^{1/2} = \Sigma_2^{1/2} = \begin{bmatrix}
1 & 0.25 \\
0.25 & 1
\end{bmatrix}
\]
as our transformations, so the resulting data are jointly multivariate normal. In the second simulation, we apply the monotone function
\[
g(z) = (\mathcal{W}_{1,1}^{-1} \circ \Phi)(z)
\]
coordinate-wise to each variable set, where \( \mathcal{W}_{1,1}^{-1} \) denotes the quantile function of the Weibull distribution with shape and scale parameter equal to 1, and \( \Phi \) denotes the standard normal CDF. The resulting data have a distribution that is a Gaussian copula, but is no longer multivariate normal. Finally, in the third simulation we apply the cyclically monotone function
\[
G(z) = U^\top (\mathcal{W}_{1,1}^{-1} \circ \Phi)(Uz)
\]
to each variable set, where the entries of \( U \) are simulated independently from \( N(0, 0.75^2) \) and \( \mathcal{W}_{1,1}^{-1} \circ \Phi \) is applied coordinate-wise. Note that because \( U \) is not diagonal, \( G \) is not coordinate-wise monotone. Therefore, the corresponding data have a distribution that is neither normal nor a Gaussian copula, but is in our model for semiparametric CCA.

We evaluate each method by comparing its estimate of the CCA parameters to the true CCA parameters using the loss criterion
\[
L_\Delta(\hat{\Delta}) = \frac{\|\hat{\Delta} - \Delta\|^2}{p_1p_2}
\]
where \( \Delta = Q_1 \Lambda Q_2^\top \). For Gaussian copula-based CCA and our method for semiparametric CCA, we use the posterior mean of \( \Delta \) as the estimator. The boxplots in Figure 1 show the distribution of \( L_\Delta \) for each method over 25 trials for \( n \in \{50, 100, 250, 500, 1000\} \). In
Figure 1: Mean squared-error for three simulation scenarios and three inference methods: traditional CCA (CCA), Gaussian copula-based CCA (GCCCA), and our method for semiparametric CCA (CMCCA). (a) Results from the first simulation. Estimation improves with sample size for all methods. (b) Results from the second simulation. Estimation with traditional CCA stops improving as \( n \) increases. (c) Results from the third simulation. Only the estimator derived from the multirank likelihood improves for \( n \geq 500 \).
the first scenario, the estimation of all three methods improves with sample size. This is expected since the data-generating distribution, the multivariate normal, falls in each of the three model families. In the second scenario, estimation with standard CCA fails to improve with sample size because the data-generating distribution is not normal. However, the data-generating distribution for the second scenario is in the Gaussian copula model and our model for semiparametric CCA, so estimation with each of the corresponding methods improves with sample size. Finally, in the third scenario estimation with standard CCA and estimation with Gaussian copula-based CCA both stop improving as \( n \) gets large. Only our method for semiparametric CCA produces estimates that improve with sample size in all three simulation scenarios.

4.2 Analysis of USDA nutrition data

We further illustrate the use of our method for semiparametric CCA by analyzing nutrition data from the USDA. In the analysis, we consider the association between the proportions of three macronutrients and four micronutrients in a sample of 576 foods from the Fruit, Vegetables, Grains, and Dairy section of the USDA’s “What We Eat in America” food categories (U.S. Department of Agriculture, Agricultural Research Service, 2020). We define the proportion of a nutrient in a food item as the amount of the nutrient per gram of food.

The plots in Figure 2 motivate the use of our model for semiparametric CCA over traditional CCA or Gaussian copula-based CCA. In the left panel, we plot pairwise scatter plots of the proportions of the macronutrients Protein, Carbohydrate, and Total Fat. From the marginal histograms alone, we can determine that the joint distribution of these macronutrients is not approximately multivariate normal. However, it is not immediately obvious
Figure 2: USDA nutrition data: (a) Pairs plots of Protein, Carbohydrate, and Total Fat macronutrients. (b) Pairs plots of same macronutrients after normal scores transformation. That the distribution of the macronutrients falls outside the Gaussian copula family. To investigate this, we apply a normal scores transformation to the macronutrient data and plot the results in the right panel of Figure 2. The normal scores transformation works by aligning the empirical quantiles of each variable with that of the standard normal distribution, transforming data with arbitrary univariate margins to have approximately standard normal margins. If the data have an empirical distribution that is approximately multivariate normal after a normal scores transformation, it would be reasonable to conclude that their distribution can be described by a Gaussian copula. However, even after the normal scores transformation, the macronutrients in this sample are still not approximately jointly normally distributed.

We apply our method for semiparametric CCA by simulating 50,000 values from a Markov Chain with stationary distribution equal to the posterior distribution of the CCA
parameters using the multirank likelihood. We discard the first 5,000 values and retain every 10\textsuperscript{th} subsequent iterate. Histograms depicting the approximate posterior distributions of $\lambda_1$, $\lambda_2$, and $\lambda_3$ are plotted in the bottom panel of Figure 3. Posterior 95\% credible intervals indicate that all three canonical correlations are non-zero, and their posterior means are 0.70, 0.48, and 0.27, respectively. These results offer strong evidence that the proportions of macronutrients and micronutrients are not independent in the food categories under consideration, and that their dependence cannot be summarized in fewer than three dimensions.

A biplot of the first two columns of $Q_1$ (Figure 3, top left panel) shows that the component of variation associated with the first canonical correlation is composed of all three macronutrients, with Protein contributing positively and Carbohydrate and Total Fat contributing negatively. The corresponding biplot of the first two columns of $Q_2$ show that the first canonical component is composed of negative contributions from the water-soluble micronutrients Vitamin C and Vitamin B6 and a positive contribution from the fat-soluble nutrient Vitamin D. The component of variation associated with the second canonical correlation is composed of macronutrients Carbohydrate and Total Fat, with opposing influences, and fat-soluble micronutrients Vitamin D and Vitamin K with negative influences. As might be expected, these micronutrients contribute to the second component of variation in the same direction as Total Fat.

5 Discussion

In this article, we have proposed a semiparametric model for CCA based on cyclically monotone transformations of jointly normal sets of variables. In contrast to existing models for CCA, our model allows the variable sets to have arbitrary multivariate marginal
Figure 3: Results from the analysis of USDA nutrition data: (a) The approximate posterior distribution of $Q_1$ depicted in a biplot. Each MCMC simulation is plotted as a transparent line. Thick lines indicate the posterior mean. (b) The approximate posterior distribution of $Q_2$. (c) The approximate posterior distribution of $\lambda_1, \lambda_2$ and $\lambda_3$. 
distributions, while retaining a parametric model of dependence. Our inference approach is based on the multirank likelihood, a type of marginal likelihood, which does not depend on the multivariate marginal distributions of the variable sets. Instead, the multirank likelihood uses information in the cyclically monotone correspondence between the observed data and the unobserved normal latent variables. To simulate values subject to the multirank likelihood’s cyclically monotone constraint, we have also introduced CMMC, which allows us to use the multirank likelihood to obtain both point estimates and confidence regions for the CCA parameters.

There are several directions of research that could extend this work. For example, much of the recent interest in CCA has been driven by applications in genomics and neuroimaging, for which the variable sets are often high-dimensional compared to the sample size. In these settings, traditional CCA may fail, so it is necessary to use regularized versions of CCA. Our approach to semiparametric CCA is amenable to extensions allowing for Bayesian inference in such high-dimensional settings. For instance, regularized CCA could be implemented via shrinkage- or sparsity-inducing prior distributions on the entries of $\Lambda$. Alternatively, the dependence between variable sets could be assumed low-rank by setting $d < \min(p_1, p_2)$. However, scaling the simulation methodology presented here to high-dimensional datasets remains a significant challenge, primarily due to the cost of simulating the orthogonal matrices $Q_1, Q_2$.

In this article we presented a coordinate-wise scheme for CMMC. However, hit-and-run schemes for CMMC are also possible, as are those that update several latent variables at once. The cost of computing the regions that preserve cyclical monotonicity remains the primary obstacle to all of these, but there may be exact or approximate CMMC algorithms that could lead to improved mixing times and applicability of CMMC to datasets with
larger sample sizes. Finally, although this article has focused on semiparametric CCA, we anticipate that our inference approach using the multirank likelihood and CMMC will be useful in other semiparametric inference problems, for instance in semiparametric regression or other hierarchical models involving cyclically monotone transformations.

Code to reproduce the figures in this article, as well as software for semiparametric CCA as described in this article is available at https://github.com/j-g-b/sbcca.
A  Proofs of propositions

A.1  Proof of Proposition 2.1

Let $P$ be a probability distributions on $\mathbb{R}^p$, and let $z \sim N(0, I_p)$. Further, let

$$\mathcal{G}^p = \{ G : \mathbb{R}^p \to \mathbb{R}^p \text{ is cyclically monotone} \}.$$

Theorems due to Brenier (1991) and McCann (1995) assert the existence of a convex function $\psi$, unique almost everywhere up to addition of a constant, such that $\nabla \psi$ pushes forward the standard normal distribution on $\mathbb{R}^p$ to $P$. Therefore, there exists an almost-everywhere unique $G = \nabla \psi$ such that

$$y = G(z) \sim P$$

It remains to verify that $G$ is cyclically monotone. This is guaranteed by Rockafellar’s Theorem (Rockafellar, 1966), which states that the subdifferentials of convex functions are cyclically monotone. Hence, there is an almost-everywhere unique $G \in \mathcal{G}^p$ so that $y \sim P$.

A.2  Proof of Proposition 2.2

Let $\theta = (G_1, G_2, Q_1, Q_2, \Lambda)$ and let $P_\theta$ denote the joint probability distribution of an observation $(y_1, y_2)$ from the model (4) with absolutely continuous $p_1$- and $p_2$-dimensional marginal distributions $P_1, P_2$. Suppose

$$P_\theta = P_{\theta'}$$

The equality of the joint probability distributions above implies that the corresponding $p_1$- and $p_2$- dimensional margins must also be equal. As before, we apply McCann’s Theorem (McCann, 1995) and Rockafellar’s Theorem (Rockafellar, 1966) to find that the transformations $G_1, G_2$ pushing forward the $p_1$- and $p_2$- dimensional standard normal distributions
to \( P_1, P_2 \), respectively, must be unique almost everywhere. Thus,

\[
G_1 = G'_1, \quad G_2 = G'_2 \quad \text{a.e.}
\]

McCann’s Theorem [McCann 1995] and Rockafellar’s Theorem [Rockafellar 1966] also guarantee the existence and almost-everywhere uniqueness of cyclically monotone functions \( H_1, H_2 \) pushing forward \( P_1, P_2 \) to the \( p_1 \)- and \( p_2 \)- dimensional standard normal distributions, respectively. Moreover, \( H_1 \circ G_1(z_1) = z_1 \) a.e. and \( H_2 \circ G_2(z_2) = z_2 \) a.e. Applying these functions to \( y_1 \) and \( y_2 \), we obtain

\[
\begin{bmatrix}
H_1(y_1) \\
H_2(y_2)
\end{bmatrix}
\sim
\begin{bmatrix}
I_{p_1} & Q_1 \Lambda Q_2^T \\
Q_2 \Lambda Q_1^T & I_{p_2}
\end{bmatrix}
\]

and, likewise,

\[
\begin{bmatrix}
H_1(y'_1) \\
H_2(y'_2)
\end{bmatrix}
\sim
\begin{bmatrix}
I_{p_1} & Q'_1 \Lambda' Q'_2^T \\
Q'_2 \Lambda' Q'_1^T & I_{p_2}
\end{bmatrix}
\]

Because \((H_1(y_1), H_2(y_2)) \overset{d}{=} (H_1(y'_1), H_2(y'_2))\), we obtain

\[
Q_1 \Lambda Q_2^T = Q'_1 \Lambda' Q'_2^T
\]

If \( \Lambda, \Lambda' \) is a diagonal matrix with strictly decreasing entries in \([0, 1]\), the uniqueness of the matrix singular value decomposition yields

\[
\Lambda = \Lambda'
\]

and

\[
Q_1 = Q'_1 S, \quad Q_2 = Q'_2 S
\]

where \( S \in \mathbb{R}^{d \times d} \) is an arbitrary diagonal matrix with diagonal entries in \([-1, 1]\). If the entries of \( \Lambda, \Lambda' \) are not strictly decreasing, then the uniqueness of the matrix singular value decomposition yields

\[
\Lambda = \Lambda'
\]
and

\[ Q_1 = Q'_1 PS, Q_2 = Q'_2 PS \]

where \( P \) is any permutation matrix with \( P_k = e_k \) if \( \lambda_k \neq \lambda_l \ \forall l \neq k \). If the entries of \( \Lambda, \Lambda' \) are strictly decreasing, then \( P = I \).

B Additional details on posterior simulation

Since we use uniform priors for each of the CCA parameters, the full conditional distributions of the CCA parameters are derived from densities proportional to the density of the latent variables \( Z_1, Z_2 \). This is the \( n \times (p_1 + p_2) \) matrix normal density truncated to the set \( \{ Z : Z \overset{cm}{\sim} Y \} \), the logarithm of which is

\[
\log \left( \Gamma_{CCA}(Z; Q_1, Q_2, \Lambda) \II[Z \overset{cm}{\sim} Y] \right) = -\frac{n}{2} \log |I - \Lambda| \\
- \frac{1}{2} \text{tr}(Z_1 Z_1^\top + Z_2 Z_2^\top) \\
- \frac{1}{2} \text{tr}(Z_1 Q_1 (\Lambda^{-2} - I)^{-1} Q_1^\top Z_1^\top + Z_2 Q_2 (\Lambda^{-2} - I)^{-1} Q_2^\top Z_2^\top) \\
- \text{tr}(Z_1 Q_1 (\Lambda - \Lambda^{-1})^{-1} Q_2^\top Z_2^\top) \\
+ \log \II[Z \overset{cm}{\sim} Y]
\]

Eliminating terms that are constant in each variable yields the full conditional distributions given in the main text.

The full conditional distribution for \( \Lambda \) has an exponential family form, but it is not immediately clear how to simulate directly from it. Therefore, we use a Metropolis-Hastings algorithm to simulate each \( \lambda_k \). We propose new values according to

\[
\lambda_k^* \sim N \left( r_k, \frac{1}{n} \left( 1 - \frac{2c_k}{a_k + b_k} \right) \right)
\]

truncated to the region \( \lambda_{k-1} \geq \lambda_k^* \geq \lambda_{k+1} \), where \( r_k \) is the real root to the cubic equation

\[
\lambda_k^3 - \frac{c_k}{n} \lambda_k^2 + \frac{a_k + b_k - n}{n} \lambda_k - \frac{c_k}{n} = 0,
\]
and \(a, b\) and \(c\) are defined as in (11) from the main text. This equation is obtained by setting the derivative of the logarithm of the full conditional density for \(\lambda_k\) to zero, so that \(r_k\) is the mode of the full conditional distribution for \(\lambda_k\).

Simulation of \(Q_1, Q_2\) is accomplished by iterating a Markov Chain for auxiliary variables \(X_1, X_2\) and taking \(Q_1, Q_2\) to be the left polar factors of these matrices at each iteration as in \cite{Jauch+2021}. Specifically, if \(X_1^*\) is a proposed value for \(X_1\), then

\[
Q_1^* = U^* V^*^\top,
\]

where \(U^*, V^*\) are the left and right singular vectors of \(X^*\). Elliptical slice sampling \cite{Murray+2010} is an MCMC method applicable to simulating from posterior distributions proportional to the product of a normal prior distribution and a likelihood function. Since the matrix normal prior distributions \(X_1 \sim N_{p_1 \times d}(0, I_d \otimes I_{p_1})\) and \(X_2 \sim N_{p_2 \times d}(0, I_d \otimes I_{p_2})\) induce uniform prior distributions on the Stiefel manifolds \(V_{p_1,d}, V_{p_2,d}\), we are able to use elliptical slice sampling to simulate new values for \(X_1, X_2\) at each iteration, where \(\log \Gamma_{CCA}(Z; Q_1, Q_2, \Lambda)\) is the log likelihood function used in the slice sampling algorithm.
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