Bayesian Copula Density Deconvolution for Zero-Inflated Data in Nutritional Epidemiology

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ABSTRACT
Estimating the marginal and joint densities of the long-term average intakes of different dietary components is an important problem in nutritional epidemiology. Since these variables cannot be directly measured, data are usually collected in the form of 24-hr recalls of the intakes, which show marked patterns of conditional heteroscedasticity. Significantly compounding the challenges, the recalls for episodically consumed dietary components also include exact zeros. The problem of estimating the density of the latent long-time intakes from their observed measurement error contaminated proxies is then a problem of deconvolution of densities with zero-inflated data. We propose a Bayesian semiparametric solution to the problem, building on a novel hierarchical latent variable framework that translates the problem to one involving continuous surrogates only. Crucial to accommodating important aspects of the problem, we then design a copula based approach to model the involved joint distributions, adopting different modeling strategies for the marginals of the different dietary components. We design efficient Markov chain Monte Carlo algorithms for posterior inference and illustrate the efficacy of the proposed method through simulation experiments. Applied to our motivating nutritional epidemiology problems, compared to other approaches, our method provides more realistic estimates of the consumption patterns of episodically consumed dietary components. Supplementary materials for this article, including a standardized description of the materials available for reproducing the work, are available as an online supplement.

1. Introduction

1.1. Problem Statement

Dietary habits are important for our general health and well-being, having been known to play important roles in the etiology of many chronic diseases. Estimating the long-term average intakes of different dietary components $X$ and their marginal and joint distributions is thus a fundamentally important problem in nutritional epidemiology.

The dietary component may be a nutrient, like sodium, vitamin A, etc., or a food group, like milk, whole grains, etc. In any case, by the very nature of the problem, $X$ can never be observed directly. Data are thus often collected in the form of 24-hr recalls of the intakes. Many of the dietary components of interest are daily consumed. Examples include total grains, sodium, etc., the recalls for which are all continuous, comprising only strictly positive intakes. Compounding the challenge, interest may additionally lie in episodically consumed components whose long-term average intake is assumed to be strictly positive but the recalls are semicontinuous, comprising positive recalls for consumption days and exact zero recalls for nonconsumption days. Examples include milk, whole grains, etc.

Since dietary patterns often vary with energy levels, measured in total caloric intake, adjustments with energy provide a way of standardizing the dietary assessments. The recalls for energy are always continuous. From a statistical viewpoint, they can thus be treated just like the regular components, and hence, with some abuse, will be referred to as such.

When the recalls are recorded within a relatively short span of time, it may be assumed that the participants’ dietary patterns $X$ will not have changed significantly over this period. Treating the recalls $Y$, like the ones shown in Table 1, to be surrogates for the latent $X$, contaminated by measurement errors $U$, the problem of estimating the joint and marginal distributions of $X$ from the recalls $Y$ then translates to a problem of multivariate deconvolution of densities with exact zero surrogates for some of the components.

Throughout we adopt the following generic notation for marginal, joint, and conditional densities, respectively. For random vectors $S$ and $T$, we denote the marginal density of $S$, the joint density of $(S, T)$, and the conditional density of $S$ given $T$, by the generic notation $f_S$, $f_{S,T}$, and $f_{S|T}$, respectively. Likewise, for univariate random variables $S$ and $T$, the corresponding densities are denoted by $f_S$, $f_{S,T}$, and $f_{S|T}$, respectively. Additional summaries of the variables and notations used can be found in Table 2.
1.2. The EATS Dataset and Its Prominent Features

The main motivation behind the research being reported here comes from the Eating at America’s Table Study (EATS) (Subar et al. 2001), a large scale epidemiological study conducted by the National Cancer Institute in which \( i = 1, \ldots, n = 965 \) participants were interviewed \( j = 1, \ldots, m_i = 4 \) times over the course of a year and their 24-hr dietary recalls were recorded.

Data on many different dietary components were recorded in the EATS study, including episodic components milk and whole grains, whose recalls involved approximately 21% and 37% exact zeros, respectively. Table 1 shows the general structure of this dataset for one regularly consumed and one episodically consumed dietary component.

Patterns of conditional heteroscedasticity are also generally very prominent in dietary recall data. See, for example, the right panels of Figure 1 which shows the plot of subject-specific means \( Y_{j,i} = \sum_{p=1}^{m_i} Y_{j,i,p}/4 \) versus subject-specific variances \( S^2_{j,i} = \sum_{p=1}^{m_i} (Y_{j,i,p} - Y_{j,i})^2/3 \) for the 24-hr recalls of sodium and energy, which provide crude estimates of the underlying true intakes \( X_{j,i} \) and the conditional measurement error variances \( \text{var}(U_{j,i|j}|X_{j,i}) \), respectively, suggesting strongly that var \( (U|X) \) increases as \( X \) increases. Similar observation can also be made for positive recalls of episodic components from the middle panels of Figure 2.

Table 1. The general structure of the EATS dataset showing the recalls for one episodically consumed and one regularly consumed dietary component.

| Subject | 24-hr recalls | Episodic component | Regular component |
|---------|---------------|--------------------|-------------------|
| 1       | \( Y_{1,1} \) | \( Y_{1,2} \) | \( Y_{1,3} \) |
| 2       | \( Y_{2,1} \) | \( Y_{2,2} \) | \( Y_{2,3} \) |
| 3       | \( Y_{3,1} \) | \( Y_{3,2} \) | \( Y_{3,3} \) |
| 4       | \( Y_{4,1} \) | \( Y_{4,2} \) | \( Y_{4,3} \) |
| ...     | ...           | ...               | ...              |
| n       | \( Y_{n,1} \) | \( Y_{n,2} \) | \( Y_{n,3} \) |

NOTE: Here, \( Y_{j,i} \) is the reported intake for the \( j \)th recall of the \( i \)th individual for the \( t \)th dietary component.

As can be seen from the right and middle panels in Figures 1 and 2, respectively, for both regular and episodic components, the variability of the positive recalls naturally decreases to zero as the average intake on consumption days decreases to zero. For all regularly consumed components, the histograms of the recalls are mildly right skewed bell shaped. The histograms for the episodically consumed components are, however, reflected J-shaped—the frequencies of the bins start with their largest value at the left end and then rapidly decrease as we move to the right. These imply that, for regularly consumed components, the distributions of the true long-term average intakes smooth out near both ends, whereas, for episodically consumed components, the distributions of the true long-term average intakes have discontinuities at zero. The right panels of Figure 2 also show that, as expected, individuals consuming an episodic component in smaller amounts also consume it less often on average.

1.3. Existing Methods and Their Limitations

The literature on univariate density deconvolution for continuous surrogates, in which context we denote the variable of interest by \( X \) and the measurement errors by \( U \), is massive. The early literature, however, focused on scenarios with restrictive assumptions, such as known measurement error distribution, homoscedasticity of the errors, their independence from \( X \), etc., which are all highly unrealistic, especially in nutritional epidemiology applications like ours. Reviews of these early methods can be found in Carroll et al. (2006) and Buonaccorsi (2010). We cite below some relatively recent ideas that are directly relevant to our proposed solution.

Bayesian frameworks can accommodate measurement errors through natural hierarchies, providing powerful tools for solving complex deconvolution problems, including scenarios where the measurement errors can be conditionally heteroscedastic. Taking such a route, Staudenmayer, Ruppert, and Buonaccorsi (2008) assumed the measurement errors to be normally distributed but allowed the variability of \( U \) to depend on \( X \),

| Notation | Description |
|----------|-------------|
| \( q \)  | Number of episodically consumed components. |
| \( p \)  | Number of regularly consumed components. |
| \( Y_{j,i} \) | Observed recall of the \( t \)th dietary component for the \( i \)th individual on the \( j \)th sampling occasion—binary for \( \ell = 1, \ldots, q \), zero if the component was not consumed, one otherwise; zero or positive continuous for \( \ell = q + 1, \ldots, 2q \), representing the reported intakes, zero when the component was not consumed, positive continuous otherwise; positive continuous for \( \ell = 2q + 1, \ldots, 2q + p \), representing the reported intakes. |
| \( W_{j,i} \) | Proxy recall of the \( t \)th dietary component for the \( i \)th individual on the \( j \)th sampling occasion—always continuous; latent for \( \ell = 1, \ldots, q \), negative if \( Y_{j,i} = 0 \), positive if \( Y_{j,i} = 1 \); latent or observed for \( \ell = q + 1, \ldots, 2q \), latent when the component was not consumed, observed and equals \( Y_{j,i} \) when a positive recall was recorded; positive for \( \ell = 2q + 1, \ldots, 2q + p \), equaling \( Y_{j,i} \), the reported positive intake. |
| \( x_{j} \) | Long-term daily average intake of the \( t \)th dietary component for the \( i \)th individual, consumption and nonconsumption days combined. Strictly positive and continuous. For \( \ell = 1, \ldots, q + p \), the observed recalls \( Y_{j,i} \) are unbiased for \( X_{j,i} \). |
| \( x_{j}^{+} \) | Long-term daily average intake of the \( t \)th dietary component for the \( i \)th individual, on consumption days only. Strictly positive and continuous. For \( \ell = 1, \ldots, q + p \), the proxy recalls \( W_{j,i} \) are unbiased for \( X_{j,i}^{+} \). |
| \( P_{j}(X_{j}) \) | Probability of reporting positive consumption on the \( t \)th dietary component by the \( i \)th individual on any sampling occasion. |
| \( \hat{X}_{j} \) | Functions of \( x_{j} \) and \( x_{j}^{+} \) such that \( W_{j,i} \) is unbiased for \( \hat{X}_{j} \). |
| \( U_{j,i} \) | Measurement errors or pseudo-errors contaminating \( X_{j,i} \) to generate \( W_{j,i} \). The \( U_{j,i} \)’s are all unbiased for \( \ell = 1, \ldots, q + p \). For \( \ell = q + 1, \ldots, 2q + p \), \( U_{j,i} \) depends on the associated \( \hat{X}_{j} \). |
| \( S_{j}^{2}(\hat{X}_{j}) \) | Variance function explaining how the conditional variability of \( U_{j,i} \) depends on the associated \( \hat{X}_{j} \) for \( \ell = q + 1, \ldots, 2q + p \). |
| \( e_{j,i} \) | Scaled measurement error or pseudo-error obtained by scaling \( U_{j,i} \) by \( s_{j}(\hat{X}_{j}) \). The \( e_{j,i} \)’s are unbiased for zero, homoscedastic, and independent of \( \hat{X}_{j} \). |
| \( Z_{j} \) | Long-term daily average normalized intake of the \( t \)th dietary component for the \( i \)th individual, normalized by energy. |
utilizing mixtures of B-splines to estimate $f_X$ as well the conditional variability $\text{var}(U|X)$. Sarkar et al. (2014) relaxed the assumption of normality of $U$, employing flexible mixtures of normals (Escobar and West 1995; Frühwirth-Schnatter 2006) to model both $f_X$ and $f_U|X$. Sarkar et al. (2018) extended the methods to multivariate settings, modeling $f_X$ and $f_U|X$ using mixtures of multivariate normals.

While Staudenmayer, Ruppert, and Buonaccorsi (2008) and Sarkar et al. (2014, 2018) provided progressively flexible frameworks for univariate and multivariate deconvolution with continuously measured surrogates, they cannot directly handle multivariate zero-inflated dietary recall data. There are several restrictive aspects of their approaches that also do not allow them to be straightforwardly extended to deconvolution problems with zero-inflated surrogates, as we outline shortly while describing our proposed approach.

The problem of estimating long-term nutritional intakes of a single episodic dietary component from zero-inflated recall data has previously been considered in Tooze, Grunwald, and Jones (2002), Tooze et al. (2006), Kipnis et al. (2009), and Zhang, Krebs-Smith, et al. (2011). These approaches all worked with component-wise Box–Cox transformed (Box and Cox 1964) positive recalls which were then assumed to decompose into a subject specific random effect component and an error or pseudo-error component. Assumed independent and homoscedastic, these components were then both

Figure 1. Exploratory plots for sodium (top row) and energy (bottom row). Left panels: Histogram of recalls $Y_{\ell,i,j}$; right panels: subject-specific means $\bar{Y}_{\ell,i,j}$ versus variances $S_{Y_{\ell,i,j}}^2$.
modeled using single component multivariate normal distributions. Estimates of the long-term consumption day intakes were then obtained via individual transformations back to the original scale. Long-term episodic consumptions were finally defined combining these estimates with probabilities of reporting nonconsumptions. As shown in Sarkar et al. (2014), Box–Cox transformations for surrogate observations have severe limitations, including almost never being able to produce transformed surrogates that conform to normality, homoscedasticity, and independence. Transformation–retransformation based methods are thus highly restrictive, even for univariate regularly consumed components.

Despite the limitations, to our knowledge, Zhang, Midthune, et al. (2011) is the only available method that can handle multivariate zero-inflated dietary recall data. It is thus also our main and only competitor.

1.4. Outline of Our Proposed Method

In this article, we develop a Bayesian semiparametric density deconvolution approach specifically designed to address problems with zero-inflated surrogates, carefully accommodating all prominent features of the EATS dataset described above. We build on an augmented latent variable framework which introduces, for each recall of the episodically consumed component, one or two latent continuous proxies, depending on whether the recall was positive or exact zero, effectively translating a deconvolution problem with zero-inflated data to one with all continuous surrogates, albeit some latent ones. This requires modeling an additional pseudo-error distribution for each episodically consumed component, but returns, as potentially useful by-products, estimates of the probabilities of reporting zero recalls for the episodically consumed dietary components. As the right panels of Figure 2 suggest, individuals who consume an episodic component less often (in other words, report more zero recalls) naturally also consume the component in smaller amounts in the long run. The probabilities of reporting zero consumptions are thus informative about the true long-term consumption amounts and conversely. Our proposed latent variable framework appropriately recognizes these features.

Even though the multivariate latent consumptions $\mathbf{X}$ and the associated multivariate errors and pseudo-errors $\mathbf{U}$ become all strictly continuous in our augmented latent variable framework, the approach of Sarkar et al. (2018) to model their distributions using mixtures of multivariate normals is still fraught with serious practical drawbacks as it does not allow much flexibility in modeling the univariate marginals $f_X$ and $f_{U|X}$, especially the marginals of the episodic components which have discontinuities at zero. The issue becomes more critical when inference is based on samples drawn from the posterior using

![Figure 2. Exploratory plots for milk (top row) and whole grains (bottom row). Left panels: Histogram of recalls $Y_{ij}$ (red) and histogram of strictly positive recalls $Y_{ij}(>0)$ (blue) superimposed on each other; middle panels: subject-specific means $\overline{Y}_{ij}$ versus subject-specific variances $S^2_{ij}$ when multiple strictly positive recalls are available; right panels: boxplots of proportion of zero recalls versus corresponding subject-specific means $\overline{Y}_{ij}$.](image-url)
Markov chain Monte Carlo (MCMC) algorithms. The latent \( X \)'s are also sampled in the process and the specific parametric form of the assumed multivariate mixture kernel may influence this step in ways that result in density estimates closely resembling its parametric form even when the shape of the true density departs from it.

As opposed to Sarkar et al. (2018) who focused on modeling the joint distributions \( f_X \) and \( f_{UX} \) first and then deriving the marginals from those estimates, we take the opposite approach of modeling the marginals \( f_{X_i} \) and \( f_{U|X} \) first and then build the joint distributions \( f_X \) and \( f_{UX} \) by modeling the dependence structures separately using Gaussian copulas. This approach allows us adopt different strategies for modeling the different components of \( f_X \) and \( f_{UX} \) which proved crucial in accommodating the important features of our motivating datasets. Following Sarkar et al. (2014), we use flexible mixtures of mean restricted normals and mixtures of B-splines to model \( f_{U|X} \)'s and the associated conditional heteroscedasticity functions. Mixtures of normal kernels, as in Sarkar et al. (2014), are, however, not suitable for modeling \( f_X \)'s. We use normalized mixtures of B-splines and mixtures of truncated normal kernels instead which are well suited to model densities with bounded supports and discontinuities at the boundaries.

The literature on copula models in measurement error-free scenarios is vast. See, for example, Nelsen (2007), Joe (2015), Shemyakin and Kniazev (2017), and the references therein. We are, however, unaware of any published work in the context of measurement error problems.

In contrast to Zhang, Midhune, et al. (2011), we model the densities of the latent consumptions and the error and pseudo-errors more directly using flexible models that can accommodate widely varying shapes with discontinuous boundaries as well as conditional heteroscedasticity. In our latent variable framework, the probability of reporting zero recalls depends directly on the latent true consumption day intake, hence informing each other. Applied to our motivating nutritional epidemiology problems, our method thus provides more realistic estimates of the intakes of the episodically consumed dietary components. Additional detailed comparisons of our method with previous approaches for zero-inflated data are presented in Section S.4 in the supplementary materials.

Compared to all previously existing density deconvolution methods, including traditional methods for strictly continuous data as well as methods designed specifically for zero-inflated data, our proposed approach is thus fundamentally novel while also being broadly applicable to both scenarios.

### 1.5. Outline of the Article

The rest of the article is organized as follows. Section 2 details the proposed Bayesian hierarchical framework. Section 3 presents results of our proposed method applied to the motivating nutritional epidemiology problems. Section 4 concludes with a discussion. A brief review of copula, a detailed comparison of our method with previous approaches to zero-inflated data, an MCMC algorithm to sample from the posterior, simulation studies comparing the proposed method with its main competitor, and some additional results are included in the supplementary materials.

## 2. Deconvolution Models

### 2.1. Latent Variable Framework

Our goal is to estimate the marginal and joint consumption patterns of \( q + p \) dietary components of which the first \( q \) are episodically consumed and the latter \( p \) are regularly consumed, including energy. There are a total of \( n \) subjects with \( m_i \) 24-hr recalls recorded for the \( i \)th subject. We let \( Y_{ij} = (Y_{1,i,j}, \ldots, Y_{q+p,i,j})^T \) denote the observed data for the \( i \)th recall of the \( i \)th individual. For \( \ell = 1, \ldots, q \), \( Y_{\ell,i,j} \) is the indicator of whether the \( \ell \)th episodic component is reported to have been consumed. For \( \ell = q + 1, \ldots, 2q \), \( Y_{\ell,i,j} \) is the reported intake of the \( \ell \)th episodically consumed component, and for \( \ell = 2q + 1, \ldots, 2q + p \), \( Y_{\ell,i,j} \) is the reported intake of the \( \ell \)th regularly consumed component. Let \( W_{ij} = (W_{1,i,j}, \ldots, W_{2q+p,i,j})^T \) denote a vector with all continuous components that are related to the observed data \( Y_{ij} \) by the relationships

\[
Y_{\ell,i,j} = 1(W_{\ell,i,j} > 0), \quad \ell = 1, \ldots, q,
\]

\[
Y_{\ell,i,j} = Y_{-(\ell-q),i,j} W_{\ell,i,j}, \quad \ell = q + 1, \ldots, 2q, \quad (1)
\]

\[
Y_{\ell,i,j} = W_{\ell,i,j}, \quad \ell = 2q + 1, \ldots, 2q + p.
\]

For \( \ell = 1, \ldots, q \), \( W_{\ell,i,j} \) indicates whether the \( \ell \)th episodic component is reported to have been consumed in the \( j \)th recall of the \( i \)th individual and is always latent except that we know whether it is positive or negative. That is, for \( \ell = 1, \ldots, q \), \( W_{\ell,i,j} \) is always latent with \( W_{\ell,i,j} < 0 \) if \( Y_{\ell,i,j} = 0 \) and \( Y_{q+\ell,i,j} = 0 \), and \( W_{\ell,i,j} \geq 0 \) if \( Y_{\ell,i,j} = 1 \) and \( Y_{q+\ell,i,j} > 0 \).

For \( \ell = q + 1, \ldots, 2q \), \( W_{\ell,i,j} \) is latent if the \( \ell \)th episodic component is reported to have not been consumed in the \( j \)th recall of the \( i \)th individual and is observed and equals the reported consumed positive amount \( Y_{\ell,i,j} \) otherwise. That is, for \( \ell = q + 1, \ldots, 2q \), \( W_{\ell,i,j} \) is latent if \( Y_{\ell-q,i,j} = 0 \) and \( Y_{\ell,i,j} = 0 \) and is observed with \( W_{\ell,i,j} = Y_{\ell,i,j} \) if \( Y_{\ell-q,i,j} = 1 \) and \( Y_{\ell,i,j} > 0 \).

For \( \ell = 2q + 1, \ldots, 2q + p \), \( W_{\ell,i,j} \) denotes the reported intake of the \( \ell \)th regular component and is always observable. That is, for \( \ell = 2q + 1, \ldots, 2q + p \), \( W_{\ell,i,j} = Y_{\ell,i,j} > 0 \).

We let \( X_i = (X_{1,i}, \ldots, X_{q+p,i})^T \) denote the latent daily average long-term intakes of the \( i \)th individual, consumption and nonconsumption days combined. We now let \( \mathbf{X}_i = (X_{1,i}, \ldots, X_{q+p,i})^T \) denote the latent daily average long-term intakes of the \( i \)th individual on consumption days only. We then define \( \mathbf{X}_i = (\mathbf{X}_{1,i}, \ldots, \mathbf{X}_{2q+p,i})^T \) as

\[
\mathbf{X}_{\ell,i} = h_{\ell}(X_{\ell,i}), \quad \ell = 1, \ldots, q,
\]

\[
\mathbf{X}_{\ell,i} = X_{-(\ell-q),i}, \quad \ell = q + 1, \ldots, 2q,
\]

\[
\mathbf{X}_{\ell,i} = X_{-(\ell-q),i}, \quad \ell = 2q + 1, \ldots, 2q + p.
\]

Here, \( h_{\ell}(\cdot) \) is an unknown function to be estimated from data. The reasons behind defining \( \mathbf{X}_i \) in this manner will be clear shortly.

For \( i = 1, \ldots, n \) and \( j = 1, \ldots, m_i \), we let \( U_{ij} = (U_{1,i,j}, \ldots, U_{2q+p,i,j})^T \) and consider the model

\[
W_{ij} = \mathbf{X}_i + U_{ij}, \quad E(U_{ij} | \mathbf{X}_i) = 0.
\]
the distribution energy-adjusted intakes. We address this latter problem in Section 2.5.

The complex nature of our problem warranted the introduction of many different variables representing the many random variables of our model. For easy reference, these variables and a few others to be introduced shortly are listed in Table 2.

2.2. Modeling the Density \( f_X \)

In this article, \( f_X \) is specified using a Gaussian copula density model

\[
f_X(X) = |R_X|^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} Y_X^{-1} (R_X^{-1} - I_{1+p}) Y_X \right\} \prod_{\ell=1}^{q+p} f_{X,\ell}(X_\ell),
\]

where \( f_{X,\ell}(X_\ell) = \Phi(Y_{X,\ell}) \) for all \( \ell \) and \( R_X \) is the correlation matrix of \( X \).

In initial attempts, we modeled the marginal densities \( f_{X,\ell} \) as flexible mixtures of truncated normal kernels \( TN(\cdot | \mu, \sigma^2, [A,B]) \) with location \( \mu \) and scale \( \sigma \) and range restricted to the interval \([A,B]\). In multivariate applications such as ours, where the components represent similar variables and have highly overlapping supports, we can greatly reduce dimension and borrow information across different dietary components, by allowing the component specific parameters of the mixture models to be shared among the variables. We thus modeled the marginal densities as

\[
f_{X,\ell}(X_\ell) = \sum_{k=1}^{K_{X,\ell}} \pi_{X,\ell,k} TN(X_\ell | \mu_{X,k}, \sigma_{X,k}^2)(A, B),
\]

where \( \mu_{X,k}, \sigma_{X,k}^2 \) are estimated “locally” utilizing only the data points associated with the corresponding mixture components. For the episodic components, the scarcity of informative observations near the left boundaries often allows the sampled latent \( X_\ell,k,i \)'s to cluster away from these boundaries, resulting in the associated \( \sigma_{X,k}^2 \)'s to be underestimated and hence the estimated densities to be peaked away from the boundaries. Setting informative lower bounds to the variance parameters solves the problem. Determining such bounds for the latent variables from their contaminated recalls, however, proved to be difficult.

For episodic components, we thus needed models that can accommodate local variations in shape but would also allow the smoothness to be learned from regions where more informative data points are available. To achieve this, we employed flexible penalized normalized mixtures of B-splines with smoothness inducing priors on the coefficients to model the densities of the episodic components. For the \( \ell \)th component, we partition the interval \([A, B]\) of interest into \( L_\ell \) subintervals using knot points \( A_\ell = t_{\ell,1} = \cdots = t_{\ell,d+1} < t_{\ell,d+2} < t_{\ell,d+3} < \cdots < \)
t_{ℓ,d+L_k} < t_{ℓ,d+L_k+1} = \cdots = t_{ℓ,2d+L_k+1} = B_ℓ. Using these knot points, \( I_ℓ = (d + L_ℓ) \) B-spline bases of degree \( d \), denoted by \( \mathbf{B}_{d,L_ℓ} = \{ b_{d,L_1}, b_{d,L_2}, \ldots, b_{d,L_d(ℓ)} \} \), can be defined through a recursion relation (see Figure 4 and Section S.2 in the supplementary materials). B-splines are nearly orthogonal and locally supported. For equidistant knot points with \( δ_ℓ = (t_ℓ, j - t_ℓ, j-1) \), the areas under these curves can be easily computed as

\[
\delta_ℓ,j = \int_{t_ℓ}^{B_ℓ} B_{d,L_ℓ}(X) dX = \begin{cases} δ_ℓ/6 & \text{for } j = 1, \ell, \\ 5δ_ℓ/6 & \text{for } j = 2, \ell - 1, \\ δ_ℓ & \text{for } j = 3, \ldots, \ell - 2. \end{cases}
\]

Mixtures of B-splines can therefore be easily normalized. A flexible model for the density functions is then obtained as

\[
f_{X,ℓ}(x_ℓ) = \mathbf{B}_{d,L_ℓ}(X_ℓ) \exp(ξ_ℓ) \left( \sum_{m=1}^{I_ℓ} \delta_ℓ,m \exp(ξ_ℓ,m) \right)^{-1},
\]

\[
(ξ_ℓ \mid J_ℓ, σ_ξ^2, ξ_0^2) ∼ \exp(2π σ_ξ^2)^{-I_ℓ/2} \exp\left( -\frac{ξ_ℓ^T P_ℓ ξ_ℓ}{2σ_ξ^2} \right), \quad σ_ξ^2, ξ_0^2 \sim \text{Inv-Ga} (a_ℓ, b_ℓ).
\]

Here, \( ξ_ℓ = (ξ_ℓ, 1, ξ_ℓ, 2, \ldots, ξ_ℓ, I_ℓ)^T \); \( \exp(ξ_ℓ) = (\exp(ξ_ℓ, 1), \exp(ξ_ℓ, 2), \ldots, \exp(ξ_ℓ, I_ℓ))^T \); and \( P_ℓ = D_ℓ^T D_ℓ \), where \( D_ℓ \) is a \((I_ℓ + 2) \times I_ℓ \) matrix such that \( D_ℓ ξ_ℓ \) computes the second-order differences in \( ξ_ℓ \). The prior \( p_ℓ (ξ_ℓ \mid ξ_0^2, σ_ξ^2) \) induces smoothness in the coefficients because it penalizes \( \sum_{j=1}^{I_ℓ} (I_ℓ^2 ξ_0^2, k)^2 = \xi_0^T P_ℓ ξ_ℓ \), the sum of squares of the second-order differences in \( ξ_ℓ \) (Eilers and Marx 1996). The parameters \( σ_ξ^2, ξ_0^2 \) play the role of smoothing parameters—the smaller the value of \( σ_ξ^2, \) the stronger the penalty and the smoother the associated variance function. The inverse-Gamma hyper-priors on \( σ_ξ^2, ξ_0^2 \) allow the data to influence the posterior smoothness and make the approach data adaptive. Importantly, the smoothness is now informed by data points across the entire range, resulting in vast improvements in the density estimates near the left boundaries.

For regularly consumed components with strictly positive recalls, we found mixtures of truncated normals to slightly outperform normalized mixtures of B-splines. This is also consistent with findings reported in Sarkar et al. (2014). For regularly consumed components, we thus still use mixtures of truncated normals with shared atoms. With densities smoothed out to zeros at the boundaries, truncations are not strictly needed for regularly consumed dietary components. We still retain the truncations to make our approach broadly applicable to other potential applications where boundary discontinuities may be present even when the recalls are all continuous.

Next, consider the problem of modeling \( \mathbf{R}_X \). The problem of modeling correlation matrices has garnered some attention in the literature (Barnard, McCulloch, and Meng 2000; Liechty, Liechty, and Müller 2004; Pourahmadi and Wang 2015; Tsay and Pourahmadi 2017). Here, we adapt the model from Zhang, Midhune, et al. (2011) based on spherical coordinate representation of Cholesky factorizations that allows the involved parameters to be treated separately of each other, simplifying posterior computation while guaranteeing the resulting matrix to always be a valid correction matrix. We prove in Section S.3.1 in the supplementary materials that the converse is also true.

That is, any correlation matrix can be represented in this form which establishes its nonparametric nature. We drop the subscript \( X \) for the rest of this subsection to keep the notation clean.

Let \( \mathbf{V}^{(q+p)×(q+p)} \) be a lower triangular matrix such that \( \mathbf{R} = \mathbf{V} \mathbf{V}^T \). The form of \( \mathbf{V} \) is

\[
\mathbf{V} = \begin{pmatrix} v_{1,1} & 0 & \cdots & 0 \\
v_{2,1} & v_{2,2} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
v_{q+p,1} & v_{q+p,2} & \cdots & v_{q+p,q+p} \end{pmatrix}.
\]

We have \( r_{ℓ,ℓ′} = \sum_{k=1}^{q+p} v_{ℓ,k} v_{ℓ′,k} \) for all \( ℓ \leq ℓ′ \). The restriction that \( \mathbf{R} \) is a correlation matrix then implies \( \sum_{k=1}^{q+p} v_{ℓ,k}^2 = 1 \) for all \( ℓ = 1, \ldots, (q+p) \). The restrictions are satisfied by the following parameterization

\[
v_{1,1} = 1,
\]

\[
v_{2,1} = b_{1,1}, \quad v_{2,2} = \sqrt{1 - b_{1,1}^2},
\]

\[
v_{3,1} = b_{2,1} \sin(\theta_{1,1}), \quad v_{3,2} = b_{2,2} \cos(\theta_{1,1}), \quad v_{3,3} = \sqrt{1 - b_{2,2}^2},
\]

\[
v_{ℓ,1} = b_{ℓ-1} \sin(\theta_{ℓ,1}), \quad v_{ℓ,2} = b_{ℓ-1} \cos(\theta_{ℓ,1}) \cos(\theta_{ℓ,1}) + \cdots + \cos(\theta_{ℓ,1}) + k - 2 \sin(\theta_{ℓ,1}) + k - 1, \quad \text{for } k = 2, \ldots, (ℓ - 2),
\]

\[
v_{ℓ,ℓ-1} = b_{ℓ-1} \cos(\theta_{ℓ-1}) \cos(\theta_{ℓ-1}) + \cdots + \cos(\theta_{ℓ-1}) + k - 1 \cos(\theta_{ℓ-1}) + \cos(\theta_{ℓ-1}),
\]

\[
v_{ℓ,ℓ} = \sqrt{1 - b_{ℓ-1}^2},
\]

where \( ℓ = 4, \ldots, (q+p), i_1(ℓ) = 1 + (1 + \cdots + (ℓ - 3)) = (ℓ^2 - 5ℓ + 8)/2 \) and \( i_2(ℓ) = i_1(ℓ) + (ℓ - 3) = (ℓ^2 - 3ℓ + 2)/2, \)

Figure 4. Plot of 9 quadratic (\( d = 2 \)) B-splines on \([A, B]\) defined using 11 knot points that divide \([A, B]\) into \( K = 6 \) equal subintervals.
Here, $\text{Unif}(a,b)$ denotes a uniform distribution with support $(a,b)$.

### 2.3. Modeling the Density $f_{\mathbf{u} \mid \mathbf{x}}$

The reported intakes of the regularly consumed components exhibit strong conditional heteroscedasticity, so do the reported intakes of the episodic components, when consumed. To accommodate conditional heteroscedasticity, we let

$$
\mathbf{U}_{ij} = \mathbf{S}(\mathbf{X}) \mathbf{e}_{ij}, \quad \text{with } \mathbb{E}(\mathbf{e}_{ij}) = \mathbf{0}, \quad \text{and}\quad \mathbf{S}(\mathbf{X}) = \text{diag}(1, \ldots, 1, s_{q+1}, \ldots, s_{2q+p}(\tilde{X}_{2q+p})).
$$

The above model implies that $\text{cov}(\mathbf{U}_{ij} \mid \mathbf{X}) = \mathbf{S}(\mathbf{X})$ and $\text{var}(\mathbf{U}_{ij} \mid \mathbf{X}) = \mathbf{S}(\mathbf{X})$, with $\mathbb{E}(\mathbf{e}_{ij})$ and $\mathbf{S}(\mathbf{X})$ being functions of $\mathbf{U}$, including its shape and correlation structure, are derived from $f_{\mathbf{e}}$. The multiplicative structural assumption arises naturally for conditionally heteroscedastic multivariate measurement errors; the model also automatically accommodates multiplicative measurement errors $W_{l,t,j} = X_{l,t,j} U_{l,t,j}$ with $E(U_{l,t,j}) = 1$ and $\tilde{U}_{l,t,j}$ independent of $\mathbf{X}_{\ell,t}$ via a simple reformulation $W_{l,t,j} = \tilde{X}_{l,t,j} (\tilde{U}_{l,t,j} - 1) = \tilde{X}_{l,t,j} + s(X_{l,t,j}) e_{l,t,j}$, where $s(X_{l,t,j}) = X_{l,t,j}$ and $e_{l,t,j} = (U_{l,t,j} - 1)$ (Sarkar et al. 2018).

As in Section 2.2.2, we use a Gaussian copula density model to specify the density $f_{\mathbf{u}}$ but the model has now satisfied many zero constraints. Specifically, we let

$$
f_{\mathbf{e}}(\mathbf{e}) = \prod_{\ell = 1}^{q} f_{\mathbf{e},\ell}(\mathbf{e}) \times |\mathbf{R}_\mathbf{e}|^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} \mathbf{e}' \mathbf{R}_\mathbf{e}^{-1} \mathbf{e} \right\}
$$

for $\ell = 1, \ldots, 2q + p$.

Here, $F_{\mathbf{e},\ell}(\mathbf{e}) = \Phi(Y_{\mathbf{e},\ell})$ for all $\ell$. The first $q$ components of $\mathbf{e}$ are independent of each other and also independent of the rest of the $q + p$ components. The latter $q + p$ components may be correlated with correlation matrix $\mathbf{R}_\mathbf{e}$.

The copula approach again allows us to use different models for the distributions of the pseudo-errors $f_{\mathbf{e},\ell}(\mathbf{e})$, $\ell = 1, \ldots, q$, and the distributions of the actual scaled measurement errors $f_{\mathbf{e},\ell}(\mathbf{e})$, $\ell = q + 1, \ldots, 2q + p$.

Here, we only model the correlation between different scaled error components $\varepsilon_{l,j,i}, \varepsilon_{l',j,i}$ for $\ell \neq \ell'$ but ignore the correlation between different sampling occasions $\varepsilon_{l,j,i}, \varepsilon_{j',j,i}$ for $j \neq j'$. The correlation between $W_{l,t,j}, W_{l',t,j}$ for $j \neq j'$ is thus explained entirely by their shared component $X_{l,t,j}$. In post model fit correlation analysis with estimated scaled "residuals," presented in Figure S.9 in the supplementary materials, we found no real evidence that the errors $\varepsilon_{l,j,i}, \varepsilon_{l',j,i}$ are significantly correlated for $j \neq j'$.

For $\ell = 1, \ldots, q$, we model the marginal densities $f_{\mathbf{e},\ell}$ as

$$
f_{\mathbf{e},\ell}(\mathbf{e}) = \text{Normal}(\varepsilon_{\mathbf{e},\ell} \mid 0, 1).
$$

This implies a probit model for the probabilities of consumptions $P_{\ell}(X_{\ell}) = \text{Pr}(U_{\ell} > -h_{\ell}(X_{\ell})) = \Phi(-h_{\ell}(X_{\ell}))$. Flexibility of this probability model thus depends on the choice of $h_{\ell}(X_{\ell})$. We discuss this issue in Section 2.4.

For $\ell = q + 1, \ldots, 2q + p$, we model the marginal densities $f_{\mathbf{e},\ell}(\mathbf{e})$ using an adaptation of the moment restricted model in Sarkar et al. (2014) but with shared normals as

$$
f_{\mathbf{e},\ell}(\mathbf{e}) = \prod_{k = 1}^{K_{\ell}} \pi_{\ell,k} f_{\mathbf{e},\ell}(\mathbf{e} \mid \mu_{\ell,k}, \sigma_{\ell,k}^2, \sigma_{\ell,k,1}^2, \sigma_{\ell,k,2}^2),
$$

with $\pi_{\ell} \sim \text{Dir}(\alpha_{\ell,k} / K_{\ell}, \ldots, \alpha_{\ell,k} / K_{\ell}), (\mu_{\ell,k}, \sigma_{\ell,k}^2, \sigma_{\ell,k,1}^2, \sigma_{\ell,k,2}^2)$.

Finally, for $\ell = q + 1, \ldots, 2q + p$, we model the variance functions $v_{\ell}(X_{\ell}) = \tilde{v}_{\ell}(X_{\ell})$ by flexible penalized mixtures of B-splines with smoothness inducing priors on the coefficients as in Staudenmayer, Ruppert, and Buonaccorsi (2008) as

$$
v_{\ell}(X_{\ell}) = \tilde{v}_{\ell}(X_{\ell}) = \sum_{j=1}^{K_{\ell}} b_{d,\ell,j} \tilde{X}_{\ell,j} \exp(\theta_{\ell,j}),
$$

subject to $E(\tilde{v}_{\ell}(X_{\ell})) = 0$, for $\ell = 1, \ldots, 2q + p$.

As before, the parameters $\sigma_{\ell,\ell}^2, \sigma_{\ell,\ell}^1$ play the role of smoothing parameter, and the inverse-Gamma hyper-priors allow them to be learned from the data themselves.
The flexibility of $h_t(X_t)$ compensates for the parametric nature of the probit link, making the model $P_t(X_t)$ robust.

The right panels of Figure 2 suggest that as $X_t$ increases, the probability of reporting a positive consumption also increases straightforwardly obtained as

\[ \Phi(h_t(X_t)), \quad W_j = \tilde{X} + U_j, \quad \mathbb{E}(U_j \mid \tilde{X}) = 0, \quad \tilde{X} = \phi(X), \]

where the functions $\psi(\cdot): \mathbb{R}^{2q+p} \rightarrow \mathbb{R}^{2q+p}$ and $\phi(\cdot): \mathbb{R}^{2q+p} \rightarrow \mathbb{R}^{2q+p}$ are easily identified from models (1) and (2). Specifically, $\phi(\cdot)$ is given by

\[ \tilde{X}_\ell = h_t(X_t), \quad \text{for } \ell = 1, \ldots, q, \]

\[ \tilde{X}_\ell = X_{\ell-q}/P_{\ell-q}(X_{\ell-q}), \quad \text{for } \ell = q + 1, \ldots, 2q, \]

(3)

where, for $\ell = 1, \ldots, q$, $P_{\ell}(X_t) = P(W_{\ell,j} > 0 \mid X_t) = \Phi(h_t(X_t))$ for some arbitrary functions $h_t(\cdot): \mathbb{R} \rightarrow \mathbb{R}$.

We state the basic assumptions needed for identifiability and our main result on identifiability below. The proof is deferred to Section S.3.2 in the supplementary materials.

**Assumption 1.**

(A1) The number of replicates $m \geq 3$.

(A2) $U_j \mid \tilde{X} \stackrel{d}{=} S(\tilde{X})e_j, \quad e_j \sim f_e, j = 1, 2, 3$, where $f_e$ has a Fourier transform that is non-vanishing everywhere.

Observe that (A2) includes the homoscedastic case, that is, when $s_t(X_t)$ is a constant function of $X_t$.

**Theorem 1.** Under (A1) and (A2), given the observed density $f_{Y_1,Y_2,Y_3}$, the equation

\[ f_{Y_1,Y_2,Y_3}(Y_1,Y_2,Y_3) = \int f_{Y_1|\tilde{X}}(Y_1 \mid \tilde{X})f_{Y_2|\tilde{X}}(Y_2 \mid \tilde{X})f_{Y_3|\tilde{X}}(Y_3 \mid \tilde{X})f_{\tilde{X}}(\tilde{X})d\tilde{X}, \]

admits a unique solution for $f_{Y_j|\tilde{X}}(Y_j \mid \tilde{X})$ for $j = 1, \ldots, 3$ and $f_{\tilde{X}}(\tilde{X})$. Furthermore, if $X$ and $\tilde{X}$ are related by (3), then $f_X(X)$ is uniquely identified from $f_{Y_j|\tilde{X}}(Y_j \mid \tilde{X})$ for $j = 1, \ldots, 3$, and $f_{\tilde{X}}(\tilde{X})$.

In practice, for identifiability, we require $m_i \geq 3$ recalls for at least some values of $i$. As long as this condition is satisfied, missing values in recall data can be simply ignored. For our motivating EATS dataset, we have $m_i = 4$ for all $i$ with no missing recalls. So the conditions are easily satisfied.
3. Applications in Nutritional Epidemiology

In this section, we discuss the results of our method applied to the EATS dataset. Specifically, we consider the problem of estimating the distributions of long-term average daily intakes of two episodic components—milk and whole grains, and two regular components—sodium and energy. The surrogates for milk and whole grains, we recall, had approximately 21% and 37% exact zeros.

Figure 5 shows the estimated marginal densities $f_{X,\ell}$ obtained by our method and the method of Zhang, Midthune, et al. (2011). For sodium and energy, there is general agreement between the estimates obtained by our method and the method of Zhang, Midthune, et al. (2011). For the episodic components milk and whole grains, on the other hand, the estimated densities look very different, especially near the left boundary. Our method shows these densities to continually increase as we approach zero from right, as is expected from Figure 2.

Figure 5. Results for the EATS datasets with sample size $n = 965$, $q = 2$ episodic components, milk and whole grains, and $p = 2$ regular components, sodium and energy, each subject having $m_i = 4$ replicates. From top to bottom, the left panels show the estimated densities $f_{X,\ell}(X)$ of milk and whole grains, sodium, and energy, respectively, obtained by our method (in blue) and the method of Zhang, Midthune, et al. (2011) (in red). The right panels show the associated distributions of the scaled errors $f_{\epsilon,q+\ell}^q(\epsilon_{q+\ell})$ and the associated variance functions $v_\ell(\tilde{X}_\ell) = s^2_\ell(\tilde{X}_\ell)$, estimated by our method.
Figure 6. Results for the EATS datasets with sample size \( n = 965 \), \( q = 2 \) episodic components, milk and whole grains, and \( p = 2 \) regular components, sodium and energy, each subject having \( m_i = 4 \) replicates. The estimated probabilities of reporting positive consumption \( P_\ell (X_\ell) \) for the episodic components milk (left panel) and whole grains (right panel), estimated by our method.

Figure 7. Results for the EATS datasets with sample size \( n = 965 \), \( q = 2 \) episodic components, milk and whole grains, and \( p = 2 \) regular components, sodium and energy, each subject having \( m_i = 4 \) replicates. From left to right, the estimated distributions of normalized intakes of milk, whole grains and sodium, normalized by total energy, estimated by our method (in blue) and by the method of Zhang, Midhune, et al. (2011) (in red).

Consistent with Figure 2, compared to milk, the distribution of whole grains is also more concentrated near zero. The estimates produced by Zhang, Midhune, et al. (2011), on the other hand, dip near zero, as was also observed in simulation scenarios.

The right panels in Figure 5 show the estimates of the densities of scaled measurement errors \( f_{\epsilon, q+1} (\epsilon_{q+1}) \) and the estimates of the variance functions \( s_\ell^2(X_\ell) \). The estimated \( f_{\epsilon, q+1} \)'s are positively skewed for all components. And, as expected from Figures 1 and 2, the estimated \( s_\ell^2 \)'s show strong patterns of conditional heteroscedasticity for all components. For the episodic components, our method also provides estimates of the probabilities of reporting positive consumptions which are shown in Figure 6. The recalls for whole grains have more zeros than the recalls for milk. Its distribution is also more concentrated near zero. The probability of reporting positive consumptions for whole grains thus increases more rapidly as its true daily average intake increases.

Figure 7 shows the distributions of normalized intakes obtained by our method and the method of Zhang, Midhune, et al. (2011). The estimates look very different, including the one for the regular component sodium. Our method provides more realistic estimates of the distribution of normalized intakes that are more concentrated near zero but are more widely spread.

Figure S.7 in the supplementary materials shows the estimated bivariate marginals for produced by our method and the method of Zhang, Midhune, et al. (2011). Figure S.8 in the supplementary materials additionally illustrates how the redundant mixture components become empty after reaching steady states in our MCMC based implementation. Figure S.8 also shows how in practice the mixture component specific parameters get shared across different dimensions in our models with shared parameters for the marginal densities.

More formal model comparisons for real data, using component wise log pseudo marginal likelihoods (Geisser and Eddy 1979) and widely applicable information criteria (WAIC) (Watanabe 2010), are discussed in Section S.9 in the supplementary materials.

4. Discussion

4.1. Summary

In this article, we considered the problem of multivariate density deconvolution when replicated proxies are available but, complicating the challenges, the proxies also include exact zeros for some of the components. The problem is important in nutritional epidemiology for estimating long-term intakes of...
episodically consumed dietary components. We developed a novel copula based deconvolution approach that focuses on the marginals first and then models the dependence among the components to build the joint densities, allowing us to adopt different modeling strategies for different marginal distributions which proved crucial in accommodating important features of our motivating datasets. In contrast to previous approaches of modeling episodically consumed dietary components, our novel Bayesian hierarchical modeling framework allows us to model the distributions of interest more directly, resulting in vast improvements in empirical performances while also providing estimates of quantities of secondary interest, including probabilities of reporting nonconsumptions, measurement errors' conditional variability, etc.

4.2. Other Potential Applications

Applications of the multivariate deconvolution approach developed here are not limited to zero-inflated data only but also naturally include data with strictly continuous recalls, as was shown in the simulations. Advanced multivariate deconvolution methods are also needed to correct for measurement errors in regression settings when multiple error contaminated predictors are needed to be included in the model.

4.3. Methodological Extensions

Other methodological extensions and subjects of ongoing research include inclusion of associated exactly measured covariates like age, sex, etc. that can potentially influence the consumption patterns, establishing theoretical convergence guarantees for the posterior, accommodation of dietary components which, unlike regular or episodic components, are never consumed by a percentage of the population, accommodation of subject specific survey weights, exploration of non-Gaussian copula classes, inclusion of additional information provided by food frequency questionnaires, etc.

4.4. HEI Index

Aside being of independent interest, episodic dietary components also contribute to the Healthy Eating Index (HEI, https://www.cnpp.usda.gov/healthyeatingindex), a performance measure developed by the US Department of Agriculture (USDA) to assess and promote healthy diets (Guenther, Reedy, and Krebs-Smith 2008; Krebs-Smith et al. 2018). The index is based on 13 energy adjusted dietary components, as many as 8 of which are episodic, and is currently calculated using the NCI method discussed in Section S.4 in the supplementary materials. The methodology developed in this article provides a much more sophisticated framework for modeling the HEI index and makes up an important component of our ongoing research.

Supplementary Materials

The supplementary materials present a brief review of copula and explicit formula of quadratic B-splines for easy reference. The supplementary materials also provide a detailed comparison of our method with previous approaches to zero-inflated data and numerical experiments comparing it with its main competitor. The supplementary materials additionally detail the choice of hyper-parameters and the MCMC algorithm used to sample from the posterior, presents some additional figures, and the results of some additional numerical experiments. R programs implementing the deconvolution methods developed in this article are included in the supplementary materials. The EATS data analyzed in Section 3 can be accessed from National Cancer Institute by arranging a Material Transfer Agreement. A simulated dataset, simulated according to one of the designs described in Section S.6 in the supplementary material, and a “readme” file providing additional details are also included in the supplementary material.

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