XPCA: Extending PCA for a Combination of Discrete and Continuous Variables

Clifford Anderson-Bergman∗
Lawrence Livermore National Laboratory
7000 East Avenue
Livermore, CA 94551-0808, USA

Tamara G. Kolda
Sandia National Laboratories
7011 East Avenue
Livermore, CA 94551-0969, USA

Abstract
Principal component analysis (PCA) is arguably the most popular tool in multivariate exploratory data analysis. In this paper, we consider the question of how to handle heterogeneous variables that include continuous, binary, and ordinal. In the probabilistic interpretation of low-rank PCA, the data has a normal multivariate distribution and, therefore, normal marginal distributions for each column. If some marginals are continuous but not normal, the semiparametric copula-based principal component analysis (COCA) method is an alternative to PCA that combines a Gaussian copula with nonparametric marginals. If some marginals are discrete or semi-continuous, we propose a new extended PCA (XPCA) method that also uses a Gaussian copula and nonparametric marginals and accounts for discrete variables in the likelihood calculation by integrating over appropriate intervals. Like PCA, the factors produced by XPCA can be used to find latent structure in data, build predictive models, and perform dimensionality reduction. We present the new model, its induced likelihood function, and a fitting algorithm which can be applied in the presence of missing data. We demonstrate how to use XPCA to produce an estimated full conditional distribution for each data point, and use this to produce to provide estimates for missing data that are automatically range respecting. We compare the methods as applied to simulated and real-world data sets that have a mixture of discrete and continuous variables.

Keywords: principal component analysis (PCA), copula component analysis (COCA), matrix completion, heterogeneous data, matrix decomposition

1. Introduction
Principal component analysis (PCA) is arguably the most popular tool in multivariate exploratory data analysis. It can be used to find latent structure in data, build predictive models, perform dimensionality reduction, and more (Jolliffe, 2002; Abdi and Williams, 2010). Given an \( m \times n \) data matrix \( X \), representing \( n \) variables for each of \( m \) objects, one use of PCA is to compute a low-rank approximation of the form \( X \approx UV^\top \). Here, \( U \) of size \( m \times k \)
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is the matrix of factor scores or loadings, $V$ of size $n \times k$ is the orthogonal matrix of principal components, and $k \ll m, n$. In this paper, we consider the question of how to handle variables that are not continuous. Specifically, we are interested in binary and discrete ordinal variables which have discontinuous cumulative distribution functions (CDFs).

To tackle this problem, we appeal to the probabilistic interpretation of PCA per Tipping and Bishop (1999) so that we can interpret the $U$ and $V$ matrices in PCA as maximum likelihood estimators (MLEs). In this interpretation, the data has a normal multivariate distribution, which implies normal marginal distributions for each column. We describe this approach in Section 2.2.

Given that PCA can be viewed as a maximum likelihood estimator under the assumption of multivariate normality, several proposals have been made to account for deviations from this assumption. Collins et al. (2002) assume the entries of a data matrix follow a distribution for the exponential family, and that the natural parameters can be estimated using low-rank matrix factorizations. Udell et al. (2016) expand this idea to allow separate distributions for each column of the data, leading to column-specific loss functions that are scaled to balance their contributions to the overall loss. Similarly, factor analysis methods model non-Gaussian random variables through the use of generalized linear latent variable models (GLLVMs) as covered in depth in Bartholomew et al. (2011). The methods we present differ from these in that there is no need to declare parametric distributions for each column of data.

Other non-likelihood based methods have been adopted for non-Gaussian data. For binary and categorical data, multiple correspondence analysis (MCA) is a very popular method. An excellent review can be found in Abdi and Valentin (2007). In short, MCA expands categorical variables into binary variables, preprocess the data and then performs PCA. Similarly, Optimal Scaling, as presented in Young (1981), is an iterative method for ordinal, categorical or interval data, in which the values are replaced with ordered values that optimize the variance explained. An excellent review can be found in Meulman et al. (2004). While commonly used, these methods lack an underlying statistical model. Recent work in Groenen and Josse (2016) has proposed a statistical model for an alternative to MCA by proposing a new estimator. In contrast, Tipping and Bishop (1999) provided were able to develop a probabilistic model that justified the already established PCA estimator. In this work, we will focus on likelihood-based methods in the framework established by Tipping and Bishop (1999).

In the case that the marginals are continuous but not normal (e.g., heavily skewed), we can appeal to the theory of copulas (Sklar, 1973; Nelsen, 2006) to separate the marginal distributions and their interactions. We describe copulas in more detail in Section 2.3. Han and Liu (2012) propose a semiparametric copula-based principal component analysis (COCA) that separates the estimation of the variable interactions and their marginals. Specifically, the interactions are still assumed to be multivariate normal so that PCA can be used on the copula, but the marginals can be any continuous distribution. COCA is asymptotically equivalent to PCA when the marginals are normal. The general idea of using semiparametric copulas can be found in Genest et al. (1995) in the sense that the marginal distributions are nonparametric and the copulas are parametric. Egger et al. (2016) show the power of COCA in the context of image analysis. COCA is ingenious in its separation of the marginals from the interactions so that PCA can be applied, but
it depends on a translation of each variable using its empirical distribution function. We review empirical distribution functions in Section 2.4. and COCA in Section 2.5. This transformation is well-behaved for continuous data but not for discrete (Hoff, 2007).

In Section 3, we present a new method we call extended PCA (XPCA) for the scenario in which one or more variables is discrete (or even semi-continuous). Like COCA, we use a Gaussian copula and nonparametric marginals. The difference is that we integrate over appropriate intervals in the likelihood to account for discrete variables and correctly compute the MLE.\(^1\) XPCA is asymptotically equivalent to COCA for continuous variables but handles discrete variables in a more appropriate manner and yields improved performance on real-world analysis tasks. PCA, COCA, and XPCA are similar in that they all assume a Gaussian copula. The difference is in the assumptions on the marginals, as illustrated in Fig. 1. PCA expects normal marginals, COCA expects continuous marginals, and XPCA can handle general marginals including semi-continuous and discrete.

We present methods for computing the XPCA model and also for inferring estimated values from it in Section 4. We demonstrate how one can derive a complete conditional distribution for every entry of the data matrix as well as a more computationally efficient method for estimating expected values. These distributions can be used to identify outliers, and the expected values can be used to fill in missing values. For binary variables, for example, the XPCA model can be used to generate the conditional probabilities for 0 and 1. In contrast, COCA would simply return a 0 or 1 with no extra information, and the value produced by PCA is hard to interpret because it could, for example, be negative or greater than 1.

In Section 5, we demonstrate the effectiveness of XPCA on both simulated and real data sets, showing significant improvements as compared to PCA and COCA. We first compare the methods on simulated data from different distributions, showing how PCA or COCA may struggle when the assumptions are violated. Then, we consider voting data from 18 years of the U.S. Senate data, covering 271 senators and 9044 votes, with 63% missing data because not all senators were in office for all votes. We show how XPCA can be used to estimate how likely a particular vote might be. We consider NBA player statistics and show

\(^1\) The idea of integrating over an interval in the context of discrete variables is used, e.g., in probit ordinal regression (Wooldridge, 2002, Chapter 15.10).
that it does a better job at estimating missing entries than the other methods, captures
relations between discrete variables missed by PCA and COCA, and present estimated
distributions of data entries conditional on the fitted model.

Our contributions may be summarized as follows:

• We propose the XPCA method, an extension to PCA/COCA that accounts for both
  continuous and discrete variables.
• We develop an algorithm to fit the XPCA model to datasets, even in the context of
  incomplete data.
• We show how the XPCA method can be used to derive a probability distribution for
  every entry of the data matrix. These distributions can in turn be used to identify
  outliers and infer missing values.
• We demonstration the benefits of XPCA on simulated and real data sets, showing
  improvements as compared to both PCA and COCA.

2. Background & Related Work

2.1 Notation

We let \( \mathbb{R} \) denote the set of real values and \( \mathbb{R}_+ = (0, +\infty) \) denote the set of strictly positive
real values. We let \( \mathbb{R}^n \) denote the set of vectors of length \( n \) and \( \mathbb{R}^{m\times n} \) denote the set of
matrices of size \( m \times n \).

We denote scalars as lowercase letters, vectors as boldface lowercase letters, and matrices
as boldface uppercase letters. The \( j \)th entry of a vector \( x \) is denoted by \( x_j \). The \((i, j)\) entry
of a matrix \( X \) is denoted as \( x_{ij} \). We use the convention that the \( i \)th row of an \( m \times n \) matrix
\( X \) is denoted as \( x_i \) and oriented as an \( 1 \times n \) object. We let \( I \) denote the identity matrix
whose size is determined by context. We use the convention \( X \succ 0 \) to denote the fact that
\( X \) is symmetric positive definite. We write \( x \leq y \) if \( x_j \leq y_j \) for all \( j \). We denote estimates
with hats; e.g., \( \hat{X} \) denotes an estimator of \( X \).

Because we are using boldface, lowercase, and uppercase letters already to distinguish
between scalars, vectors, and matrices, we instead use color to distinguish between random
variables and their realizations. Hence, if \( x \) is a random variable, then \( x \) is its realization.
We may write, for instance, \( P(x \leq x) \).

Throughout, we assume we are given a data matrix \( X \) of size \( m \times n \) which is a realization
of some multivariate random variable \( X \). The \( m \) rows correspond to objects and the \( n \)
columns correspond to variables. The data matrix \( X \) may have missing entries because not
every variable is observed for every object; therefore, we provide some notation to specify
this. We let \( \Omega_j \) denote the set of indices of known values in column \( j \) so that \((i, j) \in \Omega_j \)
if and only if \( x_{ij} \) is observed. We let \( m_j \) denote the number of known entries in column \( j \), i.e., \( m_j = |\Omega_j| \leq m \). We define \( \Omega = \bigcup_{j=1}^n \Omega_j \) to be the set of indices of all known entries.

We denote the univariate normal distribution with mean \( \mu \in \mathbb{R} \) and variance \( \sigma^2 \in \mathbb{R}_+ \)
as \( \mathcal{N}(\mu, \sigma^2) \). Its probability density function (PDF) is

\[
f(x|\mu, \sigma^2) = \frac{e^{(x-\mu)^2/2\sigma^2}}{\sqrt{2\pi}\sigma^2}.
\]
Since the distribution is continuous, the likelihood of $\mu$ and $\sigma^2$ for a given observation $x$ is simply the PDF, i.e.,
\[ L(\mu, \sigma^2|x) = f(x|\mu, \sigma^2). \]

We denote the multivariate normal distribution with mean $\mu \in \mathbb{R}^n$ and covariance $\Sigma \in \mathbb{R}^{n \times n}$ with $\Sigma > 0$ as $\mathcal{N}_n(\mu, \Sigma)$. Its joint probability density function is
\[ f(x|\mu, \Sigma) = \frac{\det(2\pi \Sigma)^{-1/2} \exp \left( -\frac{1}{2}(x - \mu)^\top \Sigma^{-1}(x - \mu) \right)}{\sqrt{(2\pi)^n \det(\Sigma)}}. \]

(2)

The likelihood of $\mu$ and $\Sigma$ for a given observation $x$ is again simply the PDF, i.e.,
\[ L(\mu, \Sigma|x) = f(x|\mu, \Sigma). \]

If $\Sigma = \sigma^2 I$, then the variables are independent and the likelihood reduces to
\[ L(\mu, \Sigma|x) = \prod_{j=1}^{n} f(x_j|\mu_j, \sigma^2). \]

We slightly abuse notation and write $X \sim \mathcal{N}_{m \times n}(\Theta, \sigma^2 I)$ to denote $x_{ij} \sim \mathcal{N}(\theta_{ij}, \sigma^2)$ for all $i = 1, \ldots, m$ and $j = 1, \ldots, n$.

Let $\phi: \mathbb{R} \to \mathbb{R}_+$ and $\Phi: \mathbb{R} \to (0,1)$ denote the probability density and cumulative distribution functions, respectively, for the univariate standard normal, i.e.,
\[ \phi(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}} \quad \text{and} \quad \Phi(x) = \int_{-\infty}^{x} \phi(t)dt. \]

(3)

We also use the inverse CDF: $\Phi^{-1} : [0,1] \to \mathbb{R} \cup \{-\infty, +\infty\}$. Writing things in terms of $\Phi$ and $\Phi^{-1}$ is convenient for implementations since routines exist to evaluate these quantities.

2.2 PCA

PCA is a standard technique for data analysis; see, e.g., Jolliffe (2002) and Abdi and Williams (2010). Tipping and Bishop (1999) provide a probabilistic interpretation that is more conducive to the low-rank matrix factorization viewpoint and is our focus here.

We assume that we are given $m$ objects, each with $n$ variables. Statistically, we represent this as a random variable $X \in \mathbb{R}^{m \times n}$. We standardize each column to define the random variable $Z$, i.e.,
\[ z_{ij} = \frac{x_{ij} - \hat{\mu}_j}{\hat{\sigma}_j}, \]

(4)

where $\hat{\mu}_j$ and $\hat{\sigma}_j$ are the estimated marginal mean and standard deviation, respectively, for the random variables in the $j$th column of $X$. This is equivalent to using the correlation matrix instead of the covariance matrix, which is generally recommended, as in Jolliffe (2002). As the notation suggests, $z_{ij}$ corresponds to the $z$-score of $x_{ij}$, i.e., the number of standard deviations that $x_{ij}$ is from its mean $\mu_j$.

In probabilistic PCA, Tipping and Bishop (1999) assume $Z$ is such that each row $z \in \mathbb{R}^{1 \times n}$ is distributed as
\[ z|u \sim \mathcal{N}_n(uV^T, \sigma^2 I) \quad \text{with} \quad V \in \mathbb{R}^{n \times k}, u \sim \mathcal{N}_k(0, I). \]

(5)
Here, \( V \) is the matrix of principal components, i.e., combinations of variables that together describe some aspect of the data and thus contribute to the correlations. We have a dependence on the random variable \( u \), which specifies the combination of the principal components. Finally, the \( \sigma^2 \) captures the variance not described by the combination of principal components.\(^2\) Tipping and Bishop (1999) show that we can integrate out the \( u \) in Eq. (5) to derive

\[
\mathbf{z} \sim \mathcal{N}_{m}(\mathbf{0}, \mathbf{\Sigma}) \quad \text{where} \quad \mathbf{\Sigma} = \mathbf{VV}^\top + \sigma^2 \mathbf{I}.
\] (6)

Then it is possible to work with \( \mathbf{Z}'\mathbf{Z} \) to obtain estimates \( \hat{\mathbf{V}} \) and \( \hat{\sigma} \). One difference between standard and probabilistic PCA is that the \( \mathbf{VV}^\top \) matrix is low rank \((k < n)\). If \( \mathbf{VV}^\top \) is full rank, then the variance term \( \sigma^2 \) is redundant and can set to zero.

We take a slightly different tact in our approach, returning to Eq. (5) and expressing it in matrix form as

\[
\mathbf{Z}|\mathbf{U} \sim \mathcal{N}_{m \times n}(\mathbf{UV}^\top, \sigma^2 \mathbf{I}) \quad \text{where} \quad \mathbf{U} \sim \mathcal{N}_{m \times k}(\mathbf{0}, \mathbf{I}).
\] (7)

Conditional on \( \mathbf{U} \), if we define \( \mathbf{\Theta} = \mathbf{UV}^\top \), then each entry of \( \mathbf{Z} \) is independent with constant variance, i.e.,

\[
z_{ij} \sim \mathcal{N}(\theta_{ij}, \sigma^2).
\]

From Eq. (1), we can write the negative log-likelihood of the entire set of observations as

\[
\text{NLL}(\mathbf{\Theta}, \sigma|\mathbf{Z}) = \sum_{(i,j) \in \Omega} \left( \frac{(z_{ij} - \theta_{ij})^2}{2\sigma^2} + \log(\sigma) \right) + c
\] (8)

where \( c \) is a constant term. We can minimize this to find the MLEs for \( \mathbf{U} \) and \( \mathbf{V} \). The optimal values of \( \mathbf{U} \) and \( \mathbf{V} \) are equivalent for all values of \( \sigma > 0 \), so \( \sigma \) can be ignored while finding \( \hat{\mathbf{U}} \) and \( \hat{\mathbf{V}} \). As such, the MLEs of \( \mathbf{U} \) and \( \mathbf{V} \) can be obtained by minimizing the standard sum of squared errors:

\[
\text{SSE}(\mathbf{\Theta}|\mathbf{Z}) = \sum_{(i,j) \in \Omega} (z_{ij} - \theta_{ij})^2.
\] (9)

Using \( \hat{\mathbf{\Theta}} = \hat{\mathbf{U}}\hat{\mathbf{V}}^\top \), then the MLE estimate of \( \sigma \) is

\[
\hat{\sigma} = \sqrt{\frac{\sum_{(i,j) \in \Omega} (z_{ij} - \hat{\theta}_{ij})^2}{|\Omega|}}.
\]

A few caveats are in order. We typically assume that \( \mathbf{V} \) is orthogonal (Abdi and Williams, 2010). If the results of the optimization are not orthogonal, then we can adjust by using the SVD factorization as follows:

\[
\hat{\mathbf{U}}\hat{\mathbf{\Sigma}}\hat{\mathbf{V}}^\top = \text{svd}(\hat{\mathbf{U}}\hat{\mathbf{V}}^\top) \quad \Rightarrow \quad \hat{\mathbf{U}} \leftarrow \hat{\mathbf{U}}\hat{\mathbf{\Sigma}}, \hat{\mathbf{V}} \leftarrow \hat{\mathbf{\Sigma}}\hat{\mathbf{V}}.
\] (10)

If there are no missing entries, then we can use the SVD to compute the best rank-\( k \) factorization of \( \mathbf{X} \) as follows: Set \( \hat{\mathbf{U}} \) to be the \( k \) leading left singular values of \( \mathbf{X} \) multiplied

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\(^2\) Tipping and Bishop (1999) allow for nonzero marginal means, but we assume they are all zero thanks to the standardization.
by the $k$ corresponding singular values, and set $\hat{\mathbf{V}}$ to be the $k$ leading right singular values. If some data is missing, then we need to apply optimization directly to Eq. (9). The PCA method is given in Algorithm 1. We can use the results of the PCA to infer values as shown in Algorithm 2, and these estimates can be used to for cross-validation, estimating missing values, or detecting outliers.

**Algorithm 1 PCA**

Let $\mathbf{X}$ be a data matrix of size $m \times n$ and $\Omega_j \subseteq \{1, \ldots, m\}$ the known entries in column $j$.

1. **for** $j = 1, \ldots, n$ **do**
2. $m_j \leftarrow |\Omega_j|$  \hspace{1cm} \triangleright \text{Number of known entries in column } j$
3. $\hat{\mu}_j \leftarrow \frac{1}{m_j} \sum_{j \in \Omega_j} x_{ij}$  \hspace{1cm} \triangleright \text{Compute marginal mean}$
4. $\hat{\upsilon}_j \leftarrow \sqrt{\frac{1}{m_j} \sum_{j \in \Omega_j} (x_{ij} - \hat{\mu}_j)^2}$  \hspace{1cm} \triangleright \text{Compute marginal standard deviation}$
5. **end for**
6. $\Omega \leftarrow \{(i, j) \mid i \in \Omega_j, j \in \{1, \ldots, n\}\}$  \hspace{1cm} \triangleright \text{Set of all known entries}$
7. **for** $(i, j) \in \Omega$ **do**
8. $z_{ij} \leftarrow (x_{ij} - \hat{\mu}_j)/\hat{\upsilon}_j$  \hspace{1cm} \triangleright \text{Standardize each column; Eq. (4)}$
9. **end for**
10. $(\hat{\mathbf{U}}, \hat{\mathbf{V}}) \leftarrow \arg \min_{\Theta} \sum_{(i, j) \in \Omega} (z_{ij} - \theta_{ij})^2 \text{ subject to } \Theta = \mathbf{U}\mathbf{V}^\top$  \hspace{1cm} \triangleright \text{MLE; see Eq. (9)}$
11. \text{If necessary, adjust } (\hat{\mathbf{U}}, \hat{\mathbf{V}}) \text{ so that } \hat{\mathbf{V}} \text{ is orthogonal} \text{ \triangleright \text{See Eq. (10)}}$

**Algorithm 2 PCA Impute**

Let $\mathcal{S}$ denote the subset of entries to be imputed, and let $\hat{\mathbf{U}}, \hat{\mathbf{V}}$ be the PCA factors.

1. **for** $(i, j) \in \mathcal{S}$ **do**
2. $\hat{\theta}_{ij} \leftarrow \sum_{k=1}^{k} \hat{u}_{i\ell} \hat{v}_{j\ell}$  \hspace{1cm} \triangleright \text{Calculate single entry of } \hat{\Theta} = \hat{\mathbf{U}}\hat{\mathbf{V}}^\top$
3. $\hat{x}_{ij} \leftarrow \hat{\theta}_{ij} \hat{v}_{j} + \hat{\mu}_j$  \hspace{1cm} \triangleright \text{Return to original scale}$
4. **end for**

2.3 Copulas

Any $n$-dimensional distribution can be expressed as a composite object: the marginal one-dimensional distribution for each of the $n$ variables and an $n$-dimensional copula, i.e., an $n$-dimensional distribution whose marginals are uniform on $[0, 1]$ (Nelsen, 2006). In this way, the marginals and their interactions can be handled separately. Specifically, Sklar’s famous result (Sklar, 1973) says that any multivariate CDF $F$ can be expressed in terms of a copula $C$ as

$$F(x) = C(y) \quad \text{where} \quad y_j = F_j(x_j) \text{ for } j = 1, \ldots, n.$$ 

Here $F_j$ represents the continuous marginal distribution of the $j$th variate. The advantage of the copula model is that this breaks up the model into two parts: the marginal distributions given by $F_j$ and the relationships between the relative percentiles given by $C$. 
There are many types of copulas. We are interested specifically in the case that $C$ is a Gaussian copula, which means

$$C(y) = \int_{-\infty}^{z} f(t \mid \mu, \Sigma) \, dt \quad \text{where} \quad z_j = \Phi^{-1}(y_j) \text{ for } j = 1, \ldots, n,$$

(11)

where $f$ is the multivariate normal PDF defined in Eq. (2). Since each $y_j$ is a standard uniform random variable, it must be the case that $z \sim \mathcal{N}(\mu, \Sigma)$.

We can consider PCA from a copula viewpoint. We are given a data matrix $X$ of size $m \times n$. We assume the marginals are Gaussian and map these to uniform marginals via the transformation:

$$y_{ij} = \Phi \left( \frac{x_{ij} - \mu_j}{v_j} \right),$$

where $\mu_j$ and $v_j$ are the mean and standard deviation of the $j$th marginal. We assume a Gaussian copula, which means that

$$Z \sim \mathcal{N}(\Theta, \Sigma^2 I) \quad \text{with} \quad z_{ij} = \Phi^{-1}(y_{ij}).$$

We note that this shows that the standard practice of normalizing each column can be seen as performing PCA with a Gaussian copula and Gaussian marginals. Of course, the $y_{ij}$ is not explicit in PCA which is why the copula interpretation may not be immediately obvious. It is worth noting that there are many other choices of copulas other than the multivariate Gaussian (see, e.g., Embrechts et al. (2001)). In general it is not straightforward how one should pick a given copula model, as discussed in Embrechts (2009). The Gaussian copula has been selected for two reasons: computational simplicity and to closer match the assumption of a probabilistic PCA model.

We subsequently describe COCA and our new XPCA, both of which also consider Gaussian copulas but have different assumptions about the marginals.

### 2.4 Empirical Distribution Function

To estimate the marginal distribution, we use the nonparametric empirical distribution function (EDF). Since we are factorizing a matrix $X$ of size $m \times n$ where each column has its own distribution, we explain the EDF in that context.

For column $j$, we assume the random variables $x_{ij}$ are drawn from an unknown distribution whose marginal CDF is $F_j : \mathbb{R} \to [0, 1]$. Note that this requires that the data be ordered (as opposed to categorical), so continuous, semi-continuous, and discrete values are allowed.

Because some of data is discrete or semi-continuous, we are likely to have repeated observations. Hence, we develop some machinery to cope with that. Let the set of distinct entries in column $j$ be

$$C_j = \{ x_{ij} \mid (i, j) \in \Omega_j \}.$$

(12)

If some values in the column are repeated, then $|C_j| < m_j$, where $m_j \leq m$ is the total number of entries (including repeats but not including missing entries) in column $j$.

We present two common methods for defining the EDF, both of which are relevant for our analysis and comparison of the methods. The first and more common way to define the
EDF is denoted here by $\hat{F}_j$ and is given by

$$\hat{F}_j(x) = \max \left\{ \frac{r_j(s)}{m_j} \mid s \leq x \text{ and } s \in C_j \right\},$$

where $r_j(s) \in \{1, ..., m_j\}$ is the rank of $s$ relative to the data in column $j$, and the maximum is used in the case of ties. If $x \leq s$ for all $s \in C_j$, then $\hat{F}_j(x) = 0$. Then the inverse is given by

$$\hat{F}_j^{-1}(y) = \begin{cases} 
\min \left\{ s \in C_j \mid \hat{F}_j(s) \leq y \right\} & \text{if } y \leq \min \left\{ \hat{F}_j(s) \mid s \in C_j \right\}, \\
\max \left\{ s \in C_j \mid \hat{F}_j(s) \leq y \right\} & \text{otherwise.}
\end{cases}$$

(14)

Observe $\hat{F}_j^{-1}: [0, 1] \to C_j$. The second way to define the EDF, which we will use for COCA, is denoted here as $\tilde{F}_j$ and is given by

$$\tilde{F}_j(x) = \max \left\{ \frac{\tilde{r}_j(s)}{m_j + 1} \mid s \leq x \text{ and } s \in C_j \right\},$$

(15)

where $\tilde{r}_j(s) \in \{1, ..., m_j\}$ is the rank of $s$ relative to the data in column $j$, and the midpoint is used in the case of ties. As with $\hat{F}$, if $x \leq s$ for all $s \in C_j$, then $\tilde{F}_j(x) = 0$. Likewise, we let $\tilde{F}_j^{-1}: [0, 1] \to C_j$ be defined analogously, replacing $\hat{F}_j$ with $\tilde{F}_j$. In both cases, the inverse maps to the set of observed values, $C_j$.

There are two differences between $\hat{F}_j$ and $\tilde{F}_j$. The first difference is the denominator: $m_j$ versus $m_j + 1$. This modification is not so unusual and can be found, for instance, in Coles et al. (2001, p. 36, Definition 2.4). Using $m_j + 1$ ensures that $\tilde{F}(x) \in (0, 1)$ for all $x \in C_j$, which is critical for COCA for reasons we explain in Section 2.5. The second difference is using the maximum versus the midpoint for breaking ties. This is an ad hoc way for COCA to handle discrete variables since, in our experiments, mapping to the midpoint yielded better results than mapping to the maximum (see Appendix B).

For continuous distributions, both $\hat{F}_j$ and $\tilde{F}_j$ are consistent nonparametric estimators of $F_j$. For discrete variables, only $\hat{F}_j$ is a consistent estimator of $F_j$. A comparison of the two definitions of the EDF is shown in Fig. 2. In the continuous case, there is little visual difference between the two definitions. In the discrete case, however, there are two major differences. First, $\tilde{F}$ never gets to 1. Second, the use of the midpoint impacts the y-values for $\tilde{F}$.

### 2.5 COCA

In PCA as described in Section 2.2, one assumption of the method is that the marginals are assumed to be normal. Han and Liu (2012) proposed COCA, a semiparametric version of PCA, to relax this assumption. The idea is to still use a parametric Gaussian copula, as in PCA, but to use nonparametric EDFs for the marginals. So, assume we are given a data matrix $X$ of size $m \times n$. We create variables with uniform marginal distribution via the transformation:

$$y_{ij} = F_j(x_{ij}),$$

where $F_j$ is the $j$th marginal EDF. As with PCA, we assume a Gaussian copula, which means that

$$Z \sim \mathcal{N}(\Theta, \sigma^2 I) \quad \text{with} \quad z_{ij} = \Phi^{-1}(y_{ij}).$$
Egger et al. (2016) applied COCA in the context of face modeling. They observed that the color intensity distributions in images were not normally distributed but rather bimodal. They compared COCA and PCA on image processing applications.

We use the version of COCA from Egger et al. (2016) in the remainder of our discussion. The procedure is given in Algorithm 3. In Line 5, it is vital that $\tilde{F}_j$ be used because it avoids an infinite $z_{ij}$ value in Line 6. If we used $\hat{F}_j$ instead, those lines would produce

$$y_{ij} = \hat{F}_j(\max_i x_{ij}) = 1 \Rightarrow \Phi^{-1}(y_{ij}) = \infty.$$ 

As such, using $\hat{F}_j$ would result in infinite values in $Z$, which would make factorizing it impossible. Genest et al. (1995) makes the observation that “this rescaling avoids difficulties arising from . . . potential unboundedness.”

The $\Theta$ estimates are then pushed through the corresponding $\tilde{F}^{-1}_j$’s to provide point estimates $\hat{x}_{ij}$, as given in Algorithm 4. In contrast to PCA, every estimate $\hat{x}_{ij}$ must be an observed value from column $j$, i.e., $\hat{x}_{ij} \in C_j$. The benefit is that we can never, for instance, estimate a negative value when there have only been nonnegative observations.
Algorithm 3 COCA
Let $X$ be a data matrix of size $m \times n$ and $\Omega_j \subseteq \{1, \ldots, m\}$ the known entries in column $j$.

1: for $j = 1, \ldots, n$ do
2: $\tilde{F}_j \leftarrow$ EDF for column $j$ per Eq. (15) $\triangleright$ Compute marginal distributions
3: end for
4: for $(i,j) \in \Omega$ do
5: $y_{ij} \leftarrow \tilde{F}_j(x_{ij})$ $\triangleright$ Transform original marginals to standard uniform
6: $z_{ij} \leftarrow \Phi^{-1}(y_{ij})$ $\triangleright$ Transform standard uniform marginals to Gaussian
7: end for
8: $(\hat{U}, \hat{V}) \leftarrow \text{argmin of Eq. (9) subject to } \Theta = UV^\top$ $\triangleright$ See Eq. (10)
9: If necessary, adjust $(\hat{U}, \hat{V})$ so that $\hat{V}$ is orthogonal

Algorithm 4 COCA Impute
Let $S$ denote the subset of entries to be estimated.

1: for $(i,j) \in S$ do
2: $\hat{\theta}_{ij} \leftarrow \sum_{\ell=1}^k \hat{u}_{i\ell} \hat{v}_{j\ell}$ $\triangleright$ Calculate single entry of $\hat{\Theta} = \hat{U}\hat{V}^\top$
3: $\hat{y}_{ij} \leftarrow \Phi(\hat{\theta}_{ij})$ $\triangleright$ Transform standard normal to standard uniform
4: $\hat{x}_{ij} \leftarrow \tilde{F}_j^{-1}(\hat{y}_{ij})$ $\triangleright$ Transform standard uniform to original distribution
5: end for

3. XPCA
We present our new method, XPCA, an extension to PCA and COCA that handles discrete variables. We present the generative model, the induced likelihood function, and two optimization approaches to find the maximum likelihood estimates.

3.1 Model
Similar to COCA, we assume a Gaussian copula model that follows a PCA generative model. In other words, we assume there is a latent variable $Z$ such that

$$Z \sim \mathcal{N}(\Theta, \sigma^2I)$$

where $\Theta$ is a low-rank matrix. The values of $Z$ are not observed exactly but rather through the transformations

$$y_{ij} = \Phi(z_{ij}) \quad \text{and} \quad x_{ij} = F_j^{-1}(y_{ij}).$$

While we assume that $Z$ comes from a multivariate Gaussian PCA model, we make no assumptions about the form of $F_j$ other than that it is a proper CDF. The key difference between XPCA and COCA is that COCA implicitly assumes that $F_j$ corresponds to a continuous random variable and so is itself continuous. In contrast, XPCA allows for jump discontinuities in $F_j$, as discussed in the next subsection.

3.2 Likelihood
We are interested in the case when $F_j$ is the CDF of a discrete random variable. In such cases, $F_j$ is not a 1-to-1 function and indeed a range of values of $z_{ij}$ (and of the corresponding
\( F(3) \)

(Figure 3: Illustrating how discrete \( x_{ij} \) values map to ranges of \( z_{ij} \) values. The value of \( x_{ij} = 3 \) is explicitly shown.)

- The value of \( y_{ij} \) will all lead to the same \( x_{ij} \). In these cases, Hoff (2007) and Li et al. (2016) suggest that we can still use standard copulas, such as the Gaussian copula, to model joint distributions of discrete random variables, but the likelihood must be computed over a range of \( y_{ij} \) values to achieve consistent estimation. Hoff (2007) was interested in examining correlation coefficients for ordinal data with a Gaussian copula, but the general principle of that work can be applied in our context as well.

- Leveraging these ideas, we can see that if the interval \((\ell_{ij}, r_{ij}]\) is the range of values of \( z_{ij} \) such that \( x_{ij} = x_{ij} \) is observed, then

\[
P(x_{ij} = x_{ij}) = \int_{\ell_{ij}}^{r_{ij}} f(t|\theta_{ij}, \sigma^2) dt = \Phi\left(\frac{r_{ij} - \theta_{ij}}{\sigma}\right) - \Phi\left(\frac{\ell_{ij} - \theta_{ij}}{\sigma}\right),
\]

where \( f \) is the PDF of a normal distribution from Eq. (1). The range of \( z_{ij} \) values corresponding to a given \( x_{ij} \) is given by \( [\Phi^{-1}(F_j(x_{ij} - \epsilon))], \Phi^{-1}(F_j(x_{ij})) \) for sufficiently small \( \epsilon \). This is illustrated in Fig. 3. Hence, the negative log-likelihood with respect to discrete random variables can be written as

\[
\text{NLL}(\Theta, \sigma, F | X) = \sum_{(i,j) \in \Omega} - \log \left[ \Phi\left(\frac{r_{ij} - \theta_{ij}}{\sigma}\right) - \Phi\left(\frac{\ell_{ij} - \theta_{ij}}{\sigma}\right) \right]
\]

where

\[
\ell_{ij} = \Phi^{-1}(F_j(x_{ij} - \epsilon)) \quad \text{and} \quad r_{ij} = \Phi^{-1}(F_j(x_{ij})).
\]

In practice, we set \( \epsilon \) to be half the distance between the closest two distinct points in any column, i.e.,

\[
\epsilon = \frac{1}{2} \min \{ \xi - \xi' \mid \xi, \xi' \in C_j, \xi > \xi', j = 1, \ldots, n \}.
\]

We observe that asymptotically, the XPCA likelihood reduces to the COCA likelihood plus a constant if all the variables are continuous. If \( F_j \) has jump discontinuities (e.g., because it corresponds to a discrete variable), then \( \ell_{ij} \neq r_{ij} \) as \( \epsilon \downarrow 0 \). However, if \( F_j \) is
continuous (because it corresponds to a continuous variable), then \( \ell_{ij} \to r_{ij} \) as \( \epsilon \downarrow 0 \) and so we see an asymptotic equivalence to COCA because

\[
\lim_{\ell_{ij} \to r_{ij}} \frac{\Phi \left( \frac{r_{ij} - \theta_{ij}}{\sigma} \right) - \Phi \left( \frac{\ell_{ij} - \theta_{ij}}{\sigma} \right)}{(r_{ij} - \ell_{ij})} = f(r_{ij}|\theta_{ij}, \sigma^2).
\]

Hence, if \( F_j \) corresponds to a continuous random variable, the contribution to the negative log-likelihood will be asymptotically equivalent, excepting the additive term \( c_{ij} = \log(r_{ij} - \ell_{ij}) \). The \( c_{ij} \) has no dependence on the parameters \( U, V, \sigma \) and so is irrelevant for the maximum likelihood estimate. As such, the XPCA solution will approach the COCA solution if all the data is continuous as we demonstrate on simulated data in Section 5.1.

A comparison of the different methods is shown in Fig. 4.

| Transformation | PCA | COCA | XPCA |
|----------------|-----|------|------|
| z_{ij} = (x_{ij} - \mu_j)/\nu_j | \( z_{ij} = \Phi^{-1}(F_j(x_{ij})) \) | \( z_{ij} = \Phi^{-1}(F_j(x_{ij})) \) | \( z_{ij} = \Phi^{-1}(F_j(x_{ij})) \) |
| Copula | \( Z \sim N(\Theta, \sigma^2 I) \) | \( Z \sim N(\Theta, \sigma^2 I) \) | \( Z \sim N(\Theta, \sigma^2 I) \) |
| Z-value | \( z_{ij} = (x_{ij} - \hat{\mu}_j)/\hat{\nu}_j \) | \( z_{ij} = \Phi^{-1}(\hat{F}_j(x_{ij})) \) | \( z_{ij} \in \left( \Phi^{-1}(\hat{F}_j(x_{ij} - \epsilon)) - \Phi^{-1}(\hat{F}_j(x_{ij})) \right) \) |
| Effective Loss | \( (z_{ij} - \theta_{ij})^2 \) | \( (z_{ij} - \theta_{ij})^2 \) | \(- \log \left[ \Phi \left( \frac{r_{ij} - \theta_{ij}}{\sigma} \right) - \Phi \left( \frac{\ell_{ij} - \theta_{ij}}{\sigma} \right) \right] \) |

Figure 4: Comparison of the underlying statistical models for PCA, COCA, and XPCA. The top line is the assumed data transformation based on the marginal distributions, the second line is the copula (same for all three), the third line is the actual computation of the z-values that should be from a Gaussian distribution, and the last line is the effective loss from the negative log likelihood.

3.3 Fitting the Model

Like COCA, we use the EDFs to estimate \( F_j \). Because the full interval \( [\ell_{ij}, r_{ij}] \) is considered, \( \hat{F}_j \) can be used instead of \( \hat{F}_j \). The parameters \( U, V \) and \( \sigma \) are then estimated using maximum likelihood estimation. With standard PCA, it is not necessary to include \( \sigma \) when solving for \( \hat{U}, \hat{V} \), because the maximum likelihood estimates of \( U \) and \( V \) do not depend on \( \sigma \). For XPCA, this is not the case and \( \sigma \) must estimated concurrently with \( U \) and \( V \).

Similar to most factorization problems, the negative log-likelihood is nonconvex as a function of \( \{U, V, \sigma\} \), but convex as a function of \( U \) conditional on \( \{V, \sigma\} \) and \( V \) conditional on \( \{U, \sigma\} \). This suggests two straightforward optimization approaches:

- All-at-once optimization, i.e., using a quasi-Newton method, or
- Alternating optimization, i.e., block coordinate descent.
Algorithm 5 XPCA

Let $X$ be a data matrix of size $m \times n$ and $\Omega_j \subseteq \{1, \ldots, m\}$ the known entries in column $j$.

1: for $j = 1, \ldots, n$ do
2: \hspace{1em} $\hat{F}_j \leftarrow$ EDF for column $j$ per Eq. (13) \texttt{▷ Compute marginal distributions}
3: end for
4: $\epsilon \leftarrow \frac{1}{2} \min \{\xi - \xi' | \xi, \xi' \in \mathcal{C}_j, \xi > \xi', j = 1, \ldots, n\}$
5: for $(i, j) \in \Omega$ do
6: \hspace{1em} $\ell_{ij} \leftarrow \Phi^{-1}(\hat{F}(x_{ij} - \epsilon))$ \texttt{▷ Lower bound of z-range}
7: \hspace{1em} $r_{ij} \leftarrow \Phi^{-1}(\hat{F}(x_{ij}))$ \texttt{▷ Upper bound of z-range}
8: end for
9: $(\hat{U}, \hat{V}, \hat{\sigma}) \leftarrow \arg\min \sum_{(i,j)\in \Omega} - \log \left[ \Phi \left( \frac{r_{ij} - \theta_{ij}}{\sigma} \right) - \Phi \left( \frac{\ell_{ij} - \theta_{ij}}{\sigma} \right) \right]$ subject to $\Theta = UV^T$
10: If necessary, adjust $(\hat{U}, \hat{V})$ so that $\hat{V}$ is orthogonal $\texttt{▷ See Eq. (10)}$

All-at-once optimization is inviting due to the simplicity of fewer hyperparameters and general speed. For this, we use L-BFGS (Nocedal, 1980; Byrd et al., 1995) as implemented in NLopt (Johnson).

Because we found that L-BFGS would occasionally have line-search failures, we also implemented a block coordinate descent algorithm that was more robust at the cost of longer computation times. Not only is the loss function convex in $U$, but the loss is independent for each row $U$ (and likewise for $V$). Thus, each iteration of our block coordinate descent algorithm updates each row of $U$ and $V$ independently, and these updates use a single step of Newton-Raphson. After $U$ and $V$ have been updated, $\sigma$ is updated. If the second derivative with respect to $\sigma$ is positive, Newton’s method with half-stepping is used to update $\sigma$; otherwise, gradient descent with a line search is used.

These approaches require the gradient and Hessian, whose formulas are given in Appendix A.

3.4 Algorithm

The XPCA method is presented in Algorithm 5. The method computes the EDFs based on the observed data. These functions are used to compute the ranges for possible $z$-values, which corresponds to the integration limits for the loss function. The optimization of the loss function is computed as described in Section 3.3. We include a final step of adjusting the factors so that $\hat{V}$ is orthogonal, but this is optional.

4. XPCA Imputation

PCA has a large number of applications. In some cases, the components themselves are of interest, in which case the factor matrices $\hat{U}$ and $\hat{V}$ are used directly or as inputs to visualization, clustering, and so on. In other cases, such as denoising or data imputation, we wish to provide estimates in the original data-space, and this is the focus of this section.

Recall that PCA uses the rescaled estimate, i.e., $\hat{x}_{ij} = \hat{\mu}_j + \hat{\theta}_{ij}\hat{v}_j$ as in Algorithm 2. COCA uses $\hat{F}^{-1}(\Phi(\theta_{ij}))$ as in Algorithm 4. XPCA can take a similar approach to COCA,
Algorithm 6 XPCA Impute via Median

Let $S$ denote the entries to be imputed and $\hat{U}, \hat{V}, \hat{\sigma}, \hat{F}_j$ be from XPCA in Algorithm 5.

1: for $(i, j) \in S$ do
   $\triangleright S$ denotes subset of entries to infer
2: $\hat{\theta}_{ij} \leftarrow \sum_{k=1}^k \hat{u}_i \hat{v}_j$\triangleright Calculate single entry of $\hat{\Theta} = \hat{U}\hat{V}^\top$
3: $\hat{y}_{ij} \leftarrow \Phi(\hat{\theta}_{ij})$\triangleright Transform standard normal to standard uniform
4: $\hat{x}_{ij} \leftarrow \hat{F}_j^{-1}(\hat{y}_{ij})$\triangleright Transform standard uniform to original distribution
5: end for

which we call median imputation and present in Section 4.1. We also present the characterization of the full distribution of $x_{ij}$ conditional on $\hat{\theta}_{ij}, \hat{\sigma}, \hat{F}_j$ as described in Section 4.2. From this information, we can infer entry means as described in Section 4.3.

4.1 Median Imputation

The simplest method of imputation for XPCA uses the median by simply evaluating

$$\hat{x}_{ij} = \hat{F}_j^{-1}(\Phi(\hat{\theta}_{ij})).$$  (18)

In fact, this is the same computation as used by COCA for a given $\hat{\Theta}$. The difference is that the loss function for the two methods is different. We refer to this as median imputation for the following reason: Because $z_{ij}$ is normally distributed (and that distribution is symmetric), $\hat{\theta}_{ij}$ represents not only the estimated mean but also the estimated median. Additionally, since $\Phi$ and $\hat{F}_j^{-1}$ are both strictly increasing functions, then we can conclude that $\hat{F}_j^{-1}(\Phi(\hat{\theta}_{ij}))$ is the estimated median of $x_{ij}$. The method is shown in Algorithm 6.

4.2 Full Distribution

One benefit of XPCA is that we can calculate the full conditional distribution for any entry. By construction, the range of $\hat{F}_j^{-1}$ is $C_j$. For every $\xi \in C_j$, our model implies

$$P(x_{ij} = \xi | \hat{\theta}_{ij}, \hat{\sigma}, \hat{F}_j) = \Phi\left(\frac{r(\xi) - \hat{\theta}_{ij}}{\hat{\sigma}}\right) - \Phi\left(\frac{\ell(\xi) - \hat{\theta}_{ij}}{\hat{\sigma}}\right),$$  (19)

where $r(\xi) = \Phi^{-1}(\hat{F}_j(\xi))$ and $\ell(\xi) = \Phi^{-1}(\hat{F}_j(\xi - \epsilon))$. (This is the same $\epsilon$ as in Eq. (17).) Evaluating this for all $\xi \in C_j$ produces the full distribution of $x_{ij}|\hat{\theta}_{ij}, \hat{\sigma}, \hat{F}_j$. This is given in Algorithm 7.

Let $d = \max_j |C_j| \leq m$ be the maximum number of distinct entries for any variable, and let $s = |S| \leq mn$ be the number of entries to impute. The computational cost of Algorithm 7 is $O((d + k)s)$. This may be prohibitively expensive if either $d$ or $s$ is large, so we present some alternatives in the next subsection.

4.3 Mean Imputation

A natural point estimate to characterize a distribution is the mean. In the case of binary variables, this fully characterizes the distribution, while the median is simply a 0 or 1 (or $\frac{1}{2}$ if there is a tie).
Algorithm 7 XPCA Impute Distributions
Let $S$ denote the entries to be imputed and $\hat{U}, \hat{V}, \hat{\sigma}, \hat{F}_j, \epsilon$ be from XPCA in Algorithm 5.

1: for $(i, j) \in S$ do
2: $\hat{\theta}_{ij} \leftarrow \sum_{\ell=1}^{k} \hat{u}_{i\ell} \hat{v}_{j\ell}$ \textcolor{gray}{$\triangleright$ Calculate single entry of $\hat{\Theta} = \hat{U}\hat{V}^T$}
3: for $\xi \in C_j$ do \textcolor{gray}{$\triangleright$ $C_j$ is the set of distinct values in column $j$ of $X$}
4: $\ell(\xi) \leftarrow \Phi^{-1}(\hat{F}_j(\xi - \epsilon))$
5: $r(\xi) \leftarrow \Phi^{-1}(\hat{F}_j(\xi))$
6: $p_{ij}(\xi) \leftarrow \Phi\left(\frac{r(\xi) - \hat{\theta}_{ij}}{\hat{\sigma}}\right) - \Phi\left(\frac{\ell(\xi) - \hat{\theta}_{ij}}{\hat{\sigma}}\right)$ \textcolor{gray}{$\triangleright P(x_{ij} = \xi | \hat{\theta}_{ij}, \hat{\sigma}, \hat{F}_j)$}
7: end for
8: end for

Algorithm 8 XPCA Impute via Mean
Let $S$ denote the entries to be imputed and $\{p_{ij}\}$ be from Algorithm 7

1: for $(i, j) \in S$ do \textcolor{gray}{$\triangleright$ $S$ denotes subset of entries to infer}
2: $\hat{x}_{ij} \leftarrow \sum_{\xi \in C_j} p_{ij}(\xi) \times \xi$
3: end for

The full conditional distribution can be used in a straightforward way to calculate the mean:

$$\mathbb{E}[x_{ij}|\hat{\theta}_{ij}, \hat{\sigma}, \hat{F}_j] = \sum_{\xi \in C_j} \xi \times P(x_{ij} = \xi | \hat{\theta}_{ij}, \hat{\sigma}, \hat{F}_j).$$ \hspace{1cm} (20)

This is given in Algorithm 8. The cost per entry is dominated by the cost of computing the distribution, i.e., $O(d+k)$. If we want to estimate every entry, then the work is $O((d+k)mn)$.

If we intend to estimate all the entries in one or more columns, then we propose an alternate strategy that may be more efficient for large $m$. The idea is to avoid computing the full distribution for every entry in a column but instead compute an estimate of the expected value function with respect to $\theta$. The expected value is a strictly increasing univariate function of $\theta$ that should be smooth. In fact, it can be viewed as a special type of kernel smoother, as it is a weighted average of all the observed values. We denote this function as $g_j(\theta)$ and define it to be

$$g_j(\theta) \equiv \mathbb{E}(x|\theta, \hat{F}_j, \hat{\sigma})$$

To estimate $g$, we evaluate the expectation at $q$ values of $\theta$ and then use linear interpolation to fill out the rest of the function. This estimate $\hat{g}$ can then be used to estimate the means, i.e., the expectations for specific values of $\theta_{ij}$ which is the imputation for $x_{ij}$. The method for all columns is shown in Algorithm 9. It still costs $O(mnk)$ to compute $\hat{\Theta}$, but we reduce the cost of the estimates from $O(dmn)$ to $O(dqn)$. By default, we use $q = m/10$.

5. Examples
We present the use of XPCA on both simulated datasets and real data sets.
Algorithm 9 XPCA Impute Means for Entire Columns

Let $\hat{U}, \hat{V}, \hat{\sigma}, \hat{F}_j$ be from XPCA in Algorithm 5.

1: $\hat{\Theta} \leftarrow \hat{U}\hat{V}^\top$
2: for $j = 1, \ldots, n$ do
3:   for $\ell = 1, \ldots, q$ do
4:     $\tau_\ell \leftarrow \Phi^{-1}((\ell - 1)/(q - 1))$
5:     $\varrho_\ell = \sum_{\xi \in C_j} \xi \times P(x = \xi|\tau_\ell, \hat{\sigma}, \hat{F}_j)$
6:   end for
7:   for $i = 1, \ldots, m$ do
8:     $\ell \leftarrow$ index such that $\hat{\theta}_{ij} \in [\tau_\ell, \tau_{\ell+1})$
9:     $\alpha \leftarrow$ value such that $\hat{\theta}_{ij} = \tau_\ell + \alpha(\tau_{\ell+1} - \tau_\ell)$
10:    $\hat{x}_{ij} \leftarrow \varrho_\ell + \alpha(\varrho_{\ell+1} - \varrho_\ell)$
11: end for
12: end for

5.1 Simulated Examples

We compare PCA, COCA, and XPCA on simplistic simulated data using different marginal distributions. First, we consider the case where all observed marginal variables are Gaussian so that all of the models have proper assumptions. Second, we consider exponential marginals so that PCA’s assumption of Gaussian marginals is violated. Third, we consider the case where 50% of the variables are binary and 50% are Gaussian, in which case only XPCA’s assumptions are valid.

In all scenarios, data was first simulated through a rank-3 PCA model with $\sigma^2 = 0.25$ (i.e., 75% of the variance in the PCA model can be explained by the low-rank structure) and then transformed by pushing through the appropriate marginal inverse CDFs. We tested on square matrices of sizes 50, 100, 200, 400 and 800, with 50% of the data masked completely at random. Each scenario was repeated 8 times. We report mean squared error (MSE) on the standardized data, for both the observed data and the underlying means that were inputs to the observed data generation. The results are shown in Fig. 5.

Based on our simulations, when the data is truly from a low-rank Gaussian copula with normal marginal distributions, PCA has the lowest MSE. This is not surprising, as PCA’s stronger assumptions of normal marginals is indeed correct in this case. When the marginal distributions are exponential, both XPCA and COCA have significantly better MSE than PCA. Even though PCA should yield the optimal MSE, this is under a linear relationship between the principal components and the data, whereas COCA and XPCA has a nonlinear relationship thanks to the EDF transforms. As expected, XPCA and COCA are very similar in performance. Finally, in the case that half the data was binary and half Gaussian, XPCA greatly outperforms both COCA and PCA.

5.2 U.S. Senate Vote Data

Our first real-world example is U.S. senate voting data from January 1989 to January 2017. This is a large span of data that covers the 101st congress through the 114th congress. We obtained the data from the Secretary of the Senate (2017). It encompasses 271 senators and
We compare all the methods for different ranks, reporting standardized MSE. Examining in-sample errors, XPCA has a slightly lower MSE than PCA, and COCA has the highest MSE.

Although these methods have comparable in-sample MSE, PCA has does much worse in cross-validation error. It severely overfits after rank-1 fit, going up to 15 MSE. For sake of completeness, we do include its error in our plot but note that it is even worse than just comparing to the mean. With XPCA and COCA, we see a much more stable imputation at these higher ranks. One could potentially argue that a rank-1 fit is all that is needed, in which case PCA would suffice. However, senators’ voting decisions are representative of a complex decision making process; although senators have a political party that they tend to vote with, they have a richer dimensionality to their decisions which both XPCA and COCA show.

Although XPCA’s mean squared error is lower than COCA, the real advantage is seen when looking deeper at the in-sample decompositions. In Fig. 7, we show the components from a rank 4 decomposition of PCA using Algorithm 2, COCA using Algorithm 4, and XPCA using Algorithm 8. Visualization of the XPCA components shows the clear separation of political party affiliation as well as bipartisan supporters. As shown in the first component in the first row of plots, XPCA demonstrates separation of senators by their political party as well as their corresponding party-dictated voting behavior. In the second component of XPCA in the second row of plots, there is a clear distinction of senators bipartisan voting behavior. In addition, there is a visible shift between red and blue approximately at bill index 2000 and again at 6000 and 9000. This represents the party control

9044 separate votes (the variables). Because different senators get voted in and out of office every two years, the data is 63% missing. The entirety of this data is discrete since senators have to either vote yes (1), no (−1), or abstain (0). Most previous works on analysis of senate data has only looked at a single session Jakulin et al. (2009); Neal (2014); Jackman (2001), so our approach adds the novelty of multiple sessions.
over the senate: if republicans had majority vote, the red points get larger values than blue. These are fundamental voting patterns not as clearly shown in PCA nor COCA. In both COCA’s and PCA’s components, there is a separation of republican vs democrats in the third component, and arguably a bipartisan voting behavior represented in the second component. However, both algorithms demonstrate a spike in value ranges for the first component contained to the 108th congress. We hypothesize that this would be fixed by regularization, but the cause of both algorithms demonstrating this behavior is unknown. The 108th congress was removed from the data and PCA no longer had this anomalous range spike, perhaps indicating that the 108th congress is unique in PCA’s analysis. However, when the 108th congress was removed and COCA analyzed this special view of the data, it moved the range spike to a different congress block. This suggests that COCA isn’t picking up on unique congressional sessions, but actually a victim of lack of regularization.

5.3 Basketball Data Set

Our next set of experiments involves statistics on NBA players from the 2015-2016 season. This dataset comprises 40 variables on 476 players. The variables include performance summaries over the entire season such as shots scored, number of offensive and defensive rebounds, and number of assists. Additionally, a few out-of-game statistics are included, such as height, weight, draft round, and draft number. Two binary variables were included: most valuable player (MVP) and defensive MVP. These were binary variables that indicated if the player had ever been voted MVP or defensive MVP in any season, up to the 2015-2016 season. The dataset is complete, i.e., no missing data and was compiled from two sources, namely National Basketball Association (2016) and Wikipedia contributors (2018b,a).

5.3.1 Data Imputation for Basketball Data Set

We examine imputation error by performing 20-fold cross validation (i.e., randomly divide the data into 20 parts and hold out on part for imputation in each test) to compute the imputation error. We compute each factorization for ranks 1 through 10 and then impute...
Figure 7: Components of a rank 4 XPCA decomposition according to Algorithm Algorithm 8. On the left hand side are the components of the 9044 bills and the right hand side are the 271 senators. XPCA shows separation of republican and democrats in both senator political parties and republican, democrat, bipartisan supported bills. The colorings for the senators is red indicates she voted only as a republican, blue indicates she voted only as a democrat, green indicates she voted as only an independent, and orange indicates inconsistent party membership. The colorings for the bills are red indicates that \( > 50\% \) of Democrats voted yes and \( > 50\% \) of Republicans voted no, blue indicates \( > 50\% \) of Republicans voted yes and \( > 50\% \) of Democrats voted no, green indicates both \( > 50\% \) of Democrats voted yes and \( > 50\% \) of Republicans voted no, black indicates both \( > 50\% \) of Democrats voted no and \( > 50\% \) of Republicans vote no, and yellow indicates the bill had no majority split.
the held out entries (using mean imputation for XPCA per Algorithm 9). As in our previous experiments, we compare the standardized MSE. The results can be seen in Table 1.

| Rank  | XPCA  | PCA  | COCA | Column Mean |
|-------|-------|------|------|-------------|
| Rank 1| 0.466 | 0.480| 0.489| 1.005       |
| Rank 2| 0.350 | 0.379| 0.364| 1.005       |
| Rank 3| 0.330 | 0.365| 0.330| 1.005       |
| Rank 4| 0.319 | 0.341| 0.377| 1.005       |
| Rank 5| 0.316 | 1.476| 0.383| 1.005       |
| Rank 6| 0.340 | 3.307| 0.430| 1.005       |
| Rank 7| 0.344 | 11.754| 0.532| 1.005      |
| Rank 8| 0.329 | 14.030| 0.653| 1.005      |
| Rank 9| 0.353 | 9.287| 0.717| 1.005       |
| Rank 10| 0.336 | 53.885| 0.717| 1.005    |

Table 1: Rescaled MSE by decomposition type

The rank-5 XPCA decomposition is the best overall MSE, with 4% improvement versus the best COCA fit and 8% improvement versus the best PCA fit. All three methods showed evidence of over-fitting by rank 6. However, PCA has more extreme problems with overfitting than either COCA or XPCA. This is most likely due to the fact that the XPCA and COCA models only impute values within the observed range for each column of data while nothing bounds the estimates produced by PCA. Interestingly, the effect of overfitting still seems much lower for XPCA than COCA, even though both only impute bounded estimates.

We examine some of individual estimates in more detail, showing the imputation results in the original dataspace. Of the 476 players in 2015-2016 season, there were six MVPs and five defensive MVPs. Table 2 shows a few examples of imputed values produced when these values were masked in the cross validation procedure. We used the rank that corresponded with best cross-validation error for a given method: rank 5 for XPCA, rank 4 for PCA, and rank 3 for COCA. We show results for three players: Kevin Durant, a former MVP; Dwight Howard, a former defensive MVP; and Anthony Morrow, a more typical NBA player.

| Kevin Durant | Dwight Howard | Anthony Morrow |
|--------------|---------------|---------------|
| MVP          | MVP           | MVP           |
| Defensive MVP| Defensive MVP | Defensive MVP |
| True Values  | 1             | 0             |
| XPCA Estimates| 0.383        | 0.048         |
| PCA Estimates | 0.142        | 0.091         |
| COCA Estimates | 0           | 0             |

Table 2: Imputed MVP Variables for Kevin Durant, Dwight Howard and Anthony Morrow

Per Algorithm 8, XPCA can only impute values within the range of possible values, and these can be interpreted as proper probabilities in this case of binary variables. In contrast, PCA’s estimate from Algorithm 2 cannot be interpreted as probabilities, as evidenced by the negative values for Anthony Morrow. COCA can only estimate observed values per
Algorithm 9, and in this case all four estimated values are zero. In fact, COCA imputed zeros for both variables for all players.

5.3.2 Components for Basketball Data Set

We examine the components from the rank-three decompositions and present the top ten variables (in absolute value) for each component in Table 3. The full components for each decomposition can be found in Appendix C.

For all three methods, the first component is strongly related to the minutes played which in turn correlates with count variables (as opposed to percentages). The second factor appears strongly related with the size of the player (i.e., height and weight), which appears to favor defensive plays (blocks, rebounds) but less favorable for more offensive statistics (three point shots). For the third factor, the methods appear to capture the value of a player, although this is a little less straightforward for PCA. The third factor for PCA does not have a clean interpretation. The third factor for COCA and XPCA seem to relate to the player value. We see that the draft number and round are the most important features, and that these are inversely related to the MVP status (XPCA also picks up DefensiveMVP). This relationship is sensible since the strongest players will generally have had the lowest draft numbers.

| PCA | PC 1 Name | PC 1 Value | PC 2 Name | PC 2 Value | PC 3 Name | PC 3 Value |
|-----|-----------|------------|-----------|------------|-----------|------------|
| 1   | MinutesPlayed | 0.208       | Weight    | 0.351      | TripleDouble | 0.402 |
| 2   | OpponentPtsDuringPlay | 0.207       | OffensiveRebound | 0.319  | GamesPlayed | -0.329 |
| 3   | ShotsMade    | 0.207       | Height    | 0.317      | TeamLosses  | -0.324 |
| 4   | Points       | 0.207       | Block     | 0.284      | DoubleDouble | 0.286 |
| 5   | Opponent2ndPts | 0.205       | ThreePtsAttempted | -0.279 | Assist | 0.222 |
| 6   | OpponentsTOPoints | 0.205       | ThreePtsMade | -0.275 | FreeThrowsMade | 0.218 |
| 7   | ShotsAttempted | 0.205       | ThreePtsPercentage | -0.242 | FreeThrowsAttempted | 0.218 |
| 8   | OpponentFastBreakPts | 0.202       | TotalRebound | 0.231 | PersonalFouls | -0.205 |
| 9   | PointsTurnOver | 0.198       | ShotsPercentage | 0.228 | TimesFouled | 0.188 |
| 10  | Turnover     | 0.196       | DoubleDouble | 0.210 | TeamWins | -0.187 |

| COCA | PC 1 Name    | PC 1 Value | PC 2 Name | PC 2 Value | PC 3 Name | PC 3 Value |
|------|--------------|------------|-----------|------------|-----------|------------|
| 1    | MinutesPlayed | 0.199       | Weight    | 0.384      | draftNumber | 0.601 |
| 2    | ShotsMade    | 0.199       | Height    | 0.374      | draftRound | 0.588 |
| 3    | MinutesPlayed | 0.199       | ThreePtsMade | -0.327 | MVP | -0.280 |
| 4    | OpponentPtsDuringPlay | 0.198       | ThreePtsAttempted | -0.324 | TeamLosses | 0.232 |
| 5    | ShotsAttempted | 0.198       | ShotsPercentage | 0.277 | TripleDouble | -0.199 |
| 6    | OpponentsTOPoints | 0.197       | ThreePtsPercentage | -0.257 | GamesPlayed | 0.170 |
| 7    | Opponent2ndPts | 0.196       | OffensiveRebound | 0.246 | PersonalFouls | 0.125 |
| 8    | PointsTurnOver | 0.194       | Block     | 0.231 | FreeThrowPercentage | -0.112 |
| 9    | TimesFouled | 0.194       | FreeThrowPercentage | -0.200 | DoubleDouble | -0.102 |
| 10   | OpponentFastBreakPts | 0.194       | DoubleDouble | 0.185 | OffensiveRebound | 0.091 |

| XPCA | PC 1 Name | PC 1 Value | PC 2 Name | PC 2 Value | PC 3 Name | PC 3 Value |
|------|-----------|------------|-----------|------------|-----------|------------|
| 1    | TripleDouble | 0.198       | Height    | 0.378      | draftRound | 0.545 |
| 2    | Points     | 0.194       | Weight    | 0.369      | draftNumber | 0.476 |
| 3    | ShotsMade  | 0.194       | DefensiveMVP | 0.331 | MVP | -0.450 |
| 4    | MinutesPlayed | 0.193       | ThreePtsMade | -0.303 | DefensiveMVP | -0.247 |
| 5    | ShotsAttempted | 0.192       | ThreePtsAttempted | -0.299 | TeamLosses | 0.207 |
| 6    | OpponentPtsDuringPlay | 0.192       | ShotsPercentage | 0.264 | FreeThrowPercentage | -0.200 |
| 7    | OpponentsTOPoints | 0.190       | OffensiveRebound | 0.221 | GamesPlayed | 0.129 |
| 8    | PointsTurnOver | 0.190       | ThreePtsPercentage | -0.210 | PersonalFouls | 0.126 |
| 9    | TimesFouled | 0.190       | Block     | 0.210 | OffensiveRebound | 0.125 |
| 10   | Opponent2ndPts | 0.189       | FreeThrowPercentage | -0.170 | ShotsPercentage | 0.104 |

Table 3: Top ten factors per decomposition method

Although in general it is difficult to argue that one set of components is definitively better than another, we contend XPCA does better at finding relations in situations where there is a heavy atom, i.e., a particular value with very high probability, e.g., 75% or higher.

Consider the influence of double and triple doubles in the first component. In basketball, a double double is when a player gets double digit statistics in two positive categories during
a single game, and a triple double is when a player gets double digit statistics in three positive categories. Hence, the double doubles must be less than or equal to the triple doubles. In our dataset, 232 of 476 players had at least one double double, while only 12 had at least one triple double. Recall that the first component was primarily about minutes played and related count variables. All three methods had moderate to heavy loadings for Double Double in this component (PCA = 0.137, COCA = 0.143 and XPCA = 0.164), but only XPCA put heavy loading on Triple Doubles (PCA = 0.067, COCA = 0.071 and XPCA = 0.198). In Fig. 8, we show correlation between minutes played and either double or triple doubles. We hypothesize that triple doubles have a heavy atom at zero, which makes it much more difficult for PCA or COCA to find the correlation between triple doubles and minutes played.

As another example, consider the defensive MVP variable in the second component. Recall that this factor seems to split defensive and offensive players, giving positive weights for defensive traits (rebounds, blocks) and negative weights for offensive traits (three-pointers, free throws). Only XPCA puts heavy positive loading onto Defensive MVP (PCA = 0.077, COCA = 0.078, XPCA = 0.331), a binary variable that should be correlated to defense-related variables and for ‘false’ is a heavy atom.

Finally, we consider the third factors for COCA and XPCA which correspond to player value in some sense since the most important characteristics are draft numbers. COCA picks up MVP (PCA = 0.173, COCA = 0.280, XPCA = 0.450) in its top ten, but XPCA gets both MVP and defensive MVP (PCA = 0.057, COCA = 0.091, XPCA = 0.247).

These examples suggest that XPCA may do a better job at finding relations between variables with a heavy atom and other variables in the dataset. The reason for the difference is that for a given $\xi$ in the set of observed values for a given column, $r(\xi)$ and $\ell(\xi)$ will be far apart. This means that the COCA and XPCA loss functions will be markedly different.

5.3.3 Conditional Distributions

Conditional on our fitted model, we can provide an estimated distribution for a given entry. For reference, we first look at the marginal distribution of points, across all players, in
Fig. 9a, in bins of size 100. Using Algorithm 7, we compute estimated conditional distributions for Kevin Durant, Dwight Howard and Anthony Morrow. These are shown in Fig. 9b, in bins of size 100. We caution that these distributions reflect the residual uncertainty conditional on the fitted parameters, rather than also incorporating the uncertainty in the parameters themselves.

6. Discussion

We consider the problem of heterogeneous variables in PCA analysis of data matrices whose rows correspond to objects or persons and whose columns correspond to features or variables. We propose XPCA, a Gaussian-copula-based decomposition method specifically targeted at datasets with a mixture of continuous and discrete variables. We develop this in a probabilistic framework and show that the XPCA factorization is a maximum likelihood solution. We provide algorithms for computing XPCA and for imputing estimates of the entries in the original data matrix. In simulations, we show that this enables us to relax the marginal assumptions built into both PCA and COCA so that discrete data can be incorporated. Additionally, we show that XPCA has advantages as compared to PCA and COCA in analysis of real data sets where some variables have heavy atoms (a specific outcome with very high probability). We have stressed the utility of XPCA for discrete variables, but XPCA is also appropriate for semi-continuous data such as zero-inflated distributions which have a heavy atom at zero.

In future work, there are potential improvements to consider. Decreasing the computation time is a priority since the computational cost of XPCA can be an order of magnitude slower than a PCA or COCA decomposition using alternating least squares, but we hypothesize that an improved optimization algorithm would alleviate most of this problem. In terms of imputation of missing data, we can potentially improve out-of-sample error by including penalization. We also want to investigate letting $\sigma$ (the residual error remaining after the low-rank decomposition) vary across columns, which would be closer to a factor analysis model. Although we can handle discrete data, we have no easy way yet of incorporating categorical data.
Acknowledgments

We thank David Hong for suggesting the U.S. Senator voting data and providing us with scripts to collect it, and Justin Jacobs for recommending the NBA player data and providing us with an initial version of the dataset. We want to acknowledge Jessica Gronski for work on a related project that helped to motivate this work.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

Appendix A. Derivatives

Recall that NLL is the loss function (i.e., negative log-likelihood) as defined in Eq. (16) and that $\Theta = UV^T$. Define the following substitutions:

\[
\bar{r}_{ij} = r_{ij} - \theta_{ij}, \quad \bar{\ell}_{ij} = \ell_{ij} - \theta_{ij}, \quad \tau = \sigma^{-1},
\]

\[
\tilde{r}_{ij} = \tau \bar{r}_{ij}, \quad \tilde{\ell}_{ij} = \tau \bar{\ell}_{ij},
\]

\[
P_{ij} = \Phi(\tilde{r}_{ij}) - \Phi(\tilde{\ell}_{ij}).
\]

Then NLL = $-\sum_{(i,j) \in \Omega} \log P_{ij}$. We need to compute derivatives of this with respect to $\sigma$, $U$, and $V$. Recall that $\Phi'(x) = \phi(x)$ and $\phi'(x) = -x\phi(x)$.

A.1 Derivatives with respect to $\sigma$

We compute the derivative with respect to $\tau = 1/\sigma$ and then use the chain rule to get the derivatives with respect to $\sigma$. The first partial derivative is

\[
\frac{\partial \text{NLL}}{\partial \sigma} = -\sum_{(i,j) \in \Omega} \frac{1}{P_{ij}} \cdot \frac{\partial P_{ij}}{\partial \tau} \cdot \frac{\partial \tau}{\partial \sigma}
\]

\[
= -\sum_{(i,j) \in \Omega} P_{ij}^{-1} \cdot \left[ \bar{r}_{ij} \phi(\tau \bar{r}_{ij}) - \bar{\ell}_{ij} \phi(\tau \bar{\ell}_{ij}) \right] \cdot \left[ -\sigma^{-2} \right]
\]

\[
= \frac{1}{\sigma^2} \sum_{(i,j) \in \Omega} \frac{1}{P_{ij}} \cdot \left[ \bar{r}_{ij} \phi(\tilde{r}_{ij}) - \bar{\ell}_{ij} \phi(\tilde{\ell}_{ij}) \right].
\]

The second partial derivative w.r.t. $\tau$ is

\[
\frac{\partial^2 \text{NLL}}{\partial \tau^2} = \sum_{(i,j) \in \Omega} P_{ij}^{-2} \cdot \left( \frac{\partial P_{ij}}{\partial \tau} \right)^2 - P_{ij}^{-1} \cdot \frac{\partial^2 P_{ij}}{\partial \tau^2}
\]

\[
= \sum_{(i,j) \in \Omega} P_{ij}^{-2} \left[ \bar{r}_{ij} \phi(\tau \bar{r}_{ij}) - \bar{\ell}_{ij} \phi(\tau \bar{\ell}_{ij}) \right]^2 + P_{ij}^{-1} \tau \left[ \bar{r}_{ij}^3 \phi(\tau \bar{r}_{ij}) - \bar{\ell}_{ij}^3 \phi(\tau \bar{\ell}_{ij}) \right].
\]
From this, we can compute the derivatives w.r.t. \( \sigma \):

\[
\frac{\partial^2 \text{NLL}}{\partial \sigma^2} = \frac{\partial^2 \text{NLL}}{\partial \tau^2} \cdot \left( \frac{\partial \tau}{\partial \sigma} \right)^2 + \frac{\partial \text{NLL}}{\partial \tau} \cdot \frac{\partial^2 \tau}{\partial \sigma^2}
\]

\[
= \frac{\partial^2 \text{NLL}}{\partial \tau^2} \cdot \frac{1}{\sigma^4} + \frac{\partial \text{NLL}}{\partial \tau} \cdot \frac{2}{\sigma^3}
\]

\[
= \frac{1}{\sigma^3} \sum_{(i,j) \in \Omega} P_{ij}^{-2} \left[ \tilde{r}_{ij} \phi(\tilde{r}_{ij}) - \tilde{\ell}_{ij} \phi(\tilde{\ell}_{ij}) \right]^2 + \frac{P_{ij}^{-1}}{\sigma^2} \left[ \tilde{r}_{ij} \phi(\tilde{r}_{ij}) - \tilde{\ell}_{ij} \phi(\tilde{\ell}_{ij}) \right]
\]

\[ - 2P_{ij}^{-1} \left[ \tilde{r}_{ij} \phi(\tilde{r}_{ij}) - \tilde{\ell}_{ij} \phi(\tilde{\ell}_{ij}) \right].\]

A.2 Derivatives with respect to \( U \) and \( V \)

If \( L_{ij} = -\log P_{ij} \) is the \((i,j)\)th summand, then \( \partial L_{ij} / \partial \theta_{k\ell} \) is zero unless \( i = k \) and \( j = \ell \); thus, we only consider \( \partial L_{ij} / \partial \theta_{ij} \). The first derivative is

\[
\frac{\partial L_{ij}}{\partial \theta_{ij}} = -\frac{1}{P_{ij}} \cdot \frac{\partial P_{ij}}{\partial \theta_{ij}} = -\frac{1}{P_{ij}} \cdot -\frac{1}{\sigma} \left[ \phi(\tilde{r}_{ij}) - \phi(\tilde{\ell}_{ij}) \right] = \frac{1}{\sigma P_{ij}} \left[ \phi(\tilde{r}_{ij}) - \phi(\tilde{\ell}_{ij}) \right].
\]

The second derivative is

\[
\frac{\partial^2 L_{ij}}{\partial \theta_{ij}^2} = P_{ij}^{-2} \cdot \left( \frac{\partial P_{ij}}{\partial \theta_{ij}} \right)^2 - P_{ij}^{-1} \cdot \frac{\partial^2 P_{ij}}{\partial \theta_{ij}^2}
\]

\[= \frac{1}{\sigma^2 P_{ij}^2} \left[ \phi(\tilde{r}_{ij}) - \phi(\tilde{\ell}_{ij}) \right]^2 + \frac{1}{\sigma^3 P_{ij}} \left[ \tilde{r}_{ij} \phi(\tilde{r}_{ij}) - \tilde{\ell}_{ij} \phi(\tilde{\ell}_{ij}) \right].\]

Now, we return to the NLL. For a given single element \( u_{i\ell} \), we have

\[
\frac{\partial \text{NLL}}{\partial u_{i\ell}} = \sum_{j: (i,j) \in \Omega} \frac{\partial L_{ij}}{\partial \theta_{ij}} \cdot \frac{\partial \theta_{ij}}{\partial u_{i\ell}}.
\]

Let \( A \) be the \( m \times n \) first-derivative matrix whose \((i,j)\) entry is \( \frac{\partial L_{ij}}{\partial \theta_{ij}} \). Then, in matrix or vector form, this looks like

\[
\frac{\partial \text{NLL}}{\partial U} = AV, \quad \text{or} \quad \frac{\partial \text{NLL}}{\partial U_i} = A_i V.
\]

These are, in turn, an \( n \times k \) matrix or a \( k \)-vector. Note that the second version is a \( 1 \times n \) vector times an \( n \times k \) matrix, so it results in a \( 1 \times k \) row vector, which makes sense for updating a row of \( U \). Using analogous reasoning, for \( V \) we have

\[
\frac{\partial \text{NLL}}{\partial V} = A^T U, \quad \text{or} \quad \frac{\partial \text{NLL}}{\partial V_j} = (A_{i\ell})^T U.
\]

For the second derivative, we have

\[
\frac{\partial^2 \text{NLL}}{\partial u_{i\ell}^2} = \sum_{j: (i,j) \in \Omega} \frac{\partial^2 L_{ij}}{\partial \theta_{ij}^2} \cdot \left( \frac{\partial \theta_{ij}}{\partial u_{i\ell}} \right)^2 + \frac{\partial L_{ij}}{\partial \theta_{ij}} \cdot \frac{\partial^2 \theta_{ij}}{\partial u_{i\ell}^2}.
\]
The second term is zero, so we look only at the first term. We can write this for a row of $U_i$ as
\[
\frac{\partial^2 \text{NLL}}{\partial U_i^2} = V^T D_i V,
\]
where $D_i$ is an $n \times n$ diagonal matrix whose $j$th diagonal entry is
\[
D_i(j,j) = \frac{\partial^2 L_{ij}}{\partial \theta^2_{ij}}.
\]
In other words, $D_i$ is the diagonal created by the $i$th row of the matrix of second derivatives w.r.t. $\theta_{ij}$. An analogous argument w.r.t. $V$ leads to
\[
\frac{\partial^2 \text{NLL}}{\partial V^2} = U^T D_j U,
\]
In this case, $D_j$ is the diagonal created by the $j$th column of the matrix of second derivatives w.r.t. $\theta_{ij}$.

Appendix B. Midpoint imputation for COCA

Han and Liu (2012) developed COCA in the context of continuous data and so do not discuss the issue of ties explicitly. A standard approach is just to use the maximum rank for ties; however, this causes problems for COCA in the case of discrete variables. Instead, we suggest using the midpoint rank.

To demonstrate that this is a good idea, we simulated an even mix of Gaussian and binary variables in the same manner as presented in section Section 5.1 for $m = n = 100$. We perform 20-fold cross validation and compare the MSE of the two methods on the held out data in Table 4. Using the midpoint rank rather than the maximum results in an 38% reduction in the MSE.

| Tie Method | MSE   | SE(MSE) |
|------------|-------|---------|
| Midpoint   | 0.2001| 0.0004  |
| Last       | 0.3254| 0.0030  |

Table 4: Comparing COCA methods for ties

Therefore, in all uses of COCA in this paper, ties are handled using the midpoint rank rather than the maximum rank.

Appendix C. Full Components for Basket Ball Data

In Section 5.3.2, we present only the top ten variable from each component. In this appendix, we show the complete data in Table 5.

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Table 5: Complete factors for rank-three decompositions of the basketball data set. The component rankings (in absolute value) are shown in parenthesis.

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