Generalized eigen, singular value, and partial least squares decompositions: The GSVD package

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Abstract

The generalized singular value decomposition (GSVD, a.k.a. “SVD triplet”, “duality diagram” approach) provides a unified strategy and basis to perform nearly all of the most common multivariate analyses (e.g., principal components, correspondence analysis, multidimensional scaling, canonical correlation, partial least squares). Though the GSVD is ubiquitous, powerful, and flexible, it has very few implementations. Here I introduce the GSVD package for R. The general goal of GSVD is to provide a small set of accessible functions to perform the GSVD and two other related decompositions (generalized eigenvalue decomposition, generalized partial least squares-singular value decomposition). Furthermore, GSVD helps provide a more unified conceptual approach and nomenclature to many techniques. I first introduce the concept of the GSVD, followed by a formal definition of the generalized decompositions. Next I provide some key decisions made during development, and then a number of examples of how to use GSVD to implement various statistical techniques. These examples also illustrate one of the goals of GSVD: how others can (or should) build analysis packages that depend on GSVD. Finally, I discuss the possible future of GSVD.

Keywords: multivariate analysis, generalized singular value decomposition, principal components analysis, correspondence analysis, multidimensional scaling, canonical correlation, partial least squares, R.

1. Introduction

The singular value decomposition (SVD; Golub and Reinsch 1971) is one of the most important tools in a multivariate toolbox. Conceptually and practically, the SVD is the core technique behind numerous statistical methods; the most common of which is principal component analysis (PCA; Jolliffe 2012; Abdi and Williams 2010; Jolliffe and Cadima 2016). A lesser known—but far more ubiquitous—tool is the generalized SVD (GSVD; Abdi 2007; Greenacre 1984; Takane 2003; Holmes 2008). The GSVD is more ubiquitous because it is the technique behind—and generalizes—many more statistical methods. The core concept behind the GSVD is that a data matrix has two companion matrices: one for the rows and one for the columns. These companion matrices are weights, constraints, or metrics imposed on the rows and columns of a data matrix. For examples, via the GSVD we can implement weighted solutions to PCA, or analyses under different metrics, such as correspondence analysis (CA: Greenacre 1984; Lebart, Morineau, and Warwick 1984; Escofier-Cordier 1965; Greenacre 2010) or canonical correlation analysis (CCA: Hotelling 1936; Abdi, Guillemot, Eslami, and Beaton 2012).
Though the GSVD generalizes—and is more flexible than—the SVD, there are few if any direct implementations of the GSVD in R. Rather, the GSVD is typically part of specific packages, and these packages are typically designed around more general analyses and broad usage. Rarely, if ever, are these GSVD implementations accessible to, or meant for, more direct access by users. Given the frequent and ubiquitous uses of the SVD and GSVD, a more accessible implementation would benefit a wide range of users.

Here I introduce a package designed around the GSVD, called GSVD. GSVD is a lightweight implementation of the GSVD and two other generalized decompositions: the generalized eigen-decomposition (GEVD) and the generalized partial least squares-SVD (GPLSSVD). GSVD was designed for a wide range of users, from analysts to package developers, all of whom would benefit from more direct access to the GSVD and similar decompositions. More importantly, the GSVD package and the idea of the GSVD provide a basis to unify concepts, nomenclature, and techniques across a wide array of statistical traditions and multivariate analyses approaches. GSVD has three core functions: geigen(), gsvd(), and gplsssvd(). These core functions provide a way for users to implement a wide array of methods including (but not limited to) multidimensional scaling, principal components analysis, correspondence analysis, canonical correlation, partial least squares, and numerous variants and extensions of the aforementioned. GSVD also helps simplify and unify concepts across techniques because, at their core, all of these techniques can be accomplished with the SVD.

In this paper, I introduce the core functions and functionality of GSVD. Furthermore, I show how the GSVD can provide a more unified nomenclature across techniques, and I show how various techniques can be implemented through geigen(), gsvd(), and gplsssvd(). Here I provide sufficient detail for the majority of users and readers. However, some readers may want to take a deeper dive into various techniques and literatures. Where possible and relevant, I point the readers to works with much more detail and substance.

This paper is outlined as follows. In Generalized decompositions I provide background on, notation for, and mathematical explanations of the three decompositions discussed here (GEVD, GSVD, and GPLSSVD), followed by some additional notes and literature. In Package description, I provide an overview of the core functions, their uses, and other development notes. In Examples of multivariate analyses I provide detailed implementations of numerous multivariate techniques, as well as variations of those techniques or variations of how to implement them with GSVD (e.g., PCA via GEVD vs PCA via GSVD). In Discussion I make some comments about the package, its uses, its potential, and possible future development.

2. Generalized decompositions

The GSVD is probably best known by way of the correspondence analysis literature (Greenacre 1984; Lebart et al. 1984; Escofier-Cordier 1965; Greenacre 2010) and, more generally, the “French way” of multivariate data analyses (Holmes and Josse 2017; Holmes 2008). There is considerable breadth and depth of materials on the GSVD and related techniques since the 1960s (and even well before then). Though such breadth and depth is beyond the scope of this paper, I provide a list of references and resources throughout the paper for any interested readers. This section instead focuses on the formulation—and to a degree the nomenclature—of the three core techniques. I first introduce notation, followed by the GEVD, the GSVD,
and then formalize and introduce the GPLSSVD.

2.1. Notation

Bold uppercase letters denote matrices (e.g., $X$). Upper case italic letters (e.g., $I$) denote cardinality, size, or length. Subscripts for matrices denote relationships with certain other matrices, for examples $Z_X$ is some matrix derived from or related to the $X$ matrix, where something like $F_I$ is a matrix related to the $I$ set of elements. When these matrices are introduced, they are also specified. Two matrices side-by-side denotes standard matrix multiplication (e.g., $XY$). Superscript $^T$ denotes the transpose operation, and superscript $^{-1}$ denotes standard matrix inversion. The diagonal operator, denoted $\text{diag}\{\}$, transforms a vector into a diagonal matrix, or extracts the diagonal of a matrix in order to produce a vector.

2.2. Generalized eigendecomposition

The generalized eigendecomposition (GEVD) requires two matrices: a $J \times J$ (square) data matrix $X$ and a $J \times J$ constraints matrix $W_X$. For the GEVD, $X$ is typically positive semi-definite and symmetric (e.g., a covariance matrix) and $W_X$ is required to be positive semi-definite. The GEVD decomposes the data matrix $X$—with respect to its constraints $W_X$—into two matrices as

$$X = QAQ^T,$$  \hspace{1cm} (1)

where $\Lambda$ is a diagonal matrix that contains the eigenvalues and $Q$ are the generalized eigenvectors. The GEVD finds orthogonal slices of a data matrix, with respect to its constraints, where each orthogonal slice explains the maximum possible variance. That is, the GEVD maximizes $\Lambda = Q^T W_X X W_X Q$ under the constraint of orthogonality where $Q^T W_X Q = I$. Practically, the GEVD is performed with the standard eigenvalue decomposition (EVD) as

$$\tilde{X} = V \Lambda V,$$  \hspace{1cm} (2)

where $\tilde{X} = W_X^{\frac{1}{2}} X W_X^{\frac{1}{2}}$ and $V$ are the eigenvectors which are orthonormal, such that $V^T V = I$. The relationship between the GEVD and EVD can be explained as the relationship between the generalized and standard eigenvectors where

$$Q = W_X^{-\frac{1}{2}} V \iff V = W_X^{\frac{1}{2}} Q.$$  \hspace{1cm} (3)

When $W_X = I$, the GEVD produces exactly the same results as the EVD because $\tilde{X} = X$ and thus $Q = V$. Analyses with the EVD and GEVD—such as PCA—typically produce component or factor scores. With the GEVD, component scores are defined as

$$F_J = W_X Q \Delta,$$  \hspace{1cm} (4)

where $\Delta = \Lambda^{\frac{1}{2}}$, which are singular values. The maximization in the GEVD can be reframed as the maximization of the component scores where $\Lambda = F_J^T W_X^{-1} F_J$, still subject to $Q^T W_X Q = I$.

2.3. Generalized singular value decomposition
The generalized singular value decomposition (GSVD) requires three matrices: an \(I \times J\) (rectangular) data matrix \(X\), an \(I \times I\) row constraints matrix \(M_X\), and a \(J \times J\) columns constraints matrix \(W_X\). For the GSVD \(M_X\) and \(W_X\) are each required to be positive semi-definite. The GSVD decomposes the data matrix \(X\)—with respect to both of its constraints \(M_X\) and \(W_X\)—into three matrices as

\[
X = P\Delta Q^T, \tag{5}
\]

where \(\Delta\) is a diagonal matrix that contains the singular values, and where \(P\) and \(Q\) are the left and right generalized singular vectors, respectively. From the GSVD we can obtain eigenvalues as \(\Lambda^2 = \Delta\). The GSVD finds orthogonal slices of a data matrix, with respect to its constraints, where each slice explains the maximum possible square root of the variance. That is, the GSVD maximizes \(\Delta = P^T M_X X W_X Q\) under the constraint of orthogonality where \(P^T M_X P = I = Q^T W_X Q\). Typically, the GSVD is performed with the standard SVD as

\[
\tilde{X} = U\Delta V, \tag{6}
\]

where \(\tilde{X} = M_X^{1/2} X W_X^{1/2}\), and where \(U\) and \(V\) are the left and right singular vectors, respectively, which are orthonormal such that \(U^T U = I = V^T V\). The relationship between the GSVD and SVD can be explained as the relationship between the generalized and standard singular vectors where

\[
P = M_X^{-1/2} U \iff U = M_X^{1/2} P \tag{7}
\]
\[
Q = W_X^{-1/2} V \iff V = W_X^{1/2} Q.
\]

When \(M_X = I = W_X\), the GSVD produces exactly the same results as the SVD because \(\tilde{X} = X\) and thus \(P = U\) and \(Q = V\). Analyses with the SVD and GSVD—such as PCA or CA—typically produce component or factor scores. With the GSVD, component scores are defined as

\[
F_I = M_X P \Delta \text{ and } F_J = W_X Q \Delta, \tag{8}
\]

for the left (rows) and right (columns) of \(X\), respectively. The optimization in the GSVD can be reframed as the maximization of the component scores where \(F_I^T M_X^{-1} F_I = \Lambda = F_J^T W_X^{-1} F_J\), still subject to \(P^T M_X P = I = Q^T W_X Q\). Note how the optimization with respect to the component scores shows a maximization for the eigenvalues.

### 2.4. Generalized partial least squares singular value decomposition

The generalized partial least squares-singular value decomposition (GPLSSVD) is a reformulation of the PLSSVD. The PLSSVD is a specific type of PLS from the broader PLS family (Tenenhaus 1998). The PLSSVD has various other names—for example, PLS correlation (Krishnan, Williams, McIntosh, and Abdi 2011)—but canonically comes from the psychology (Ketterlinus, Bookstein, Sampson, and Lamb 1989) and neuroimaging literatures (McIntosh, Bookstein, Haxby, and Grady 1996), though it traces its origins to Tucker’s interbattery factor analysis (Tucker 1958). Recently, with other colleagues, I introduced the idea of the GPLSSVD as it helped us formalize a new version of PLS for categorical data (Beaton, Dunlop, and Abdi 2016; Beaton, Saporta, Abdi, and others 2019). However, the GPLSSVD also allows us to generalize other methods, such as canonical correlation analysis (see Supplemental Material of Beaton et al. 2019).
The GPLSSVD requires six matrices: an \( N \times I \) (rectangular) data matrix \( X \) with its \( N \times N \) row constraints matrix \( M_X \) and its \( I \times I \) (rectangular) data matrix \( Y \) with its \( N \times N \) row constraints matrix \( M_Y \) and its \( J \times J \) columns constraints matrix \( W_Y \). For the GPLSSVD all constraint matrices are required to be positive semi-definite. The GPLSSVD decomposes the relationship between the data matrices, with respect to their constraints, and expresses the common information as the relationship between latent variables. The goal of partial least squares-SVD (PLSSVD) is to find a combination of orthogonal latent variables that maximize the relationship between two data matrices. PLS is often presented as \( \arg\max(\langle x^\ell, y^\ell \rangle) = \arg\max \text{cov}(\langle x^\ell, y^\ell \rangle) \), under the condition that \( \langle x^\ell, y^{\ell'} \rangle = 0 \) when \( \ell \neq \ell' \). This maximization can be framed as

\[
L_X^T L_Y = \Delta, \tag{9}
\]

where \( \Delta \) is the diagonal matrix of singular values, and so \( \Delta^2 = \Lambda \) which are eigenvalues. Like with the GSVD, the GPLSSVD decomposes the relationship between two data matrices into three matrices as

\[
[(M_X^\frac{1}{2} X)^T(M_Y^\frac{1}{2} Y)] = P \Delta Q^T, \tag{10}
\]

where \( \Delta \) is the diagonal matrix of singular values, and where \( P \) and \( Q \) are the left and right generalized singular vectors, respectively. Like the GSVD and GEVD, the GPLSSVD finds orthogonal slices of \( (M_X^\frac{1}{2} X)^T(M_Y^\frac{1}{2} Y) \) with respect to the column constraints. The GPLSSVD maximizes \( \Delta = P^T W_X [(M_X^\frac{1}{2} X)^T(M_Y^\frac{1}{2} Y)] W_Y Q \) under the constraint of orthogonality where \( P^T W_X P = I = Q^T W_Y Q \). Typically, the GPLSSVD is performed with the SVD as

\[
\tilde{X}^T \tilde{Y} = U \Delta V, \tag{11}
\]

where \( \tilde{X} = M_X^\frac{1}{2} X W_X^\frac{1}{2} \) and \( \tilde{Y} = M_Y^\frac{1}{2} Y W_Y^\frac{1}{2} \), and where \( U \) and \( V \) are the left and right singular vectors, respectively, which are orthonormal such that \( U^T U = I = V^T V \). The relationship between the generalized and standard singular vectors are

\[
P = W_X^{-\frac{1}{2}} U \iff U = W_X^\frac{1}{2} P \tag{12}
\]

\[
Q = W_Y^{-\frac{1}{2}} V \iff V = W_Y^\frac{1}{2} Q. \tag{12}
\]

When all constraint matrices are \( I \), the GPLSSVD produces exactly the same results as the PLSSVD because \( \tilde{X} = X \) and \( \tilde{Y} = Y \) and thus \( P = U \) and \( Q = V \).

The latent variables are then expressed with respect to the constraints and generalized singular vectors as \( L_X = (M_X^\frac{1}{2} X W_X P) \) and \( L_Y = (M_Y^\frac{1}{2} Y W_Y Q) \). These latent variables maximize the weighted covariance (by way of the constraints) subject to orthogonality where

\[
L_X^T L_Y = (M_X^\frac{1}{2} X W_X P)^T (M_Y^\frac{1}{2} Y W_Y Q) = (\tilde{X} U)^T (\tilde{Y} V) = U^T \tilde{X}^T \tilde{Y} V = \Delta. \tag{13}
\]

We will see in the following section that the “weighted covariance” could be the correlation, which allows us to use the GPLSSVD to perform various types of “cross-decomposition”
techniques. Like with the GEVD and GSVD, the GPLSSVD produces component or factor scores. The component scores are defined as

$$F_I = W_X P \Delta$$ and $$F_J = W_Y Q \Delta$$,

(14)

for the columns of $X$ and the columns of $Y$, respectively. The optimization in the GPLSSVD can be reframed as the maximization of the component scores where $F_I^T W_X^{-1} F_I = \Lambda = F_J^T W_Y^{-1} F_J$ where $\Lambda$ are the eigenvalues, and this maximization is still subject to $P^T W_X P = I = Q^T W_Y Q$.

2.5. Decomposition tuples

For simplicity, the GSVD is often referred to as a “triplet” or “the GSVD triplet” (Husson, Josse, and Saporta 2016; Holmes 2008) comprised of (1) the data matrix, (2) the column constraints, and (3) the row constraints. We can use the same concept to also define “tuples” for the GEVD and GPLSSVD. To note, the traditional way to present the GSVD triplet is in the above order (data, column constraints, row constraints). However, here I present a different order for the elements in the tuples so that I can (1) better harmonize the tuples across the three decompositions presented here, and (2) simplify the tuples such that the order of the elements within the tuples reflects the matrix multiplication steps. Furthermore, I present two different tuples for each decomposition—a complete and a partial—where the partial is a lower rank solution. The complete decomposition tuples are:

- The complete GEVD 2-tuple: GEVD($X, W_X$)
- The complete GSVD decomposition 3-tuple: GSVD($M_X X, X, W_X$)
- The complete GPLSSVD decomposition 6-tuple: GPLSSVD($M_X X, X, W_X, M_Y Y, W_Y$).

Additionally, we can take the idea of tuples one step further and allow for the these tuples to also define the desired returned rank of the results referred to as “partial decompositions”. The partial decompositions produce (return) only the first $C$ components, and are defined as:

- The partial GEVD decomposition 3-tuple: GEVD($X, W_X, C$)
- The partial GSVD decomposition 4-tuple: GSVD($M_X X, X, W_X, C$)
- The partial GPLSSVD decomposition 7-tuple: GPLSSVD($M_X X, X, W_X, M_Y Y, W_Y, C$).

Overall, these tuples provide short and convenient ways to express the decompositions. And as we will see in later sections, these tuples provide a simpler way to express specific techniques under the same framework (e.g., PLS and CCA via GPLSSVD).

2.6. Restrictions and limitations

In general, GSVD was designed around the most common analyses that use the GSVD, GEVD, and GPLSSVD. These techniques are, typically, multidimensional scaling (GEVD), principal components analysis (GEVD or GSVD), correspondence analysis (GSVD), partial least squares (GSVD or GPLSSVD), reduced rank regression (GSVD or GPLSSVD), canonical
correlation analysis (GSVD or GPLSSVD), and numerous variants and extensions of all the
amforementioned (and more).

One of the restrictions of these generalized decompositions is that any constraint matrix must
be positive semi-definite. That means, typically, these matrices are square symmetric ma-
trices with non-negative eigenvalues. Often that means constraint matrices are, for examples,
covariance matrices or diagonal matrices. GSVD performs checks to ensure adherence to
positive semi-definiteness for constraint matrices.

Likewise, many techniques performed through the GEVD or EVD also assume positive semi-
definiteness. For example, PCA is the EVD of a correlation or covariance matrix. Thus in
GSVD, there are checks for positive semi-definite matrices in the GEVD. Furthermore, all
decompositions in GSVD check for eigenvalues below a precision level. When found, these
very small eigenvalues are effectively zero and not returned by any of the decompositions in
GSVD. However, this can be changed with an input parameter to allow for these vectors to
be returned (I discuss these parameters in the following section).

2.7. Other and related decompositions.

To note, the GSVD discussed here is not the same as another technique referred to as the
“generalized singular value decomposition” (Van Loan 1976). The Van Loan generalized SVD
has more recently been referred to as the “quotient SVD (QSVD)” to help distinguish it from
the GSVD defined here (Takane 2003). Furthermore, there are numerous other variants of
the EVD and SVD beyond the GEVD and GSVD presented here. Takane (2003) provides a
detailed explanation of those variants as well as the relationships between the variants.

2.8. Other packages of note

There are multiple packages that implement methods based on the GSVD or GEVD, where
some of do in fact make use of a GSVD or GSVD-like call. Generally, though, the GSVD calls
in these packages are meant more for internal (to the package) use instead of a more external
facing tool like GSVD. A core (but by no means comprehensive) list of those packages follows.

There are at least four packages designed to provide interfaces to specific GSVD techniques,
and each of those packages has an internal function meant for GSVD-like decomposition.

- **ExPosition** which includes the function `genPDQ` (Beaton, Fatt, and Abdi 2014). As
the author of ExPosition, I designed `genPDQ` under the most common usages which are
generally diagonal matrices (or simply just vectors). I regret that design choice, which
is one of the primary motivations why I developed GSVD.

- **FactoMineR** (Lé, Josse, Husson, and others 2008) includes the function `svd.triplet`,
which also makes use of vectors instead of matrices because the most common (con-
ceptual) uses of the GSVD is that the row and/or column constraints are diagonal
matrices.

- **ade4** (Dray, Dufour, and others 2007) which includes a function called `as.dudi` that is
the core decomposition step. It, too, makes use of vectors.

- **amap** (Lucas 2019) which includes the function `acp` which, akin to the previous 3 pack-
ages listed, also only makes use of vectors for row and column constraints.
However, there are other packages that also more generally provide methods based on GSVD, GEVD, or GPLSSVD approaches however, they do not necessarily include a GSVD-like decomposition. Instead they make more direct use of the SVD or eigendecompositions, or alternative methods (e.g., alternating least squares). Those packages include but are not limited to:

- **MASS** (Venables and Ripley 2002) includes `MASS::corresp` which is an implementation of CA,
- **ca** which includes a number of CA-based methods (Nenadic and Greenacre 2007),
- **CAvariants** is another package that includes standard CA and other variations not seen in other packages (Lombardo and Beh 2016),
- **homals**, and **anacor**, are packages each that address a number of methods in the CA family (Leeuw and Mair 2009; de Leeuw and Mair 2009),
- **candisc** focuses on canonical discriminant and correlation analyses (Friendly and Fox 2020),
- **vegan** that includes a very large set of ordination methods with a particular emphasis on cross-decomposition or canonical methods (Oksanen, Blanchet, Friendly, Kindt, Legendre, McGlinn, Minchin, O’Hara, Simpson, Solymos, Stevens, Szöecs, and Wagner 2019), and
- **rgcca** also presents a more unified approach to CCA and PLS under a more unified framework that also includes various approaches to regularization (Tenenhaus and Guillemot 2017; Tenenhaus and Tenenhaus 2014).
- **ics** is a package for invariant coordinate selection, which can obtain unmixing matrices (i.e., as in independent components analysis) (Nordhausen, Oja, and Tyler 2008; Tyler, Critchley, Dümbgen, and Oja 2009).

### 3. Package description: core functions and features

The **GSVD** package has three primary “workhorse” functions:

- **geigen(X, W, k = 0, tol = sqrt(.Machine$double.eps), symmetric)**,
- **gsvd(X, LW, RW, k = 0, tol = .Machine$double.eps)**, and
- **gplssvd(X, Y, XLW, YLW, XRW, YRW, k = 0, tol = .Machine$double.eps)**

In `geigen()` or `gsvd()` each there is one data matrix `X`, whereas `gplssvd()` has two data matrices `X` and `Y`. In `geigen()` there is a single constraint matrix `W`. In `gsvd()` there are two constraint matrices, `LW` or “left weights” for the rows of `X` and `RW` or “right weights” for the columns of `X`. The “left” and “right” references are used because of the association between these weights and the left and right generalized singular vectors. In `gplssvd()` there are two
Table 1: Mapping between arguments (input) to functions (rows) and notation for the analysis tuples (columns).

| Function  | X | Y | M_X | W_X | M_Y | W_Y | C |
|-----------|---|---|-----|-----|-----|-----|---|
| geigen()  | X | - | -   | W   | -   | -   | k |
| gsvd()    | X | - | LW  | RW  | -   | -   | k |
| gplssvd() | X | Y | XRW | XLW | YRW | YLW | k |

constraint matrices per data matrix (so four total constraint matrices): XLW and XRW for X’s “left” and “right” weights, and YLW and YRW for Y’s “left” and “right” weights. The geigen() includes the argument symmetric to indicate if X is a symmetric matrix; when missing X is tested via isSymmetric(). The symmetric argument is eventually passed through to, and is the same as, symmetric in base::eigen(). All three functions include k which indicates how many components to return. Finally, all three functions include a tolerance argument tol, which is passed through to tolerance_svd() or tolerance_eigen(). These functions are the same as base::svd() and base::eigen(), respectively, with the added tolerance feature. In both cases, the tol argument is used to check for any eigenvalues or singular values below the tolerance threshold. Any eigen- or singular values below that threshold are discarded, as they are effectively zero. These values occur when data are collinear, which is common in high dimensional cases or in techniques such as Multiple Correspondence Analysis. However, the tol argument can be effectively turned off with the use of NA, NULL, Inf, -Inf, NaN, or any value < 0. In this case, both tolerance_svd() and tolerance_eigen() simply call base::svd() and base::eigen() with no changes. When using the tol argument, eigenand singular values are also checked to ensure that they are real and positive values. If they are not, then geigen(), gsvd(), and gplssvd() stop. The motivation behind this behavior is because the geigen(), gsvd(), and gplssvd() functions are meant to perform routine multivariate analyses—such as MDS, PCA, CA, CCA, or PLS—that require data and/or constraint matrices assumed to be positive semi-definite.

Data matrices are the minimally required objects for geigen(), gsvd(), and gplssvd(). All other arguments (input) either have suitable defaults or are allowed to be missing. For example, when any of the constraints (“weights”) are missing, then the constraints are mathematically equivalent to identity matrices (i.e., I) which contain 1s on the diagonal with 0s off-diagonal. Table 1 shows a mapping between our (more formal) notation above and our more intuitively named arguments for the functions. The rows of Table 1 are the three primary functions—geigen(), gsvd(), and gplssvd()—where the columns are the elements used in the formal notation (and also used in the tuple notation).

Additionally, there are some “helper” and convenience functions used internally to the geigen(), gsvd(), and gplssvd() functions that are made available for use. These include sqrt_psd_matrix() and invsqrt_psd_matrix() which compute the square root (sqrt) and inverse square root (invsqrt) of positive semi-definite (psd) matrices (matrix), respectively. The GSVD package also includes helpful functions for testing matrices: is_diagonal_matrix() and is_empty_matrix(). Both of these tests help minimize the memory and computational footprints for, or check validity of, the constraints matrices.

Finally, the three core functions in GSVD—geigen(), gsvd(), and gplssvd()—each have their own class objects but provide overlapping and identical outputs. The class object is
What it is             Notation  geigen  gsvd  gplssvd  
\(d\)             k singular values           \(\Delta\)               ✓               ✓               ✓               ✓  
\(d_{\text{full}}\)           all singular values            \(\Delta\)               ✓               ✓               ✓               ✓  
\(l\)             k eigenvalues             \(\Lambda\)               ✓               ✓               ✓               ✓  
\(l_{\text{full}}\)           all eigenvalues            \(\Lambda\)               ✓               ✓               ✓               ✓  
\(u\)             k Left singular/eigen vectors           \(U\)               ✓               ✓               ✓               ✓  
\(v\)             k Right singular/eigen vectors           \(V\)               ✓               ✓               ✓               ✓  
\(p\)             k Left generalized singular/eigen vectors           \(P\)               ✓               ✓               ✓               ✓  
\(q\)             k Right generalized singular/eigen vectors           \(Q\)               ✓               ✓               ✓               ✓  
\(f_i\)             k Left component scores           \(F_i\)               ✓               ✓               ✓               ✓  
\(f_j\)             k Right component scores           \(F_j\)               ✓               ✓               ✓               ✓  
\(l_x\)             k Latent variable scores for \(X\)           \(L_X\)               ✓               ✓               ✓               ✓  
\(l_y\)             k Latent variable scores for \(Y\)           \(L_Y\)               ✓               ✓               ✓               ✓  

Table 2: Mapping of values (output from functions; rows) to their conceptual meanings, notation used here, and which GSVD functions have these values.

Hierarchical from a list, to a package, to the specific function: \(c("\text{geigen","GSVD","list"})\), \(c("\text{gsvd","GSVD","list"})\), and \(c("\text{gplssvd","GSVD","list"})\) for \text{geigen()}, \text{gsvd()}, and \text{gplssvd()} respectively. Table 2 lists the possible outputs across \text{geigen()}, \text{gsvd()}, and \text{gplssvd()}. The first column of Table 2 explains the returned value, where the second column provides a mapping back to the notation used here. The last three columns indicate—with an ‘X’—which of the returned values are available from the \text{geigen}, \text{gsvd}, or \text{gplssvd} functions.

Different fields and traditions use different nomenclature, different descriptions, or different ways of framing optimizations. But conceptually and mathematically, numerous multivariate techniques are much more related than they appear, especially when solved with the EVD and SVD. The GSVD package provides a single framework to unify common multivariate analyses by way of three generalized decompositions. The arguments (function inputs) and values (function outputs) help reinforce the mathematical and conceptual equivalence and relationships between techniques, and now via the GSVD package, we see this unification programmatically and through analyses. Therefore the common names—across the core functions—for the values in Table 2 was an intentional design choice.

Finally, this package is “lightweight” in that it is written in base R, with no dependencies, and has a minimal set of functions to achieve the goals of GSVD. Furthermore, a number of strategies were employed in order to minimize both memory and computational footprints. For example, when constraints matrices are available, they are checked for certain conditions. Specifically, if a matrix is a diagonal matrix it is transformed into a vector, which decreases memory consumption and speeds up some computations (e.g., multiplication). If that same vector is all 1s, then the matrix was an identity matrix, and is then ignored in all computation.

4. Examples of multivariate analyses

In this section, I present many of the most commonly used multivariate analyses, and how they can be performed through the GSVD package, as well as how these methods can be
framed in various ways. Here, I focus primarily on what are likely the most common: principal components analysis, multidimensional scaling, correspondence analysis (and some of its variations), partial least squares, reduced rank regression (a.k.a. redundancy analysis or multivariable multivariate regression; Van Den Wollenberg 1977; De la Torre 2012), and canonical correlation analysis. As I introduce these methods, I also introduce how to use various functions (and their parameters) in GSVD.

There are other very common multivariate techniques, such as log and power CA methods (Greenacre 2010, 2009), and various discriminant analyses. I forgo the descriptions of these latter cases because they tend to be specific or special cases of techniques I do highlight. For examples: log-linear CA requires additional transformations and then performs CA, and various discriminant analyses reduce to special cases of PLS, RRR, or CCA.

The GSVD package contains several toy or illustrative data sets that work as small examples of various techniques. There is also a larger and more realistic data set in the package that I use in the following examples. That data set is a synthetic data set modeled after data from the Ontario Neurodegenerative Disease Research Initiative (ONDRI; https://ondri.ca/). The synthetic data were generated from real data, but were “synthesized” with the synthpop package (Nowok, Raab, and Dibben 2016). This synthetic data set—synthetic_ONDRI—contains 138 rows (observations) and 17 columns (variables). See https://github.com/ondri-nibs for more details. The synthetic_ONDRI data set is particularly useful because it contains a variety of data types, e.g., some quantitative such as cognitive or behavioral scores that are continuous, and brain volumes that are strictly positive integers, as well as categorical and ordinal variables (typically demographic or clinical measures). For each of the following illustrations of techniques, I use particular subsets of the synthetic_ONDRI data most relevant or appropriate for those techniques (e.g., continuous measures for PCA, distances for MDS, cross-tabulations of categories for CA).

4.1. Principal components analysis

Generally, there are two ways to approach PCA: with a covariance matrix or with a correlation matrix. First, I show both of these PCA approaches on a subset of continuous measures from the synthetic_ONDRI dataset. Then I focus on correlation PCA, but with an emphasis on (some of) the variety of ways we can perform correlation PCA with generalized decompositions. PCA is illustrated with a subset of continuous measures from cognitive tasks.

We can perform a covariance PCA and a correlation PCA with the generalized eigendecomposition as:

```r
R> continuous_data <- synthetic_ONDRI[,c("TMT_A_sec", "TMT_B_sec",
+ "Stroop_color_sec", "Stroop_word_sec",
+ "Stroop_inhibit_sec", "Stroop_switch_sec")]

R> cov_pca_geigen <- geigen( cov(continuous_data) )
R> cor_pca_geigen <- geigen( cor(continuous_data) )
```

In these cases, the use here is no different—from a user perspective—of how PCA would be performed with the plain eigen. For now, the major advantage of the geigen approach is that the output (values) also include component scores and other measures common to these
decompositions, such as singular values, as seen in the output. The following code chunk shows the results of the \texttt{print} method for \texttt{geigen}

\begin{verbatim}
R> cov_pca_geigen

**GSVD package object of class type 'geigen'.**
geigen() was performed on a matrix with 6 columns/rows
Number of total components = 6.
Number of retained components = 6.
The 'geigen' object contains:
$d_full Full set of singular values
$l_full Full set of eigen values
$d Retained set of singular values (k)
$l Retained set of eigen values (k)
$v Eigen/singular vectors
$q Generalized eigen/singular vectors
$fj Component scores
\end{verbatim}

R> cor_pca_geigen

**GSVD package object of class type 'geigen'.**
geigen() was performed on a matrix with 6 columns/rows
Number of total components = 6.
Number of retained components = 6.
The 'geigen' object contains:
$d_full Full set of singular values
$l_full Full set of eigen values
$d Retained set of singular values (k)
$l Retained set of eigen values (k)
$v Eigen/singular vectors
$q Generalized eigen/singular vectors
$fj Component scores

A more comprehensive approach to PCA is the analysis of a rectangular table—i.e., the observations by the measures—as opposed to the square symmetric matrix of relationships between the variables. The more comprehensive approach to PCA can be performed with \texttt{gsvd}, as shown below, with its \texttt{print} method to show the output from \texttt{gsvd}. For this example of correlation PCA, we introduce a set of constraints for the rows. For standard PCA, the row constraints are just $1^T$ where $I$ is the number of rows in the data matrix.

\begin{verbatim}
R> scaled_data <- scale(continuous_data, center = T, scale = T)
R> degrees_of_freedom <- nrow(continuous_data)-1
\end{verbatim}
R> row_constraints <- rep(1/(degrees_of_freedom), nrow(scaled_data))
R>
R> cor_pca_gsvd <- gsvd( scaled_data, LW = row_constraints )
R>
R> cor_pca_gsvd

**GSVD package object of class type 'gsvd'.**

gsvd() was performed on a matrix with 138 rows and 6 columns.
Number of components = 6.
Number of retained components = 6.

The 'gsvd' object contains:
$ d_full Full set of singular values
$ l_full Full set of eigen values
$ d Retained set of singular values (k)
$ l Retained set of eigen values (k)
$ u Left singular vectors (for rows of DAT)
$ v Right singular vectors (for columns of DAT)
$ p Left generalized singular vectors (for rows of DAT)
$ q Right generalized singular vectors (for columns of DAT)
$ fi Left component scores (for rows of DAT)
$ fj Right component scores (for columns of DAT)

In the next code chunk, we can see that the results for the common objects—the singular and eigenvalues, the generalized and plain singular vectors, and the component scores—are all identical between geigen and gsvd.

R> all(
+ all.equal(cor_pca_geigen$l_full, cor_pca_gsvd$l_full),
+ all.equal(cor_pca_geigen$d_full, cor_pca_gsvd$d_full),
+ all.equal(cor_pca_geigen$v, cor_pca_gsvd$v),
+ all.equal(cor_pca_geigen$q, cor_pca_gsvd$q),
+ all.equal(cor_pca_geigen$fj, cor_pca_gsvd$fj)
+ )

[1] TRUE

The use of row constraints helps illustrate the GSVD triplet. The previous correlation PCA example is GSVD($\frac{1}{\sqrt{I}} I, X, I$) where $\frac{1}{\sqrt{I}} I$ is a diagonal matrix of $\frac{1}{\sqrt{I}}$ with $I$ as the number of rows of $X$ and $I$ is the identity matrix. In this particular case, the row constraints are all equal and thus a simple scaling factor. Alternatively, we could just divide by that scalar as gsvd( scaled_data / sqrt(degrees_of_freedom)) which is equivalent to geigen( cor(continuous_data) ).

The previous PCA triplet—GSVD($\frac{1}{\sqrt{I}} I, X, I$)—helps us transition to an alternative view of correlation PCA and an expanded use of the GSVD triplet. Correlation PCA can be reframed
as covariance PCA with additional constraints imposed on the columns. Let’s first compute PCA with row and column constraints via `gsvd`, then go into more detail on the GSVD triplet and its computation.

```r
R> centered_data <- scale(continuous_data, scale = F)
R> degrees_of_freedom <- nrow(centered_data)-1
R> row_constraints <- rep(1/(degrees_of_freedom), nrow(centered_data))
R> col_constraints <- degrees_of_freedom / colSums( (centered_data)^2 )
R>
R> cor_pca_gsvd_triplet <- gsvd(centered_data,
+ LW = row_constraints,
+ RW = col_constraints)
```

First, let’s test the equality between the previous correlation PCA and this alternative approach.

```r
R> mapply(all.equal, cor_pca_gsvd, cor_pca_gsvd_triplet)
```

We can see that almost everything is identical, with two exceptions: q and fj. That’s because the decomposed matrix is identical across the two, but their constraints are not. The commonalities and the differences stem from how the problem was framed. Let’s unpack what we did for the three versions of PCA shown. Let’s assume that $X$ is a matrix that has been column-wise centered. The covariance matrix for $X$ is $\Sigma = X^T(1/n - 1/I)X$, where $d = \text{diag}\{\Sigma\}$, which are the variances per variable, and $D = \text{diag}\{d\}$ which is a diagonal matrix of the variances. Each of the three correlation PCA approaches can be framed as the following generalized decompositions:

- GEVD($D^{-1/2}SD^{-1/2}, I$)
- GSVD($1/n - 1/I, XD^{-1/2}, I$)
- GSVD($1/n - 1/I, X, D^{-1}$)

The second way of framing PCA—GSVD($1/n - 1/I, XD^{-1/2}, I$)—is the canonical “French way” of presenting PCA via the GSVD: a centered data matrix ($X$) normalized/scaled by the square
root of the variances \((\mathbf{D}^{-\frac{1}{2}})\), with equal weights of \(\frac{1}{r}\) for the rows and an identity matrix for the columns.

Though not always practical for simple PCA computation, the use of constraints in a GEVD doublet and GSVD triplet shows that we can frame (or re-frame) various techniques as decompositions of data with respect to constraints. In the case of PCA, the the constraint-based decompositions highlight that we could perform PCA with any (suitable) constraints applied to the rows and columns. So for example, we may have \textit{a priori} knowledge about the observations (rows) and elect to use different weights for each observation (we’ll actually see this in the MDS examples). We could also use some known or assumed population variance as column constraints instead of the sample variance, or use column constraints as a set of weights to impose on the variables in the data.

4.2. (Metric) Multidimensional scaling

Metric multidimensional scaling (MDS) is a technique akin to PCA, but specifically for the factorization of distance matrix (Torgerson 1952; Borg and Groenen 2005). MDS, like PCA, is also an eigen-technique. Like the PCA examples, I show several ways to perform MDS through the generalized approaches; specifically all through the GEVD. But for this particular example we will (eventually) make use of some known or \textit{a priori} information as the constraints. First we show how to perform MDS as a plain EVD problem and then with constraints as a GEVD problem. In these MDS illustrations, I use a conceptually simpler albeit computationally more expensive approach. For example, I use centering matrices and matrix algebra (in \texttt{R}) to show the steps. Much more efficient methods exist. In these examples we use the same measures as in the PCA example.

\begin{verbatim}
R> data_for_distances <- synthetic_ONDRI[, +   c("TMT_A_sec", "TMT_B_sec", +   "Stroop_color_sec", "Stroop_word_sec", +   "Stroop_inhibit_sec","Stroop_switch_sec")]
R> scaled_data <- scale(data_for_distances, center = T, scale = T)
R> distance_matrix <- as.matrix( dist( scaled_data ) )
R> row_weights <- rep(1/nrow(distance_matrix), nrow(distance_matrix))
R> centering_matrix <- diag(nrow(distance_matrix)) - + ( rep(1,nrow(distance_matrix)) %o% row_weights )
R> matrix_to_decompose <- centering_matrix %*% + (-(distance_matrix^2)/2) %*% + t(centering_matrix)
R> mds_geigen <- geigen(matrix_to_decompose)

The results from \texttt{geigen(matrix_to_decompose)} produce a variety of outputs that align with the concept of eigenvectors, generalized eigenvectors, and component scores. But, more specifically, the results of \texttt{base::cmdscale(distance_matrix)} are identical to \texttt{mds_geigen$fj[,1:2]};
\end{verbatim}
that is, MDS scores as viewed through geigen are component scores.
However, the generalized approach allows us to include constraints. In the following example, we can now include a weighting factor per observation as a constraint to impose on that observation. Here we use the inverse of age, so that we effectively downweight older individuals and upweight younger individuals.

\[
R> \text{row_weights} \leftarrow \frac{1}{\text{synthetic\_ONDRI\$AGE}}
\]

\[
R> \text{centering_matrix} \leftarrow \text{diag(nrow(distance_matrix))} - (\text{rep(1,nrow(distance_matrix)) \%\% (row_weights/sum(row_weights))})
\]

\[
R> \text{matrix\_to\_decompose} \leftarrow -(\text{centering_matrix} \%\% (distance_matrix^2) \%\% t(\text{centering_matrix}))/2
\]

\[
R> \text{mds\_weighted\_geigen} \leftarrow \text{geigen( matrix\_to\_decompose , W = row_weights, tol = NA )}
\]

In mds_weighted_geigen we require the use of tol=NA. This is because matrix_to_decompose is not positive semi-definite. Recall that one of the key principles of the GSVD package is that we require positive semi-definite matrices for the constraints, and that the design of geigen also—by default—assume positive semi-definite matrices. This is because most multivariate analyses—from the eigendecomposition perspective—require correlation or covariance matrices which are by definition positive semi-definite. If we were to run geigen(matrix_to_decompose, diag(row_weights)) we would get an error. In fact, we are unable to set an appropriate tolerance parameter in this case because the last few eigenvalues have large negative values. But the use of tol=NA allows for a direct computation of the eigendecomposition, without dropping any of the dimensions (e.g., those below tolerance). For such an analysis, it is typical to discard dimensions with such eigenvalues (which is why it is a default in the package). However, some standard analyses do violate those assumptions. For examples: the weighted MDS here, principal axis factoring, and other approaches to factor analysis where, for example, the diagonal of a correlation matrix is loaded with the communalities. So the GSVD package accommodates these approaches by effectively ignoring the tolerance requirement for eigenvalues.

The weighted version of MDS produces the same kind of results as vegan::wcmdscale, but there exist differences the computation of scores. From the perspective of GSVD the scores are the generalized singular vectors, scaled by the singular values per component, and with respect to a metric (i.e., the constraints). Thus—as we’ve seen in the previous section—the component scores are \( W_X Q \Delta \). Many SVD and eigen-based analyses have numerous ways of presenting and visualizing results. In fact, the vegan package presents a slightly different version of the weighted MDS scores compared to GSVD. From the GSVD perspective, vegan produces scores computed from the generalized singular vectors scaled by their respective singular values, or \( Q \Delta \). We can see this in Figure 1, which shows the first two components from MDS and the weighted MDS, with component 1 on the horizontal axis and component 2 on the vertical axis. Figures 1a, c, and e each show the standard MDS solution where Figures
1b, d, and f show the weighted (constrained) MDS solution. Figures 1a and b show the eigen/singular vectors scaled by the singular values ($V\Delta$), Figures 1c and d show the weighted generalized eigen/singular vectors scaled by the singular values ($WXQ\Delta$), and Figures 1c and d show the generalized eigen/singular vectors scaled by the singular values ($Q\Delta$). Note that, in general, component scores (e.g., Figures 1e and f) should show axes proportion to their eigen or singular values (Nguyen and Holmes 2019). This is true for virtually all analyses shown in this paper. However, for simplicity and to help with comparisons, here I do not scale the axes. We can see in Figure 1 that the standard form of MDS produces sets of scores that show no differences in their pattern, but that the weighted version does across the various scores. Furthermore, we can also see that each weighted version set provides a slightly different perspective compared to the standard MDS.

4.3. Correspondence analysis

Correspondence analysis (CA) is one of—if not the—prototypical GSVD triplet method. CA is like PCA, but was originally designed for two-way contingency tables, and was then expanded into multiple correspondence analysis (MCA) for N-way contingency tables (Greenacre 1984; Lebart et al. 1984; Escoufier-Cordier 1965; Greenacre 2010; Greenacre and Blasius 2006). MCA is more like PCA in that the rows are typically observations and the columns are measures, where the data are transformed into “complete disjunctive coding” (a.k.a. nominal coding, dummy coding, one-hot encoding, and a variety of other names). CA methods can be thought of as a “$\chi^2$ PCA”. Prior to decomposition, the data matrix for CA methods are preprocessed in a way to make the data table analogous to that of a $\chi^2$ table, where we decompose the (weighted) deviations under the assumption of independence.

The next section goes through three forms of CA. Each form helps highlight the utility and flexibility of the GSVD and make use of various forms of weights. Each illustration is one of the many well-established derivatives of CA. The first example illustrates standard CA (on a two-way contingency table). The second example illustrates MCA on multiple categorical variables, which is then followed by—and compared with—the third example, a regularized MCA of the same data.

Let’s begin with standard CA—which is applied to a two-way contingency table. Here we’ll use genotypes from two genes: ApoE and MAPT. Both are risk factors in neurodegenerative disorders.

```r
R> observed_matrix <- mapt_by_apoe_table / sum(mapt_by_apoe_table)
R> row_probabilities <- rowSums(observed_matrix)
R> col_probabilities <- colSums(observed_matrix)
R> expected_matrix <- row_probabilities %o% col_probabilities
R> deviations_matrix <- observed_matrix - expected_matrix
R>
R> ca_gsvd <- gsvd( deviations_matrix,
+                  LW = 1/row_probabilities,
+                  RW = 1/col_probabilities )
```

In CA, the primarily and almost exclusively visualized items are the component scores: $fi$ and $fj$. Recall that the components scores are the generalized singular vectors, scaled by the singular values, under the metric defined by the constraints, or $MXP\Delta$ and $WXP\Delta$. The
Figure 1: Metric multidimensional scaling (MDS). Panels A, C, and E show standard MDS where panels B, D, and F show weighted MDS. Panels A and B show the singular vectors, panels C and D show the generalized singular vectors, and panels E and F show the component scores. Note how the configuration of the observations change in the weighted MDS through the different sets of scores (panels B, D, and F).
Figure 2: Row and column component scores for Correspondence Analysis (CA). Panel A shows the row component scores, where panel B shows the column component scores.

Table 3: Illustration of complete disjunctive coding (a.k.a. dummy coding, one-hot encoding) where each level of a categorical variable is represented. A value of ‘1’ indicates the presence of that level for that row (‘0’ otherwise).

|              | MAPTH1H1 | MAPTH1H2 | MAPTH2H2 | APOEE32 | APOEE33 |
|--------------|----------|----------|----------|---------|---------|
| OND01_SYN_0001| 0        | 0        | 1        | 0       | 0       |
| OND01_SYN_0011| 1        | 0        | 0        | 0       | 1       |
| OND01_SYN_0021| 0        | 1        | 0        | 0       | 1       |
| OND01_SYN_0041| 1        | 0        | 0        | 0       | 1       |
| OND01_SYN_0083| 1        | 0        | 0        | 0       | 1       |


The reason behind the scores as visuals in CA is that the scores reflect the $\chi^2$ distance. The CA component scores are shown in Figure 2.

Next I show MCA, which generalizes standard CA to multiple categorical variables. Here we use four variables: MAPT and ApoE like before, and now also include sex, and a clinical measure with a few ordinal levels (but here we treat those as levels of a categorical variable). The computation for MCA is exactly the same as CA, but now the data are disjunctive (see Table 3). However, MCA is more akin to PCA with observations on the rows and measures on the columns, as opposed to standard CA which has measures on both the rows and columns. The results of MCA are shown in Figure 3, where Figure 3a shows the component scores for the rows (observations) and Figure 3b shows the columns (measures, some of which are seen in Table 3).

```r
R> observed_matrix <- disjunctive_data / sum(disjunctive_data)
R> row_probabilities <- rowSums(observed_matrix)
R> col_probabilities <- colSums(observed_matrix)
R> expected_matrix <- row_probabilities %o% col_probabilities
R> deviations_matrix <- observed_matrix - expected_matrix
```
Figure 3: Row and column component scores from Multiple Correspondence Analysis (MCA). Here, the row component scores (panel A) are observations, where the column component scores (panel B) are levels of categorical variables.

R>
R> mca.gsvd <- gsvd( deviations_matrix,
+ LW = 1/row_probabilities,
+ RW = 1/col_probabilities)

Up until this point, all constraints matrices have been diagonal matrices. The next example serves two purposes: (1) use a well-established method that has more sophisticated constraints than simple vectors (or diagonal matrices), and (2) highlight a particular ridge regularization approach to show how the GSVD easily incorporates such techniques. Takane (Takane and Hwang 2006) introduced a variation of MCA called regularized MCA (RMCA) that uses a ridge-like approach. The ridge-like approach requires a cross product matrix for the row (observation) constraints, and a block-diagonal matrix for the column (measures) constraints. The next block of code shows how the procedure works through the GSVD. When the regularization parameter—\(\omega\)—is 0, then this is the same as standard MCA (within a scaling factor). Also note that for each iteration of RMCA, we now make use of the \(k\) parameter where \(\text{gsvd}(\ldots, k = 2)\), so that we only return a subset of possible results. All sets of vectors and scores are just the first two components, with the exception of \$d_full and \$l_full which return the full set of singular and eigenvalues, respectively. Note the small changes in the output object that indicate how many full (possible) components exist, and also how many were returned (\(k=2\)).

R> omegas <- c(0, 1, 2, 3, 4, 5, 10, 25, 50)
R> rmca_results <- vector("list",length(omegas))
R>
R> centered_data <- scale(disjunctive_data,scale=F)
R> projmat <- t(centered_data) %*% MASS::ginv( tcrossprod(centered_data) ) %*% centered_data
R> for(i in 1:length(omegas)){
+ LW <- diag(nrow(centered_data)) +
+ (omegas[i] * MASS::ginv(tcrossprod(centered_data))
+ RW <- diag(colSums(disjunctive_data)) + (omegas[i] * projmat)
+ invRW <- t(MASS::ginv(RW))
+ rownames(LW) <- colnames(LW) <- rownames(centered_data)
+ rownames(invRW) <- rownames(RW)
+ colnames(invRW) <- colnames(RW)
+ rmca_results[[i]] <- gsvd(centered_data, LW = LW, RW = invRW, k = 2)
+ }

R> rmca_results[[1]]

**GSVD package object of class type 'gsvd'.**

gsvd() was performed on a matrix with 138 rows and 15 columns
Number of components = 11.
Number of retained components = 2.

The 'gsvd' object contains:
  $d_full Full set of singular values
  $l_full Full set of eigen values
  $d Retained set of singular values (k)
  $l Retained set of eigen values (k)
  $u Left singular vectors (for rows of DAT)
  $v Right singular vectors (for columns of DAT)
  $p Left generalized singular vectors (for rows of DAT)
  $q Right generalized singular vectors (for columns of DAT)
  $fi Left component scores (for rows of DAT)
  $fj Right component scores (for columns of DAT)

So what does this regularization do? In Figure 4 we show a partial view of how this regularization works. In Figures 4a and b we see the scree plots, which is the explained variance (eigenvalues) per component. In Figure 4c and d we see the component scores for the columns. Figure 4a and c show the standard MCA where Figure 4b and d show each iteration of the RMCA, where the \( \omega \) parameter is used to color the eigenvalues and component scores on a gradient scale (via `ggplot::scale_color_gradient(...,trans="log1p")`). Figure 4 shows that as the regularization parameter increases, we see that explained variance for the higher dimensions decreases, and that in general, the component scores approach zero. Figure 4d in particular also shows us that stable measures do not change much under regularization (e.g., SEXfemale) where as rare and relatively unstable measures approach zero and see substantial changes in their component scores (e.g., MAPTH2H2 or APOEE42).
The CA-based approaches make use of each element in the GSVD. The implementations here show that standard CA and MCA use vectors—algebraically these are diagonal matrices—where RMCA requires more sophisticated matrices than simple diagonal matrices. RMCA illustrates two key concepts: (1) with appropriate sets of constraints, the GSVD—and all of the generalized methods presented here—provides an easy pathway to ridge regularization, and (2) constraints matrices are not always simple diagonal matrices: an important point expanded upon in the next section.

4.4. Partial least squares, reduced rank regression, and canonical correlation

So far, we have seen various examples of the GEVD and GSVD. The GEVD and GSVD are well-established concepts. Recently, I introduced an extension of the GEVD and GSVD concept to “two (data) table techniques”, and called this new extension the “GPLSSVD” (Beaton et al. 2019), which is short for the “generalized partial least squares-singular value decomposition”. The GPLSSVD provides the same base concepts as the GEVD or GSVD, but specifically for scenarios wherein there are two data matrices. The most common two-table techniques are canonical correlation analysis (CCA), reduced rank regression (RRR; sometimes called redundancy analysis, RDA), and a specific form of partial least squares (PLS) called the PLSSVD, “partial least squares correlation” (PLSC), and a variety of other names. This particular form of PLS traces its history to Tucker’s interbattery factor analysis.

The GPLSSVD requires at minimum two data matrices, and allows for the inclusion of positive semi-definite constraints matrices for the rows and columns of both data matrices. Here, I illustrate four methods that make use of the GPLSSVD. All of these examples emphasize the expression of latent variables, though do recall that at their core, these methods make use of the SVD. Each method makes use of different sets of constraints: (1) PLS-SVD/PLSC which uses no constraints, (2) RRR/RDA which uses one set of constraints, (3) CCA which uses two sets of constraints, and finally (4) partial least squares-correspondence analysis (PLS-CA; Beaton et al. (2019); Beaton et al. (2016)) which makes use of all four sets of constraints.

The first three methods—PLS, RRR, and CCA—are methods used to analyze numeric, or data that are generally assumed to be continuous values. The final method—PLS-CA—was initially designed for analysis of two data sets that are categorical, but easily extends to a variety of data types (Beaton et al. 2019). With that in mind, the first three examples will all make use of exactly the same data sets. This helps highlight the similarities and differences between PLS, RRR, and CCA, and shows how the same data can be viewed in multiple ways by imposing various constraints.

In the PLS/RRR/CCA examples, we have two data matrices of generally continuous data. One matrix contains age, total gray matter volume (in percentage of total intracranial volume), and total white matter volume (in percentage of total intracranial volume). The other matrix contains the cognitive tasks seen in the PCA and MDS examples. Here, the respective GPLSSVD models for each method are:

- PLS: GPLSSVD(I_N, X, I_I, I_N, Y, I_J)
- RRR: GPLSSVD(I_N, X, (X^T X)^-1, I_N, Y, I_J)
- CCA: GPLSSVD(I_N, X, (X^T X)^-1, I_N, Y, (Y^T Y)^-1)
Figure 4: MCA (panels A and C) vs. Regularized MCA (panels B and D). Panels A and B show scree plots, which reflect the amount of explained variance per component (and thus decreases as components increase). RMCA shows multiple overlaid scree plots because there exists one version for each run with $\omega$. Panels C and D show the column component scores (levels of categorical variables) in the plain MCA and as the scores change through the iterations of RMCA. Only the first two components are shown, with the first component on the horizontal axis, and the second component on the vertical axis. Note that the initial RMCA ($\omega = 0$) is equivalent to MCA.
Before an illustration of these techniques, it is worth noting that PLS, RRR, and CCA are multivariate extensions of univariate concepts. PLS emphasizes the covariance between $X$ and $Y$, RRR emphasizes the least squares fit (i.e., regression) of $Y$ onto space defined by $X$, and CCA emphasizes the correlation between $X$ and $Y$. For the first illustrations of PLS, RRR, and CCA, I use column-wise centered and scaled $X$ and $Y$ matrices.

```r
R> X <- synthetic_ONDRI[, + c("TMT_A_sec", "TMT_B_sec", + "Stroop_color_sec","Stroop_word_sec", + "Stroop_inhibit_sec","Stroop_switch_sec")]
R> Y <- synthetic_ONDRI[,c("AGE","NAGM_PERCENT","NAWM_PERCENT")]
R> R> scaled_X <- scale(X, center = T, scale = T)
R> scaled_Y <- scale(Y, center = T, scale = T)
R> R> pls_gplssvd <- gplssvd(scaled_X, scaled_Y)
R> rrr_gplssvd <- gplssvd(scaled_X, scaled_Y, + XRW = MASS::ginv(crossprod(scaled_X)))
R> cca_gplssvd <- gplssvd(scaled_X, scaled_Y, + XRW = MASS::ginv(crossprod(scaled_X)), + YRW = MASS::ginv(crossprod(scaled_Y)))
```

All three approaches provide the same types of outputs: singular and eigenvalues, latent variable scores (for the participants), standard and generalized singular vectors, and component scores. The output object is identical for all three approaches because they all make use of `gplssvd()`, so let’s only look at one of the objects, `cca_gplssvd`. Like both the `geigen()` and `gsvd()` outputs, we have many common objects (e.g., vectors, scores, eigenvalues). However `gplssvd()` also provides the latent variable scores—$l_x$ and $l_y$—which are row scores—for $X$ and $Y$, respectively—with respect to the singular vectors. For reference, see also Tables 1 and 2.

```r
R> cca_gplssvd

**GSVD package object of class type 'gplssvd'.**

gplssvd() was performed on an X matrix with 138 rows and 6 columns and a Y matrix with 138 rows and 3 columns.
Number of total components = 3.
Number of retained components = 3.

The 'gplssvd' object contains:
$d_{full}$ Full set of singular values
$l_{full}$ Full set of eigen values
$d$ Retained set of singular values (k)
$l$ Retained set of eigen values (k)
$u$ Left singular vectors (for columns of $X$)  
$v$ Right singular vectors (for columns of $Y$)  
$p$ Left generalized singular vectors (for columns of $X$)  
$q$ Right generalized singular vectors (for columns of $Y$)  
$fi$ Left component scores (for columns of $X$)  
$fj$ Right component scores (for columns of $Y$)  
$lx$ Left ($X$) latent variable scores (for rows of $X$)  
$ly$ Right ($Y$) latent variable scores (for rows of $Y$)

Before visualizing the results of these three approaches, let’s first establish the connections between framing the methods via the GPLSSVD and the more typical ways. Let’s do so by pointing out the relationship between base::cancor and the results in cca_gplssvd. From cca_gplssvd, the canonical correlations are the singular values. Recall also that the optimization when framed through the GPLSSVD is that the singular values are also $\text{diag}(L^T_X L_Y)$, so $\text{diag}(t(\text{cca_gplssvd}$lx$)% *% cca_gplssvd$ly$) are also the canonical correlations. So from the perspective of GPLSSVD, the relationship between the latent variables also maximize for the canonical correlations. Furthermore, the coefficients (per set of variables) from base::cancor(scaled_X, scaled_Y) are equal to $W_X P$ and $W_Y Q$ in the GPLSSVD model or alternatively also $F_I \Delta^{-1}$ or $F_J \Delta^{-1}$. The primary difference between the GPLSSVD approach and various implementations of canonical correlation (including base::cancor()) is that all sets of scores from the GPLSSVD are limited to the rank of the decomposed matrix. That is, if $X$ has fewer variables than $Y$, then all sets of scores associated with $Y$ will be only span the vectors determined by the rank of the relationship between those matrices. Likewise, in reduced rank regression (a.k.a. redundancy analysis) there exist $\beta$ coefficients which are expressed through the GPLSSVD model above as $P \Delta$ or $\text{rrr_gplssvd}$p %*% diag(rrr_gplssvd$d$). Finally, it is worth noting that the above approaches to RRR and CCA are not the only ways to frame these techniques through the GPLSSVD. There are multiple and, in some cases, computationally simpler alternatives; however those approaches are conceptually more abstract than how I framed them here. Plus, the GSVD framework highlights how these techniques stem from the same core methods.

Let’s now visually compare the results from the GPLSSVD for PLS, RRR, and CCA. First let’s look at the latent variable scores, which expresses the maximization in GPLSSVD as scores for the rows (observations) of each data matrix.

Figure 5 shows the latent variable scores for all three of the analyses. Latent variable scores are the expression of the rows of each data matrix with respect to the components (a.k.a. latent variables). Each data matrix—i.e., $X$ and $Y$—has a set of latent variable scores per component. Typically in PLS, the latent variables for each matrix are plotted against one another, that is, the first column of $L_X$ vs. the first column of $L_Y$. Plotting the latent variables reflects what the GPLSSVD maximizes (i.e., $L^T_X L_Y$). So we show these latent variables scores for all of the GPLSSVD approaches (PLS, RRR, and CCA).

Figure 5 shows that the results are highly similar for the latent variable scores across approaches (a point I revisit soon). That is, these techniques show an approximately equivalent perspective of how the rows (observations) express themselves with respect to the latent variables. What about the variables of each data set? Figure 6 shows the component scores from these same analyses. Figure 6 shows some clear differences in how variables are related across the techniques—in particular Figure 6a from PLS. The similarities and differences in Figure
Figure 5: Latent variable scores for PLS, RRR, and CCA where with data matrices are column-wise centered and scaled. The latent variable scores for the rows of each data matrix, with the row items of $X$ on the horizontal axes and with the row items of $Y$ on the vertical axes. Panels A, C, and E show the first latent variable ($X$ vs. $Y$) and panels B, D, and E show the second latent variable ($X$ vs. $Y$). Panels A and B show PLS, panels C and D show RRR, and panels E and F show CCA.
Figure 6: Component scores for PLS, RRR, and CCA where with data matrices are column-wise centered and scaled. Panels A, C, and E show the variables from the \(X\) matrix, where panels B, D, and E show the variables from the \(Y\) matrix. The horizontal axes are the first component, where the vertical axes are the second component. Panels A and B show PLS, panels C and D show RRR, and panels E and F show CCA.

6 highlight that while these techniques are very related, they do not necessarily express the relationships between \(X\) and \(Y\) in the same way.

Recall that for these analyses, GPLSSVD optimizes for the maximum common information between the two data sets—with respect to their constraints—where
\[
L_X^T L_Y = \Delta = P^T W_X (M_X^2 X)^T (M_Y^2 Y) W_Y Q.
\]
Now let’s look at these same approaches but where the data matrices are column-wise centered but not scaled. Figures 7 and 8 show the latent variable scores and the component scores where the data are only column-wise centered. Now the analyses show much more apparent differences. The differences are because the data transformations in conjunction with the constraints, each play an important role in the results, and thus critical roles for the interpretation of those results.

Finally, let’s look at a GPLSSVD approach that makes use of all data and constraint matrices: PLS-CA. PLS-CA was initially designed as a PLS approach for categorical data (Beaton et al.
Figure 7: Latent variable scores for PLS, RRR, and CCA, but now with data only column-wise centered. The latent variable scores for the rows of each data matrix, with the row items of $X$ on the horizontal axes and with the row items of $Y$ on the vertical axes. Panels A, C, and E show the first latent variable ($X$ vs. $Y$) and panels B, D, and F show the second latent variable ($X$ vs. $Y$). Panels A and B show PLS, panels C and D show RRR, and panels E and F show CCA.
Figure 8: Component scores for PLS, RRR, and CCA, but now with the data only column-wise centered. Panels A, C, and E show the variables from the $X$ matrix, where panels B, D, and E show the variables from the $Y$ matrix. The horizontal axes are the first component, where the vertical axes are the second component. Panels A and B show PLS, panels C and D show RRR, and panels E and F show CCA.
2016) but can accommodate virtually any data type (Beaton et al. 2019). Here, let’s just focus on the problem of two categorical tables. The data for PLS-CA are processed in the same way they are for MCA, except now there are two tables. For the PLS-CA example, we have genetics in one table and age plus a clinical measure in the other table. All of these measures are categorical or ordinal. In this example and for simplicity, the ordinal data are treated as distinct levels instead of ordered levels.

R> plsca_gplssvd <- gplssvd(
+ X = deviations_matrix_X,
+ Y = deviations_matrix_Y,
+ XLW = 1/row_probabilities_X,
+ YLW = 1/row_probabilities_Y,
+ XRW = 1/col_probabilities_X,
+ YRW = 1/col_probabilities_Y
+
)

Like the other GPLSSVD techniques, PLS-CA also produces latent variable scores. But we forgo visualizing those in favor of highlighting the singular vectors and scores. That’s because PLS-CA is one particular method where we can much more clearly see the differences between the singular vectors, the generalized singular vectors, and the component scores. Figure 9 shows all sets of these scores. Figures 9a, c, and e show the scores associated with the columns of one data matrix, whereas Figure 9b, d, and f show the scores for the other data matrix. Figures 9a and b show the singular vectors, Figures 9c and d show the generalized singular vectors, and Figures 9e and f show the component scores. Figures 9 shows component 1 on the horizontal axis with component 2 on the vertical axis for all subfigures.

4.5. Final notes

There are several influential factors that drive the core principles that motivated the design and implementation of the GSVD package. These influences span the “French way” of data analyses (Holmes and Josse 2017; Holmes 2008), the relationships between various decompositions (Takane 2003). Furthermore, many of the most common multivariate techniques perform these non-arbitrary transformations via (positive semi-definitive) metrics used as constraints (see Takane GEVD & GSVD). The metrics used for constraints include, for example, χ² distances for Correspondence Analysis, Mahalanobis distances for CCA and related methods. At its core, the GSVD package provides the three primary bases—geigen(), gsvd(), and gplssvd()—of the most common multivariate techniques and numerous variants of those techniques. The package provides a radically simplified way to approach these methods: users generally need only to know what their constraints and (transformed) data should be, instead about how to perform the necessary steps (e.g., matrix multiplication, square roots of matrices).

The eigen() and svd() functions—and many of their analogs and extensions—provide a very simplified set of outputs. However, with respect to core analysis and interpretation principles, the GSVD package provides comprehensive output common to the numerous eigen-based multivariate techniques. The component scores are examples of important and comprehensive outputs from the GSVD package. The component scores provide a view of the results with respect to (1) the constraints, and (2) the length of the components (singular values).
Figure 9: Singular vectors, generalized singular vectors, and component scores from partial least squares-correspondence analysis (PLS-CA). The horizontal axes are the first component, and the vertical axes are the second component. Panels A and B show the singular vectors, panels C and D show the generalized singular vectors, and Panels E and D show the component scores. Panels A, C, and E show the columns from the $X$ matrix, where panels B, D, and F show the columns from the $Y$ matrix. Each visual helps reflect the types and amount of information we can obtain from GPLSSVD methods that make use of various sets of weights.
The component scores—and the fact that these are weighted and “stretched” versions of the
generalized vectors—means that interpretation and visualization requires caution and care.
Nguyen and Holmes (2019) provide a comprehensive view of decompositions, but most im-
portantly make suggestions on how to more appropriately show and interpret visuals. The
visuals presented here did not stretch the axis according to the proportions of the singular or
eigenvalues. That stretching is important for interpretation, but here many of the visuals are
either simple illustrations of output or for simple comparisons.

Finally, it is worth noting that many techniques can be performed with any of these decom-
positions. For examples, PLS, RRR, and CCA could be performed with the GSVD (or
even with two GEVDs one for each set of variables). Likewise, one-table techniques (e.g., CA,
or PCA) could be performed as the GSVD or GEVD (as presented earlier here with PCA).
However, the direct interfaces of these methods provide a simpler conceptual framework for
the techniques than some of these alternative approaches (e.g., CCA as two separate GEVDs).

5. Discussion

The GSVD package provides a core and minimal set of functions designed around a common
framework and nomenclature. More importantly, GSVD also conceptually unifies a large ar-
ray of multivariate techniques. Above, I show only a handful of standard and very common
multivariate approaches, and how they conceptually fit into generalized decomposition ap-
proaches as well as how to perform them with the GSVD package. The intent and design
of GSVD was to provide a unified core for those analysis approaches. Though users could
directly perform analyses with the GSVD package, there is likely more benefit to developers
and analysts to build analysis methods and packages on top of GSVD. The primary moti-
vations to build upon GSVD (i.e., use GSVD as a dependency) are because (1) GSVD only
provides a minimal set of classes and objects for S3 methods, and more importantly (2) nu-
merous multivariate techniques benefit from additional information; for examples, PCA and
CA require preprocessing steps that are necessary for external or out of sample data, and
thus require such external information (e.g., column centers, or row weights).

Though only a relatively small set of multivariate techniques were shown here, the GSVD
package was designed for virtually any variation of some of the methods presented here. Such
methods include discriminant techniques that generally fall under specific instances of PLS,
RRR, or CCA. There are also numerous variations of CA that make use of different—and
sometimes asymmetric—sets of weights (Gimaret-Carpentier, Chessel, and Pascal 1998), use
power transformations or various centers (Greenacre 2009), alternate metrics such as the
Hellinger distance (Rao 1995), and numerous other alternatives (see, e.g., Beh and Lombardo
2012) Even broader families of techniques that decompose multiple tables also fit within the
framework established here. These multi-table techniques are often ways of structuring and
transforming sets of tables, and then concatenating them in a way to produce a larger data
matrix (with rows and columns). These multi-table techniques also routinely make use of
constraints or weights imposed on the columns and rows. Some of those methods include, for
examples, constrained PCA (Takane 2013) and multiple factor analysis (Abdi, Williams, and
Valentin 2013; Bécue-Bertaut and Pagès 2008; Escofier and Pagès 1994)

Finally, the use of returned rank is highly beneficial to statistical learning and machine learn-
ing strategies such as sparsification techniques such as the penalized matrix decomposition
(Witten, Tibshirani, and Hastie 2009) or the constrained SVD (Guillemot, Beaton, Gloaguen, Löfstedt, Levine, Raymond, Tenenhaus, and Abdi 2019). Lower rank solutions is even more common for iterative algorithms like partial least squares regression (PLSR). The most common implementations of PLSR use a rank 1 SVD solution, followed by deflation of both the $X$ and $Y$ matrices. To see such PLSR implementations that depend on GSVD, please see another package I have developed that focuses on two-table/“cross-decomposition” methods (Beaton et al. (2019) see also https://github.com/derekbeaton/gpls).

In its current form, the GSVD package is lightweight, has zero dependencies, and is written in base R. The general goals of the GSVD package is both to remain lightweight—with minimal yet core functionality from a user perspective—and as a “workhorse” package. The GSVD package should be the core dependency in an analysis package, as opposed to being used as the analysis package. Given that, I plan to provide a substantial overhaul of the ExPosition (Beaton et al. 2014) family of packages in the (near) future, and GSVD is the first step towards that overhaul. Though the GSVD package is intentionally minimal with no dependencies, there are possible benefits to some dependencies in the future. For example, there are numerous packages and tools that could make the GSVD package more memory and computationally efficient. So the future of GSVD could make use the Matrix (Bates and Maechler 2019) for storage (memory) and other tools for faster decompositions themselves. Specifically, the eigen and singular value decompositions at the core of tolerance_eigen() and tolerance_svd() could be sped up and or be more memory efficient with the usage of RcppArmadillo (Eddelbuettel and Sanderson 2014), RcppEigen (Bates and Eddelbuettel 2013), or RSpectra (Qiu and Mei 2019).

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