Multiset Canonical Correlation Analysis

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Abstract

The Burt matrix collects all bivariate cross tables, and/or covariance matrices, of m variables in a single matrix. Various forms of canonical analysis based on the Burt matrix are discussed.

Contents

Note: This is a working paper which will be expanded/updated frequently. One way to think about this paper is as an update of De Leeuw (1982), using more modern computing and reporting machinery. The directory deleeuwpdx.net/pubfolders/burt has a pdf copy of this article, the complete Rmd file with all code chunks, and R and C files with the code.

1 Basic Theory

1.1 Definition

Suppose $X_1, \cdots, X_m$ are data matrices, where X_j is $n \times k_j$. Define $X := \begin{bmatrix} X_1 \mid \cdots \mid X_m \end{bmatrix}$ and $C := X'X$. The matrix C has $k_j \times k_\ell$ submatrices $C_{j\ell} = X_j' X_\ell$. Also define D as the direct sum $D := D_1 \oplus \cdots \oplus D_m$, where $D_j := C_{jj}$. From now on we suppose that all D_j are non-singular.

For $m = 3$, for example, we have

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix},$$

and

$$D = \begin{bmatrix} D_1 & 0 & 0 \\ 0 & D_2 & 0 \\ 0 & 0 & D_3 \end{bmatrix}.$$

Multiset Canonical Correlation Analysis (MCCA) finds one or more solutions of the generalized eigenequation

$$CY = mDY\Lambda, \tag{1}$$

with the generalized eigenvectors normalized by $Y'DY = I$. Also see Tenenhaus and Tenenhaus (2011) and Van der Velden and Takane (2012).

Here is a small artificial example with three matrices. It shows uses the function `listTable()`, which constructs C and D from a list of matrices.

```
set.seed (12345)
x1 <- matrix (rnorm (300), 100, 3)
x2 <- matrix (rnorm (200), 100, 2)
x3 <- matrix (rnorm (300), 100, 3)
x <- list (x1, x2, x3)
f <- listTable (x)
f$c
```

```
##             [,1]       [,2]       [,3]       [,4]        [,5]       [,6]
## [1,] 129.0320238  12.738789  -5.578408  20.334906  -0.3360786   6.820853
## [2,]  12.7387892 101.442761 -12.031152  15.647845 -13.9436246  11.774335
## [3,]  -5.5784082 -12.031152  86.270839 -27.152383   2.8396161   2.854388
## [4,]  20.3349065  15.647845 -27.152383  97.908355 -11.8448756  10.106362
## [5,]  -0.3360786 -13.943625   2.839616 -11.844876  77.9628982  12.827916
## [6,]   6.8208532  11.774335   2.854388  10.106362  12.8279157 117.839426
## [7,]  -5.4455739  -9.098341  -7.395909  -6.212267 -16.4610676   0.273929
## [8,]  18.4183132  10.929051  -8.278757   6.278734 -25.5588589 -18.025705
##            [,7]       [,8]
## [1,]  -5.445574  18.418313
## [2,]  -9.098341  10.929051
## [3,]  -7.395909  -8.278757
## [4,]  -6.212267   6.278734
## [5,] -16.461068 -25.558859
## [6,]   0.273929 -18.025705
## [7,] 107.079262   2.524830
## [8,]   2.524830 101.613899
```

```
f$d
```

```
## NULL
```

The `listTable()` function has some additional arguments, which can be used to optionally center, standardize, or orthonormalize the matrices in the list.

```
formals("listTable")
```

```
## $x
##
##
## $center
## [1] FALSE
##
## $standardize
## [1] FALSE
##
## $orthonormalize
## [1] FALSE
```

1.2 MCCA Eigenvalues

All eigenvalues of equation (1) satisfy $0 \leq \lambda \leq 1$. Clearly $m\lambda_s = y'Cy$, which shows that $\lambda \geq 0$ and $\lambda = 0$ if and only if $Cy = 0$ if and only if $Xy = 0$. The number of zero eigenvalues of (1) is consequently the nullity of X. To show that $\lambda \leq 1$ observe that

$$\sum_{j=1}^m (X_j y_j - \frac{1}{m}\sum_{j=1}^m X_j y_j)'(X_j y_j - \frac{1}{m}\sum_{j=1}^m X_j y_j) \geq 0,$$

which can be written as

$$y'Dy - \frac{1}{m}y'Cy \geq 0.$$

This proves $\lambda \leq 1$ and $\lambda = 1$ if and only if all $X_j y_j$ are equal.

The following chunk computes the eigenvalues in our small example with three matrices.

```
library (geigen)
dim(f$c)
```

```
## [1] 8 8
```

```
dim(f$d)
```

```
## NULL
```

```
#h <- geigen (f$c / 3, f$d, s = TRUE)
#rev (h$values)
```

Define Z as $\left[X_1 D_1^{-\frac{1}{2}} \mid \cdots \mid X_m D_m^{-\frac{1}{2}}\right]$ and $E := Z'Z$. Thus $E_{j\ell} = D_j^{-\frac{1}{2}} C_{j\ell} D_\ell^{-\frac{1}{2}}$ and $E_{jj} = I$ for all j.

For $m = 3$ we have

$$E = \begin{bmatrix} I & D_1^{-\frac{1}{2}} C_{12} D_2^{-\frac{1}{2}} & D_1^{-\frac{1}{2}} C_{13} D_3^{-\frac{1}{2}} \\ D_2^{-\frac{1}{2}} C_{21} D_1^{-\frac{1}{2}} & I & D_2^{-\frac{1}{2}} C_{23} D_3^{-\frac{1}{2}} \\ D_3^{-\frac{1}{2}} C_{31} D_1^{-\frac{1}{2}} & D_3^{-\frac{1}{2}} C_{32} D_2^{-\frac{1}{2}} & I \end{bmatrix}$$

The eigenvalues of $\frac{1}{m}E$ are the same as those of (1). It follows that

$$\mathbf{tr}\ \Lambda = \frac{1}{m}\sum_{j=1}^{m} k_j.$$

The sum of squares of the eigenvalues is $\frac{1}{m^2}\mathbf{tr}\ E'E$.

The matrix $D_j^{-\frac{1}{2}}$ can be the inverse of the symmetric square root of D_j, or the inverse of the triangular factor in the QR decomposition of X_j. In fact it can be any nonsingular T such that $T'D_jT = I$. Solutions for T differ only by a rotation matrix (a square orthonormal), and thus the choice of T does not change the eigenvalues of E.

The matrix E can be created by using `listTable()` with argument `orthonormal=TRUE`. It uses the Gram-Schmidt code in De Leeuw (2015a) for the orthonormalization.

```
f <- listTable (x, o = TRUE)
f$c
```

```
##               [,1]          [,2]          [,3]          [,4]          [,5]
## [1,]  1.000000e+00 -3.773024e-17  3.599551e-17  1.809187e-01  2.137444e-02
## [2,] -3.773024e-17  1.000000e+00  7.356312e-17  1.377245e-01 -1.400175e-01
## [3,]  3.599551e-17  7.356312e-17  1.000000e+00 -2.713240e-01 -2.183805e-02
## [4,]  1.809187e-01  1.377245e-01 -2.713240e-01  1.000000e+00  7.459311e-17
## [5,]  2.137444e-02 -1.400175e-01 -2.183805e-02  7.459311e-17  1.000000e+00
## [6,]  5.531522e-02  1.021675e-01  4.425189e-02  9.408917e-02  1.479562e-01
## [7,] -4.646289e-02 -8.290192e-02 -9.053349e-02 -6.090152e-02 -1.905037e-01
## [8,]  1.735305e-01  1.107133e-01 -6.072594e-02  8.107887e-02 -2.557320e-01
##               [,6]          [,7]          [,8]
## [1,]  5.531522e-02 -4.646289e-02  1.735305e-01
## [2,]  1.021675e-01 -8.290192e-02  1.107133e-01
## [3,]  4.425189e-02 -9.053349e-02 -6.072594e-02
## [4,]  9.408917e-02 -6.090152e-02  8.107887e-02
## [5,]  1.479562e-01 -1.905037e-01 -2.557320e-01
## [6,]  1.000000e+00 -1.040834e-17  2.602085e-17
## [7,] -1.040834e-17  1.000000e+00  2.775558e-17
## [8,]  2.602085e-17  2.775558e-17  1.000000e+00
```

```
eigen (f$c / length (x), symmetric = TRUE, only.values = TRUE)$values
```

```
## [1] 0.4967371 0.4448935 0.3852558 0.3440331 0.3295966 0.2575979 0.2217012
## [8] 0.1868515
```

Matrices $\tilde{X}'\tilde{X}$ and $\tilde{X}\tilde{X}'$ have the same non-zero eigenvalues, the squares of the singular values of $\tilde{X}$. Thus the non-zero λ_s are also the non-zero eigenvalues of

$$P_\bullet := \frac{1}{m}\sum_{j=1}^{m} P_j,$$

where $P_j := X_j(X_j'X_j)^{-1}X_j'$. Note that P_j does not change if X_j is replaced by X_jT with T nonsingular.

```
p <- tcrossprod (f$g) / 3
eigen (p, symmetric = TRUE, only.values = TRUE)$values[1:8]
```

```
## [1] 0.4967371 0.4448935 0.3852558 0.3440331 0.3295966 0.2575979 0.2217012
## [8] 0.1868515
```

1.3 Least Squares Loss Function

For computational purposes, especially if we incorporate optimal scaling in MCCA as in Gifi (1990), it is convenient to formulate the technique as minimization of a least squares loss function. This formulation originates with Carroll (1968). The loss function is

$$\sigma(H;Y_1,\cdots,Y_m)=\frac{1}{m}\sum_{j=1}^m\mathbf{tr}\ (H-X_jY_j)'(H-X_jY_j),$$

which we minimize over the Y_j and over all H satisfying $H'H=I$. We choose the dimensionality p. Since

$$\min_{Y_1,\cdots,Y_m}\sigma(H;Y_1,\cdots,Y_m)=\frac{1}{m}\sum_{j=1}^m\mathbf{tr}\ H'(I-P_j)H,$$

we see that the minimizing H are the eigenvectors corresponding to the p largest eigenvalues of $P_\bullet$, and

$$\min_{H'H=I}\min_{Y_1,\cdots,Y_m}\sigma(H;Y_1,\cdots,Y_m)=\sum_{s=p+1}^m(1-\lambda_s).$$

For the corresponding optimum Y_j we find $D_j^{\frac{1}{2}}Y_j=Z_j'H$, and thus $Y'DY=mH'P_\bullet H=m\Lambda$. We have $CY=mDY\Lambda$, but the columns of Y are normalized to the size of the eigenvalues.

2 Multiple Correspondence Analysis

2.1 The Burt Table

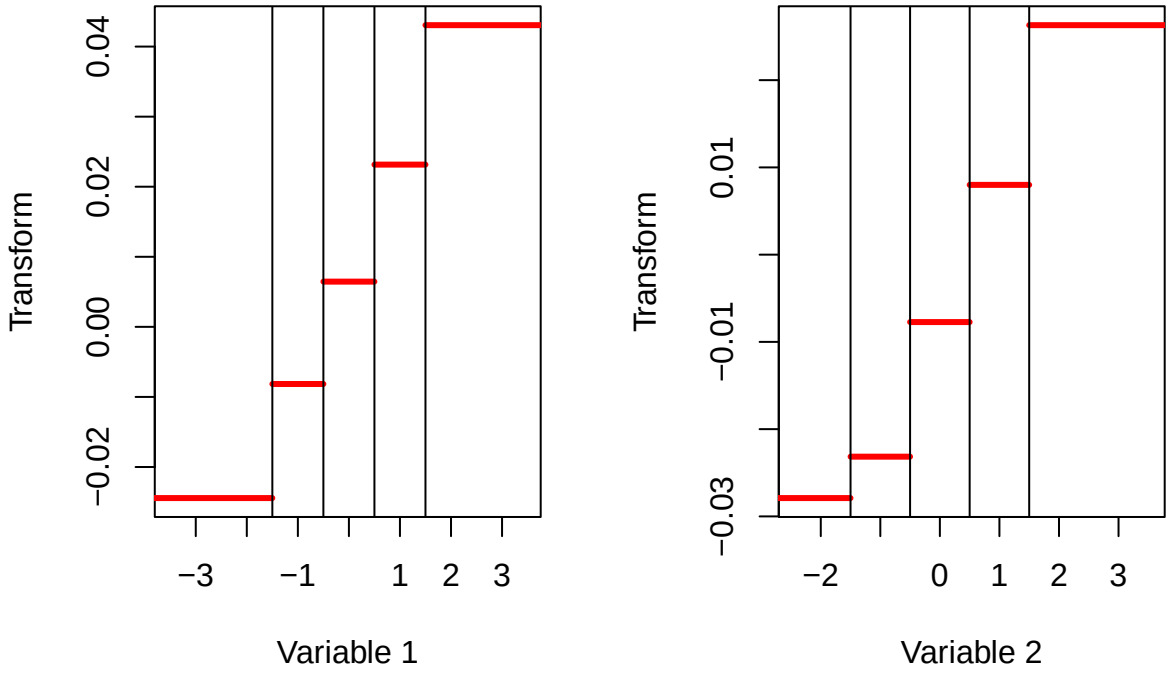
In the special case in which the X_j are indicator matrices, i.e. non-negative matrices with rows that add up to one, our MCCA technique becomes Multiple Correspondence Analysis (MCA). In this case the matrix C is called the *Burt Table*. For a detailed discussion, see Greenacre and Blasius (2006) and specifically De Leeuw (2006).

Two different cases can be distinguished. The indicator matrices can be binary, also known as *crisp*, in which case they obviously have a single nonzero element equal to one in each row, or they can be *fuzzy indicators*, discussed in detail in Rijckevorsel and De Leeuw (1988). The `burtTable()` function handles both cases by using the B-spline code in De Leeuw (2015c). The number of nonzero elements in each row of the indicator matrix is determined by the degree of the spline, with degree zero defining the *crisp* indicator. The number of columns of X_j is determined, in addition, by the number of interior knots of the spline. There is a special provision to generate crisp indicators from categorical, possibly non-numerical, variables by setting the degree equal to a negative number and by ignoring the knots argument.

In the following example we generate a sample from a four-variable standard multinormal with correlations $\frac{1}{2}$, rounded to integers. All four variables generate indicators by using knots at $-1.5,-.5,+.5$ and $+1.5$, the first three have spline degree zero and the fourth has spline degree two Thus there are three crisp indicators and one fuzzy indicator.

```
set.seed (12345)
x <- ceiling ( (matrix (rnorm (4000), 1000, 4) + rnorm (1000)) / sqrt (2))
x <- center (x)
n <- c(-1.5, -.5, .5, 1.5)
k <- list (n, n, n, n)
fp <- burtTable (x, c (0, 0, 0, 2), k)
dp <- blockSelect (fp$c, fp$ord)
hp <- geigen (fp$c / 4, dp, symmetric = TRUE)
rev (hp$values[-c(1,2,3)])[-1]
```

```
##  [1] 0.5970850 0.4037270 0.3107367 0.2823285 0.2720878 0.2638761 0.2562212
##  [8] 0.2477486 0.2387625 0.2340783 0.2222054 0.2105898 0.2042858 0.1867432
## [15] 0.1765546 0.1399286 0.1279515 0.1250894
```



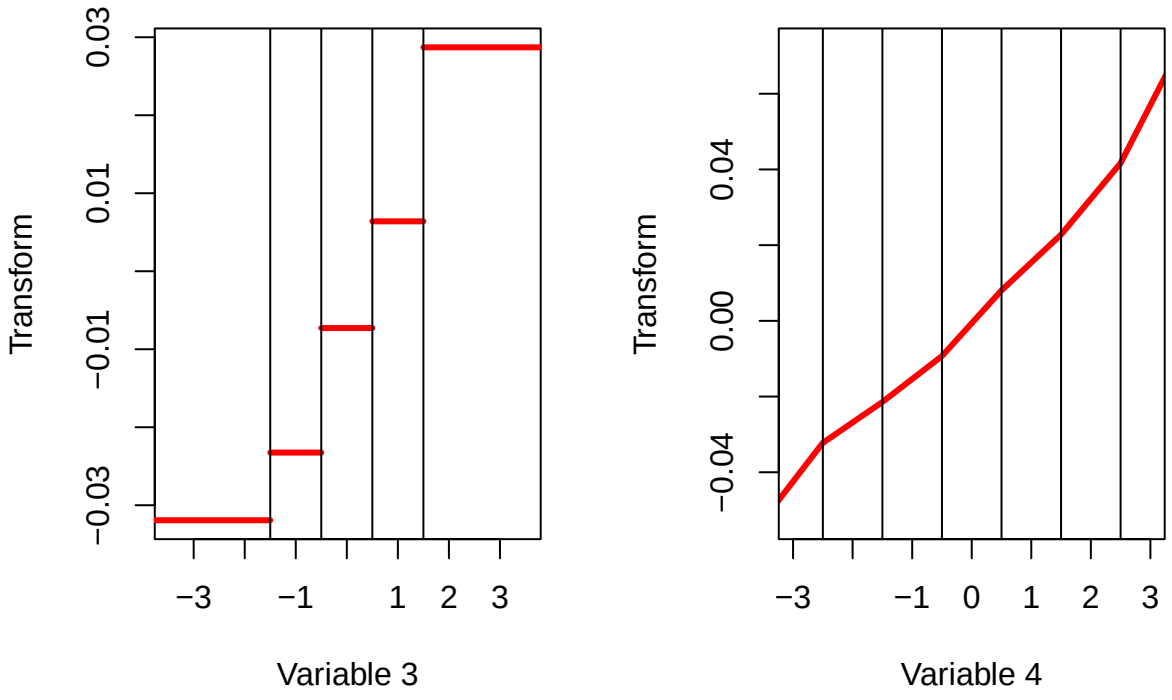


Figure 1: MCA - PCA Option

In MCA we typically use the indicator matrices to define one X_j each. But in the Gifi system De Leeuw (2015b) we can group the indicators into sets of variables to emulate other forms of multivariate analysis. In the next analysis we use two blocks, one consisting of the first variable and one of the remaining three. This makes the technique a form of regression analysis, where the first variable is predicted from the rest.

```
fr <- burtTable (x, c (0, 0, 0, 2), k, center = TRUE)
dr <- blockSelect (fr$c, c(fr$ord[1], sum (fr$ord[-1])))
hr <- geigen (fr$c / 2, dr, symmetric = TRUE)
sort (2 * hr$values - 1, decreasing = TRUE)[1:4]
```

```
## [1] 0.5916795 0.3531064 0.1975003 0.1061619
```

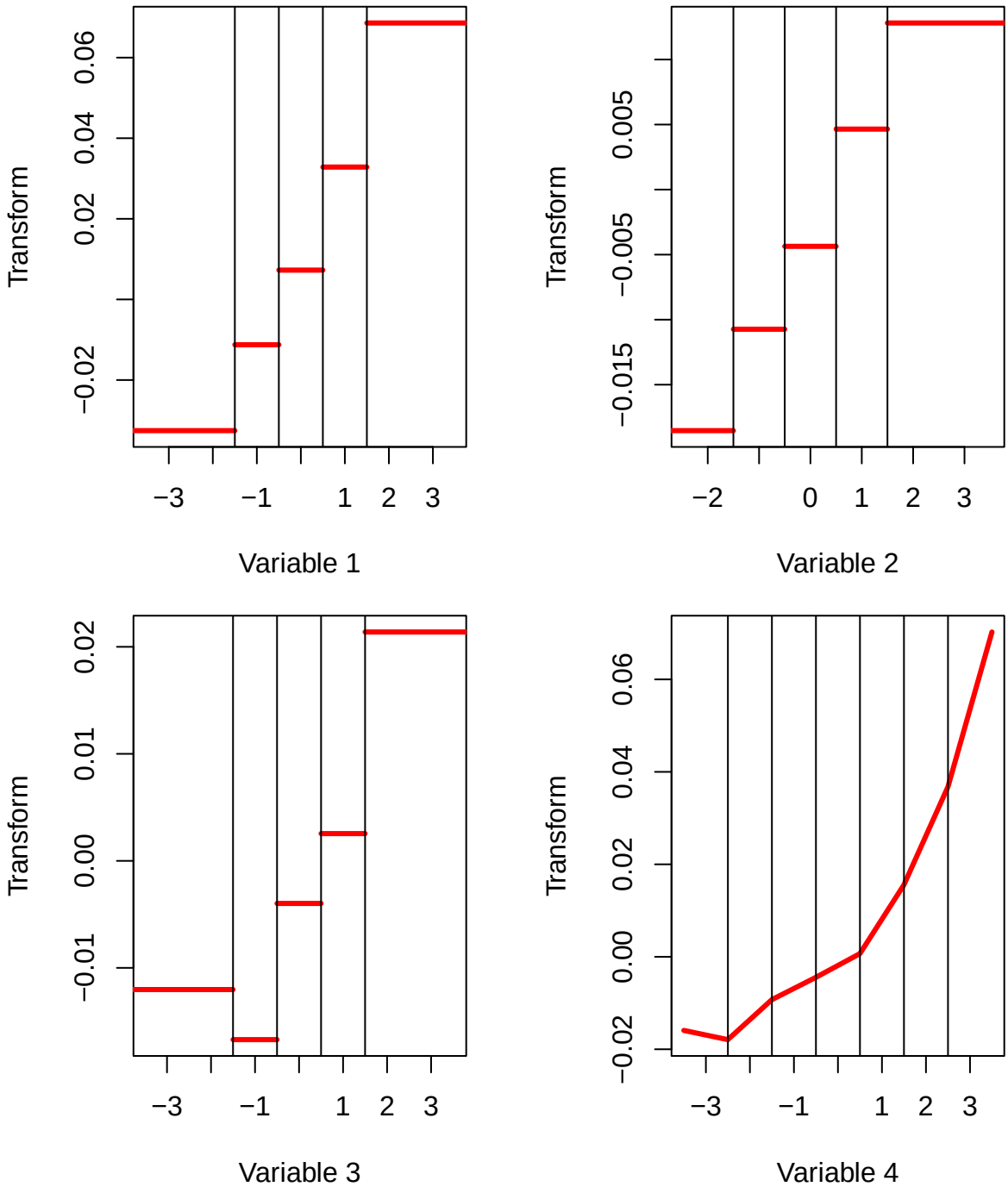


Figure 2: MCA - Regression Option

2.2 Using Homogeneity

The MCCA problem can be formulated as finding stationary values of

$$\lambda(y_1, \cdots, y_m) = \sum_{j=1}^{m} \sum_{\ell=1}^{m} y_j' C_{j\ell} y_\ell$$

over the y_j satisfying $\sum_{j=1}^m y_j' D_j y_j = m$.

Alternatively we can look for stationary values of

$$\lambda(\alpha_1, \cdots, \alpha_m, \eta_1, \cdots, \eta_m) = \sum_{j=1}^m \sum_{\ell=1}^m \alpha_j \alpha_\ell \eta_j' C_{j\ell} \eta_\ell$$

over α_j satisfying $\sum_{j=1}^m \alpha_j^2 = m$ and η_j satisfying $\eta_j' D_j \eta_j = 1$ for all j.

If we define $R(\eta_1, \cdots, \eta_m)$ with elements $r(\eta_1, \cdots, \eta_m)_{j\ell} = \eta_j' C_{j\ell} \eta_\ell$ then we want stationary values of $\alpha' R(\eta_1, \cdots, \eta_m)\alpha$ over $\alpha'\alpha = m$.

2.3 Induced Correlation Matrices

```
print (r <- inducedR (fp$c, yp[, sum(fp$ord) - 1], fp$ord))
```

```
##           [,1]      [,2]      [,3]      [,4]
## [1,] 1.0000000 0.4484230 0.4828116 0.4649239
## [2,] 0.4484230 1.0000000 0.4462666 0.4766192
## [3,] 0.4828116 0.4462666 1.0000000 0.4575092
## [4,] 0.4649239 0.4766192 0.4575092 1.0000000
```

```
eigen(r)$values / 4
```

```
## [1] 0.5970850 0.1433047 0.1307759 0.1288345
```

```
print (r <- inducedR (fp$c, yp[, sum(fp$ord) - 2], fp$ord))
```

```
##           [,1]      [,2]      [,3]      [,4]
## [1,] 1.0000000 0.1657850 0.2323857 0.2654327
## [2,] 0.1657850 1.0000000 0.2021524 0.1658702
## [3,] 0.2323857 0.2021524 1.0000000 0.1922082
## [4,] 0.2654327 0.1658702 0.1922082 1.0000000
```

```
eigen(r)$values / 4
```

```
## [1] 0.4037270 0.2170939 0.1980885 0.1810906
```

```
inducedR (fr$c, yr[,sum(fr$ord)], c(fr$ord[1], sum (fr$ord[-1])))
```

```
##           [,1]      [,2]
## [1,] 1.0000000 0.5916795
## [2,] 0.5916795 1.0000000
```

```
inducedR (fr$c, yr[,sum(fr$ord) - 1], c(fr$ord[1], sum (fr$ord[-1])))
```

```
##           [,1]      [,2]
## [1,] 1.0000000 0.3531064
## [2,] 0.3531064 1.0000000
```

2.4 Binary Variables

2.5 On Being Normal

3 Linked Singular Value Decompositions

3.1 Pairwise Canonical Correlation Analysis

If we define the $K \times K$ matrix Γ by replacing each $E_{j\ell}$ by the diagonal matrix $\Gamma_{j\ell}$ of the canonical correlations between X_j and X_ℓ, then

$$\sum_{s=1}^{K} \lambda_s^2 = \frac{1}{m^2}\mathbf{tr}\ E'E = \frac{1}{m^2}\mathbf{tr}\ \Gamma'\Gamma.$$

The canonical correlations are the singular values of the matrices $E_{j\ell}$. The matrix Γ is as follows.

```
##           [,1]      [,2]       [,3]     [,4]       [,5]      [,6]       [,7]
## [1,] 1.0000000 0.0000000 0.00000000 0.336463 0.00000000 0.2219902 0.00000000
## [2,] 0.0000000 1.0000000 0.00000000 0.000000 0.14069690 0.0000000 0.12082589
## [3,] 0.0000000 0.0000000 1.00000000 0.000000 0.00000000 0.0000000 0.00000000
## [4,] 0.3364630 0.0000000 0.00000000 1.000000 0.00000000 0.3541990 0.00000000
## [5,] 0.0000000 0.1406969 0.00000000 0.000000 1.00000000 0.0000000 0.09977141
## [6,] 0.2219902 0.0000000 0.00000000 0.354199 0.00000000 1.0000000 0.00000000
## [7,] 0.0000000 0.1208259 0.00000000 0.000000 0.09977141 0.0000000 1.00000000
## [8,] 0.0000000 0.0000000 0.02100453 0.000000 0.00000000 0.0000000 0.00000000
##           [,8]
## [1,] 0.00000000
## [2,] 0.00000000
## [3,] 0.02100453
## [4,] 0.00000000
## [5,] 0.00000000
## [6,] 0.00000000
## [7,] 0.00000000
## [8,] 1.00000000
```

Indeed, both $\mathbf{tr}\ E'E$ and $\mathbf{tr}\ \Gamma'\Gamma$ are equal to 8.6654679. Although the sum and the sum of squares of the eigenvalues of E and Γ are the same, the individual eigenvalues differ. For $\frac{1}{3}\Gamma$ they are

```
## [1] 0.5372982 0.4138783 0.3403348 0.3263318 0.3009372 0.2851846 0.2595023
## [8] 0.2031994
```

We do see, however, that the two vectors of eigenvalues are quite close. This phenomenon is studied in more detail in a later section of the paper.

For now we merely observe that we can permute rows and columns of Γ so that it becomes the direct sum of three matrices R_1, R_2 and R_3. Think of Γ as a supermatrices with nine submatrices, all diagonal. Matrix R_1 consists of all $(1,1)$ elements of the submatrices of Γ, matrix R_2 has the $(2,2)$ elements, and R_3 the $(3,3)$ elements. The utility function `partPerm()` does just that.

```
print (rm <- kplPerm (gm, c(3,2,3))$pcp)
```

```
##           [,1]     [,2]      [,3]      [,4]       [,5]       [,6]       [,7]
## [1,] 1.0000000 0.336463 0.2219902 0.0000000 0.00000000 0.00000000 0.00000000
```

```
## [2,] 0.3364630 1.000000 0.3541990 0.0000000 0.00000000 0.00000000 0.00000000
## [3,] 0.2219902 0.354199 1.0000000 0.0000000 0.00000000 0.00000000 0.00000000
## [4,] 0.0000000 0.000000 0.0000000 1.0000000 0.14069690 0.12082589 0.00000000
## [5,] 0.0000000 0.000000 0.0000000 0.1406969 1.00000000 0.09977141 0.00000000
## [6,] 0.0000000 0.000000 0.0000000 0.1208259 0.09977141 1.00000000 0.00000000
## [7,] 0.0000000 0.000000 0.0000000 0.0000000 0.00000000 0.00000000 1.00000000
## [8,] 0.0000000 0.000000 0.0000000 0.0000000 0.00000000 0.00000000 0.02100453
##           [,8]
## [1,] 0.00000000
## [2,] 0.00000000
## [3,] 0.00000000
## [4,] 0.00000000
## [5,] 0.00000000
## [6,] 0.00000000
## [7,] 0.02100453
## [8,] 1.00000000
```

The eigenvalues of this rearranged matrix are the same as those of Γ, and they are the direct sum of the eigenvalues of R_1, R_2 and R_3. Or, to put is slightly differently, we can find the eigenvalues of Γ by first permuting to block diagonal form and then finding the eigenvalues of the blocks. This gives the eigenvalues in the order determined by the block structure (ordered within blocks).

```
##           [,1]      [,2]      [,3]      [,4]      [,5]      [,6]      [,7]
## [1,] 0.5372982 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
## [2,] 0.0000000 0.2595023 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
## [3,] 0.0000000 0.0000000 0.2031994 0.0000000 0.0000000 0.0000000 0.0000000
## [4,] 0.0000000 0.0000000 0.0000000 0.4138783 0.0000000 0.0000000 0.0000000
## [5,] 0.0000000 0.0000000 0.0000000 0.0000000 0.3009372 0.0000000 0.0000000
## [6,] 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.2851846 0.0000000
## [7,] 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.3403348
## [8,] 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
##           [,8]
## [1,] 0.0000000
## [2,] 0.0000000
## [3,] 0.0000000
## [4,] 0.0000000
## [5,] 0.0000000
## [6,] 0.0000000
## [7,] 0.0000000
## [8,] 0.3263318
```

Using pairwise canonical correlations, followed by permutation to block diagonal form, cannot be recommended as a general MCCA technique. There is no obvious loss function that is minimized, and it is not clear how the canonical correlations in the different blocks should be ordered.

3.2 Two Sets of Variables

If there are only two sets the generalized eigenvalue problem for the Burt matrix becomes

$$\begin{bmatrix} D_1 & C_{12} \\ C_{21} & D_2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = 2\lambda \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix},$$

which we can rewrite as

$$C_{12}a_2 = (2\lambda - 1)D_1a_1,$$
$$C_{21}a_1 = (2\lambda - 1)D_2a_2,$$

from which we see that MCCA finds the canonical correlations between X_1 and X_2. We also see that at a solution $a_1'D_1a_1 = a_2'D_2a_2 = \frac{1}{2}$, and the canonical correlations are given by $\rho = 2\lambda - 1$. See also Van der Velden (2012).

3.3 KPL Diagonalization

In the section on pairwise canonical correlation analysis we saw that permuting pairwise canonical correlations to block diagonal form can give a decent approximation of the eigenvalues of MCCA. Here we describe the nature of this approximation in more detail, following De Leeuw (1982), Bekker and De Leeuw (1988), and De Leeuw (1988).

In MCCA we have $A'CA = m\Lambda$ and $A'DA = I$. Or, alternatively, $K'EK = m\Lambda$ with $K'K = KK' = I$, i.e. $E = mK\Lambda K'$. In CCA we have $E_{j\ell} = K_{j\ell}\Gamma_{j\ell}L_{j\ell}'$.

Let's first look at the same MCA example as before, but now with all variable bases defined by splines of degree zero (i.e. all indicators are crisp). We first compute the eigenvalues and then the approximations.

```
set.seed (12345)
x <- round ( (matrix (rnorm (4000), 1000, 4) + rnorm (1000)) / sqrt (2))
f <- burtTable (x, c (0,0,0,0), list (c (-1.5, 1.5), c (-1.5, 1.5), c (-1.5, 1.5), c (-1.5, 1.5)))
e <- makeE (f$c, c(3, 3, 3, 3))
eigen (e)$values[1:9] / 4
```

```
## [1] 1.0000000 0.4519489 0.3527894 0.2367481 0.2098061 0.2043497 0.1926123
## [8] 0.1786254 0.1731200
```

```
h <- kplSVD (e, c(3, 3 ,3, 3))
```

```
## Iteration      1 ssq      13.10653878
## Iteration      2 ssq      13.10701043
## Iteration      3 ssq      13.10727417
## Iteration      4 ssq      13.10737974
## Iteration      5 ssq      13.10742536
## Iteration      6 ssq      13.10744491
## Iteration      7 ssq       13.1074533
## Iteration      8 ssq       13.1074569
## Iteration      9 ssq      13.10745844
## Iteration     10 ssq      13.10745911
```

```
p <- kplPerm (h$kek, c(3, 3, 3 ,3))
eigen (blockSelect (p$pcp, p$ord))$values[1:9] / 4
```

```
## [1] 1.0000000 0.4518596 0.3525997 0.2361880 0.2093469 0.2018654 0.1933701
## [8] 0.1811957 0.1735746
```

```
x <- list(x1, x2, x3)
e <- listTable (x, o = TRUE)$c
eigen (e)$values / 3
```

```
## [1] 0.4967371 0.4448935 0.3852558 0.3440331 0.3295966 0.2575979 0.2217012
## [8] 0.1868515
```

```
h <- kplSVD (e, c(3, 2, 3))
```

```
## Iteration      1 ssq     0.4307643907
## Iteration      2 ssq     0.4307649187
```

```
p <- kplPerm (h$kek, c(3, 2, 3))
eigen (blockSelect (p$pcp, p$ord))$values / 3
```

```
## [1] 0.4805455 0.3908237 0.3696209 0.3392870 0.3273796 0.2902927 0.2395554
## [8] 0.2291618
```

4 Appendix: Code

```
dyn.load("gs.so")
dyn.load("splinebasis.so")

bsplineBasis <-
  function (x, degree, innerknots, lowknot = min(x,innerknots) - 1e-6, highknot = max(x,innerknots) + 1e
  innerknots <- unique (sort (innerknots))
  knots <-
  c(rep(lowknot, degree + 1), innerknots, rep(highknot, degree + 1))
  n <- length (x)
  m <- length (innerknots) + 2 * (degree + 1)
  nf <- length (innerknots) + degree + 1
  basis <- rep (0,  n * nf)
  res <- .C(
  "splinebasis", d = as.integer(degree),
  n = as.integer(n), m = as.integer (m), x = as.double (x), knots = as.double (knots), basis = as.double
  )
  basis <- matrix (res$basis, n, nf)
  basis <- basis[,which(colSums(basis) > 0)]
  return (basis)
  }

gs<-function(x) {
n<-dim(x)[1]; m<-dim(x)[2];
q<-matrix(0,n,m); r<-matrix(0,m,m)
qr<-.C("gsc",as.double(x),as.double(q),as.double(r),as.integer(dim(x)[1]),
    as.integer(dim(x)[2]))
return(list(q=matrix(qr[[2]],n,m),r=matrix(qr[[3]],m,m)))
}
```

```
center <- function (x) {
   return (apply (x, 2, function (z)
    z - mean (z)))
}

standardize <- function (x) {
  return (apply (x, 2, function (z) z / sqrt (sum (z ^ 2))))
}

listTable <- function (x, center = TRUE, standardize = TRUE, orthonormalize = FALSE) {
    n <- nrow (x[[1]])
    m <- length (x)
    g <- matrix (0, n, 0)
    l <- rep (0, m)
    for (j in 1:m) {
         h <- x[[j]]
         if (center) {
            h <- center (h)
         }
         if (standardize) {
            h <- standardize (h)
         }
         if (orthonormalize) {
            h <- gs (h)$q
         }
         g <- cbind (g, h)
         l[j] <- ncol (h)
    }
    return (list(c = crossprod (g),  g = g, ord = l))
}

burtTable <- function (x, degrees = rep (-1, ncol (x)), knots = NULL, center = FALSE, standardize = FALS
    n <- nrow (x)
    m <- ncol (x)
    g <- matrix (0, n, 0)
    l <- rep (0, m)
    for (j in 1:m) {
        z <- x[,j]
        if (degrees[j] < 0) {
            h <- ifelse (outer (z, unique (z), "=="), 1, 0)
        }
        else {
            h <- bsplineBasis (z, degrees [j], knots [[j]])
        }
        if (center) {
            h <- center (h)[, -1]
        }
        if (standardize) {
            h <- standardize (h)
        }
        if (orthonormalize) {
            h <- gs (h)$q
        }
```

```
        g <- cbind (g, h)
        l[j] <- ncol (h)
     }
    return (list(c = crossprod (g), g = g, ord = l))
}

kplPerm <- function (cc, k) {
  kl<-unlist (sapply (k, function (i) 1:i))
  p <- ifelse (outer (1:sum (k), order (kl), "=="), 1, 0)
  return (list (pcp = t(p) %*% cc %*% p, perm = p, ord = as.vector (table (kl))))
}

makeE <- function (cc, k) {
    dd <- mInvSqrt (blockSelect (cc, k))
    return (dd %*% cc %*% dd)
}

mInvSqrt <- function (x) {
    ex <- eigen (x)
    ew <- abs (ex$values)
    ev <- ifelse (ew == 0, 0, 1 / sqrt (ew))
    ey <- ex$vectors
    return (ey %*% (ev * t (ey)))
}

blockSelect <- function (cc, k) {
    l <- unlist (lapply (1:length (k), function(i) rep (i,k[i])))
    return (cc * ifelse (outer (l, l, "=="), 1, 0))
}

directSum <- function (x) {
    m <- length (x)
    nr <- sum (sapply (x, nrow))
    nc <- sum (sapply (x, ncol))
    z <- matrix (0, nr, nc)
    kr <- 0
    kc <- 0
    for (i in 1:m) {
        ir <- nrow (x[[i]])
        ic <- ncol (x[[i]])
        z[kr + (1:ir), kc + (1:ic)] <- x[[i]]
        kr <- kr + ir
        kc <- kc + ic
    }
    return (z)
}

kplSVD <- function (e, k, eps = 1e-6, itmax = 500, verbose = TRUE, vectors = TRUE) {
    m <- length (k)
    sk <- sum (k)
    ll <- kk <- ww <- diag (sk)
    itel <- 1
    ossq <- 0
```

```
    klw <- 1 + cumsum (c (0, k))[1:m]
    kup <- cumsum (k)
    ind <- lapply (1:m, function (i) klw[i]:kup[i])
    for (i in 1:m)
        kk[ind[[i]],ind[[i]]] <- t (svd (e[ind[[i]], ])$u)
    kek <- kk %*% e %*% t(kk)
    for (i in 1:m) for (j in 1:m)
        ww[ind[[i]],ind[[j]]] <- ifelse(outer(1:k[i],1:k[j],"=="),1,0)
    repeat {
        for (l in 1:m) {
            if (k[l] == 2) next()
            li <- ind[[l]]
            for (i in (klw[l] + 1):(kup[l]-1)) for (j in (i+1):kup[l]) {
                bi <- kek[i,-li]
                bj <- kek[j,-li]
                wi <- ww[i,-li]
                wj <- ww[j,-li]
                acc <- sum(wi*bi^2)+sum(wj*bj^2)
                acs <- sum((wi-wj)*bi*bj)
                ass <- sum(wi*bj^2)+sum(wj*bi^2)
                u <- eigen(matrix(c(acc,acs,acs,ass),2,2))$vectors[,1]
                c <- u[1]
                s <- u[2]
                kek[-li,i] <- kek[i,-li] <- c*bi+s*bj
                kek[-li,j] <- kek[j,-li] <- c*bj-s*bi
                if (vectors) {
                    ki <- kk[i,li]; kj <- kk[j,li]
                    kk[i,li] <- c*ki+s*kj
                    kk[j,li] <- c*kj-s*ki
                    }
                }
            }
        nssq <- sum (ww * kek ^ 2) - sum (diag (kek) ^ 2)
        if (verbose)
            cat("Iteration ",formatC(itel,digits=4),"ssq ",formatC(nssq,digits=10,width=15),"\n")
        if (((nssq - ossq) < eps) || (itel == itmax)) break()
        itel <- itel + 1
        ossq <- nssq
        }
    return(list(kek = kek, kk = kk, itel = itel, ssq = nssq))
}

inducedR <- function (c, y, k) {
  m <- length (k)
  l <- unlist (lapply (1:m, function(i) rep (i,k[i])))
  g <- ifelse (outer (l, 1:m, "=="), 1, 0)
  s <- g * matrix (y, length(y), m)
  r <- crossprod (s, c %*% s)
  e <- abs (diag (r))
  d <- ifelse (e == 0, 0, e)
  return (r / sqrt (outer (d, d)))
}
```

5 Appendix: NEWS

0.01 11/15/15

- First working version posted

0.02 11/18/15

- least squares loss function
- code for listTables and burtTables
- pairwise canonical correlations

0.03 11/21/15

- code for burt permutations
- more on pairwise CCA
- MCA case
- Two sets case

0.04 11/21/15

- KPL example

0.05 11/24/15

- refactored KPL code
- changed some sections around

0.06 11/25/15

- added some sections (empty for now)
- changed listTable() and burtTable() code

0.07 11/27/15

- induced correlation example
- induced correlation code
- more empty sections added
- made normal example somewhat bigger

0.08 12/01/15

- improved plots
- many edits
- homogeneity section (to be combined with induced correlations)

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