psychometrika-vol. 42, no. 2 june, 1977

REDUNDANCY ANALYSIS AN ALTERNATIVE FOR CANONICAL CORRELATION ANALYSIS

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A component method is presented maximizing Stewart and Love's redundancy index. Relationships with multiple correlation and principal component analysis are pointed out and a rotational procedure for obtaining bi-orthogonal variates is given. An elaborate example comparing canonical correlation analysis and redundancy analysis on artificial data is presented.

Key words: principal components, generalized multiple correlation analysis, cross battery principle component analysis.

1. Introduction

In canonical correlation analysis components are extracted from two sets of variables simultaneously in such a way as to maximize the correlation, μ , between these components. Mathematically, the criterion to be maximized under restrictions is

(1)
$$w'R_{xy}v - \frac{1}{2}\mu(w'R_{xx}w - 1) - \frac{1}{2}\nu(v'R_{yy}v - 1),$$

where μ and ν are Lagrange multipliers. Elaboration then leads to the following eigenvalue eigenvector equations [Anderson, 1958]:

(2)
$$(R_{xx}^{-1}R_{xy}R_{yy}^{-1}R_{yx} - \mu^2 I) w = 0,$$

and

(3)
$$(R_{yy}^{-1}R_{yx}R_{xx}^{-1}R_{xy} - \nu^2 I) v = 0$$

The eigenvalues μ^2 and ν^2 are equal, and are also equal to the squared canonical correlation coefficient. After extraction of the first pair of canonical variates, a second pair can be determined having maximum correlation, with the restriction that the variates are uncorrelated with all other canonical variates except with their counterparts in the other set, and so forth.

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A Fortran IV program for the method of redundancy analysis described in this paper can be obtained from the author upon request.

Whereas in bivariate correlation and multiple correlation analysis the squared correlation coefficient is equal to the proportion of explained variance of the variables under consideration, this is not the case for the canonical correlation coefficient. Canonical correlation actually gives no information about the explained variance of the variables in one set given the other, since no attention is paid to factor loadings. Two minor components might correlate very highly, while the explained variance of the variables is very low, because of the near zero loadings of the variables on those components. As a high canonical correlation does not tell us anything about the communality of two sets of variables, it is as such an analytical tool which is hard to interpret.

As an addition to canonical correlation analysis, Stewart and Love [1968] introduced the redundancy index, which is the mean variance of the variables of one set that is explained by a canonical variate of the other set. That is, in the present notation,

(4)
$$\Re_{y_i} = \mu_i^{2*} \frac{1}{m_y} * f_{y \hat{y_i}'} f_{y \hat{y_i}},$$

and

(5)
$$\Re_{y} = \sum_{l} \Re_{y_{l}},$$

where \Re_{y_i} is the redundancy of the critieria given the i^{th} canonical variate of the predictors (\Re_y is the overall redundancy). The symbol m_y stands for the number of criteria; μ_i is the i^{th} canonical correlation, while $f_{y'y_i} = v_i' R_{yy}$ is the vector of loadings of the y-variables on their i^{th} canonical component.

Unlike canonical correlation, redundancy is non-symmetric. Thus in general, given a canonical correlation coefficient, the associated redundancy of the *Y*-variables will be different from that of the *X*-variables. (Since the redundancy of the *X*-variables given the *Y*-variables is completely analogous to that of the *Y*-variables given the *X*-variables, we will only discuss the latter one.)

The redundancy formula can be looked upon as a two-step explained variance formula, in which μ^2 is the explained variance of the canonical variate of one set, given its counterpart in the other set whereas the second part of the formula is the mean explained variance of the variables by their i^{th} canonical component.

In terms of this two-step explained variance approach, canonical correlation analysis only maximizes one part of the redundancy formula. It would seem reasonable, however, to try and maximize redundancy per se.

2. The Method

To maximize redundancy it is convenient to rewrite the index. From the derivation of the canonical correlation coefficient we know [Anderson, 1958, p. 291] that,

$$R_{yx}w - \mu R_{yy}v = 0,$$

and

(7)
$$R_{yx}w = \mu R_{yy}v$$

So,

(8)
$$\Re_{y_i} = \frac{1}{m_y} * \mu_i * f_{yy_i} f_{yy_i} * \mu_i$$

(9)
$$= \frac{1}{m_y} * \mu_i * v_i' R_{yy} R_{yy} v_i * \mu_i$$

(10)
$$= \frac{1}{m_y} w_i' R_{xy} R_{yx} w_i = \frac{1}{m_y} f_{yx_i'} f_{yx_i'}$$

where $f_{y\hat{x}_i}$ is the vector of loadings of the Y-variables on the i^{th} canonical component of the X-variables. Therefore redundancy can also be looked upon as the mean squared loading of the variables of one set on the canonical variate under consideration of the other set.

Given two sets of variables X and Y standardized to zero mean and unit variance, we seek a variate $\xi = Xw$ with unit variance such that the sum of squared correlations of the Y variables with that variate is maximal, and a variate $\zeta = Yv$ for which the same holds in the reverse direction. The correlation of the Y-variables with the variate ξ is given by the column vector (1/N)Y'Xw; the sum of squared correlations is equal to the minor product moment. So we have to maximize

(11)

$$\Phi = \frac{1}{N^2} w' X' Y Y' X w - \mu(\frac{1}{N} w' X' X w - 1),$$

$$\Psi = \frac{1}{N^2} v' Y' X X' Y v - \nu(\frac{1}{N} v' Y' Y v - 1),$$
or

or

(12)

$$\Phi = w'R_{xy}R_{yx}w - \mu(w'R_{xx}w - 1),$$

$$\Psi = v'R_{yx}R_{xy}v - \nu(v'R_{yy}v - 1)$$

Setting the partial derivatives with respect to w and v equal to zero we get

(13)

$$\frac{\delta\Phi}{\delta w} = R_{xy}R_{yx}w - \mu R_{xx}w = 0,$$

$$\frac{\delta\Phi}{\delta v} = R_{yx}R_{xy}v - \nu R_{yy}v = 0,$$

which can be written as two general characteristic equations:

(14)
$$(R_{xy}R_{yx} - \mu R_{xx})w = 0,$$
$$(R_{yx}R_{xy} - \nu R_{yy})v = 0.$$

The numerical solution to this problem is formally identical to that for the case of canonical correlation, since both the matrix products $R_{xy}R_{yx}$ and $R_{yx}R_{xy}$ and the matrices R_{xx} and R_{yy} are real symmetric matrices. However, the eigenvalues μ and ν are not equal, as in the case of canonical correlation analysis, so one has to compute both eigenstructures. We can interpet μ as m_y times the mean variance of the Y-variables that is explained by the first canonical variate of the X-variables. We will return to this point later.

When subsequent redundancy variates are determined we want them to be uncorrelated with the preceding variates extracted from the same set. It is not, in general, possible to have *bi-orthogonal* components in redundancy analysis, i.e. the components in the one set are not necessarily orthogonal to the components in the other set, since Xw and Yv are determined separately (in canonical correlation analysis the canonical components are determined biorthogonally).

The functions to be maximized when the j^{th} variates are determined are

 $\Phi_{j} = w_{j}' R_{xy} R_{yx} w_{j} - \mu_{j} (w_{j}' R_{xx} w_{j} - 1) - 2 \sum_{i} \alpha_{i} w_{j}' R_{xx} w_{i},$

$$\Psi_{j} = v_{i}' R_{yx} R_{xy} v_{j} - v_{j} (v_{j}' R_{yy} v_{j} - 1) - 2 \sum_{i} \beta_{i} v_{j}' R_{yy} v_{i},$$

for $i = 1, \dots, j - 1$.

Differentiating and setting equal to zero, leads to

(16)
$$\begin{cases} \frac{\delta \Phi_j}{\delta w_j} = R_{xy} R_{yx} w_j - \mu_j R_{xx} w_j - \sum_i \alpha_i R_{xx} w_i = 0 \\ \frac{\delta \Psi_j}{\delta v_j} = R_{yx} R_{xy} v_j - \nu_j R_{yy} v_j - \sum_i \beta_i R_{yy} v_i = 0 \end{cases}$$

Premultiplication by w_i and v_i respectively for every *i* gives us

(17)
$$w_i' R_{xy} R_{yx} w_j - \alpha_i = 0,$$
$$v_i' R_{yx} R_{xy} v_i - \beta_i = 0.$$

Because $w_i' R_{xy} R_{yx}$ is equal to $\mu_i w_i' R_{xx}$ (cf. the characteristic equation for the first variate) and $v_i' R_{yx} R_{xy}$ is equal to $v_i v_i' R_{yy}$, we have

(18)
$$\mu_i w_i' R_{xx} w_j - \alpha_i = 0 \rightarrow \alpha_i = 0,$$
$$\nu_i v_i' R_{yy} v_j - \beta_i = 0 \rightarrow \beta_i = 0,$$

which leaves us with the same characteristic equation that we found for the first variates. In other words, the vectors w_j and v_j satisfying the above restrictions are proportional to the j^{th} eigenvectors of the characteristic equations

(19)
$$(R_{xy}R_{yx} - \mu R_{xx})w = 0,$$
$$(R_{yx}R_{xy} - \nu R_{yy})v = 0.$$

Norming the eigenvector w_j so as to satisfy $w_j' R_{xx} w_j = 1$, we have the j^{th} factor of the predictors explaining a maximum of variance in the criteria (and vice versa).

3. Multiple Correlation as a Special Case of Redundancy Analysis.

When we take a closer look at the matrix product $R_{xx}^{-1}R_{xy}R_{yx}$, we can see that there is some resemblance with multiple correlation. When we think of just one Y-variable, then $R_{xx}^{-1}R_{xy}$ is the column vector of β -weights in the multiple regression of that variable. Now, however, it is not the row vector of β -weights which is postmultiplied with the column vector of correlations of that variable with the predictors to give a scalar, but rather the reverse is true, to yield a matrix. In this matrix, the diagonal elements are the β -weights of the corresponding predictor in the multiple regression of the criterion times its correlation with the criterion; in other words, the partial regression coefficient of the given predictor in the multiple regression of the criterion. The trace of that matrix is the total proportion of variance of the criterion accounted for by all predictors (the multiple correlation squared). From this it is obvious that canonical redundancy analysis includes as special cases multiple and bivariate correlation. The equations are, for only one Y-variable,

(20)
$$(R_{xx}^{-1}r_{xy}r_{yx} - \mu I)w = 0,$$

or

(21)
$$(\beta r_{yx} - \mu I)w = 0.$$

When $R_{y,x}^2$ is substituted for μ , and β for w, one can show that the characteristic equation still holds:

(22)
$$\beta r_{yx} R_{xx}^{-1} r_{xy} - R_{y,x}^{2} \beta = 0;$$

(23)
$$\beta (R_{y,X}^2 - R_{y,X}^2) = 0.$$

So in the case of one criterion, μ is the multiple correlation squared and w is the vector of β -weights.

When we generalize to more Y-variables, the j^{th} diagonal element in $R_{xx}^{-1}R_{xy}R_{yx}$ is the sum of contributions of the j^{th} X-variable to the multiple correlation of all Y-variables with the set of X-variables. Thus it is possible to look at those diagonal elements as a kind of overall canonical partial regression coefficients. The trace of the matrix product under consideration is as expected equal to the sum of the redundancies of the variables of the other set.

So, when all redundancy components of the X-variables are determined, the explained variance of the Y-variables is equal to their respective squared multiple correlation with the X-variables. This is also true for canonical correlation analysis of which multiple correlation is a special case.

When there are residual dimensions (X and Y have a different rank) for one of the two sets, the variables of the other set will have zero loadings on them. This then implies that both analyses, when all possible components are determined, span the same space, though in a different way.

4. Principal Component Analysis as a Special Case.

When the two sets upon which redundancy analysis is performed are the same, (19) leads to

(24)
$$(R_{xx}^{-1}R_{xx}R_{xx} - \mu I)w = 0,$$

or

(25)
$$(R_{xx} - \mu I)w = 0,$$

which is the characteristic equation of principal component analysis.

The characteristic equation (2) of canonical correlation analysis performed on two identical sets of variables contains an identity matrix, out of which the components are to be extracted. This is obvious in this case where all pairs of canonical variates correlate perfectly. Thus principal component analysis can be looked upon as a special case of redundancy analysis, but not, however, as a special case of canonical correlation analysis.

5. Bi-orthogonality

When a redundancy analysis is performed, extracting from each set p factors, for example, the explained variance of the variables in each set is a maximum, but the sets of variates spanning maximal redundant spaces are not bi-orthogonal. That is to say, the correlation matrices of variates within sets $(\Phi_{xx} \text{ and } \Phi_{yy})$ are identity matrices, but the matrix of intercorrelations between sets of variates Φ_{xy} ($w'R_{xy}v$) is not a diagonal one. For some applications bi-orthogonality could be a desirable property.

Thus we seek orthogonal rotation matrices T and S such that $\Xi^* = \Xi T$ and $Z^* = ZS$ are sets of variates that are bi-orthogonal, where Ξ is the matrix of redundancy variates ξ of the X-variables and Z is the matrix of redundancy variates ζ of the Y-variables. This now can be done by performing a canonical correlation analysis upon the redundancy variates Ξ and Z.

The characteristic equation (see [2]) becomes

(26)
$$(\Phi_{xx}^{-1}\Phi_{xy}\Phi_{yy}^{-1}\Phi_{yx} - \alpha^2 I)t = 0.$$

Because Φ_{xx} and Φ_{yy} are identity matrices this reduces to

$$(27) \qquad (\Phi_{xy}\Phi_{yx} - \alpha^2 I)t = 0$$

As in canonical correlation analysis, s can be found as a function of t:

(28)
$$s = \Phi_{yx} t/\alpha,$$

and α^2 is the squared correlation between the variates Ξt and Zs.

The whole procedure can be summarized as

(29)
$$(\Phi_{xy}\Phi_{yx}-\alpha^2 I)T=0,$$

and

$$S = A^{-1}\Phi_{yx}T,$$

where A^{-1} is the diagonal matrix of inverses of the correlations between pairs of variates. It is possible to view T and S as orthogonal rotation matrices, containing the sines and cosines between old redundancy variates and new (biorthogonal) redundancy variates.

6. An Example with Artificial Data

Of four X-variables and four Y-variables the intercorrelation matrices R_{xx} and R_{yy} were constructed by means of orthogonal pattern matrices F and G; $R_{xx} = FF'$, $R_{yy} = GG'$. The matrices F and G are given in Table 1a. The matrix R_{xy} was constructed with the same loadings and a more or less arbitrary matrix of intercorrelations between the components of the two sets. This matrix and the resulting total correlation matrix can be found in Table 1b and 1c respectively.

In Table 2 the matrix-products $R_{xx}^{-1}R_{xy}R_{yx}$ and $R_{yy}^{-1}R_{yx}R_{xy}$ are given. The diagonal entries of these matrices are interesting as they can be looked upon as a kind of overall canonical partial regression coefficients (above). For example, .643 is the sum of partial regression coefficients of the first X-variable in the multiple regression of each of the Y-variables on the set of X-variables. In Table 3 the beta-weights for the construction of the variates are given for canonical correlation analysis and redundancy analysis respectively. In Table 4 the loadings are given of the X- and Y-variables on both the canonical and redundancy variates. So all in all, we have eight sets of factor loadings.

Table 5 gives the redundancies as obtained by canonical correlation analysis and redundancy analysis respectively. As the complete set of factors is determined, the total redundancies are the same for both types of analysis (above). Differences between both methods can be easily seen by deleting, for example, the last component of both.

The redundancy (explained variance) per variable can be obtained by summating the squared loadings (as given in Tables 4a and 4b) of a variable on the components of the other set. In Table 6 the correlations between the sets of variates are given, illustrating the lack of bi-orthogonality for the case of redundancy analysis.

When the rotational procedure described above is performed on the complete set of redundancy factors given above, the canonical correlation solution will result, as in this case where both methods span the same space (above). However if only the first two factors are retained, the solution will be definitely different from that for canonical correlation retaining just two fac-

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TABLE 1
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Matrices in the construction procedure

	= # 2 5 1						**=====	
(a) fa	actor patte	ern F facto	ors		G factors			
2 3	+(.50 ^{1/2}) -	$(.40^{\frac{1}{2}}) + (.40^{\frac{1}{2}}) -$	$(.07^{\frac{1}{2}}) + (.07^{\frac{1}{2}}) +$	(.03 ^{1/2}) (.D3 ^{1/2})	$+(.40^{\frac{1}{2}}) - (.30^{\frac{1}{2}}) + (.20^{\frac{1}{2}}) + (.10^{\frac{1}{2}})$			- (.10 ^{1/2}) + (.10 ^{1/2}) + (.10 ^{1/2})
(b) co	mponent ir	tercorrel	lations					·····
		Y-compo	onents					
X-compone	ents 1	2	3	4				
1	.70	.10	10	.10				
2	10	.75	.10	10				
3	+.10	10	.80	.10				
4	10	+.10	10	.85				
(c) re	sulting co	orrelation	matrix	<u> </u>				
	1	2	3	4	5	8	7	
2	.800							
3	.140	.060						
4	.060	.140	.800					
5	003	.062	.422	.710				
6	.265	.203	.714	.440	.400			
7	.404	.709	142	.089	.200	.000		
8	.723	,461	012	037	.000	,200	,400	

tors. In Table 7 the rotation matrices T and S are given, which rotate the two pairs of variates in bi-orthogonal form.

By postmultiplication of the original sets of loadings by the appropriate rotation matrix, the loadings on the bi-orthogonal redundancy variates are found. These are presented in Table 8, while the diagonal matrix of intercorrelations between rotated X- and Y-variates is finally given in Table 9.

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TABLE 2
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	Matrix products $R_{xx}^{-1}R_{xy}R_{yx}$ and $R_{yy}^{-1}R_{xy}R_{xy}$										
^R × ^{−1} ^R ×y ^R yx						R ⁻¹ R yy ^y y	x ^R xy		-		
.643	.273	.054	.004		.517	.347	140	189			
.146	.518	031	.085		.435	.657	.175	.234			
079	213	.612	.111		024	.081	.582	.451			
.128	.261	.113	.606		082	.097	.349	.509			
				<u> </u>					-		

A more or less substantive evaluation of the above example can be given by assuming that the X- and Y-variables are intelligence tests. The canonical correlation method finds as first factors those that are maximally correlated, but unimportant in the sense of explained variance. The test batteries resemble

			TABLE	3					
		Beta we	ights fo	r canonica	1				
		correla	tion- an	d redundan	cy analysis				
									= =
		canonic variate				reduno varia			
	1,182	-1,047	.781	395	.508	.184	0.842	-1.503	
x-	-1.334	1.201	.102	152	.413	.210	530	+1.662	
variables	-1.585	790	307	162	266	834	1.029	+1.197	
	1,524	.619	-,330	 667	.606	161	-1.157	-1.235	
		canonic variate				redun varia	-		
	.867	.185	485	530	-,101	.620	480	.823	
Y-	955	360	125	494	559	.391	.451	796	
variables	555	.915	.337	-,208	473	416	728	613	
	.644	~ .558	.705	279	392	~,367	.531	.855	

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TABLE 4a
```

Factor loadings in canonical correlation analysis

		X-var	iates			Y-varia	tes	
	016	159	.799	580	014	130	.615	415
	271	.403	.661	571	237	.330	.509	409
X-	281	370	455	760	245	-,302	350	543
variables	.140	.092	514	841	.122	.075	-,395	602
	.327	.183	360	550	.374	.224	467	769
	419	326	137	545	480	398	178	761
Y− variables	108	.596	.402	~.304	124	.729	.522	425
	.202	216	.627	329	.231	264	.815	460

each other to a high degree, but in quite minor facets. The first two intelligence dimensions of the X-battery yield mean explained variances of 10.0% for the X-variables and 8.9 percent for the Y-variables. The situation is not as bad for the first two factors of Y. Here the results are 31.2 and 21.9 respectively.

By contrast, the first two redundancy factors of X explain 85.7 percent of

TABLE 4b										
Factor loadings in redundancy analysis										
				*=======						
		x-	variate	S		Y-var:	iates			
	.837	.226	.492	080	.343	454	-,423	264		
	.888	.285	.043	+,359	.295	575	.341	.251		
X- variables	.315	925	.189	+.099	.590	.328	-,289	.291		
Variables	.482	-,788	358	135	.538	.246	.395	289		
	622	332	.211	.157	419	.693	-,445	.382		
	636	346	210	151	678	.565	.366	-,295		
Y- variables	370	.604	.217	144	650	439	612	106		
VOLTOUIES	345	.589	227	.148	693	455	.330	.451		

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TABLE 5
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Redundancies for canonical correlation analysis (C.C.A.) and redundancy analysis (R.A.)

	С,	.C.A.	R.A.	
;	X-variables	Y-variables	X-variables	Y-variables
	.033	.084	.262	.210
	.056	.135	.235	.176
	.229	.176	.047	.133
	.249	.200	.023	.075
tota	.567	.595	.567	.595
-			*******	<u></u>

the variance of the X-variables and 49.7 percent for the Y-variables. Given the first two Y-variates, the two figures are 68.4 and 38.6 respectively.

The danger of obtaining highly correlated, but unimportant factors in a canonical correlation analysis is especially present when there are two variables, one in each set, which are not characteristic for the whole set, but yet highly correlated with each other. Then one can find a factor pair of essentially unique factors as the first canonical factors.

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TABLE 6
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Correlation matrices of X- and Y-variates

 (Φ_{xy}) for both types of analysis

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C.C.A.
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R.A.
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.873	.000	.000	.000	689	115	175	.146
.000	.818	.000	.000	.116	733	150	.094
.000	.000	.769	.000	168	156	.774	107
.000	.000	.000	,715	138	081	~. 126	-,842

TABLE 7

Rotation matrices T (for X-variables)

and S (for Y-variables)

	Т	S	
.0667	.9978	0943	.9955
.9978	0667	.9955	.0943

TABLE 8

Loadings after rotation to bi-orthogonality

	X-var	iates	Y-variates						
	.281	.820		430	.372				
X	.343	.867		554	.333				
variables	902	.376		.366	.566				
	754	.533		.281	.521				
	272	651		.729	651				
Y~	285	665		.627	~.665				
variables	.636	311		376	311				
	.619	288		388	288				

,

TABLE 9

Correlation matrix of the new redundancy variates after rotation. Y-variates -.7420 .0000 X-variates .0000 -.6986

In redundancy analysis it is not necessary to extract factors from both sets. This has an important advantage. When we have a set of dependent and independent variables, the predictive qualities of the independent set are found in the redundancy factors without the complication of taking into account the factors of the other set. It is easily seen that the Y-variates can explain more variance of the X-variates, than the other way around. However, the predictive power of the X-battery with respect to the other battery is almost entirely concentrated in the first two factors. This is less the case for the Y-set.

Retaining the first two dimensions of each battery, the resulting spaces are optimal in the redundancy sense. When one wants to interpret the factors as intelligence dimensions, bi-orthogonality could be desirable. Doing a rotation towards bi-orthogonality does not influence the explained variances for the total space; however, a different distribution of explained variance over factors will result. As a result the factor pairs can be interpreted irrespective of all the other intelligence factors of both sets.

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Manuscript received 7/9/75 Final Version received 5/24/76