ANNALES DE LA FACULTÉ DES SCIENCES DE TOULOUSE

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Annales de la faculté des sciences de Toulouse 6e série, tome 11, nº 4 (2002), p. 469-483
<http://www.numdam.org/item?id=AFST_2002_6_11_4_469_0>

Annales de la Faculté des Sciences de Toulouse Vol. XI, n° 4, 2002
pp. 469–483

Biplots for matched two-way tables [*]

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RÉSUMÉ. — Cet article a pour objet l'analyse exploratoire de tableaux appariés à deux entrées et leur représentation par des « biplots ». Ce faisant, nous revoyons la décomposition en valeurs singulières des matrices réelles et complexes. Il est montré comment des méthodes classiques, initialement introduites pour analyser des tableaux carrés, s'étendent à ce cadre plus général. L'interprétation en terme de modèle de ces « biplots » est aussi tirée au clair.

ABSTRACT. — This paper is an investigation into the exploratory analyses of matched two-way tables and their biplot visualizations. In doing so, we revisit the singular value decomposition of real and complex matrices. It is shown how standard methods, initially derived for the analysis of square tables, extend to this more general setting. The modeling interpretation of these biplots is also elicited.

(*) Reçu le 18 septembre 2001, accepté le 18 septembre 2002
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1. Introduction

A central concept in the analysis of square tables is that of symmetry and, consequently, that of departure from symmetry (Caussinus [2]). This is illustrated in several analyses: some are model based (Caussinus [2], and van der Heijden and Mooijaart [20]), some are matrix based (Constantine and Gower [5], Escoufier and Grorud [8], and Greenacre [14]), some are mixed (van der Heijden *et al.* [19]). In the exploratory approaches the square table under consideration, possibly pre-processed, is split into two matrices, a symmetric part and a skew-symmetric part. In the generalized linear modeling approach, analogous decompositions are considered for the predictor (see van der Heijden and Mooijaart [20]).

A similar decomposition can be elaborated for a set of two matched two-way tables. The concept of symmetry translates into the concept of a "common" part, while departure from symmetry into departure from the common part, that is the "specific" part. Most statistical analyses addressed to square tables can then be extended. As expected by the aficionados of square tables, it turns out that descriptive and modeling points of view are closely intertwined.

What follows is an investigation into the exploratory analysis of a set of two matched two-way tables and their biplot visualizations. It is shown how standard methods, initially derived for the analysis of square tables, extend to this more general setting. This is illustrated on a data set that we present in section 2. The concepts of extended symmetry (the "common" part) and extended skew-symmetry (the "specific" part) are defined in section 3. In section 4, we consider the singular value decomposition of real and complex matrices for the analysis of extended symmetry and extended skew-symmetry. The corresponding biplot visualizations and interpretations are presented in section 5. As expected, these descriptive techniques develop into intermediate models in a hierarchy of well-known linear models. The last section is devoted to this development.

2. Data

We consider the results of the two referenda held in New Caledonia in 1988 and 1998 taken from an article of Jean-Louis Saux in "*Le Monde*" dated Tuesday 10 November 1998 (see Table 1). The size of this data set is rather small but this is intended to balance the intricacy of the statistical interpretation of the biplots that we present here.

2.1. Matched two-way tables

Table 1 exemplifies the situation where a set of two matched two-way tables is of interest: the potential voters are cross-classified according to their vote (*abstention, blanc, oui, non*) and their province (*Îles, Nord, Sud*) on these two occasions. This will appear as a simple extension of the concept of square tables, namely two-way tables which are cross-classified according to two homologous factors (with levels in one-to-one relationship). However in our case, nothing is square except for the unobserved geographical mobility table and voting transition table which would be of great interest! A similar but simpler situation is investigated in McCullagh and Nelder [17, subsection 9.3.3] where the estimation of voter transition probabilities from marginal frequencies is considered. Here, the analysis aims at detecting vote $(I) \times$ province (J) interactions and, possibly, their evolutions over occasion $(T = 1, 2)$.

Table 1. — Referenda in New Caledonia in 1988 and 1998.

	1988			1998		
Province :	Sud	Nord	Îles	Sud	Nord	Îles
Vote						
abstention	19061	6973	6292	12612	6831	8049
blanc	3932	606	46	1687	377	51
oui	14049	10624	4613	32185	16031	7203
non	18765	2493	808	18909	2439	342

2.2. Pre-processing

Since we are dealing with count data, it is quite natural to keep in mind a Poisson kernel. Approximate normality is then derived by using the square root transformation. Such a pre-processing provides two matched matrices, the entries of which are normally distributed with constant variance of $\frac{1}{4}$. Normality and matrix form are here of special interest since we want to use least-square methods, namely the singular value decomposition of matrices.

Finally, each table is double-centred to filter (additive) main effects while preserving higher order interactions. A model based interpretation of this pre-processing will be given in section 6.

In passing we note that the square root transformation has been also advocated on different grounds for the singular value decomposition of a matrix of row profiles (Domenges and Volle [6]).

3. Extended symmetry and extended skew-symmetry

Let A and B denote the resulting matched matrices. Let $C = \frac{1}{2}A + \frac{1}{2}B$ and $D = \frac{1}{2}A - \frac{1}{2}B$. Matrix C is interpreted as the "common" part of the matched tables A and B while D $(-D)$ is the "specific" part of A over B (B over A).

It is easily seen that these extend both concepts of symmetry and skew-symmetry for a square matrix. If A is a square matrix, possibly pre-processed, let $B = A'$, the transpose of A. Then C and D reduce to the decomposition of a square matrix A into its symmetric and skew-symmetric parts: $C = \frac{1}{2}A + \frac{1}{2}A'$ and $D = \frac{1}{2}A - \frac{1}{2}A'$ with $D = -D'$.

Considering a square table A as a set of matched tables A and A' is not new: this "trick" is used in a modeling context for fitting quasi-symmetry (see the "three dimensional representation of quasi-symmetry" in Bishop, Fienberg and Holland [1]). It turns out that it can also be used to fit reduced rank models (Falguerolles [9] and Falguerolles and van der Heijden [12]).

The "common" matrix C and the "specific" matrix D for the example are given in Table 2.

Table 2. — Matrices C and D for the example.

	C			D		
Province :	Sud	Nord	Îles	Sud	Nord	Îles
Vote						
abstention	-11.21	-4.90	16.11	-9.90	2.19	7.71
blanc	-13.87	4.68	9.19	-6.12	1.72	4.40
oui	-3.24	11.06	-7.82	13.82	-5.21	-8.61
non	28.32	-10.84	-17.48	2.20	1.30	-3.50

4. Singular values decompositions

Biplot visualizations for a given data matrix M are derived from reduced rank approximations obtained by (generalized) singular value decomposition, where these approximations are least-squares optimal (Gabriel [13]). We review some of the singular value decompositions which can be considered for the joint analysis of tables A and B (or of C and D). We omit all discussion pertaining to metric choice in the possible use of generalized singular value decomposition although we recognize that these potentially affect the visual aspects of associated biplots.

4.1. Concatenating A and B

One obvious strategy is to analyse the (pre-processed) block matrices:

$$M = \begin{pmatrix} A \\ B \end{pmatrix} \quad \text{or} \quad M = \begin{pmatrix} A & B \end{pmatrix}$$

In the example the first analysis may reveal the change of vote categories for fixed provinces and the second the difference between provinces for fixed vote categories. This approach is not pursued further, mainly for its lack of symmetry with respect to the cross-classifying factors I and J.

4.2. Extended Constantine–Gower decomposition

This approach concentrates on separate analyses of C, the "common" part, and D, the "specific" part. See Constantine and Gower [5] for the analysis of a square table A where $C = \frac{1}{2}A + \frac{1}{2}A'$ and $D = \frac{1}{2}A - \frac{1}{2}A'$. Indeed, we have $||A||^2 + ||B||^2 = ||C||^2 + ||D||^2$ (for the Frobenius norm).

In the example, since C and D are double-centred (by heredity) and since they each have smallest dimension equal to 3, C and D have maximal order 2 which is here the case.

Applying the singular value decomposition to matrices C and D, it turns out that C has general form:

$$s_1^C u_1^C (v_1^C)' + s_2^C u_2^C (v_2^C)'$$

while D has:

$$s_1^D u_1^D (v_1^D)' + s_2^D u_2^D (v_2^D)'$$

with standard notation. The ranks of C and D being 2, each singular value decomposition gives rise to a two-dimensional biplot which fully visualizes its corresponding matrix.

Table 3. — The squared singular values of C and D.

matrix	squared first singular value	squared second singular value	total
C	1795.41	331.89	2127.30
D	522.49	10.62	533.11
total			2660.41

The squared singular values of C and D are reported in Table 3 as well as their total. The modeling interpretation of the latter will be given in section 6. The first singular value of D is quite large and even larger than the second singular value of C. This indicates significant changes between the two referenda. This was noted in "*Le Monde*" where Jean-Louis Saux stated that "*l'évolution est donc considérable*".

Note that the singular value decomposition of the block matrix:

$$M = \begin{pmatrix} A & B \\ B & A \end{pmatrix}$$

collects the singular elements of both C and D, thus ordering the dimensions attributable to each aspect (Greenacre [14, 15]).

4.3. Extended complex decomposition

The idea is to analyse the complex matrix $C + iD$ by complex singular value decomposition (Steward [18]). We have now $||C + iD||^2 = ||C||^2 + ||D||^2$, and complex singular value decomposition provides complex left and right singular vectors and real positive singular values. Note that each pair of associated complex left and right singular vectors are given up to a product by complex conjugate scalars with unit norm. This lack of identifiability is overcome by introducing one constraint. Escoufier and Grorud [8] used this approach for the analysis of a square table A where $C = \frac{1}{2}A + \frac{1}{2}A'$ and $D = \frac{1}{2}A - \frac{1}{2}A'$. See also Chino, Grorud and Yoshino [4].

Again, considerations of dimensions and calculations show that $C+iD$ is of order 2. The squared real singular values obtained in the complex singular decomposition of $C+iD$ are given in Table 4 as well as their sum of squared values.

Table 4. — The singular values of $C + iD$.

matrix	squared first singular value	squared second singular value	total
$C + iD$	2348.20	312.21	2660.41

The order one complex approximation of $C + iD$ is :

$$s_1(u_1 + iu_2)(v_1 - iv_2)' \tag{1}$$

which can be rewritten as:

$$s_1\left(u_1v_1' + u_2v_2'\right) + is_1\left(u_2v_1' - u_1v_2'\right). \tag{2}$$

In (2), the real part approximates C, the "common" part, while the imaginary part approximates D, the "specific" part. Interestingly, it turns out that the entries of the approximation of C can be read as an inner product in a two-dimensional Euclidean space while the entries of the approximation of D as signed areas in the same space. Remember that D is the "specific" part of A over B and $-D$ the "specific" part of B over A: this sign change translates as an orientation change when interpreting corresponding areas in the biplot (see Figure 3).

Thus the I levels and the J levels will be represented in the form of a unique biplot with two readings: one for the "common" part C, and one for the "specific" parts D (and $-D$).

Note that the singular elements of $C+iD$ can be obtained by performing the singular value decomposition of

$$M = \begin{pmatrix} C & -D \\ D & C \end{pmatrix}$$

(see Durand [7, page 33–34], Chakak *et al.* [3] and Grorud [16]). The singular values occur in constant pairs and the order 2 approximation of M has the following structure:

$$s_1 \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \begin{bmatrix} v_1' & v_2' \end{bmatrix} + s_1 \begin{bmatrix} -u_2 \\ u_1 \end{bmatrix} \begin{bmatrix} -v_2' & v_1' \end{bmatrix}.$$

The complex order 1 reconstruction of $C + iD$ obtained in (1) can thus be easily recovered. In other words, the **order one** complex approximation of $C + iD$ is nothing else but the **order two** real approximation of the block matrix M.

Thus, in a single operation, either the complex singular value decomposition of $C + iD$ or the real singular value decomposition of M produces reduced rank approximations for C and D. In these, a one-dimensional complex singular element of $C + iD$ provides bi-dimensional elements for the approximation of C and D.

5. Biplot visualizations

We consider biplot visualizations for the example and discuss their practical use.

5.1. Example

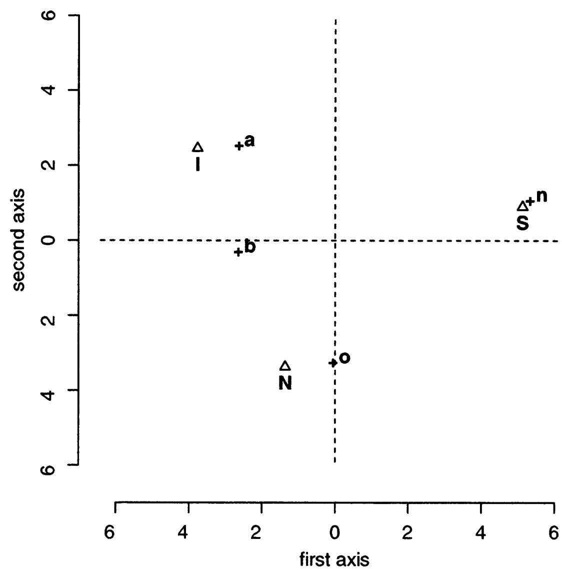

Figure 1. — Biplot of C: I, N, S are province categories ($\triangle$) and a, b, n, n vote categories ($+$).

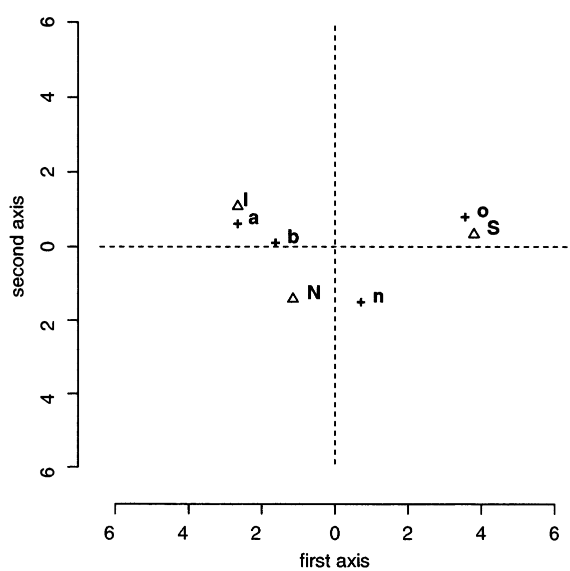

Figure 2. — Biplot of D.

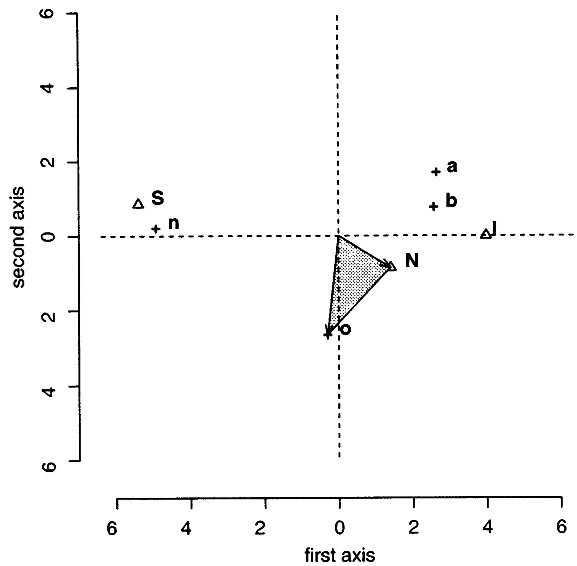

Figure 3. — Biplot of the approximations of C and D given by the first order approximation of $C + iD$: the first bi-dimension.

The rank 2 biplots for C and D are given in Figure 1 and Figure 2. The rank 1 biplot for $C + iD$ is given in Figure 3.

All visualizations, Figure 1 and Figure 2 on the one hand and Figure 3 on the other, tell basically the same story. And, given the small size of the example, the story could have been read directly from Table 2: the overall strong *non* attitude and lack of *abstention* and *blanc* in the *Province du Sud*, with an increase in *oui* and a decrease of *abstention* from 1988 to 1998; the overall strong *abstention* attitude and lack of *non* in the *Province des Îles*, with an increase of *abstention* and decrease of *oui* from 1988 to 1998 ...

As an illustration of the reading of the complex biplot (see Figure 3), we consider the vote *oui* in the *Province du Nord*. The corresponding values in Table 2 are 11.06 for matrix C (a positive attitude in both referenda) and -5.21 for matrix D (a declining attitude in 1998 compared to 1988). An approximation of these two numbers can be recovered from the complex biplot (Figure 3). The reading goes as follows. Let O be the origin. For the "common" part, it is the inner product between $\vec{ON}$ and $\vec{Oo}$ which approximates 11.06; the acute angle tells the positivity of the corresponding value and it turns out that the approximation is equal to 1.85. For the "specific" part it is twice the area of triangle ONo which approximates

-5.21; The fact that we go clockwise from N to o tells the negativity of the corresponding values and it turns out that the approximation is equal to -3.99. These different readings on a common biplot are visualized on Figure 3.

5.2. Two for one better than one for two?

Are two different readings on the same biplot better than the same reading on two different biplots?

Firstly, we note that the comparison between biplots of Figure 1 and Figure 2 on the one hand, and of Figure 3 on the other is biased: a fair comparison would oppose two rank 1 biplots, one for C and one for D, to the rank 1 biplot of $C + iD$ which is represented in dimension 2!

Table 5. — Constantine–Gower approach: order 1 approximations of matrices C and D for the example.

	C			D		
Province :	Sud	Nord	Îles	Sud	Nord	Îles
Vote						
abstention	-13.50	3.60	9.90	-10.10	3.05	7.05
blanc	-13.58	3.62	9.96	-6.16	1.86	4.30
oui	-0.28	0.07	0.20	13.56	-4.09	-9.47
non	27.37	-7.29	-20.07	2.69	-0.81	-1.88

Table 6. — Escoufier–Grorud approach: order 1 approximations of matrices C and D for the example.

	C			D		
Province :	Sud	Nord	Îles	Sud	Nord	Îles
Vote						
abstention	-12.83	2.28	10.55	-11.38	4.65	6.73
blanc	-13.24	2.97	10.27	-6.34	3.29	3.05
oui	-0.67	1.85	-1.19	14.56	-3.99	-10.57
non	26.73	-7.11	-19.62	3.15	-3.94	0.79

Table 5 and 6 report the numerical values of the approximations given by the first singular elements for both methods. An overall measure of residual error for each approach is the total of two sums of squared differences: the sum of squared differences between C and its order 1 approximation and the sum of squared differences between D and its order 1 approximation. The Constantine–Gower approach gives 342.51 while the Escoufier–Grorud 312.21. In this example, the complex biplot is winning by a hair's breadth!

This is certainly factual. The natural bi-dimensionality of biplots constructed under the complex approach is more important in this comparison: biplots are best displayed in two-dimensions. But the price to pay is the provocative constraint to look at one picture with two different pairs of glasses.

6. The modeling connection

In this section, a modeling point of view is taken up for comparing the two approaches.

As already mentioned in subsection 2.2, under a Poisson kernel for the initial data, the square root transformation gives data which are approximately Gaussian with constant variance $\frac{1}{4}$. The design is complete and balanced: there is one observation for each cell of the $I \times J \times T$ classification where I denotes the vote categories, J the Province categories and T the two occasions.

In this Gaussian context with complete and balanced design:

1. the double centring of each table is nothing else but considering the residuals of an $I * T + J * T$ model fitted under the identity link,

2. the "common" part C contains the $I \times J$ interaction.

3. the "specific" parts D and $-D$ contain residuals from the model $I * T + J * T + I * J$ of all two-way interactions.

The biplot analyses of C and D are interleaved in the above-mentioned linear models and correspond to bilinear models (see Falguerolles and Francis [11] and Falguerolles [10]). In particular, twice the sum of squared singular values of C (and D) is equal to the difference of sum of squared residuals between models $I * T + J * T + I * J$ and $I * T + J * T$ ($I * J * T$ and $I * T + J * T + I * J$). This factor of 2 occurs since the size of the data set (A and B) is twice the number of entries in either C, D or $C + iD$.

The biplot analysis of $C + iD$ is also interleaved in the linear models $I * T + J * T$ and $I * J * T$. But now, the complex singular value decomposition of $C + iD$ gives rise to two bi-dimensions, each bi-dimension defining an approximation of C and D. Due to the identifiability constraints, the introduction of the kth order complex singular elements to previous elements results in the specification of $2 * (I + J - d_k)$ new independant parameters where $d_k = d_{k-1} + 2$ if $k > 1$ and $d_1 = 3$.

The usual goodness-of-fit measures are summarized in Table 7 which presents in a modeling context the results already obtained in the biplot exploration of the data (compare Table 3 and Table 4).

Although sandwiched between the linear models $I*T+J*T$ and $I*J*T$, the model obtained by adding the predictors derived from the first order approximation of C and D to the baseline linear model $I * T + J * T$ is not included in Table 7. Its sum of squared residuals is equal to 685.02 $(663.78 + 21.24)$ with 4 degrees of freedom. But it turns out that a slightly better fit is obtained with the model where the predictors derived from the first order approximation of $C+iD$ are added to to the baseline linear model $I*T+J*T$: as seen in Table 7, the sum of squared residuals is then equal to 624.43 with 4 degrees of freedom. Twice the hair's breadth of subsection 5.2!

In passing we note that the modeling approach is best suited when there are missing or structural values in the data. In this case, real or complex singular value decompositions cannot be directly applied and iterative methods must be considered.

7. Concluding remarks

The central trick in this paper is the Gaussian assumption with identity link in a balanced design. Under these assumptions, a reduced rank approximation for both the "common" part and the "specific" part can be simultaneously attempted: the singular elements are embedded. It is well-known that this property does not hold in other settings. In particular, for square tables and under a Poisson assumption with log link, a more rigid point of view is often recommended:

- If quasi-symmetry is rejected then only departure from quasi-symmetry is to be modelled by a reduced rank model.
- If quasi-symmetry is accepted then only the symmetric part is to be modelled by a reduced rank model.

Table 7. — A model based summary: In the upper part, the singular value decompositions of C and D provide the reduced rank approximations which are introduced in intermediate models (see also Table 3). In the lower part, the complex singular value decomposition of $C + iD$ provides the reduced rank approximations which are introduced in intermediate models (see also Table 4). Degrees of freedom are enclosed in parentheses.

Modeling based on separate analysis of C and D

Model	Sum of squared residuals	(df)	Source of variation	Sum of squares difference	(df)
1	52615.79	(23)	–	–	(–)
$I*T+J*T$	5320.82	(12)	$I*T+J*T-1$	47294.97	(11)
$I*T+J*T+s_1^C u_1^C (v_1^C)'$	1730.00	(8)	$s_1^C u_1^C (v_1^C)'$	3590.82	(4)
$I*T+J*T+I*J$	1066.22	(6)	$s_2^C u_2^C (v_2^C)'$	663.78	(2)
$I*T+J*T+I*J+(-1)^T s_1^D u_1^D (v_1^D)'$	21.24	(2)	$(-1)^T s_1^D u_1^D (v_1^D)'$	1044.98	(4)
$I*J*T$	0	(0)	$(-1)^T s_2^D u_2^D (v_2^D)'$	21.24	(2)

Modeling based on the analysis of $C + iD$

Model	Sum of squared residuals	(df)	Source of variation	Sum of squares difference	(df)
1	52615.79	(23)	–	–	(–)
$I*T+J*T$	5320.82	(12)	$I*T+J*T-1$	47294.97	(11)
$I*T+J*T+$ $s_1\left\{(u_1v_1'+u_2v_2')+(-1)^T(u_2v_1'-u_1v_2')\right\}$	624.43	(4)	$s_1\left\{(u_1v_1'+u_2v_2')+(-1)^T(u_2v_1'-u_1v_2')\right\}$	4696.39	(8)
$I*J*T$	0	(0)	$s_2\left\{(u_3v_3'+u_4v_4')+(-1)^T(u_4v_3'-u_3v_4')\right\}$	624.43	(4)

See, for example, the discussions in van der Heijden and Mooijart [20], Greenacre [14] and Falguerolles and van der Heijden [12] which can easily be extended to matched tables. A more flexible approach is to keep the spirit of complex conjoint approximation of C and D but this is another debate which is similar to that of type I, II and III sum of squares in variance analysis.

The two for one approach seems hard to generalize further than the Gaussian case. In principle, Escoufier–Grorud decomposition (see subsection 4.2) could be incorporated in the predictor on top of the baseline linear model $I * T + J * T$. But estimation procedures are not available at the moment.

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