

**APPLICATIONS OF THE MODIFIED LEVERRIER-FADDEEV
ALGORITHM FOR THE CONSTRUCTION OF EXPLICIT MATRIX
SPECTRAL DECOMPOSITIONS AND INVERSES**

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APPLICATIONS OF THE MODIFIED LEVERRIER-FADDEEV ALGORITHM FOR THE CONSTRUCTION OF EXPLICIT MATRIX SPECTRAL DECOMPOSITIONS AND INVERSES

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ABSTRACT. The Leverrier-Faddeev algorithm, as modified by Gower [1], provides a powerful tool for constructing explicit matrix inverses and spectral decompositions, especially for classes of matrices that exhibit certain kinds of defined structure. The derivation of some standard results illustrates the method and some new applications are given stemming from the field of multidimensional scaling.

1. Introduction.

Explicit spectral decompositions and inverses of matrices are often required to model ideal situations and to express large matrix problems in terms of smaller problems. Generally, progress can be made only when the matrices concerned exhibit some definite structure and then their decompositions and inverses often exhibit related structure. When presented with a putative inverse or an eigenvector, it is usually a trivial matter to confirm its validity, but, unless one can produce these things through inspiration or through some deep insight, methods for their construction are essential. Gower [1] extended the Leverrier-Faddeev algorithm and showed how it could be used to construct inverses, generalized inverses and spectral decompositions of a very wide class of matrices. The results are especially useful when the Jordan form of the $n \times n$ matrix \mathbf{A} , $\mathbf{J} = \mathbf{TAT}^{-1}$, is diagonal; this includes most cases of practical importance: all square matrices with distinct eigenvalues, all symmetric matrices, all Hermitian matrices and all skew-symmetric matrices. Gower [2] discussed the specialized details required for skew-symmetry and gave an explicit example. Indeed, the motivation for the original work of [1] was to handle skew-symmetric matrices \mathbf{S} . With skew-symmetry \mathbf{S}^2 is symmetric with equal eigenvalues occurring in pairs, a property causing the original Leverrier-Faddeev algorithm to fail. It has become clear to us that the modified algorithm is of even more value than was thought originally, and in the following we give some further examples that demonstrate its use both in theoretical studies and in developing efficient numerical algorithms. We start by recapitulating the main results that will be used in the examples.

Consider the sequence

$$(1.1) \quad \begin{aligned} \mathbf{Y}_0 &= \mathbf{A} \\ \mathbf{Y}_i &= \mathbf{AY}_{i-1} + p_i \mathbf{A}, \quad i = 1, \dots, n \end{aligned}$$

where $p_i = -(1/i)\text{Tr}(\mathbf{Y}_{i-1})$ and n is the order of \mathbf{A} . This sequence stops after n steps, with $\mathbf{Y}_n = \mathbf{0}$. The numbers p_i turn out to be the coefficients of the characteristic polynomial of \mathbf{A} . For any eigenvalue λ define the matrix

$$(1.2) \quad \mathbf{Y} = \sum_{i=0}^{n-1} \lambda^{n-i-1} \mathbf{Y}_i$$

then in [1] it was shown that $\mathbf{A}\mathbf{Y} = \lambda\mathbf{Y}$ so that the columns of \mathbf{Y} are right-eigenvectors of \mathbf{A} . When λ is a simple eigenvalue, then \mathbf{Y} is necessarily of unit rank and all its columns are equivalent eigenvectors. Similarly the rows of \mathbf{Y} give the left-eigenvectors of \mathbf{A} . When λ is not a simple eigenvalue, then \mathbf{Y} will be null. However if the quantities p_i are replaced by q_i , the coefficients of the minimal polynomial of degree m of \mathbf{A} , then the sequence corresponding to (1.1) stops after $i = m$ steps and

$$(1.3) \quad \begin{aligned} \mathbf{X} &= \sum_{i=0}^{m-1} \lambda^{m-i-1} \mathbf{X}_i, & \lambda \neq 0 \\ \mathbf{X} &= \mathbf{X}_{m-2} + q_{m-1} \mathbf{I}, & \lambda = 0. \end{aligned}$$

Normally \mathbf{X} has rank equal to the multiplicity of λ . The only case of difficulty is when λ is associated with more than one Jordan block and these have different sizes. Then the rank of \mathbf{X} is equal to the number of associated Jordan blocks of maximal size, in which case, the eigenvectors associated with the smaller blocks are not contained in \mathbf{X} ; this eventuality does not arise in the following. An important difference between the sequences (1.1) and (1.3) is that whereas the coefficients p_i are found iteratively, the coefficients q_i require an *a priori* knowledge of the coefficients of the minimal polynomial. However it will be seen below that this is not necessarily a constraint for using (1.3) as a basis for constructing spectral decompositions or inverses of patterned matrices, as a knowledge of the q_i is often not essential for making progress. If the q_i are required, see Krylov's method and Gantmacher's modification of it (volume 1, chapter 4, section 8 of [9]).

The results for inverses, either obtained directly in [1] or as straightforward extensions, are as follows. When \mathbf{A} is non-singular then

$$(1.4) \quad \mathbf{A}^{-1} = -\frac{1}{p_n}(\mathbf{Y}_{n-2} + p_{n-1}\mathbf{I}).$$

When \mathbf{A} is of rank r and $p_r \neq 0$, then

$$(1.5) \quad \mathbf{A}^- = -\frac{1}{p_r}(\mathbf{Y}_{r-2} - \frac{p_{r-1}}{p_r} \mathbf{Y}_{r-1})$$

gives a reflexive generalized inverse of \mathbf{A} which, when symmetric, is the Moore-Penrose inverse. Similarly

$$(1.6) \quad \mathbf{A}^- = -\frac{1}{q_m}(\mathbf{X}_{m-2} - \frac{q_{m-1}}{q_m} \mathbf{X}_{m-1}).$$

When $r = n$ these expressions give ordinary inverses.

It is obvious that these results may be used directly when a matrix has a minimal polynomial of low degree. However, their real value emerges when \mathbf{A} has some regular pattern that is preserved under addition and multiplication. Then it follows from (1.1) - (1.6) that this pattern is preserved in \mathbf{Y} , \mathbf{X} and the three inverse formulae (1.4) - (1.6). Often, pattern may be expressed in terms of a few unknown parameters which may be evaluated by substitution into the standard spectral and inverse matrix conditions. Then not only is there no need to know the minimal equation, but also the rank of \mathbf{X} , after substitution of the parameter values, gives the multiplicity of each eigenvalue as well as all associated eigenvectors. The following examples illustrate the power of the method.

2. Examples.

2.1 The matrix of constant correlations.

To fix ideas and to illustrate various aspects of the method in their most simple form, consider the matrix of constant correlations

$$\mathbf{A} = \rho \mathbf{1}\mathbf{1}' + (1-\rho)\mathbf{I}.$$

Then $\mathbf{A}^2 = (n\rho^2 + 2\rho - 2\rho^2)\mathbf{1}\mathbf{1}' + (1-\rho)^2\mathbf{I}^2$ and provided that $\rho \neq 0$ the minimal equation is $\mathbf{A}^2 - (n\rho+2-2\rho)\mathbf{A} + (1-\rho)(n\rho-\rho+1)\mathbf{I} = \mathbf{0}$, giving $q_1 = -(n\rho+2-2\rho)$ and $q_2 = (1-\rho)(n\rho-\rho+1)$, and hence the sequence

$$\begin{aligned} \mathbf{X}_0 &= \mathbf{A} \\ \mathbf{X}_1 &= \mathbf{A}^2 + q_1\mathbf{A} = -q_2\mathbf{I} \\ \mathbf{X}_2 &= \mathbf{0}. \end{aligned}$$

Thus for any eigenvalue λ

$$\mathbf{X} = \lambda\mathbf{X}_0 + \mathbf{X}_1 = \lambda\mathbf{A} - q_2\mathbf{I}.$$

We may write $\mathbf{A} = \alpha\mathbf{N} + \beta(\mathbf{I} - \mathbf{N})$ where $\alpha = (n-1)\rho + 1$, $\beta = 1 - \rho$ and $\mathbf{N} = \mathbf{1}\mathbf{1}'/n$, and hence $q_1 = \alpha + \beta$, $q_2 = \alpha\beta$. Thus

$$\mathbf{X} = \alpha(\lambda - \beta)\mathbf{N} + \beta(\lambda - \alpha)(\mathbf{I} - \mathbf{N}).$$

It follows that when $\lambda = \alpha$, then $\mathbf{X} = \alpha(\alpha-\beta)\mathbf{N}$ which has unit rank, so that α is a simple eigenvalue corresponding to a vector $\mathbf{1}$. When $\lambda = \beta$, then $\mathbf{X} = \beta(\beta-\alpha)(\mathbf{I} - \mathbf{N})$ with rank $(n-1)$, so that β is a multiple eigenvalue of order $(n-1)$ corresponding to vectors that are orthogonal to $\mathbf{1}$.

The inverse of \mathbf{A} may be obtained from (1.6) as

$$\begin{aligned} \mathbf{A}^{-1} &= -\frac{1}{q_2}(\mathbf{X}_0 - \frac{q_1}{q_2}\mathbf{X}_1) \\ &= -\frac{1}{\alpha\beta}(\mathbf{A} - q_1\mathbf{I}) \\ &= \frac{1}{\alpha\beta}(\beta\mathbf{N} + \alpha(\mathbf{I} - \mathbf{N})). \end{aligned}$$

These expressions may be simplified and obtained by other methods; they are presented here to illustrate the use of (1.1) - (1.6). Unlike more ad hoc approaches, this method may be readily used with more complicated examples.

The above has depended on a knowledge of the minimal equation but, as with this example, such knowledge is not always essential. Clearly

$$\mathbf{A}^i = \alpha^i\mathbf{N} + \beta^i(\mathbf{I} - \mathbf{N})$$

and so this structure is preserved throughout the sequence (1.3) and hence is the structure of \mathbf{X} for every eigenvalue λ , i.e. there exist constants γ, δ such that

$$\mathbf{X} = \gamma\mathbf{N} + \delta(\mathbf{I} - \mathbf{N}).$$

To find γ, δ it is sufficient to substitute in $\mathbf{A}\mathbf{X} = \lambda\mathbf{X}$ to give

$$\alpha\gamma\mathbf{N} + \beta\delta(\mathbf{I} - \mathbf{N}) = \lambda\gamma\mathbf{N} + \lambda\delta(\mathbf{I} - \mathbf{N}).$$

This shows that either (i) $\lambda = \alpha$ and $\delta = 0$ so that $\mathbf{X} = \gamma\mathbf{N}$, or (ii) $\lambda = \beta$ and $\gamma = 0$ so that $\mathbf{X} = \delta(\mathbf{I} - \mathbf{N})$, which leads to the results found previously.

Similarly, \mathbf{A}^{-1} must also have the form $\gamma\mathbf{N} + \delta(\mathbf{I} - \mathbf{N})$ so that $\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$ gives $\alpha\gamma\mathbf{N} + \beta\delta(\mathbf{I} - \mathbf{N}) = \mathbf{I}$, so that $\gamma = 1/\alpha$ and $\delta = 1/\beta$ as is required.

2.2 Circulant matrices.

Suppose \mathbf{A} is a circulant matrix, then \mathbf{A}^j is also a circulant and the circulant structure is preserved throughout the sequence (1.3), so \mathbf{X} also is a circulant. Suppose the eigenvalues of \mathbf{A} are simple, then \mathbf{X} must be a circulant matrix of unit rank with first row $(1, x_1, \dots, x_{n-1})$, say, and hence second row $(x_{n-1}, 1, x_1, \dots, x_{n-2})$. Because \mathbf{X} has unit rank, the second row must be a multiple of the first, giving, $x_j = x_1^j$ and $x_1^n = 1$. Thus x_1 is one of the n th roots of unity and \mathbf{X} is a matrix, all of whose elements are roots of unity. The root ω gives an eigenvector $(1, \omega, \omega^2, \dots, \omega^{n-1})$ with corresponding eigenvalue $\sum_{j=1}^n a_j \omega^{j-1}$ where (a_1, a_2, \dots, a_n) is the first row of \mathbf{A} . All n eigenvalues are obtained by letting ω take the values of all n roots of unity, including $\omega = 1$. Note that in the above it was not necessary to know that the eigenvalues of \mathbf{A} are distinct;

it was merely *assumed* that they were. On this assumption we arrived at n independent eigenvectors of \mathbf{A} , incidently proving that the eigenvalues *are* distinct unless $\sum_{j=1}^n a_j \omega^{j-1}$ happens to have the same value for different settings of ω . In the following, we use the standard notation, defining a circulant in terms of its first row as $\mathbf{A} = \text{circ}(a_1, a_2, \dots, a_n)$.

2.3 Block-circulants.

Results similar to those of section 2.2 follow when \mathbf{A} is a block-circulant matrix with $p \times p$, say, blocks, each of order n . Writing $(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \dots, \mathbf{A}_p)$ for the first row of blocks of \mathbf{A} , a block circulant matrix is defined by constructing subsequent rows of blocks by cyclic permutation, in the usual manner for circulants. Neither \mathbf{A} itself nor any component block is necessarily a circulant (see Davis [8] for a general discussion of circulants, including block-circulants). However the sum of two block-circulant matrices is clearly another block-circulant and so is their product. Thus every eigenvector of \mathbf{A} that corresponds to a simple eigenvalue spans a matrix \mathbf{X} , which is a block-circulant with unit rank. For \mathbf{X} to have unit rank, its blocks must have the form $\mathbf{X}_{jk} = \{\mathbf{x}_j \mathbf{y}_k'\}$ for $j, k = 1, 2, \dots, p$. For the block-circulant property to hold, the first two rows of blocks must be related by

$$\mathbf{x}_2 \mathbf{y}_j' = \mathbf{x}_1 \mathbf{y}_{j-1}' \quad j = 1, 2, \dots, p$$

where \mathbf{y}_0 is understood to be a synonym for \mathbf{y}_p . Therefore

$$\mathbf{y}_j = \rho^{j-1} \mathbf{y}_1 \text{ where } \rho = (\mathbf{x}_2 \mathbf{x}_1') / (\mathbf{x}_2 \mathbf{x}_2')$$

giving $\mathbf{y}_1 = \rho \mathbf{y}_0$, $\mathbf{y}_p = \rho^{p-1} \mathbf{y}_1$ and hence $\rho^p = 1$, so that $\rho = \omega$, one of the p -th roots of unity. Similarly $\mathbf{x}_j = \sigma^{j-1} \mathbf{x}_1$ where $\sigma = \omega^{-1}$. Thus $\mathbf{X}_{jk} = \{\omega^{k-j} \mathbf{x}_1 \mathbf{y}_1'\}$ defines a matrix \mathbf{X} corresponding to a left-eigenvector $\mathbf{u} = (\mathbf{x}_1', \omega \mathbf{x}_1', \omega^2 \mathbf{x}_1', \dots, \omega^{p-1} \mathbf{x}_1')$ and a right-eigenvector $\mathbf{v} = (\mathbf{y}_1', \omega^{-1} \mathbf{y}_1', \omega^{-2} \mathbf{y}_1', \dots, \omega^{-(p-1)} \mathbf{y}_1')$. The vector \mathbf{y}_1 may be found from the first term of $\mathbf{A} \mathbf{v} = \lambda \mathbf{v}$ to give $(\mathbf{A}_1 + \omega^{-1} \mathbf{A}_2 + \omega^{-2} \mathbf{A}_3 + \dots + \omega^{-(p-1)} \mathbf{A}_p) \mathbf{y}_1 = \lambda \mathbf{y}_1$; the other rows lead to the same eigenvalue problem. Thus (λ, \mathbf{y}_1) are an eigenvalue and right-vector of $\sum_{j=1}^p \omega^{-(j-1)} \mathbf{A}_j$. Similarly (λ, \mathbf{x}_1) are an eigenvalue and left-vector of $\sum_{j=1}^p \omega^{j-1} \mathbf{A}_j$. For each of the p roots ω , these give n eigenvalues and associated vectors, a total of np solutions. These expressions cannot be simplified further, unless of course the matrices $\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \dots, \mathbf{A}_p$ themselves exhibit some special structure. For example, when each \mathbf{A}_j is itself a circulant then \mathbf{x}_1 and \mathbf{y}_1 are given by the results of section 2.2.

2.4 Symmetric circulants.

For this section, a more developed version of the notation of section 2.2 is required. We now define $\omega = \cos \theta + i \sin \theta$, where $\theta = 2\pi/n$, rather than any other root of unity; the other roots will have the form ω^j . The associated eigenvectors will be written

$\mathbf{w}'_j = (1, \omega^j, \omega^{2j}, \dots, \omega^{(n-1)j})$ for $j = 1, 2, \dots, n$. Thus $\mathbf{w}_n = \mathbf{1}$. When n is even then $\mathbf{w}_{n/2} = (1, -1, 1, \dots, -1)' = \boldsymbol{\alpha}$ (say) gives another real eigenvector. The eigenvalue λ_j corresponding to \mathbf{w}_j is given by $\lambda_j = \mathbf{a}'\mathbf{w}_j$ where $\mathbf{a}' = (a_1, a_2, \dots, a_n)$.

It may be verified that $\text{circ}(a_1, a_2, \dots, a_n)$ is symmetric if and only if

$$a_j = a_{n-j+2} \quad j = 1, 2, \dots, n$$

where we define $a_{n+1} = a_1$. Recognizing that symmetric circulants have fewer parameters than unrestricted circulants, we shall write a symmetric circulant as $\text{symcirc}(a_1, a_2, \dots, a_m)$ where $m = (n+1)/2$ for n odd and $m = (n+2)/2$ for n even. Thus:

$$\text{symcirc}(a_1, a_2, \dots, a_m) = \text{circ}(a_1, a_2, a_3, \dots, a_m, \dots, a_3, a_2)$$

where the "central value" a_m is repeated twice when n is odd.

When $j \neq n$, or $j \neq n/2$ (n even) then:

$$\lambda_j = \lambda_{n-j} = a_1 + \delta(-1)^j a_m + \sum_{k=2}^{m-\delta} a_k (\omega^{j(k-1)} + \omega^{j(n-k+1)})$$

where $\delta = 0$ when n is odd and $\delta = 1$ when n is even. Now

$$\omega^{j(k-1)} + \omega^{j(n-k+1)} = \omega^{j(k-1)} + \omega^{-j(k-1)} = 2\cos \{(k-1)j\theta\}$$

so, as is required for a real symmetric matrix, all eigenvalues are real, and for symmetric circulants they occur in equal pairs, except for λ_n and $\lambda_{n/2}$ (n even).

Writing $\mathbf{w}_j = \mathbf{u}_j + i\mathbf{v}_j$, then $\mathbf{A}\mathbf{w}_j = \lambda_j\mathbf{w}_j$ shows that \mathbf{u}_j and \mathbf{v}_j are a real pair of eigenvectors corresponding to the double root λ_j . Thus $\mathbf{u}'_j = \{1, \cos(j\theta), \cos(2j\theta), \dots, \cos(n-1)j\theta\}$ and $\mathbf{v}'_j = \{0, \sin(j\theta), \sin(2j\theta), \dots, \sin(n-1)j\theta\}$. Some algebraic manipulation leads to

$$(2.4.1) \quad \mathbf{W}_j = \mathbf{u}_j \mathbf{u}'_j + \mathbf{v}_j \mathbf{v}'_j = \text{symcirc}\{1, \cos(j\theta), \cos(2j\theta), \dots, \cos(m-1)j\theta\}.$$

Because the symmetric circulant property is preserved under addition and multiplication, this form for \mathbf{W}_j could have been deduced directly from (1.3), noting that for the double roots \mathbf{X} must be a symmetric circulant of rank two. It may be verified that \mathbf{W}_j is the general form for a rank two symmetric circulant, just as $\mathbf{w}_j \mathbf{w}'_j$ is the general form for a rank one ordinary circulant.

Before we can complete the spectral decomposition of \mathbf{A} we require the normalized and independent forms of the eigenvectors. For the eigenvectors $\mathbf{1}$ and $\boldsymbol{\alpha}$ we have that $\mathbf{1}'\mathbf{1} = \boldsymbol{\alpha}'\boldsymbol{\alpha} = n$; because \mathbf{A} is symmetric both must be orthogonal to all vectors $\mathbf{u}_j, \mathbf{v}_j$. For the same reason $\mathbf{u}'_j \mathbf{u}_k = \mathbf{u}'_j \mathbf{v}_k = \mathbf{v}'_j \mathbf{v}_k = 0$ for all $j \neq k$, establishing the independence of all vectors except, perhaps, of each $\mathbf{u}_j, \mathbf{v}_j$ pair.

Define $\mathbf{w}_j^* = \mathbf{u}_j - i\mathbf{v}_j = \mathbf{w}_j$ to be the vector conjugate to \mathbf{w}_j . Then:

$$\begin{aligned} \mathbf{w}_j' \mathbf{w}_j^* &= n & \text{and} \\ \mathbf{w}_j' \mathbf{w}_j &= 0. \end{aligned}$$

Expanding these equations gives:

$$\begin{aligned} (\mathbf{u}_j' \mathbf{u}_j + \mathbf{v}_j' \mathbf{v}_j) &= n & \text{and} \\ (\mathbf{u}_j' \mathbf{u}_j - \mathbf{v}_j' \mathbf{v}_j) + i(\mathbf{u}_j' \mathbf{v}_j + \mathbf{v}_j' \mathbf{u}_j) &= 0. \end{aligned}$$

Hence $\mathbf{u}_j' \mathbf{v}_j = 0$ and $\mathbf{u}_j' \mathbf{u}_j = \mathbf{v}_j' \mathbf{v}_j = n/2$, establishing both the required normalization and that all pairs $\mathbf{u}_j, \mathbf{v}_j$ are orthogonal. Thus the spectral decomposition of \mathbf{A} is:

$$(2.4.2) \quad \mathbf{A} = \frac{1}{n} \{ \lambda_n \mathbf{1}\mathbf{1}' + \delta \lambda_{m-1} \boldsymbol{\alpha} \boldsymbol{\alpha}' + 2 \sum_{j=1}^p \lambda_j \mathbf{W}_j \}$$

where $p = m-1$ for n odd and $p = m-2$ for n even. Thus $\mathbf{A} = (1/n) \text{symcirc}(b_1, b_2, \dots, b_m)$ where:

$$(2.4.3) \quad b_k = \lambda_n + \delta \lambda_{m-1} \alpha_k + 2 \sum_{j=1}^p \lambda_j \cos(k-1)j\theta.$$

Similarly $\mathbf{A}^{-1} = (1/n) \text{symcirc}(c_1, c_2, \dots, c_m)$ where:

$$(2.4.4) \quad c_k = \lambda_n^{-1} + \delta \lambda_{m-1}^{-1} \alpha_k + 2 \sum_{j=1}^p \lambda_j^{-1} \cos(k-1)j\theta.$$

This formula gives an efficient way for evaluating the inverse of a symmetric circulant matrix. It requires the calculation of only p trigonometric functions $\cos(j\theta)$ $j = 1, 2, \dots, p$ which are used repeatedly in the evaluation of the m values c_k and of the eigenvalues very much as with more conventional fourier transforms.

2.5. Block symmetric-circulants.

When the block-circulant $\mathbf{A} = \text{bcirc}(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_p)$ satisfies $\mathbf{A}_j = \mathbf{A}_{p-j+2}$ ($j = 1, 2, \dots, p$) where $\mathbf{A}_{p+1} = \mathbf{A}_1$ then, in analogy with section 2.4, \mathbf{A} will be termed a block symmetric-circulant. Thus block symmetric-circulants are normally neither symmetric nor circulants.

In section 2.3 it was shown that the eigenvectors of \mathbf{A} may be derived from the root and vector pairs (λ, \mathbf{y}_1) of $\sum_{j=1}^p \omega^{-(j-1)} \mathbf{A}_j = \mathbf{B}(\omega)$, (say). When \mathbf{A} is a block symmetric-circulant then

$$\begin{aligned} \omega^{-(j-1)} \mathbf{A}_j + \omega^{-(p-j+1)} \mathbf{A}_{p-j+2} &= \omega^{-(j-1)} \mathbf{A}_j + \omega^{(j-1)} \mathbf{A}_j' \\ &= (\mathbf{A}_j + \mathbf{A}_j') \cos(j-1)\theta. \end{aligned}$$

Hence $\mathbf{B}(\omega)$ is real, but symmetric only if \mathbf{A}_1 and $\mathbf{A}_{p/2+1}$, p even, are symmetric. Because $\mathbf{B}(\omega) = \mathbf{B}(\omega^{-1})$ the same pairs (λ, \mathbf{y}_1) arise from different settings of ω ; however these induce different eigenvectors of \mathbf{A} . When $\mathbf{B}(\omega)$ is symmetric, the real and imaginary components of the eigenvectors of \mathbf{A} associated with a common eigenvalue may be separated to give real eigenvectors, as in section 2.4. For the special case when each \mathbf{A}_j is a symmetric circulant (see section 4.2), then $\mathbf{B}(\omega)$ is itself a symmetric circulant and its spectral decomposition, and hence inverse, is given by section 2.4, and may be used directly to give an explicit inverse of \mathbf{A} .

3. *The spectral decomposition of a linear mapping arising in metric scaling.*

Suppose we are given a symmetric matrix \mathbf{D} of order n whose (i,j) th element is the squared Euclidean distance between two points that may be labelled P_i and P_j . The diagonal values of \mathbf{D} are all zero. In classical metric scaling there is an interest in the linear mapping

$$\mathbf{B} = -\frac{1}{2}(\mathbf{I} - \mathbf{N})\mathbf{D}(\mathbf{I} - \mathbf{N}) \text{ and its inverse mapping } \mathbf{D} = \mathbf{E}\mathbf{1}\mathbf{1}' + \mathbf{1}\mathbf{1}'\mathbf{E} - 2\mathbf{B}, \text{ where}$$

$\mathbf{E} = \text{diag}(\mathbf{B})$. Here b_{ij} has the geometrical interpretation of being the inner-product $\Delta(P_i)\Delta(P_j)\cos(\theta_{ij})$ where θ is the angle subtended by P_i and P_j at the centroid. The diagonal values of \mathbf{B} are non-negative but they are redundant, in the sense that they may be easily evaluated from the other row or column members because \mathbf{B} has zero row and column sums. In theoretical studies (see e.g.[3] and [4]) there is interest in regarding the sub-diagonal elements of \mathbf{D} and \mathbf{B} as vectors \mathbf{d} and \mathbf{b} in $m = \frac{1}{2}n(n-1)$ dimensional Euclidean space. The above mappings may then be written $\mathbf{b} = \mathbf{T}\mathbf{d}$ with inverse $\mathbf{d} = \mathbf{K}\mathbf{b}$. Critchley [3] gives the matrix forms of the $m \times m$ matrices \mathbf{T} and \mathbf{K} and also gives their spectral decompositions. We now show how these decompositions may be constructed using the modified Leverrier-Faddeev decomposition (1.3).

Either by direct inspection or from [3], we have that

$$(3.1) \quad \mathbf{T} = -\frac{1}{2}\left(\mathbf{I} - \frac{1}{n}\mathbf{R}\mathbf{R}' + \frac{2}{n^2}\mathbf{1}\mathbf{1}'\right)$$

and $\mathbf{K} = -(2\mathbf{I} + \mathbf{R}\mathbf{R}')$

where \mathbf{R} is an $m \times n$ matrix given by

$$(3.2) \quad \mathbf{R}' = \left| \begin{array}{cccc|c} \mathbf{1}'_{n-1} & \mathbf{0}' & \dots & \mathbf{0}' & 0 \\ & \mathbf{1}'_{n-2} & \dots & \mathbf{0}' & 0 \\ & & & \vdots & \vdots \\ \mathbf{I}_{n-1} & & & \mathbf{0}' & 0 \\ & \mathbf{I}_{n-2} & & \vdots & \vdots \\ & & \dots & \mathbf{1}'_2 & 0 \\ & & & \mathbf{I}_2 & 1 \\ & & & & 1 \end{array} \right|$$

From (3.2) it is easy to derive the following basic identities where the size of unit matrices \mathbf{I} and of vectors of units $\mathbf{1}$ is to be understood from context to be conformable with the dimensions of \mathbf{R} .

$$(3.3) \quad \begin{aligned} \mathbf{R}'\mathbf{R} &= (n-2)\mathbf{I} + \mathbf{1}\mathbf{1}' \\ \mathbf{R}\mathbf{1} &= 2\mathbf{1} \\ \mathbf{R}'\mathbf{1} &= (n-1)\mathbf{1} \end{aligned}$$

from which it is easy to verify that $\mathbf{TK} = \mathbf{KT} = \mathbf{I}$. Further useful identities follow easily from (3.3) to give

$$(3.4) \quad \begin{aligned} \mathbf{R}\mathbf{R}'\mathbf{1} &= 2(n-1)\mathbf{1} \\ \mathbf{R}\mathbf{R}'\mathbf{R}\mathbf{R}' &= (n-2)\mathbf{R}\mathbf{R}' + 4\mathbf{1}\mathbf{1}' \\ \mathbf{1}\mathbf{1}'\mathbf{R} &= (n-1)\mathbf{1}\mathbf{1}' \\ \mathbf{1}\mathbf{1}'\mathbf{R}' &= 2\mathbf{1}\mathbf{1}' \\ (\mathbf{R}'\mathbf{R})^{-1} &= \frac{1}{(n-2)}\left(\mathbf{I} - \frac{1}{2(n-1)}\mathbf{1}\mathbf{1}'\right). \end{aligned}$$

Using (3.3) and (3.4) it follows easily that

$$\mathbf{K}^r = \alpha_r\mathbf{I} + \beta_r\mathbf{1}\mathbf{1}' + \gamma_r\mathbf{R}\mathbf{R}'$$

for some constants $\alpha_r, \beta_r, \gamma_r$ and hence that this structure is preserved throughout the sequence (1.3). Therefore the eigenvectors of \mathbf{K} span a matrix of the same form

$$(3.5) \quad \mathbf{X} = \alpha\mathbf{I} + \beta\mathbf{1}\mathbf{1}' + \gamma\mathbf{R}\mathbf{R}'.$$

Substituting into $\mathbf{K}\mathbf{X} = \lambda\mathbf{X}$ yields, after extensive use of the identities,

$$(3.6) \quad -2\alpha\mathbf{I} - 2(n\beta + 2\gamma)\mathbf{1}\mathbf{1}' - (n\gamma + \alpha)\mathbf{R}\mathbf{R}' = \lambda(\alpha\mathbf{I} + \beta\mathbf{1}\mathbf{1}' + \gamma\mathbf{R}\mathbf{R}').$$

Equating coefficients gives

$$\begin{aligned} \frac{n\beta + 2\gamma}{\alpha} &= \frac{\beta}{\alpha}, & \text{which implies that } \alpha = 0 \text{ or } (n-1)\beta + 2\gamma = 0 \\ \text{and } \frac{n\gamma + \alpha}{2\alpha} &= \frac{\gamma}{\alpha}, & \text{which implies that } \alpha = 0 \text{ or } (n-2)\gamma + \alpha = 0. \end{aligned}$$

Hence either (i) $\alpha = 0$, in which case returning to (3.6) gives

$$\frac{n\gamma}{2(n\beta + 2\gamma)} = \frac{\gamma}{\beta},$$

which implies that $\gamma = 0$ or $n\beta + 4\gamma = 0$, or (ii) $\alpha = \frac{1}{2}(n - 1)(n - 2)\beta$, $\gamma = -\frac{1}{2}(n - 1)\beta$. Thus there are three possibilities

$\alpha = \gamma = 0$	corresponding to	$\lambda_1 = -2n$
$\alpha = 0, \gamma = \frac{-n\beta}{4}$	$\lambda_2 = -n$
$\alpha = \frac{1}{2}(n - 1)(n - 2)\beta, \gamma = -\frac{1}{2}(n - 1)\beta$	$\lambda_3 = -2.$

Substituting into the expression for \mathbf{X} gives eigenvalues with the matrices spanned by the corresponding eigenvectors as

$$(3.7) \quad \begin{aligned} \lambda_1 &= -2n, & \mathbf{X}_1 &= \mathbf{1}\mathbf{1}' \\ \lambda_2 &= -n, & \mathbf{X}_2 &= 4\mathbf{1}\mathbf{1}' - n\mathbf{R}\mathbf{R}' \\ \lambda_3 &= -2, & \mathbf{X}_3 &= \frac{1}{2}(n - 1)(n - 2)\mathbf{I} + \mathbf{1}\mathbf{1}' - \frac{1}{2}(n - 1)\mathbf{R}\mathbf{R}'. \end{aligned}$$

Normalizing to get suitable projection matrices $\mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3$ gives

$$(3.8) \quad \begin{aligned} \mathbf{H}_1 &= \frac{1}{m} \mathbf{1}\mathbf{1}' = \frac{2}{n(n - 1)} \mathbf{1}\mathbf{1}' \\ \mathbf{H}_2 &= \frac{1}{n(n - 2)} (n\mathbf{R}\mathbf{R}' - 4\mathbf{1}\mathbf{1}') \\ \mathbf{H}_3 &= \mathbf{I} + \frac{2}{(n - 1)(n - 2)} \mathbf{1}\mathbf{1}' - \frac{1}{(n - 2)} \mathbf{R}\mathbf{R}'. \end{aligned}$$

It may be verified that these are indeed idempotent and mutually orthogonal. Further

$$\begin{aligned} \mathbf{H}_1 + \mathbf{H}_2 + \mathbf{H}_3 &= \mathbf{I} \\ -(2n\mathbf{H}_1 + n\mathbf{H}_2 + 2\mathbf{H}_3) &= \mathbf{K} \end{aligned}$$

and, by inversion $-(\frac{1}{2n}\mathbf{H}_1 + \frac{1}{n}\mathbf{H}_2 + \frac{1}{2}\mathbf{H}_3) = \mathbf{T}$.

The eigenvectors themselves are easily obtained from the projection matrices

- (i) Corresponding to \mathbf{H}_1 is the eigenvector $\mathbf{V}_1 = \mathbf{1}$
- (ii) We have that $n\mathbf{R}\mathbf{R}' - 4\mathbf{1}\mathbf{1}' = n\mathbf{R}(\mathbf{I} - \mathbf{N})\mathbf{R}'$ so that corresponding to \mathbf{H}_2 are eigenvectors given by the columns of $\mathbf{R}(\mathbf{I} - \mathbf{N})$. This matrix has rank $n-1$ and hence non-independent columns. A set of independent eigenvectors which span the whole space, but are not orthogonal, may be obtained by setting $\mathbf{V}_2 = \mathbf{R}(\mathbf{I} - \mathbf{N})\mathbf{I}_n^{(n-1)}$, where $\mathbf{I}_p^{(q)}$ denotes the matrix formed from the first q columns of \mathbf{I}_p
- (iii) Some manipulation of the identities (3.3) and (3.4) shows that $\mathbf{H}_3 = \mathbf{I} - \mathbf{R}(\mathbf{R}'\mathbf{R})^{-1}\mathbf{R}'$ with $\mathbf{V}_3 = (\mathbf{I} - \mathbf{R}(\mathbf{R}'\mathbf{R})^{-1}\mathbf{R}')\mathbf{I}_m^{(m-n)}$.

4. Block designs in multidimensional scaling.

Multidimensional scaling (MDS) is a technique used for finding a spatial representation of points whose distances should match as closely as possible a symmetric dissimilarity matrix. For an introduction to MDS see Kruskal and Wish [6]. The SMACOF algorithm for MDS (De Leeuw and Heiser [7], [8]) needs the Moore-Penrose inverse of a matrix

$$\mathbf{V} = \frac{1}{2} [\text{diag}(\mathbf{1}'(\mathbf{W} + \mathbf{W}')) - (\mathbf{W} + \mathbf{W}')]$$

where \mathbf{W} is a matrix of weights with zero diagonal elements. Because $\mathbf{1}'\mathbf{V} = \mathbf{0}$ the symmetric matrix \mathbf{V} has $\mathbf{1}$ as a null vector and its Moore-Penrose inverse is given by $\mathbf{V}^- = (\mathbf{V} + \mathbf{1}\mathbf{1}')^{-1} - c\mathbf{1}\mathbf{1}'$. Here $c = n^{-2}$ but its value is irrelevant in SMACOF as \mathbf{V}^- is subsequently multiplied by a matrix orthogonal to $\mathbf{1}$. Hence we focus attention on the inverse of $\mathbf{A} = \mathbf{V} + \mathbf{1}\mathbf{1}'$. In certain applications only a part of the whole dissimilarity matrix is used, particularly when n is large, and it is then convenient to use \mathbf{W} to define a design matrix, whose elements are zero when a dissimilarity is absent and, usually, unity when it is not. In the following we assume that \mathbf{V} represents a block design with $k \times k$ blocks, where all elements in block i, j of \mathbf{A} have equal values ξ_{ij} . Thus a block $\xi_{ij}\mathbf{1}\mathbf{1}'$ of \mathbf{A} is associated with a weight $1 - \xi_{ij}$ in the corresponding block of the design \mathbf{V} ; a block with zero weight corresponds to $\xi_{ij} = 1$. Clearly \mathbf{A} has the pattern

$$\begin{bmatrix} \alpha_1 \mathbf{I}_1 & & & \\ & \alpha_2 \mathbf{I}_1 & & \\ & & \dots & \\ & & & \alpha_k \mathbf{I}_k \end{bmatrix} + \begin{bmatrix} \xi_{11} \mathbf{1}\mathbf{1}' & \xi_{12} \mathbf{1}\mathbf{1}' & \dots & \xi_{1k} \mathbf{1}\mathbf{1}' \\ \xi_{12} \mathbf{1}\mathbf{1}' & \xi_{22} \mathbf{1}\mathbf{1}' & \dots & \xi_{2k} \mathbf{1}\mathbf{1}' \\ \dots & \dots & \dots & \dots \\ \xi_{1k} \mathbf{1}\mathbf{1}' & \xi_{2k} \mathbf{1}\mathbf{1}' & \dots & \xi_{kk} \mathbf{1}\mathbf{1}' \end{bmatrix}$$

where $\alpha_i = \sum_s (1 - \xi_{is}) n_s$ and the length of the vectors $\mathbf{1}$ are conformable with the block-sizes n_1, n_2, \dots, n_k . Let \mathbf{Z} be a matrix with the same pattern as \mathbf{A} , defined by the diagonal blocks $\theta_i \mathbf{I}_i$ and $\varphi_{ij}\mathbf{1}\mathbf{1}'$. The result of \mathbf{AZ} is again a block-matrix, with block ij given by

$$(4.1) \quad (\alpha_i \varphi_{ij} + \theta_j \xi_{ij} + \sum_{s=1}^k n_i \xi_{is} \varphi_{sj}) \mathbf{1}\mathbf{1}' \quad \text{for } i \neq j$$

$$(4.2) \quad (\alpha_i \varphi_{ii} + \theta_i \xi_{ii} + \sum_{s=1}^k n_i \xi_{is} \varphi_{si}) \mathbf{1}\mathbf{1}' + \alpha_i \theta_i \mathbf{I}_i \quad \text{for } i = j.$$

This shows that matrices with the pattern of \mathbf{A} preserve this pattern when multiplied by another matrix of the same pattern. Consequently $\mathbf{A}^2, \mathbf{A}^3, \dots, \mathbf{A}^p$ all have the same pattern. From section 1 we know that \mathbf{A}^{-1} shares this same pattern. In the following, this fact is used to simplify the computation of \mathbf{A}^{-1} . In the sequel let \mathbf{Z} represent \mathbf{A}^{-1} . Obviously \mathbf{AZ} must be equal to \mathbf{I} so that (4.1) must vanish and (4.2) must be the same as \mathbf{I}_i . Premultiplication of both sides of (4.2) by any unit vector \mathbf{u}_i orthogonal to $\mathbf{1}$, i.e. $\mathbf{u}_i' \mathbf{u}_i = 1$ and $\mathbf{u}_i' \mathbf{1} = 0$, shows that $\theta_i = 1/\alpha_i$ and hence the coefficient of $\mathbf{1}\mathbf{1}'$ in (4.2) must be zero. Thus

$$\alpha_i \varphi_{ij} + \sum_{s=1}^k n_i \xi_{is} \varphi_{sj} = -\theta_j \xi_{ij} \quad \text{for all pairs } i,j.$$

This set of equations can be written in terms of matrices as

$$\begin{bmatrix} \varphi_{11} & \varphi_{12} & \dots & \varphi_{1k} \\ \varphi_{12} & \varphi_{22} & \dots & \varphi_{2k} \\ \dots & \dots & \dots & \dots \\ \varphi_{1k} & \varphi_{2k} & \dots & \varphi_{kk} \end{bmatrix} \begin{bmatrix} n_1 \\ n_2 \\ \dots \\ n_k \end{bmatrix} \begin{bmatrix} \alpha_1/n_1 + \xi_{11} & \xi_{12} & \dots & \xi_{1k} \\ \xi_{12} & \alpha_2/n_2 + \xi_{22} & \dots & \xi_{2k} \\ \dots & \dots & \dots & \dots \\ \xi_{1k} & \xi_{2k} & \dots & \alpha_k/n_k + \xi_{kk} \end{bmatrix} \\ = - \begin{bmatrix} \xi_{11} & \xi_{12} & \dots & \xi_{1k} \\ \xi_{12} & \xi_{22} & \dots & \xi_{2k} \\ \dots & \dots & \dots & \dots \\ \xi_{1k} & \xi_{2k} & \dots & \xi_{kk} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \dots \\ \theta_k \end{bmatrix}.$$

or $\Phi \text{diag}(\mathbf{n}) \mathbf{A}_r = -\Xi \Theta$, in which the only unknown matrix is Φ , which is equal to $-\Xi \Theta \mathbf{A}_r^{-1} (\text{diag}(\mathbf{n}))^{-1}$. This shows that it suffices to invert a $k \times k$ matrix \mathbf{A}_r to find the original inverse. For large design matrices, not uncommon in MDS, this gives an important gain in speed. However, for some special designs the inversion of the $k \times k$ matrix can be simplified even further; some important examples are discussed in the next section.

4.1 Block tridiagonal designs.

A fast computational method for the inverse for block tridiagonal designs can be formulated by making use of the sparseness of Ξ . Such a design consists of blocks on the diagonal and both adjacent subdiagonals. In this case the elements of Ξ are restricted to be 0 or 1 indicating if the block is present or absent. The second and higher subdiagonals of \mathbf{A}_r have unit values. As a first step towards finding the inverse of \mathbf{A}_r it is convenient to subtract the rank one matrix $\mathbf{1}\mathbf{1}'$ to obtain a sparse tridiagonal matrix

$$\mathbf{B} = \mathbf{A}_r - \mathbf{1}\mathbf{1}' = \begin{bmatrix} \beta_1 & -1 & \dots & 0 & 0 \\ -1 & \beta_2 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \beta_{k-1} & -1 \\ 0 & 0 & \dots & -1 & \beta_k \end{bmatrix}$$

with $\beta_1 = n_2/n_1$, $\beta_i = (n_{i-1} + n_{i+1})/n_i$ and $\beta_k = n_{k-1}/n_k$. For k larger than 3 \mathbf{B} is more sparse than \mathbf{A}_r . However, because $\mathbf{B}\mathbf{n} = \mathbf{0}$, the matrix $\mathbf{A}_r = \mathbf{B} + \mathbf{1}\mathbf{1}'$ cannot be inverted from knowledge of \mathbf{B}^{-1} . To modify \mathbf{B} to be of full rank, while retaining its tridiagonal form, we may proceed as follows. Let \mathbf{e} be the unit vector, zero everywhere except for its final position which has value one. Then for any valid design $\mathbf{e}'\mathbf{n} \neq 0$ and we may write:

$$\mathbf{A}_r = \mathbf{1}\mathbf{1}' - \mathbf{e}\mathbf{e}' + \mathbf{T}$$

where $\mathbf{T} = \mathbf{B} + \mathbf{e}\mathbf{e}'$. \mathbf{T} is tridiagonal and of full rank, with $\mathbf{T}\mathbf{n} = (\mathbf{e}'\mathbf{n})\mathbf{e}$, so that

$$(4.3) \quad \mathbf{T}^{-1}\mathbf{e} = \mathbf{n}/(\mathbf{e}'\mathbf{n}) .$$

Using result (4.3) and after some manipulations:

$$(4.3) \quad \mathbf{A}_r^{-1} = \left(\mathbf{I} - \frac{\mathbf{n}\mathbf{1}'}{\mathbf{1}'\mathbf{n}} \right) \mathbf{T}^{-1} \left(\mathbf{I} - \frac{\mathbf{1}\mathbf{n}'}{\mathbf{1}'\mathbf{n}} \right) + \frac{\mathbf{n}\mathbf{n}'}{\mathbf{1}'\mathbf{n}} .$$

Thus to invert \mathbf{A}_r it is only necessary to invert the tridiagonal matrix \mathbf{T} . The Cholesky decomposition \mathbf{LDL}' of \mathbf{T} may be used to find \mathbf{T}^{-1} , where the lower triangular matrix \mathbf{L} is

$$\begin{bmatrix} 1 & 0 & \dots & 0 & 0 \\ -1/d_1 & 1 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & -1/d_{k-1} & 1 \end{bmatrix}$$

and the diagonal matrix \mathbf{D} has non-zero elements $d_1 = \beta_1$, $d_i = \beta_i - d_{i-1}^2$ for $i = 2, 3, \dots, k-1$ and $d_k = 1$. The inverse of \mathbf{T} is given by $(\mathbf{L}^{-1})'\mathbf{D}^{-1}\mathbf{L}^{-1} = \mathbf{M}'\mathbf{D}^{-1}\mathbf{M}$, where the lower triangular matrix \mathbf{M} has diagonal elements unity and subdiagonal elements

$$m_{ij} = \left(\prod_{s=j}^{i-1} d_s \right)^{-1} .$$

One important characteristic of the block tridiagonal design is that the associated inverse can be computed relatively fast. The gain of speed when using this method depends on the number of blocks and the size of the blocks, but it can be considerable.

4.2 Circular designs.

An important class of designs is when Ξ denotes a symmetric circulant design (see Spence [10]). In general \mathbf{A}_r will not be a symmetric circulant because the values α_i are not constant and then \mathbf{A}_r seems to need full inversion. However there are two important cases where advantage can be taken of the explicit results of section 2.4. These are (i) when $\mathbf{n} = n/k \mathbf{1}$, which requires that n is a multiple of k , and (ii) when $n_s = 1$ for all s so that $\alpha_i = \sum_s (1 - \xi_{is})$, which is a constant because the rows of the circulant Ξ have constant sum. Case (i) merely requires the inverse of the $k \times k$ symmetric circulant \mathbf{A}_r . Case (ii) is especially important because although the block-structure is lost (all the blocks are of size 1×1), the ξ 's may be chosen such that $\Xi = \text{symcirc}(1, 1, 0, \dots, 0)$ which gives a tridiagonal design with a single element in

positions $(1,n)$ and $(n,1)$ or we may choose a band design $\Xi = \text{symcirc}(1,1,1,\dots,1,0,\dots,0)$ supplemented by extra cells in the upper-right and lower-left corner. Other choices such as $\Xi = \text{symcirc}(1,1,0,1,0,\dots,0)$ determine a more interlocking type of design. Note that because $\mathbf{1}$ is an eigenvector of every circulant matrix, we may operate on $\mathbf{A} - \mathbf{1}\mathbf{1}'$ and then, omitting the term in λ_n^{-1} , (2.4.4) gives the generalized inverse required by MDS. All such designs may be analysed very efficiently by the methods of section 2.4, especially when many of the ξ 's are zero.

When Ξ is a symmetric block-circulant with constant row sums, case (ii) may be handled by the method outlined in section 2.5. Although this may seem a very specialized result, it has practical importance because it includes the case when each $\Xi_j = \mathbf{1}\mathbf{1}'$ or $\mathbf{0}$ which gives block forms of design analogous to the augmented diagonal designs mentioned immediately above. These may be handled much more efficiently than other designs of case (ii).

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