A THEOREM ON MATRICES OF 0'S AND 1'S

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In this note we define two types of matrices, called "special" and "quasi-special", which we first discuss in their own rights; it turns out that the quasi-special matrices have a canonical representation (under permutational similarity) in terms of special matrices. We show how this fact can, essentially, be expressed in the language of graph theory, and we also use it to give a new proof of a theorem of Goldberg [**1**] on matrices with real roots. We shall be concerned, specifically, with the following properties of an $n \times n$ matrix $A = (a_{ij})$:

DEFINITION 1. We call A *special* if $a_{ij} \neq 0$ implies $a_{ji} \neq 0$.

DEFINITION 2. Given any integer s with[1] $3 \leqq s \leqq n$, we call A *s-special* if, for every ordered set $(i) = (i_1, \cdots, i_s)$ of integers i_r in the range $1 \leqq i_r \leqq n$ $(r = 1, \cdots, s)$, the statement

$$\mathrm{N}_A(i): \quad a_{i_1 i_2} \neq 0, \ \cdots, \ a_{i_{s-1} i_s} \neq 0 \ , \quad a_{i_s i_1} \neq 0$$

implies

$$\mathrm{N}_{A'}(i): \quad a_{i_2 i_1} \neq 0, \ \cdots, \ a_{i_s i_{s-1}} \neq 0 \ , \quad a_{i_1 i_s} \neq 0 \ .$$

For example, every symmetric matrix is special (and the same is true of hermitian matrices over any ring with involution). Also, obviously, every special $n \times n$ matrix is s-special for each $s = 3, \cdots, n$, and it will be convenient to call any matrix with this latter property *quasi-special*. Thus every special matrix is quasi-special. The converse of this is easily seen to be false: e.g.

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix}$$

is 3-special (since $\mathrm{N}_A(i_1, i_2, i_3)$ is always false), hence quasi-special, but this A is evidently not special. Nevertheless, every quasi-special matrix does have certain special matrices associated with it. More precisely, our main result is

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[1] Clearly $s = 1, 2$ would lead to properties enjoyed by every matrix A, and so we need not consider these values of s.

THEOREM. (1) *Given any $n \times n$ matrix of the lower-triangular block form*

$$B = \begin{pmatrix} B_{11} & 0 & 0 & \cdots & 0 \\ B_{21} & B_{22} & 0 & & 0 \\ \vdots & & & \ddots & \vdots \\ B_{m1} & B_{m2} & B_{m3} & \cdots & B_{mm} \end{pmatrix}$$

where each block B_{kk} occuring on the diagonal of B is special (in particular, square), and given any $n \times n$ permutation matrix P, then the matrix $A = PBP^{-1}$ is always quasi-special.

(2) *Conversely, every quasi-special $n \times n$ matrix A can be expressed in the form $A = PBP^{-1}$, with B, P as in* (1).

For matrices over any integral domain, of course $\mathrm{N}_A(i)$ becomes simply $a_{i_1 i_2} \cdots a_{i_s i_1} \neq 0$. However, our Theorem is essentially combinatorial, in that its proof involves no genuinely algebraic operations on the elements of the matrices A, B, which may consequently be of quite arbitrary nature. All that we need is that there be given some classification of these elements into two disjoint subsets, say Z and N (standing for "zero" and "nonzero"), in which case we must replace each inequality $a_{i_r i_{r+1}} \neq 0$ occurring in $\mathrm{N}_A(i)$ by a corresponding statement $a_{i_r i_{r+1}} \in N$ (or, equivalently, by a relational statement $i_r\, R i_{r+1}$). Since our arguments will not require any further properties of Z or N we might, with no real loss of generality, equally well have stated the theorem for matrices whose elements are all 0 or 1 (hence our title). Nevertheless, for the sake of its application in a Corollary below, where the elements will be complex numbers, we have preferred to state the result in the apparently (but rather illusorily) more general from above.

Proof of (1). This is relatively trivial. Since the property of being quasi-special (or not) is clearly preserved under similarity transformation by any permutation matrix P, we need only prove that a matrix of the type B must itself be quasi-special. To this end, let $(i) = (i_1, \cdots, i_s)$ (where $3 \leqq s \leqq n$) be any sequence for which $\mathrm{N}_B(i)$ holds. We shall show first that this can happen only if each of the $b_{i_r i_{r+1}}$ (where we define $i_{s+1} = i_1$ conventionally) lies in some diagonal block B_{kk} (and indeed all in the same block, though this is not vital to our argument).

For, since $\mathrm{N}_B(i)$ requires all the $b_{i_r i_{r+1}}$ to be nonzero, each $b_{i_r i_{r+}}$

must lie in some block B_{uv} with $v \leqq u$ (where u, v depend on r). Among all those B_{uv} which contain a $b_{i_r i_{r+1}}$, choose one with minimum u; without loss of generality, we may suppose that the corresponding $r = 1$, i.e. that $b_{i_1 i_2} \in B_{uv}$ with u minimum and $v \leqq u$. Then, since all the B_{kk} are square, $b_{i_2 i_3} \in B_{vw}$ for some w, and, by the minimality of u, we must have $v = u$, i.e. $b_{i_1 i_2} \in B_{uu}$. Repeating the argument, we see that $b_{i_2 i_3} \in B_{uu}, \cdots, b_{i_{s-1} i_s} \in B_{uu}, b_{i_s i_1} \in B_{uu}$.

Thus all the $b_{i_r i_{r+1}}$ corresponding to any sequence (i) for which $N_B(i)$ holds must belong to the same diagonal block B_{uu}. Since each such B_{uu} is given to be special (even quasi-special would be enough for our present purpose) and since all the $b_{i_r i_{r+1}}$ are nonzero (by $N_B(i)$), it follows that all the $b_{i_{r+1} i_r}$ are nonzero too, i.e. $N_{B'}(i)$ holds. To summarize, $N_B(i)$ implies $N_B(i)$, so that B, and hence A, is indeed quasi-special, as required.

Proof of (2). If A is not itself special, i.e. if for some u, v we have $a_{uv} = 0$, $a_{vu} \neq 0$, then, since of course $u \neq v$, by applying a suitable permutational similarity (specifically, the one that interchanges the first row with the uth and the vth with the nth, and the columns similarly), we may take $u = 1$, $v = n$, i.e. we may suppose throughout that

$$(*) \qquad a_{1n} = 0 \; , \qquad a_{n1} \neq 0 \; .$$

We now apply a double induction, first on the order n of A and secondly on the row index i within A. Thus, supposing the theorem already proved for all square matrices of order $<n$, we let A be as stated, assume by way of contradiction that A can *not* be transformed to the form B by permutation, and take as our "inner" inductive hypothesis the proposition

H_i: *there exist an* $n \times n$ *permutation matrix* Q_i, *and integers* $k_1, \cdots, k_i$ *satisfying* $1 \leqq k_1 \leqq k_2 \leqq \cdots \leqq k_i < n$ *such that, for each* $h = 1, \cdots, i$, *we have*

$$c_{hj} \neq 0 \, (k_{h-1} < j \leqq k_h) \; , \qquad c_{hj} = 0 \quad (k_h < j \leqq n) \; ,$$

and also $c_{n1} \neq 0$, *where* $C = (c_{hj})$ *denotes the matrix* $Q_i^{-1} A Q_i$ *and we interpret* $k_0 = 1$.

We wish to prove first that H_i is true for each $i = 1, \cdots, n-1$, and our chief task in so doing will be to deduce H_i from H_{i-1}. Suppose then, for some i with $1 < i < n$, that H_{i-1} holds. Since the property of being quasi-special is unaffected under similarity transformation by a permutation matrix, and since any product of permutation matrices is itself a permutation matrix, we may assume with no loss of generality that Q_{i-1} is just the unit matrix (so that we may speak of A rather than C).

Given H_{i-1}, if $k_{i-1} \leqq i-1$, then A would have an $(i-1) \times (n-i+1)$ block of zeroes in its upper right hand corner. Also the leading $(i-1) \times (i-1)$ block of A and its complementary $(n-i+1) \times (n-i+1)$ submatrix are both quasi-special, of order at most $n-1$, and so, by our inductive hypothesis on n, we could find an $n \times n$ permutation matrix P (of the form $P = \text{diag.}(P_1, P_2)$, where P_1, P_2 are permutation matrices of orders $i-1$, $n-i+1$ respectively) transforming A to the form B, which is contrary to assumption.

Thus the only possibility is that each $k_{i-1} \geqq i$. Let us now permute the columns of A to the right of the k_{i-1}th, but omitting the nth (i.e. $n - k_{i-1} - 1$ columns in all), among themselves so that, in the set of elements where these columns intersect the ith row, the nonzero elements (if any) are brought to the left, and the zeroes (if any) to the right (while, by the definition of $k_1, \cdots, k_{i-1}$, such a permutation of columns leaves the first $i-1$ rows unaffected); and define an integer k_i (clearly in the desired range $k_{i-1} \leqq k_i < n$) by writing the number of these nonzero elements as $k_i - k_{i-1}$.. Then, since $k_{i-1} \geqq i$, we may perform a corresponding permutation on the $(k_{i-1}+1)$th through $(n-1)$st rows without interfering with any of the first i rows (or the nth, so that a_{n1} is left nonzero), i.e., with this k_i, we have constructed a permutational similarity taking A into just the form prescribed in H_i, *provided only that* $a_{in} = 0$.

To prove that we do always in fact have $a_{in} = 0$, we proceed indirectly, and shall first consider the elements of the ith column which lie above the ith row. For $i > 1$, if $a_{pi} = 0$ for each $p = 1, \cdots, i-1$, then this would imply $i > k_{i-1}$, a contradiction. Hence there must be some integer i_1 in the range $i > i_1 \geqq 1$ such that $a_{i_1 i} \neq 0$. By repeating this argument, we can find a sequence of integers $i > i_1 > i_2 > \cdots > i_t > i_{t+1} = 1$ such that $a_{i_1 i} \neq 0, a_{i_2 i_1} \neq 0, \cdots, a_{i_t i_{t-1}} \neq 0$, $a_{1 i_t} \neq 0$ (where we interpret $t = 0$ if $i_1 = 1$, in which case we need only the fact that $a_{1i} \neq 0$). But then, if $a_{in} \neq 0$, we should have (since $a_{n1} \neq 0$ by H_{i-1}) a $(t+3)$-cycle of nonzero elements

$$a_{1i_t} \neq 0 \,, \quad a_{i\ i\ -1} \neq 0 \,, \quad \cdots \,, \quad a_{i_2 i_1} \neq 0 \,, \quad a_{i_1 i} \neq 0 \,, \quad a_{in} \neq 0 \,, \quad a_{n1} \neq 0 \,,$$

whence, since A is quasi-special and $t + 3 \leqq i + 1 \leqq n$, it would follow that (in particular) $a_{1n} \neq 0$, contrary to H_{i-1} (at least for $n \geqq 3$); hence $a_{in} \neq 0$ cannot occur, i.e. H_i holds in its entirety.

Thus, to sum up, given the truth of (2) for all matrices A of order $<n$, where $n \geqq 3$, we have proved, for each i with $1 < i < n$, that H_{i-1} implies H_i. Since H_1 always holds (as is easily verified, given $(*)$), it follows that H_{n-1} holds. But, since $k_{n-1} < n$, this would imply that (after a suitable permutational transformation) the nth column of A (excepting perhaps the (n, n) element) consisted entirely of zeroes, so that, by our ("outer") inductive hypothesis on n, it would follow that A could, after all, be permuted into the form B, which contradiction completes our inner induction argument.

Thus for $n \geqq 3$, the required assertion (2) about any $n \times n$ quasi-special matrix A is implied by the corresponding assertion about all quasi-special matrices of order $<n$; the cases $n = 1, 2$ being trivial, (2) now follows at once by induction on n.

Though the proof we have given is in a sense quite direct, it is also possible to regard our Theorem as being just an algebraic formulation of a geometrically almost self-evident result in the theory of graphs; and, in the process, our apparently somewhat exotic Definitions 1, 2 above will now appear in a more natural light.

We suppose given a directed graph G, i.e. a set of *vertices* (denoted $p, q, p_1, p_2, \cdots$) and a binary relation R on this set (so that, for given vertices p, q, then pRq may or may not hold); we may think of the vertices of G as points in a plane, with a directed segment from p to q for each pair p, q satisfying pRq. By convention, pRp is always false[2]. By a *cycle* of G we shall mean any ordered subset $p_1, \cdots, p_s$ of its vertices such that $p_1Rp_2, \cdots, p_{s-1}Rp_s, p_sRp_1$; we call such a cycle *reversible* if $p_s, p_{s-1}, \cdots, p_1$ is also a cycle. If G has no cycles, we call G *acyclic*. If, for arbitrary $p, q \in G$, pRq implies qRp, then we call G *symmetric*. If, for arbitrary $p, q \in G$ with $p \neq q$, there is always a sequence $q_1, \cdots, q_s$ of vertices of G such that $q_1 = p, q_s = q$ and also, for each $i = 2, \cdots, s$, either $q_{i-1} Rq_i$ or q_iRq_{i-1}, then we call G *connected*.

The concept of a subgraph is clear, and we can also define quotient graphs by factoring G with respect to any prescribed identifications of its vertices. More precisely, given any equivalence relation S on the vertices of G, inducing equivalence classes denoted by $G_{h(h=1,2\ \cdots)}$, then we may regard the G_h as vertices of a new graph $\mathfrak{G}$ by defining $\mathfrak{R}$ on $\mathfrak{G}$ by the rule that $G_h \mathfrak{R} G_k$ (for $h \neq k$) if and only if there exist $p \in G_h$, $q \in G_k$ such that pRq. We call $\mathfrak{G}$ the *quotient graph of G by S*, and write $\mathfrak{G} = G/S$. We can now state

LEMMA. (1) *Given any directed graph G and a quotient graph G/S of it which is acyclic and of which every vertex is a symmetrical subgraph of G, then every cycle of G is reversible.*

[2] For definiteness, it is desirable to adopt either this convention or its opposite, and in the present connection this alternative seems the more convenient. However, there is no general agreement on the point: e.g. Harary uses the opposite convention in [**2**], but in effect also uses ours in [**3**].

(2) *Conversely, if every cycle of a directed graph G is reversible, then there is a factoring G/S such that G/S is acyclic and each vertex G_h of G/S is a symmetrical connected subgraph of G.*

Proof of (1). By the acyclic nature of G/S, any cycle in G can involve only vertices from a single equivalence class G_h under S; and, since each such G_h is given to be symmetric, any cycle in G_h is certainly reversible.

Proof of (2). We define a binary relation S on G by the rule that, for $p, q \in G$, we have pSq whenever either $p = q$ or there is a cycle of G containing both p and q. We see at once that S is an equivalence. It is also a trivial matter to check that the induced equivalence classes are connected and (by our hypothesis on G) symmetric with respect to the given relation R on G, and, finally, that G/S is acyclic.

So transparent a lemma as this deserves stating only for the sake of its applications, and presumably various forms of the same result have appeared in the literature; for example, a somewhat more general version is implicit in [3]. However, it seems desirable here to have an explicit account in a terminology adapted to our present concerns.

In both parts of the Lemma, clearly G is connected if and only if G/S and all its vertices G_h are. The two parts of the Lemma are in close analogy with those of our Theorem, and in fact we can set up a one-one correspondence between directed graphs of n vertices (numbered in some specified order) on the one hand, and $n \times n$ matrices of 0's and 1's with zero diagonal on the other (we shall suppose n finite, for conformity with our statement of the Theorem, but this is not really necessary). Specifically, given G, with vertices $p_1 \cdots$, p_n, we define $a_{ij} = 1$ if $p_i R p_j$, and $a_{ij} = 0$ otherwise; conversely, given any $n \times n$ matrix A of 0's and 1's with zero diagonal, we can reverse this to obtain a unique numbered graph G of order n. Thus we may write $A = M(G)$, $G = M^{-1}(A)$. We verify at once that A is special if and only if G is symmetric, that A is quasi-special if and only if the cycles of G are reversible, and that A is lower-triangular (i.e. $a_{ij} = 0$ whenever $i < j$) if and only if $p_i R p_j$ implies $i > j$ (in particular, this makes G acyclic). The restriction that A have zero diagonal is purely a technicality, since the diagonal elements have no effect on the properties of being special or quasi-special.

Also, given any equivalence S on G, there is a simple relationship between the matrix A corresponding to G and those corresponding to G/S and its vertices G_h. For the matrix $M(G_h)$, relative to the ordering induced on G_h by the prescribed numbering of G, is just the submatrix of A formed by the intersections of the rows and columns of A corresponding to those vertices of G which lie in G_h. Also, if the numbering of G is chosen so that all the vertices of G_1 come first (in some arbitrary order), then those of G_2, and so on, and if we partition A accordingly, then each G_h will have as its matrix the hth diagonal block of A; and G/S will have as its matrix (e_{hk}), where $e_{hk} = 1$ if $h \neq k$ and there exist $p \in G_h, q \in G_k$ with pRq, and where $e_{hk} = 0$ otherwise.

Finally, similarity transformation of A by a permutation matrix P corresponds to re-numbering the vertices of G according to the permutation defined by P, while G is connected if and only if there is no such P transforming A into a diagonal sum of smaller matrices.

Thus our correspondence $A = M(G) \leftrightarrow G = M^{-1}(A)$ embraces all the concepts involved in the Theorem and the Lemma, and it is a routine matter (the only point constituting a minor exception is that we need to show that any finite acyclic graph can be numbered in such a way that its matrix is triangular) to check that the various hypotheses and conclusions of the two parts of the Theorem translate, under this correspondence, into those of the Lemma. Thus (at the cost of introducing several additional concepts and definitions) our lemma and its proof provide an alternative and more intuitive proof for the Theorem. This second approach shows also that the set of diagonal blocks B_{kk} appearing in the Theorem is uniquely determined by A (up to permutational similarities applied to the B_{kk} themselves).

We conclude with our promised application: this could be established as a direct consequence of the Lemma, but seems more naturally obtained from the theorem. We first need some terminology analogous to that in Definition 2 above.

DEFINITION 3. Given any complex $n \times n$ matrix A and an integer s with $3 \leqq s \leqq n$, we call A *s-hermitian* if, for every ordered index set (i) (as in Definition 2), we have

$$a_{i_1i_2} \cdots a_{i_{s-1}i_s}a_{i_si_1} = \overline{a_{i_2i_1} \cdots a_{i_si_{s-1}}a_{i_1i_s}} .$$

If A is s-hermitian for each $s = 3, \cdots, n$, then we call A *quasi-hermitian*. Thus every quasi-hermitian matrix is quasi-special.

COROLLARY. *If, for a given $n \times n$ quasi-hermitian matrix A, we have*

(P): *all $a_{ij}a_{ji}$ are real and non-negative $(i, j = 1, \cdots, n)$, then A has all its eigenvalues real.*

This result is due to Goldberg [1], whose own proof was by explicitly exhibiting a certain hermitian matrix having the same principal minors (and hence the same characteristic function) as A.

Proof. By part (2) of our Theorem, A is permutationally similar to a matrix of the form B. Since (P) and the property of being quasi-hermitian are preserved under any permutational similarity, consequently B, and hence each of its diagonal blocks B_{kk}, again satisfies the hypotheses of the Corollary; thus, since the eigenvalues of the B_{kk} are collectively just those of A, it will be enough to prove that all of the eigenvalues of these B_{kk} are real. In other words, we need only prove the Corollary for the case of a *special* matrix; accordingly, we may suppose from the outset that A is itself special.

We now introduce an $n \times n$ matrix D coinciding with A except where A has zeroes, in which places we let D have 1's; i.e., more formally, let

$$d_{ij} = \begin{cases} a_{ij} \text{ when } a_{ij} \neq 0 , \\ 1 \text{ when } a_{ij} = 0 . \end{cases}$$

Since A is special and satisfies (P), we have $d_{ij}d_{ji}$ real and strictly positive ($i, j = 1, \cdots, n$). Define also, for all u, v with $1 \leqq u < v \leqq n$,

$$\begin{aligned} f_{uv} &= d_{u,u+1}d_{u+1,u+2} \cdots d_{v-1,v} , \\ g_{uv} &= d_{u+1,u}d_{u+2,u+1} \cdots d_{v,v-1} , \\ f_{uu} &= g_{uu} = 1 , \end{aligned}$$

and write

$$t_i = |g_{1i}|^2\overline{f_{in}g_{in}} \qquad (i = 1, \cdots, n)$$

Now, since the d_{ij} are all nonzero by definition, certainly each $g_{1i} \neq 0$, while also, for any u, v with $u < v$, we have

$$f_{uv}g_{uv} = (d_{u,u+1}d_{u+1,u}) \cdots (d_{v-1,v}d_{v,v-1}) ,$$

so that each $f_{uv}g_{uv}$ is real and strictly positive. In particular $f_{in}g_{in} > 0$ for all $i < n$, while this is trivially true for $i = n$. Thus all the t_i are strictly positive real numbers.

We wish to show next that $t_ja_{ij} = t_i\overline{a_{ji}}$ ($i, j = 1, \cdots, n$), to which end it will be convenient to write the t_i in the equivalent form $t_i = \overline{g_{1n}}g_{1i}\overline{f_{in}}$. There being no loss of generality (since the t_i are real) in supposing that $i < j$, it will suffice to prove that

$$g_{1j}\overline{f_{jn}}a_{ij} = g_{1i}\overline{f_{in}a_{ji}} \qquad (1 \leqq i < j \leqq n) .$$

But, under our assumption $i < j$, clearly $g_{1j} = g_{1i}g_{ij}$, $f_{in} = f_{ij}f_{jn}$, and so we need only verify that $g_{ij}a_{ij} = \overline{f_{ij}a_{ji}}$, which, on being translated back in terms of the a_{ij}, is an immediate consequence of our assumption that A is special, quasi-hermitian and satisfies (P).

Thus we have produced positive real $t_1, \cdots, t_n$ such that $t_j a_{ij} = t_i \overline{a_{ji}}$ $(i, j = 1, \cdots, n)$, i.e. $AT^2 = T^2A^*$, where $T = \text{diag.}\,(t_1^{1/2}, \cdots, t_n^{1/2})$ is hermitian and non-singular, and we use an asterick to denote the conjugate transposed. Thus $T^{-1}AT = (T^{-1}AT)^*$, so that A is similar to the hermitian matrix $T^{-1}AT$; in particular, the eigenvalues of A must be real, as required.

In conclusion, we note that, by considering matrices of the form

$$\begin{pmatrix} 0 & a_{12} & a_{13} \\ a_{21} & 0 & 0 \\ a_{31} & 0 & 0 \end{pmatrix},$$

with characteristic function $x(x^2 - a_{12}a_{21} - a_{13}a_{31})$, it is clear that a special quasi-hermitian matrix A can have its eigenvalues all real even if (P) fails (in particular, A need not be hermitian).

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