On Moore Graphs with Diameters 2 and 3

Abstract: This note treats the existence of connected, undirected graphs homogeneous of degree $d$ and of diameter $k$, having a number of nodes which is maximal according to a certain definition. For $k = 2$ unique graphs exist for $d = 2, 3, 7$ and possibly for $d = 57$ (which is undecided), but for no other degree. For $k = 3$ a graph exists only for $d = 2$. The proof exploits the characteristic roots and vectors of the adjacency matrix (and its principal submatrices) of the graph.

1. Introduction

In a graph of degree $d$ and diameter $k$, having $n$ nodes, let one node be distinguished. Let $n_i$, $i = 0, 1, \cdots, k$ be the number of nodes at distance $i$ from the distinguished node. Then $n_0 = 1$ and

$$n_i \leq d(d - 1)^{i-1} \text{ for } i \geq 1. \tag{1}$$

Hence

$$\sum_{i=0}^{k} n_i = n \leq 1 + d \sum_{i=1}^{k} (d - 1)^{i-1}. \tag{2}$$

E. F. Moore has posed the problem of describing graphs for which equality holds in (2). We call such graphs “Moore graphs of type $(d, k)$”. This note shows that for $k = 2$ the types $(2, 2)$, $(3, 2)$, $(7, 2)$ exist and there is only one graph of each of these types. Furthermore, there are no other $(d, 2)$ graphs except possibly $(57, 2)$, for which existence is undecided. For $k = 3$ only $(2, 3)$ exists; this is the 7-gon.

The results of Section 2 and Eq. (3) are due to Moore, who has also shown the nonexistence of certain isolated values of $(d, k)$ using methods of number theory.

2. Elementary properties

Moore observed that in graphs for which equality holds in (2) every node is of degree $d$, since it necessitates that equality hold in (1) for each $i$. Furthermore, since no node has degree exceeding $d$, each node counted in $n_i$ is joined with $(d - 1)$ nodes counted in $n_{i+1}$, for $i = 1, \cdots, k - 1$. Hence no arc joins two nodes equally distant from some distinguished node, except when both are at distance $k$ from the distinguished node.

Thus if arcs joining nodes at distance $k$ from the distinguished node are deleted the residual graph is a hierarchy, as in Fig. 1. The same hierarchy results from distinguishing any node.

Figure 1

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3. Notation

The discussion deals with matrices of various orders, and with some which are most clearly symbolized as arrays of matrices or blocks of lower order. We will not attempt to indicate orders by indices, but rather to indicate them explicitly or implicitly in the context.

The following symbols denote particular matrices throughout:

- \( I \) is the identity matrix
- \( 0 \) is the zero matrix
- \( J \) is the matrix all of whose elements are unity
- \( K \) is a matrix of order \( d(d-1) \) which is a \( d \times d \) array of diagonal blocks of \( J \)'s of order \( d-1 \).

Thus

\[
K = \begin{bmatrix}
J & 0 & \cdots & 0 \\
0 & J & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots \\
0 & 0 & \cdots & J
\end{bmatrix}
\]

0 is used also for a vector all of whose elements are zero.
- \( u \) is a vector all of whose elements are unity.
- \( e_i \) is a vector whose \( i \)-th element is unity and the remainder are zero.

We use prime (') to indicate the transpose of a matrix. An unprimed vector symbol is a column vector, a primed vector symbol is a row vector. Thus

\[
u = \begin{bmatrix}
1 \\
1 \\
\vdots \\
1
\end{bmatrix}
\]

The subset of nodes of tier \( k \), Fig. 1, which are joined to the \( i \)-th node of tier \( (k-1) \) is designated \( S_i \). The arcs joining nodes of tier \( k \), which are omitted from the hierarchy, are called re-entering arcs.

4. Diameter 2

Consider a Moore graph with \( k = 2 \). Then \( n = 1 + d^2 \). Let \( A \) be its adjacency matrix. That is, with the nodes of the graph given any numbering,

\[
a_{ij} = \begin{cases}
1 & \text{if nodes } i \text{ and } j \text{ have an arc in common} \\
0 & \text{otherwise}
\end{cases}
\]

From the elementary properties, each pair of nodes is at most joined by one path of length 2. The second order adjacencies (i.e., the pairs of nodes joined by paths of length 2 without retracing any arcs) are given by \( A^2 - dI \). Using the 0th, 1st and 2nd order adjacencies,

\[
A^2 + A - (d-1)I = J. \quad (3)
\]

Since \( J \) is a polynomial in \( A \), \( A \) and \( J \) have a common set of eigenvectors. One of these is \( u \), and \( Ju = nu \), \( Au = du \).

For this eigenvector, (3) supplies the relation which is already known,

\[
(1 + d^2)u = nu.
\]

Let \( v \) be any other eigenvector of \( A \) corresponding to eigenvalue \( r \). Then \( JV = 0 \), \( AV = rv \).

Using (3),

\[
T + r - (d-1) = 0.
\]

The values of \( d \) which satisfy this equation are:

- \( d = 0 \), for which \( n = 1 \). This is a single node, which does not have diameter 2.
- \( d = 2 \), for which \( n = 5 \). This is the pentagon, clearly a Moore graph of type (2, 2), and clearly the only one of that type.

The values of \( d \) for which the \( r \)'s of (4) are rational are those for which \( 4d - 3 \) is a square integer, \( s^2 \), since any rational eigenvalues of \( A \) are also integral. Let \( m \) be the multiplicity of \( r_1 \). Then the sum of the eigenvalues is

\[
d + \frac{(n-1)}{2} (r_1 + r_2) = d - \frac{d^2}{2} = 0.
\]

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\[
d + m \frac{s-1}{2} + (n-1-m) = \frac{s-1}{2} = 0.
\]

Using \( n = 1 = d^2 \) and \( d = (s^2 + 3)/4 \),

\[
s^2 + s^2 + 6s^2 - 2s^2 + (9 - 32m)s - 15 = 0. \quad (5)
\]

Since (5) requires solutions in integers the only candidates for \( s \) are the factors of 15. The solutions are:
The case \( d = 7 \) has an exemplar which is shown later.

The case \( d = 57 \) is undecided.

The uniqueness of Moore graphs \((3, 2)\) and \((7, 2)\) is shown in the next section.

5. Uniqueness

Let the nodes be numbered as follows:

No. 0: any node,
Nos. 1 to \( d \): the nodes adjacent to No. 0 in arbitrary order,
Nos. \((d + 1)\) to \((2d - 1)\): the nodes of \( S_1 \) in arbitrary order,

\[
\begin{array}{ccccccc}
0 & 11 & 01 & 01 & 10 & 10 & 10 \\
1 & 01 & 01 & 01 & 01 & 01 & 01 \\
& & & & & & 01 \, 01 \, 01 \, 01 \, 01 \, 01 \, 01 \\
& & & & & & 01 \, 01 \, 01 \, 01 \, 01 \, 01 \, 01 \\
& & & & & & 01 \, 01 \, 01 \, 01 \, 01 \, 01 \, 01 \\
& & & & & & 01 \, 01 \, 01 \, 01 \, 01 \, 01 \, 01 \\
& & & & & & 01 \, 01 \, 01 \, 01 \, 01 \, 01 \, 01 \\
\end{array}
\]

The adjacency matrix \( A \) then has the form of Fig. 2.

The \( P_{ij} \) are matrices of order \((d - 1)\), as indicated by the tabulation of the number of rows in each block. The argument will concern several of the principal submatrices of \( A \). Consider first the principal submatrix of order \( d(d - 1) \) in the lower right, outlined in heavy rules, which shows the adjacency relations between the tier 2 nodes through the re-entering arcs. Let it be designated \( B \). We give further form to \( B \) in the following theorems, which are rather obvious consequences of the hierarchy of Fig. 1.

- **Theorem 1**

  No cycle of length less than 5 exists in the graph.

  If there were such a cycle, designate one of its nodes as the distinguished node. Then equality would not hold in (1) for some \( i \).

- **Theorem 2**

  The diagonal blocks of \( B \) are 0.

  Let two nodes of tier 2, \( a \) and \( b \), be members of the same subset \( S_i \). If they were adjacent, then \( a, b \) and the \( i \)-th node of tier one would form a cycle of length 3.

- **Theorem 3**

  The blocks \( P_{ij} \) of \( B \) are permutation matrices.

  Let node \( a \) be a member of \( S_i \) and \( b \) and \( c \) be members of \( S_j \). If \( a \) were adjacent to both \( b \) and \( c \), then \( a, b, c \) and the \( j \)-th node of tier one would form a cycle of length 4. Hence any node of tier 2 is adjacent to at most one node in any of the subsets designated \( S_i \). Since such a node is adjacent to \((d - 1)\) other nodes of tier 2 through the re-entering arcs, and
since there are \((d - 1)\) subsets \(S_i\) other than the one of which it is itself a member, each node of tier 2 is adjacent to exactly one node in each of the other subsets. Hence each row and each column of each \(P_{ij}\) in \(B\) contains exactly one 1.

* Theorem 4

The nodes may be so numbered that \(P_{ij} = P_{ji} = I\).

In arriving at the form for \(A\) shown in Fig. 2 no order was prescribed for the nodes within each \(S_i\) of tier 2. Let any order be given to the nodes of \(S_i\). Each node of \(S_i\) is adjacent to one node of each other subset. If each node of \(S_i\) is given the order number of its adjacent node in \(S_i\), then \(P_{ii} = I\).

Note that the orders of nodes in tier 1 and in \(S_i\) are still arbitrary. This fact will be used later.

When the nodes are numbered so that \(A\) has the form of Fig. 2 with the further arrangement of Theorem 4, \(A\) is said to be in canonical form. By using the canonical form of \(A\) in (3) one finds that \(B\) satisfies

\[
B' + B - (d - 1)I = J - K.
\]

Then from Eq. (6),

For \(j \neq 1\), \(\sum \limits_i P_{ij} = J_j\);

and \(P_{ik} + \sum \limits_j P_{ij}P_{jk} = J\) if \(i \neq k\).

An analysis similar to that given for \(A\) shows that the eigenvalues of \(B\) and their multiplicities are:

<table>
<thead>
<tr>
<th>eigenvalue</th>
<th>multiplicity</th>
</tr>
</thead>
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<tr>
<td>2</td>
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</tr>
<tr>
<td>-1</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
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<td>6</td>
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<tr>
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<td>56</td>
</tr>
<tr>
<td>7</td>
<td>1672</td>
</tr>
<tr>
<td>-8</td>
<td>1463</td>
</tr>
</tbody>
</table>

* Theorem 5

The Moore graph \((3, 2)\) is unique.

In the canonical form

\[
B = \begin{bmatrix}
0 & I & I \\
I & 0 & P \\
I & P & 0
\end{bmatrix}
\]

\(P\) cannot be \(I\), for this would mean that \(\sum \limits_i P_{ii} = 2I\), violating (7). Hence

\[
P = \begin{bmatrix}
0 & 1 \\
1 & 0
\end{bmatrix}
\]

and this is unique.

The submatrix \(B\) for a Moore graph of type \((7, 2)\) in canonical form is shown in Fig. 3. Only
the upper triangle is represented in the Figure, since $B$ is symmetric. To show that by appropriate numbering of the nodes the adjacency matrix for any graph $(7, 2)$ may be made to correspond with that shown, and hence that there is only one such graph, requires several steps. We first show that all $P_{ii}$ are involutions.

• Theorem 6

The principal submatrix of $A$ for type $(7, 2)$,

$$M = \begin{bmatrix} 0 & I & I \\ I & 0 & P_{23} \\ I & P_{23}' & 0 \end{bmatrix}$$

has an eigenvalue 2 of multiplicity 3.

The argument involves the invariant vector spaces corresponding to eigenvalue 2 of $A$, and some of the other principal submatrices of $A$. A set of vectors forming a basis for the invariant vector space of $A$ corresponding to the characteristic root 2 is shown below. For notation, the components are segregated according to the blocks shown for $A$ in Fig. 2. The first 8 components are written out and the last 42 components are shown as 7 vectors of dimension 6. The vectors are numbered at the left for ease of reference later.

The last 42 components of (I) form an eigenvector for $B$ for eigenvalue 6, and the last 42 components of numbers (II) through (VII) are eigenvectors for $B$ for eigenvalue $-1$. Hence there remain 21 independent vectors whose first eight components are 0 and whose last 42 components form a basis for the eigenspace corresponding to 2 of $B$. We symbolize these as

(VIII) $0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ v_i' \ v_i' \ v_i' \ v_i' \ v_i' \ v_i' \ v_i'$.

Because as eigenvectors of $B$ they correspond to different eigenvalues,

$$u'v_i = 0.$$ 

We now consider the upper left principal submatrix $L$ of $A$, of order 26, and the submatrix $L^*$ of order 27 obtained through augmenting $L$ by one column and the corresponding row,

$$L = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & u' & 0' & 0' \\ 1 & 0' & u' & 0' \\ 1 & 0' & 0' & u' \\ 1 & 0' & 0' & 0' \\ 1 & 0' & 0' & 0' \\ 1 & 0' & 0' & 0' \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & I & I \\ 0 & u & 0 & 0 & 0 & 0 & 0 & I & 0 & P_{23} \\ 0 & 0 & u & 0 & 0 & 0 & 0 & I & P_{23}' & 0 \end{bmatrix},$$

$$L^* = L_u + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} e_k + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} e_i + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} e_j$$

where the augmenting column for $L^*$ comes from the fourth block, and $h, i$ and $j$ are unspecified.
Since the eigenspace for eigenvalue 2 of $A$ has dimension 28 (see the solutions of (5)) a subspace of this eigenspace of dimension at least 4 lies in the subspace corresponding to $L$. By inspection of the exhibited vectors a basis for such a 4-space is given above in Fig. 4 for some unspecified $v_i$.

If $L$ be augmented by one column and row, as shown in $L^*$ above, then a subspace of dimension at least 5 of eigenvectors for eigenvalue 2 of $A$ lies in the subspace of $L^*$. The four vectors above, being characteristic vectors for $A$, are characteristic vectors for $L^*$.

A fifth vector for the basis of this 5-space is independent of the eigenvectors (IV), (V), (VI) and (VII) of $A$ exhibited earlier, since any such dependence would introduce a component proportional to $u$ in at least one of the last four blocks (last 24 components). But in the block containing the augmenting column the vector may have at most one nonzero component, and in the other blocks all its components are zero. Hence the fifth vector is of the form of (VIII)

$$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ w'_i \ w'_i \ w'_i \ 0' \ 0'. $$

But $u'w_i = 0$, and $u_i$ has at most one nonzero component.

Of the five eigenvectors for $L^*$ exhibited above, the two containing $v$'s and $u$'s are zero in all the components not corresponding to the principal submatrix $M$ in the statement of the theorem. Hence they are eigenvectors for an eigenvalue 2 of $M$. They are mutually independent, and are also independent of (being orthogonal to) a vector

$$(u' \ u' \ u')$$

for $M$. The latter is, by inspection, an eigenvector for eigenvalue 2 of $M$. Hence the eigenvalue 2 of $M$ has multiplicity at least 3. We can now show that $P_{23}$ is an involution. For if we rewrite $P_{23}$ as $P$, then $M$ becomes

$$
\begin{pmatrix}
0 & I & I \\
I & 0 & P \\
I & P' & 0
\end{pmatrix}.
$$

Let us denote by $x$, $y$, $z$ the three parts of a characteristic vector of $M$ corresponding to 2. Then

$$y + z = 2x$$
$$x + Pz = 2y$$
$$x + P'y = 2z.$$

Substituting for $x$ in the last two equations, we obtain

$$-3y + (I + 2P)z = 0$$
$$(I + 2P')y - 3z = 0.$$ 

So the multiplicity of 2 as an eigenvalue of $M$ equals the multiplicity of 3 as an eigenvalue of

$$
\begin{pmatrix}
0 & I + 2P \\
I + 2P' & 0
\end{pmatrix}.
$$

Now any real matrix of the form

$$
\begin{pmatrix}
0 & T \\
T' & 0
\end{pmatrix},
$$

where all submatrices are square, has for its eigenvalues the square roots of the eigenvalues of $TT'$ and their negatives. Hence the multiplicity of 2 as an eigenvalue of $M$ is the multiplicity of 9 as an eigenvalue of

$$(I + 2P)(I + 2P') = 5I + 2(P + P').$$

Thus the multiplicity of 2 as an eigenvalue of $M$ is the multiplicity of 2 as an eigenvalue of $P + P'$,

and it is clear that this is in turn equal to the number of disjoint cycles in $P$. So $P = P_{23}$ is composed of three disjoint cycles. Thus we have

- **Theorem 7**

  In the canonical form for Moore graphs of type $(7, 2)$ all $P_{ii}$, $i \neq 1$ and $i \neq j$, are involutions.

  We adopt the notation

  $$P_{ii} = 0.$$

- **Theorem 8**

  In a Moore graph of type $(7, 2)$ in canonical form

  $P_{ii}P_{kn}P_{ki} = P_{kn}$ if $i \neq j, \ i \neq k, \ jk \neq 1.$

  If $i = 1$ the theorem is trivial. We consider $i = 1$ and write the involutions as three transpositions.
Let $P_{ij} = (ab)(cd)(ef)$. In $P_{ik}$ the companion of $a$ must come from one of $(cd)$ or $(ef)$, and the companion of $b$ from the other, because of (7). Let $P_{ik} = (ac)(be)(df)$, which is completely general. Then $P_{ij}P_{jk} = (aeb)(bdf)$.

Since $P_{ik}$ is in a row with $P_{ij}$ and in a column with $P_{ik}$ it may have no substitution of terms, which is the same as any substitution appearing in any of $P_{ij}$, $P_{ik}$ or $P_{ij}P_{ik}$. The only involution with this property is $P_{ik} = (af)(be)(ce)$. Evaluating the product $P_{ij}P_{jk}$ proves the theorem.

If all of $i$, $j$ and $k$ are different, the expression in Theorem 8 may be multiplied on the left by $P_{ik}$ and on the right by $P_{jk}$, and we have

- **Theorem 9**

$P_{ij}P_{jk}P_{ik} = P_{ik}$ if $i$, $j$, $k$ are all different and $j, k \neq 1$.

- **Theorem 10**

$P_{ij} \neq P_{kl}$ if $i$, $j$, $k$ and $l$ are all different.

If any subscript is unity the theorem is trivial. For ease of presentation, we prove the theorem for a particular set of subscripts, none unity, but it obviously extends to the general case.

Suppose $P_{23} = P_{45}$. Then

$$P_{23}P_{34}P_{45} = P_{34}P_{45}P_{23} = P_{24}$$

by Theorem 9. Also,

$$P_{23}P_{34}P_{45} = P_{45}P_{34}P_{23} = P_{35}$$

Hence $P_{35} = P_{34}$.

Similarly $P_{25} = P_{54}$.

Hence

$$P_{23} + P_{24} + P_{26} = P_{32} + P_{34} + P_{35} = P_{42} + P_{43} + P_{45}.$$  

Hence by Eq. (7),

$$P_{26} + P_{27} = P_{36} + P_{37} = P_{46} + P_{47}.$$  

But $P_{26} + P_{27} = P_{36} + P_{37}$ implies $P_{36} = P_{37}$. Similarly, $P_{26} + P_{27} = P_{46} + P_{47}$ implies $P_{46} = P_{47}$. Therefore, $P_{36} = P_{46}$, violating (7).

- **Theorem 11**

The Moore graph $(7, 2)$ is unique.

There are 15 different $P_{ij}$, $2 \leq i < j$. There are fifteen different involutions of order 6 without fixed points. Hence, for any Moore graph $(7, 2)$ in canonical form, the involution $(12)(34)(56)$ appears once. By an appropriate numbering of the nodes of tier 1 it may be brought to the $P_{23}$ position.

Because of Eq. (7), in the remaining $P_{23}$, $j > 2$, the first row of each is one of $e_1', e_2', e_3', e_4'$, and each of these appears once. By an appropriate numbering of nodes 4, 5, 6, 7 of tier 1 the $P_{23}$ may be brought to the sequence of Fig. 3.

With $P_{23} = (12)(34)(56)$, because of Eq. (7), and the numbering of nodes of tier 1 already assigned, $P_{24}$ might be only $(13)(25)(46)$ or $(13)(26)(45)$. The order of the fourth and fifth nodes of $S_1$ may be transposed, if necessary, to achieve $(13)(25)(46)$. The remaining $P_{23}$ are then uniquely determined. The argument is similar to that used in Theorem 8.

The second row of $B$ having been determined, all other $P_{ij}$ are uniquely determined by the relation of Theorem 9, with $j = 2$. Hence, any $(7, 2)$ graph may be numbered to have the adjacency matrix of Fig. 4.

6. Diameter 3

- **Theorem 12**

If the polynomial which is characteristic of Moore graphs of type $(d, k)$, $k \geq 2$, is irreducible in the field of rational numbers, then no such graphs exist unless $d = 2$.

The polynomials $F_i(x)$ satisfy the difference equation

$$F_{i+1} = xF_i - (d - 1)F_{i-1}$$

$$F_i = x + 1, \quad F_2 = x^2 + x - (d - 1)$$

and the equation for the adjacency matrix for diameter $k$ is

$$F_k(A) = J,$$

similar to (3). An adjacency matrix satisfying this equation has the number $d$ as one of its eigenvalues, and it has exactly $k$ distinct other eigenvalues which are the roots of the irreducible $F_i(x)$. Let those roots be $r_i$, $i = 1, \ldots, k$.

The first and second coefficients of $F_k$, $k \geq 2$, are both unity. Hence

$$\sum_{i=1}^k r_i = -1.$$  

If $F_k$ is irreducible its roots have equal multiplicity as eigenvalues of $A$. The number of nodes in a Moore graph of diameter $k$, if $d > 2$, is

$$n = 1 + d \frac{(d - 1)^k - 1}{d - 2}$$

and hence the multiplicity of each $r_i$ is 503
\[ m = \frac{d^k - 1}{k(d - 2)} \]

Since the trace of \( A \) is 0,

\[ d + m \sum_{i=1}^{k} r_i = 0. \]

Substituting for \( m \), this reduces to

\[(d - 1)^k - k(d - 1) + (k - 1) = 0.\]

Considering this as a polynomial in \((d - 1)\), and remarking \( k \geq 2 \), by the rule of signs it has at most two positive roots. Since it has a double root at \( d - 1 = 1 \), no \( d > 2 \) satisfies it.

Of course, \( d = 2 \) corresponds to the \((2k + 1)\)-gon, which is a Moore graph.

**Theorem 13**

The only Moore graph of diameter 3 is \((2, 3)\).

The polynomial equation for \( k = 3 \) is

\[ x^3 + x^2 - 2(d - 1)x - (d - 1) = 0. \]

If a graph \((d, 3)\) exists, \( d > 2 \), where \( d \) of course is an integer, then the above equation has at least one root which is an integer. Let \( r \) be such a root. Then

\[ d - 1 = \frac{r^2(r + 1)}{2r + 1}. \]

Now \( 2r + 1 \) is relatively prime to both \( r \) and \( r + 1 \). Hence the denominator is 1 or \(-1\), and for both of these \( d = 1 \), but the type \((1, 3)\) does not exist.

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