

Rank of the Model Matrix for Linear Compartmental Models

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Abstract This paper will show that the rank of the model matrix of a closed, n compartmental model with k sinks is $n-k$. This statement will be extended to include open compartmental models as a part of theorem.

Keyword : Model Matrix, Compartmental Model, Digraph, Subgraph.

1. Introduction

An increasing amount of discussion in the literature has been developed to the complete observability(CO) and complete controllability(CC) of the linear, time-invariant models described by

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y &= Cx \end{aligned} \tag{1.1}$$
$$x \in R^n, y \in R^p, u \in R^m$$

which incorporate a priori structural information of the system being modeled as parameterization of the model matrix A and other matrices B and C (Bellman (1970), Cobelli et al.(1987), Godfrey(1983), Godfrey et al.(1987), and Simon et al. (1991)). The analysis is related respectively to complete controllability (CC) and complete observability(CO) relies heavily on the rank of the model matrix (Grewal et. al.(1976), Jacquez(1985), Kalman(1963), and Lee(1995)). The area, involving the rank of the model matrix, requires some standard representation of the model matrix so that general statements regarding its rank can be made. Using the results of the graphical decomposition of Lee(1995) along with the polynomial matrix results, this paper will show that the rank of the model matrix of a closed, n compartmental model with k sinks is $n-k$.

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This statement will be extended to include open compartmental models as a part of theorem 2.1.

2. Analysis of the Model Matrix

The model matrix for any closed compartmental model can be written in the form,

$$A = -N\bar{K}\tilde{N}^T \quad (2.1)$$

where N = incidence matrix of the model's digraph

$\tilde{N} = N$ with all -1's set equal to zero

\bar{K} = diagonal matrix whose elements correspond to the flow parameters of the arcs.

Equation (2.1) can be justified in the following manner. Let q_i be the number of arcs directed away from vertex i . Arrange the incidence matrix, N , by designating the first q_1 columns of N for arcs leaving vertex 1, etc. Furthermore, arrange the rows of N so that row i , N_i , of N corresponds to vertex ($i = 1, 2, \dots, n$). Let k_i be a ($q_i \times 1$) vector of flow rate parameters for arcs leaving vertex i with the parameters arranged to correspond with the order of the arcs in N . Then equation (1.3) can be written as (assuming zero input for convenience),

$$\dot{x}_i = -N_i[k_1x_1, k_2x_2, \dots, k_nx_n]^T \quad i = 1, 2, \dots, n. \quad (2.2)$$

Also equation (2.2) can be written in the form,

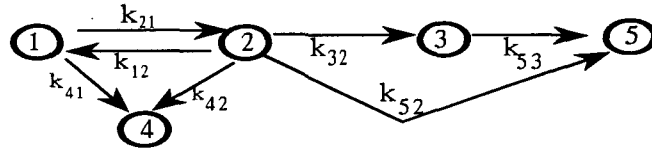
$$\dot{x}_i = -N_i\bar{K}[x_1 \cdots x_1, x_2 \cdots x_2, \dots, x_n \cdots x_n]^T \quad (2.3)$$

where the diagonal elements of \bar{K} are arranged to correspond with their positions in equation (2.2). Next equation (2.3) can be written as

$$\dot{x}_i = -N_i\bar{K}\tilde{N}^T x \quad (2.4)$$

where the first q_1 elements of the first column of \tilde{N}^T are 1's and the remaining elements zeros; the next q_2 elements of column 2 are 1's and all other elements are zero; etc. Therefore, \tilde{N}^T is precisely the transpose of N with all -1 elements set equal to zero. Since equations (2.2) through (2.4) are valid for $i = 1, 2, \dots, n$, equation (2.1) follows.

Example 2.1. Consider the following closed model.



Then the model matrix A , can be written in the form,

$$A = \begin{bmatrix} 1 & 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 \end{bmatrix} \begin{bmatrix} k_{21} \\ k_{41} \\ k_{12} \\ k_{32} \\ k_{42} \\ k_{52} \\ k_{53} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

Note that $q_1=2, q_2=4, q_3=1, q_4=q_5=0$. Also, $k_1=[k_{21}, k_{41}]$, $k_2=[k_{12}, k_{32}, k_{42}, k_{52}]$ and $k_3=[k_{53}]$.

Let n = number of vertices (or compartments) and q = number of arcs (flow channels). Then the dimensions of N , \tilde{N}^T , and \bar{K} are $(n \times q)$, $(q \times n)$, and $(q \times q)$ respectively. Furthermore, since

$$r(A) = r(N\bar{K}\tilde{N}^T), \tag{2.6}$$

it follows from Busacker et al. (1965) that

$$r(N) + r(\bar{K}) + r(\tilde{N}^T) - 2q \leq r(A) \leq \min\{n-1, r(\tilde{N}^T)\} \tag{2.7}$$

However, for connected digraphs, $r(N) = n-1$ and $r(K) = q \geq n-1$ (a connected graph with n vertices must have at least $n-1$ arcs). Then inequality (2.7) can be reduced to

$$r(\tilde{N}) + n - q \leq r(A) \leq \min\{n-1, r(\tilde{N})\} \tag{2.8}$$

and for a digraph with $n-1$ arcs,

$$r(A) = r(\tilde{N}) \tag{2.9}$$

for all nonzero flow rate parameters.

Proposition 2.1. Given a closed compartmental model which has a digraph with n vertices, $n-1$ arcs, and no more than one arc is directed away from a vertex. Then the rank of the model matrix, A , is $n-1$.

Proof. From equation (2.9), $r(A) = r(\tilde{N})$. Since no more than one arc is directed away from a vertex, there is at most one zero element in each column of \tilde{N}^T . Also, there is exactly one nonzero element in each row of \tilde{N}^T corresponding to each arc in the digraph. Therefore, $r(\tilde{N}^T) = n - 1$ and, consequently $r(A) = n - 1$. \square

The next proposition concerns the rank of the model matrix for a closed compartmental model having a digraph, D_1 , and the rank of the model matrix for a closed compartmental model having a digraph, D_2 , which can be constructed from D_1 by adding an arc between vertices of D .

Let A_1 be the model matrix corresponding to the digraph, D_1 , and A_2 be the model matrix corresponding to the digraph, D_2 . Let q_1 equal the number of arcs in D_1 , and k_{ji} be the flow rate parameter of the arc added to D_1 to the form D_2 .

Proposition 2.2. If $r(A_1) = n - 1$ on a dense subset of R^{q_1} , then $r(A_2) = n - 1$ on a dense subset of R^{q_1+1} .

Proof. Let k be a q_1 vector of flow rate parameters in D_1 . If the added arc is directed away from vertex i to vertex j and the flow rate parameter for the arc is k_{ji} , then

$$A_1 + A_2 = K_{ji} \quad (2.10)$$

with $K_{ji} = k_{ji}(e_j - e_i)e_i^T$ and e_i is a vector of appreciate dimension having the i th element (which equals one) as the only nonzero element. Since A_1 and A_2 are model matrices for closed compartmental models,

$$f^T A_1 = f^T A_2 = 0 \quad (2.11)$$

then $r([A_1, f]) = n$ on a dense subset of R^{q_1} . Now from equation (2.10),

$$[A_2, f][A_2, f]^T = [A_1, f][A_1, f]^T + A_1 K_{ji}^T + K_{ji} A_1^T + K_{ji} K_{ji}^T \quad (2.12)$$

Since $r([A_2, f]) = n$ clearly, $r(A_2) = n - 1$ on a dense subset of R^{q_1+1} . \square

Combining propositions 2.1 and 2.2, the following important proposition can be obtained.

Proposition 2.3. The model matrix, A , of a closed compartmental model with a strongly connected digraph has $r(A) = n - 1$ on a dense subset of R^q ($q =$ number of flow rate parameters).

Proof. Select a vertex, n_1 , in the strongly connected digraph, D . Since the digraph is strongly connected, every vertex in D has a path which leads to n_1 . Therefore it is always possible to construct a directed subgraph of D which

satisfies the hypothesis of proposition 2.1. Let the model matrix corresponding to this directed subgraph be \hat{A} . Then by proposition 2.1, $r(\hat{A}) = n - 1$. Now D can be constructed from the directed subgraph by adding arcs. By proposition 2.2, $r(A) = n - 1$ on a dense subset of R^q . \square

This proposition provides a mean of assessing the contribution of sinks to the rank of the overall model matrix. However, the strongly connected subgraphs corresponding to sources and transits always have an arc directed away from one of their vertices toward a vertex in another subgraph. This introduces an extra term in the model matrix of the strongly connected subgraph (note the difference between A_{SC} and \tilde{A}_{SC} or A_T and \tilde{A}_T in equations of Lee (1995)). The following proposition accounts for the effect of this added parameter.

Proposition 2.4. If A is the model matrix of a closed compartmental model with a strongly connected digraph having n vertices and q arcs, then

$$r(A - \bar{K}_0) = n \tag{2.14}$$

where $\bar{K}_0 = k_0 e_i e_i^T$, k_0 is an independent parameter, and $i = 1, 2, \dots, n - 1$, or n .

Proof. Let D be the strongly connected digraph with n vertices, q arcs, and corresponding model matrix, A By proposition 2.3, $r(A) = n - 1$. Construct a new digraph, \hat{D} , with $n+1$ vertices, by adding an arc from vertex i of D to a new vertex, zero. Let the flow rate parameter of the new arc be k_0 . Then the model matrix, \hat{A} , corresponding to \hat{D} is

$$\hat{A} = \begin{bmatrix} \tilde{A} & 0 \\ k_0 e_i^T & 0 \end{bmatrix} \tag{2.15}$$

Where $\tilde{A} = A - \bar{K}_0$ and e_i is a zero vector except for a one in the i th position. From proposition 2.3, there is a directed subgraph of D which has n vertices, $n-1$ arcs, and no more one arc is directed away from a vertex. Furthermore, the directed subgraph may be selected so that vertex i has no arcs leaving it. Then, the new digraph, \hat{D} , contains a subgraph satisfying the hypothesis of proposition 2.1. Then by proposition 2.1, $r(\hat{A}) = n$. Since $f^T \hat{A} = 0$, any n rows of \hat{A} are independent. Therefore, $r(\hat{A}) = n$ on a dense subset of R^{q+1} . \square

Finally, the conclusions of propositions 2.3 and 2.4, along with the standard form of the model matrix A (p.57 Lee(1995)) can be used to prove the directed statement regarding the rank of the model matrix.

Theorem 2.5. A compartmental model with n compartments and a total of k

sinks, l of which have excretions, has a model matrix, A with $r(A) = n - k + 1$.

Proof. Consider a closed compartmental model and equation (1.1). Every source and transit has at least one arc directed away from its subgraph. Then, by propositions 2.4, $r(\tilde{A}_{SCi}) = n_{SCi}$ where n_{SCi} = number of vertices in i th source, and $r(\tilde{A}_{Ti}) = n_{Ti}$ where n_{Ti} = number of vertices in the i th transit. Then from equations of Lee (p. 57-58, 1995),

$$r(\tilde{A}_{SC}) = \sum_{i=1}^j n_{SCi} \quad \text{and} \quad r(\tilde{A}_T) = \sum_{i=1}^h n_{Ti} \quad (2.16)$$

Each sink has no leaving arcs. By Proposition 2.3, $r(\tilde{A}_{SCi}) = n_{SCi} - 1$ where A_{SCi} = number of vertices in i th sink.

Then from Lee (p58, 1995),

$$r(A_{SK}) = \sum_{i=1}^k (n_{SKi} - 1) = \left(\sum_{i=1}^k n_{SKi} \right) - k \quad (2.17)$$

Therefore, for closed compartmental models,

$$\begin{aligned} r(A) &= r(\tilde{A}_{SC}) + r(\tilde{A}_T) + r(A_{SK}) \\ &= \left(\sum_{i=1}^j n_{SCi} \right) + \sum_{i=1}^h n_{Ti} + \left(\sum_{i=1}^k n_{SKi} \right) - k \\ &= n - k \end{aligned}$$

For open compartmental models, the rank of A will increase by one for every sink which has an excretion. Therefore, $r(A) = n - k + 1$. \square

3. Conclusions

We conclude that the rank of the model matrix of a closed, n compartmental model with k sinks is $n-k$.

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