Which Linear Compartmental Systems Contain Traps?

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This paper will prove the following result which was stated without proof by Dr. John Jacquez: A linear compartmental system has a trap if and only if the associated system of differential equations has a zero eigenvalue. It will then use this result to prove an approximation theorem which says roughly that a linear compartmental system has an approximate trap if and only if the associated system of differential equations has an eigenvalue which is approximately zero.

Let $S$ represent a linear compartmental system consisting of compartments $C_1, C_2, \ldots, C_n$ and $q_j$ be the amount of material in $C_j$. Let $f_{i,j}$ be the fractional exchange coefficient so that the rate of flow of material from $C_j$ to $C_i$ is $f_{i,j}q_j$; and let $f_{0,j}q_j$ be the rate of flow of material from $C_j$ to the environment. The total outflow from $C_j$ is $(f_{0,j} + \sum_{i \neq j} f_{i,j})q_j$ which we will write as $f_{j,i}q_j$. This leads us to consider the system of differential equations,

$$\dot{q}_j = \sum_{i \neq j} f_{i,j}q_i - f_{j,i}q_j, \quad j = 1 \ldots n, \quad (1)$$

where we write $\sum'$ for $\sum_{i \neq j}$. Equation (1) may be written

$$\dot{q} = Fq, \quad (2)$$

where $q$ is the column vector whose entries are $q_1, \ldots, q_n$ and $F$ is the matrix given by

$$F_{i,j} = \begin{cases} f_{i,j} & \text{if } i \neq j \\ -f_{j,i} & \text{if } i = j. \end{cases} \quad (3)$$

$\lambda$ is an eigenvalue of Eq. 2 just if $\det(F - \lambda I) = 0$. Thus $\lambda = 0$ is an eigenvalue just if $\det(F) = 0$.

What do we mean by a trap? We mean a subsystem with no output (to things outside itself). Suppose $T \subseteq S$ and renumbering compartments need be, $T = C_m, \ldots, C_n(m \leq n)$. $T$ is a trap if and only if $f_{i,j} = 0$ for all $(i,j)$ such that $j \geq m$ and $i < m$ (including $i = 0$).

In stating the above it was convenient to renumber the compartments of $S$. What does this do to the matrix $F$? Re numbering amounts to applying some permutation $P$ to the subscripts of $C_1, \ldots, C_n$. The new matrix
representing the new system is obtained by applying \( P \) to both the rows and the columns of the old matrix \([1]\). This is easy to see in case \( P \) merely switches the names of two compartments. Since any permutation can be written as a series of switches the result follows.

**THEOREM 1**

\( S \) has a trap if and only if either:

(a) each column of \( F \) sums to zero or,

(b) There is a permutation which can be applied to the rows and columns of \( F \) to give a matrix of the form \[
\begin{pmatrix}
U & 0 \\
Q & R
\end{pmatrix}
\]

where \( 0 \) consists only of zeros, \( U \) and \( R \) are square and each column of \( R \) sums to zero.

"a" corresponds to the case \( T = S \) and "b" to the case \( T \subset S \).

**Proof**

The following are all equivalent.

i. \( T \subseteq S \) is a trap (and may be written \( T = C_m, \ldots, C_n \))

ii. \( f_{i,j} = 0 \) for all \((i, j)\) such that \( j = m, \ldots, n \) and \( i = 0, \ldots, m - 1 \).

iii. \( F_{i,j} = 0 \) for all \((i, j)\) such that \( j = m, \ldots, n \) and \( i = 1, \ldots, m - 1 \)
and (Eq. 3 plus \( f_{0,j} = 0 \)) \( F_{j,j} = -\sum_i F_{i,j}, j = m, \ldots, n \).

iv. Statement "b" if \( m > 1 \) or statement "a" if \( m = 1 \).

**THEOREM 2**

\( S \) has a trap if and only if zero is an eigenvalue of Eq. (2).

**Proof**

Recall that zero is an eigenvalue of Eq. 2 if and only if \( \det(F) = 0 \). Suppose \( S \) has a trap \( T \). If \( T = S \) then from theorem 1 each column of \( F \) sums to zero so \( \det(F) = 0 \). If \( T \subset S \) permute \( F \) to get it in the form mentioned in theorem 1 part b. Each column of \( R \) sums to zero so \( \det(R) = 0 \).

Hence the columns of \( R \) are linearly dependent. So are the columns of \( F \) which pass through \( R \) since \( 0 \) consists of zeros only. Hence \( \det(F) = 0 \).

Suppose \( \det(F) = 0 \). From Eq. 3 and the definition of \( f_{i,j} \) we see that \( \Sigma_i F_{i,j} = 0 \) just if \( |F_{j,j}| = \Sigma_i |F_{i,j}| \). Finally, since \( f_{i,j} \geq 0 \), \( |F_{j,j}| \geq \Sigma_i |F_{i,j}| \).

We will show that a matrix with the above three properties must satisfy "a" or "b" of theorem 1 and this will complete the proof. The lemma is a restatement of a result given by O. Tausky [2].

Let \( A = (a_{i,j}) \) be an \( n \times n \) real or complex matrix and \( A_j = \Sigma_i |a_{i,j}| \).

Let \( x = (x_1, \ldots, x_n) \). We will say \( |x_j| \) is maximal if \( |x_j| \geq |x_i| \), all \( i \neq j \).
**Lemma**

Suppose

1. \( \det(A) = 0 \) and
2. \( |a_{j,i}| \geq A_j \) all \( j \).

Then either

**I.** \( |a_{i,i}| = A_i \) for all \( i \) or,

**II.** \( A \) can be transformed to the form \( \begin{pmatrix} U & 0 \\ Q & R \end{pmatrix} \) by the same permutation of its rows and columns where \( U \) and \( R \) are square matrices and \( 0 \) consists entirely of zeros. For those columns \( t \) which fall in \( R \) we also have \( |a_{t,t}| = A_t \).

Recall that II is equivalent to \( b \) of theorem 1 because of the second property mentioned above.

**Proof of lemma**

Since \( \det(A) = 0 \) there is a nonzero \( X = (x_1, \ldots, x_n) \) solving \( AX = 0 \). We may permute the rows of \( A \) (and the columns of \( A \) the same way) so that \( |x_1| \leq |x_2| \leq \ldots \leq |x_n| \). Suppose all \( |x_i| \) are maximal. From the \( i \)th equation of \( AX = 0 \) we have

\[
-x_i a_{i,i} = \sum_j x_j a_{j,i},
\]

(4)

\[
|x_i| |a_{i,i}| \leq \sum_j |x_j| |a_{j,i}|,
\]

(5)

and since all \( |x_j| \) are equal

\[
|a_{i,i}| = \sum |a_{j,i}| = A_i.
\]

(6)

With "2" this gives \( |a_{i,i}| = A_i \) (for all \( i \)).

The other possibility is that (at least) \( |x_1| < |x_2| \leq \ldots \leq |x_n| \). Let \( m \) be the lowest index for which \( |x_m| = |x_n| \). If \( t \geq m \) we see as we did before that

\[
|x_i| |a_{i,i}| \leq \sum_j |x_j| |a_{j,i}|.
\]

(7)

Hence, \( |a_{t,t}| < \sum_j |a_{j,t}| \) (contradicting 2) unless all the \( a_{i,t} \) for which \( |x_i| < |x_t| \) are zero. Thus \( a_{i,t} = 0 \), \( i = 1, \ldots, m - 1 \) and this is true for all \( t = m, \ldots, n \). This gives the required block of zeros.

If column \( t \) falls in \( R \) (i.e. if \( t \geq m \)) then Eq. 7 applies. The first \( n - 1 \) terms in the sum are zero. For the rest \( |x_j| = |x_t| \) so \( \sum_j |a_{j,i}| \geq |a_{i,t}| \) and as before this gives \( A_t = |a_{i,t}| \).

We will now use the above theorem to prove an approximate result which will say that under broad conditions \( \det(F) \) is approximately zero if and only if \( F \) has an eigenvalue which is approximately zero and this happens if and only if \( S \) has a subsystem which is approximately a trap. In order to state and prove such a result we will need to introduce some additional notation.

For a given set \( C_1, \ldots, C_n \) we can consider \( \mathcal{S} \), the set of all compartmental systems on \( C_1, \ldots, C_n \), and \( \mathcal{F} \), the set of all matrices of such
systems. Since a choice of particular system $S \in \mathcal{S}$ is equivalent to a choice of a set of fractional transfer coefficients there is an obvious one to one correspondence between $\mathcal{S}$ and $\mathcal{F}$. In $\mathcal{F}$ we will say as usual that a sequence of matrices $F_j$ converges to a given matrix $F_0$ ($F_j \to F_0$) if and only if each entry of $F_j$ converges to the corresponding entry of $F_0$. The determinant is then a continuous function from $\mathcal{F}$ to the real numbers $R$.

$S \in \mathcal{S}$ has an approximate trap if it has a subsystem whose total output is small. More formally let $T \subseteq \{C_1, \ldots, C_n\}$. Without loss of generality $T = \{C_m, \ldots, C_n\}$. Then for any $S \in \mathcal{S}$ we define

$$L_T(S) = \sum_{j > m} \sum_{i < m} f_{i,j},$$

so that $L_T$ is the sum of the fractional coefficients for transfer out of $T$. We have the following picture

$$\begin{array}{c}
\mathcal{S} \\
\downarrow \uparrow u \\
R \\
\leftarrow \mathcal{F} \supseteq \mathcal{F} \rightarrow R, \\
\downarrow \uparrow v \\
\leftarrow L_T(S) \rightarrow \mathcal{S} \\
\uparrow K_T \\
\leftarrow R
\end{array}$$

where $u$ and $v$ give the correspondence between $\mathcal{S}$ and $\mathcal{F}$ and $K_T = L_T \cdot v$. $K_T$ is a continuous function from $\mathcal{F}$ to $R$ for each $T$.

Let $K(F) = \min_T K_T(F)$ taking the minimum over all nonempty $T \subseteq \{C_1, \ldots, C_n\}$. $K$ is a continuous function from $\mathcal{F}$ to $R$. We have the picture

$$\begin{array}{c}
\mathcal{S} \\
\downarrow \uparrow u \\
R \\
\leftarrow \mathcal{F} \rightarrow R \\
\downarrow \uparrow v \\
\leftarrow R \downarrow \uparrow K \\
\leftarrow \mathcal{F} \rightarrow \det
\end{array}$$

By Theorem 2, $K(F) = 0$ if and only if $\det(F) = 0$.

**THEOREM 3**

Suppose $\{F_j\}$ is a sequence of matrices in $\mathcal{F}$ and $F_j \to F_0$. Then $\det(F_j) \to 0$ if and only if $K(F_j) \to 0$.

**Proof**

$\det(F_j) \to \det(F_0)$ so $\det(F_j) \to 0$ if and only if $\det(F_0) = 0$. Similarly $K(F_j) \to 0$ if and only if $K(F_0) = 0$. $K(F_0) = 0$ if and only if $\det(F_0) = 0$.

A set of matrices is said to be bounded if the set of all the entries in all the matrices is a bounded set of numbers. It is a standard result that any closed bounded set of $n \times n$ matrices is compact.

**THEOREM 4**

Suppose $\{F_j\}$ is a bounded sequence of matrices in $\mathcal{F}$. Then $\det(F_j) \to 0$ if and only if $K(F_j) \to 0$. 
Suppose the contrary. By compactness we can choose a convergent subsequence with the same property. This contradicts theorem 3.

Finally, we should point out that for $F$ bounded, $\det(F)$ is approximately zero if and only if $F$ has an eigenvalue which is approximately zero. To see this let $\Lambda_j$ be the set of eigenvalues of $F_j$. The product of all the $\lambda$'s in $\Lambda_j$ is $\det(F_j)$ so at least one $\lambda$ in $\Lambda_j$ is no bigger than $|\det(F_j)|^{1/n}$. On the other hand if $M$ is the bound on the entries of the matrices it is easy to see that each $\lambda$ in $\Lambda_j$ must satisfy $|\lambda| \leq nM$. If $\lambda$ is in $\Lambda_j$ we have $|\det(F_j)| \leq (nM)^{n-1}\lambda$. Thus $\det(F_j) \to 0$ if and only if $\min\{|\lambda|\text{ such that } \lambda \in \Lambda_j\} \to 0$.

This is the result we were after except for the requirement that the sequence be bounded. The following example shows that the boundedness condition cannot simply be dropped.

Let $S_j$ be given by

$$F_j = \begin{pmatrix} -j & 1/j \\ 0 & -1/j \end{pmatrix}$$

$C_2 \rightarrow_i C_1 \rightarrow_j$.

$$K(F_j) = \min(1/j, j) = 1/j,$$ so $K(F_j) \to 0$.

On the other hand $\det(F_j) = 1$ for all $j$.

My attempts to construct an example in which $K(F_j)$ stayed away from zero and $\det(F_j) \to 0$ were frustrated. The core of the trouble was that according to theorem 4 any such sequence must be unbounded. However, if we notice that in evaluating $\det(F_j)$ all terms have the same sign and if we notice that $K(F_j)$ is a minimum of several sums of positive terms, it becomes clear that any unbounded sequence in which $K(F_j)$ stays away from zero and $\det(F_j) \to 0$ can be replaced by a bounded sequence with the same properties. (The terms which grow unboundedly can simply be replaced by suitable nonzero constants.) Thus no such example exists. The reader who prefers ending on a positive note may restate this as a theorem.

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REFERENCES