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Which Linear Compartmental Systems Contain Traps?

DANIEL FIFE
University of Michigan Medical School, Ann Arbor, Michigan, 48104

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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 $(f_{0,j} + \Sigma_{i\neq j} f_{i,j})q_j$ which we will write as $f_{j,j}q_j$. This leads us to consider the system of differential equations,

$$\dot{q}_j = \Sigma' f_{j,i}q_i - f_{j,j}q_j, \qquad j = 1 \ldots n, \tag{1}$$

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

$$\dot{q} = Fq, \tag{2}$$

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

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

λ 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, $T = C_m, \ldots, C_n (m \leqslant n)$. T is a trap if and only if $f_{i,j} = 0$ for all (i, j) such that $j \geqslant m$ 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? Renumbering 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 $f_{0,j} = 0$) $F_{j,j} = -\Sigma_i F_{i,j}$, $j = m, \ldots, n$.

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 $f_{i,j} \geqslant 0$, $|F_{j,j}| \geqslant \Sigma_i' |F_{i,j}|$. 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 $|x_j| \geqslant |x_i|$, all $i \neq j$.

LEMMA

Suppose

(1) $\mathrm{Det}(A) = 0$ *and*

(2) $|a_{j,j}| \geqslant A_j$ *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 $XA = 0$. We may permute the rows of A (and the columns of A the same way) so that $|x_1| \leqslant |x_2| \leqslant \ldots \leqslant |x_n|$. Suppose all $|x_i|$ are maximal. From the ith equation of $XA = 0$ we have

$$- x_i a_{i,i} = \Sigma_j' x_j a_{j,i}, \tag{4}$$

$$|x_i|\,|a_{i,i}| \leqslant \Sigma_j' |x_j|\,|a_{j,i}|, \tag{5}$$

and since all $|x_j|$ are equal

$$|a_{i,i}| \leqslant \Sigma' |a_{j,i}| = A_i. \tag{6}$$

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

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

$$|x_t|\,|a_{t,t}| \leqslant \Sigma_j |x_j|\,|a_{j,t}|. \tag{7}$$

Hence, $|a_{t,t}| < \Sigma_j' |a_{j,t}|$ (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 $t \geqslant m$) then Eq. 7 applies. The first $n - 1$ terms in the sum are zero. For the rest $|x_j| = |x_t|$ so $\Sigma_j' |a_{j,t}| \geqslant |a_{t,t}|$ and as before this gives $A_t = |a_{t,t}|$.

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 $\mathscr{S}$, the set of all compartmental systems on $C_1, \ldots, C_n$, and $\mathscr{F}$, the set of all matrices of such systems. Since a choice of particular system $S \in \mathscr{S}$ is equivalent to a choice of a set of fractional transfer coefficients there is an obvious one to one correspondence between $\mathscr{S}$ and $\mathscr{F}$. In $\mathscr{F}$ 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 $\mathscr{F}$ to the real numbers R.

$S \in \mathscr{S}$ 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 $S \in \mathscr{S}$ we define

$$L_T(S) = \Sigma_{\substack{i<m \\ j \geqslant m}} f_{i,j}, \tag{8}$$

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

$$\overset{\xleftarrow{\qquad K_T \qquad}}{R \xleftarrow[L_T]{} \mathscr{S} \underset{v}{\overset{u}{\rightleftarrows}} \mathscr{F} \xrightarrow{\det} R,}$$

where u and v give the correspondence between $\mathscr{S}$ and $\mathscr{F}$ and $K_T = L_T . v$. K_T is a continuous function from $\mathscr{F}$ 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 $\mathscr{F}$ to R. We have the picture

$$\begin{array}{c} \mathscr{S} \\ {\scriptstyle u}\downarrow\uparrow{\scriptstyle v} \\ R \xleftarrow[K]{} \mathscr{F} \xrightarrow[\det]{} R \end{array}$$

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

THEOREM 3

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

Proof

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 Λ_j be the set of eigenvalues of F_j. The product of all the λ's in Λ_j is $\det(F_j)$ so at least one λ in Λ_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 λ in Λ_j must satisfy $|\lambda| \leqslant nM$. If λ is in Λ_j we have $|\det(F_j)| \leqslant (nM)^{n-1}\lambda$. 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

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

$$C_2 \overset{1/j}{\rightarrow} C_1 \overset{j}{\rightarrow}$$

$K(F_j) = \min(1/j, j) = 1/j$, 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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