# ON THE ONE-DIMENSIONAL MULTI-GROUP DIFFUSION EQUATIONS

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November 1st 2010

**Introduction.**

In [1] I discussed among other things the one-dimensional multi-group diffusion equations in a particular simple (but often used) form. I showed that the associated eigenvalues were positive real. This note contains supplementary remarks to the proof, and also the details of an earlier proof (referred to in [1]) of the same fact for a much used discrete approximation to these equations (actually providing an alternative proof of the above by going to the limit).

**Remarks to** [1, pages 20–23]**.**

We discuss the system of differential equations

$$\begin{aligned} -\frac{d}{dx}(d_1(x)\frac{d}{dx}\phi_1(x)) + a_1(x)\phi_1(x) =& \lambda\sigma_1(x)\phi_n(x) \\ -\frac{d}{dx}(d_j(x)\frac{d}{dx}\phi_j(x)) + a_j(x)\phi_j(x) =& \sigma_j(x)\phi_{j-1}(x), \quad (2 \le j \le n) \end{aligned}$$

valid in a certain finite interval, with suitable boundary conditions (for these, and the conditions on the coefficients, see [1]. We shall here assume that the coefficients are positive, and that the diffusion coefficients $d_j$ have a positive lower bound).

The possibility that $\lambda = |\lambda| e^{i\theta}$ with $0 < \theta < 2\pi$ is investigated. The corresponding set of eigenfunctions are $\phi_j(x) = |\phi_j(x)| \exp(i\psi_j(x))$.

Taking the real part of the differential equations just means replacing $\phi_j(x)$ with $|\phi_j(x)| \cos(\psi_j(x))$ in equations $2, 3, \ldots, n$, while the source term in equation 1 becomes $|\lambda|\sigma_1(x)|\phi_n(x)| \cos(\psi_n(x) + \theta)$.

Now, if, for some $j$, $|\phi_j(x)| \cos(\psi_j(x)) \equiv 0$, the same is true for all of the functions with greater index. However, it may happen that $|\phi_n(x)| \cos(\psi_n(x) + \theta)$ is not identically equal to 0 (then $\theta \neq \pi$). But, expanding the cosine, we see that $\sin(\psi_n(x))$ is not identically equal to 0, and so, if we alter all $\psi_k(x)$ by adding an arbitrary common constant $\alpha \in (0, \pi)$, none of the functions $|\phi_j(x)| \cos(\psi_j(x))$ can be identically equal to zero. Consider this done. For simplicity, the functions $|\phi_k(x)| \cos(\psi_k(x))$ are now just called $f_k(x)$.

For each $k$ we can then divide the reactor interval into a minimal number of subintervals inside each of which $f_k(x)$ (if not identically zero) has constant sign and so also has an extremum away from zero (actually just a point where $|f_k(x)|$ is maximal). In such a point the term $-\frac{d}{dx}(d_k(x)\frac{d}{dx}f_k(x))$, if non-zero, has the same sign as $f_k(x)$, and so also $f_{k-1}(x)$ has this sign, thus giving an injection of the set of subintervals of $f_k$ into that of $f_{k-1}$. In particular, we get an injection of the set of subintervals of $|\phi_n(x)|\cos(\psi_n(x))$ into that of $|\phi_n(x)|\cos(\psi_n(x)+\theta)$.

This fact is used in several ways in the remaining part of the proof given in [1].

First it is used to show that because of the positive lower bounds for the functions $d_k(x)$, none of the functions $f_k$can have an infinite number of subintervals. Actually, it was shown that otherwise the zeros of $\cos(\psi_n(x))$ would have a limit point $y$ belonging to the closed reactor interval. But then this would be true (with the same value of $y$) for $\cos(\psi_n(x)+\alpha)$ with arbitrary phase $\alpha$, implying $\cos(\psi_n(y)+\alpha)=0$ for every $\alpha$, an impossibility.

It then follows that we have the same number of subintervals for all $k$, and that, for instance, the signs of all $f_k(x)$ in the leftmost subinterval are the same. This is true for all values of the phase $\alpha$, except possibly for the few values we have excluded. But then the two functions $|\phi_n(x)|\cos(\psi_n(x))$ and $|\phi_n(x)|\cos(\psi_n(x)+\theta)$ also have the same sign in this subinterval. This easily is shown to give a contradiction for suitable values of $\alpha$, q.e.d.

**The difference equations.**

They have the form

$$\begin{aligned}(D_1-L_1-U_1)\underline{\phi}_1 &= \lambda F_1\underline{\phi}_n\\ (D_j-L_j-U_j)\underline{\phi}_j &= F_j\underline{\phi}_{j-1}, \quad (2\le j\le n)\end{aligned}$$

where the matrices all have the same order $m$. For $1\le j\le n$: The diagonal matrices $D_j$ all have positive elements, and the diagonal matrices $F_j$ have non-negative elements. The matrices $L_j$ are sub-diagonal, i.e. the element $l_{j,r,s}$ in row $r$ and column $s$ is different from 0, in fact non-negative, only if $r-s=1$. Similarly, the matrices $U_j$ are non-negative super-diagonal matrices. The matrices $M_j=D_j-L_j-U_j$ are irreducible, their row sums are non-negative (positive for at least one row). These properties together ensure that each matrix $M_j$ is invertible. Our equations can then be written

$$(\prod_{j=n}^{1} M_j^{-1}F_j)\underline{\phi}_n=\frac{1}{\lambda}\underline{\phi}_n.$$

This reformulation is of interest for the following, because it shows that the set of eigenvalues depends continuously on the elements of the matrices $F_j$, simply because the set of solutions to an algebraic equation depends continuously on its coefficients. The problem is that the diagonal matrices $F_j$ may have zero elements (in the diagonal). But the following discussion is much simplified if all their diagonal elements can be assumed to be positive (which we shall do). The original problem is then obtained by taking the limit, which, in the worst case, can result in a zero eigenvalue, and this can be ruled out since the $M_j$ are invertible.

Since we can now assume the matrices $F_j$ invertible, the original equations can be rewritten as

$$(\prod_{j=1}^{n} F_j^{-1}M_j)\underline{\phi}_n=\lambda\underline{\phi}_n.$$

The next step is to show that each matrix $M_j$ can be written as a product of bidiagonal matrices. Actually (in obvious notation)

$$D-L-U=(D'-L')(I-U')$$

gives

$$\begin{aligned} L =& L' \\ U =& D'U' \\ D =& D' + L'U', \end{aligned}$$

from which the elements of $L'$, $D'$, and $U'$ can be determined. The details: We have

$$d'_{1,1} = d_{1,1}$$

and, for $1 \le j \le n-1$,

$$\begin{aligned} u'_{j,j+1} =& \frac{u_{j,j+1}}{d'_{j,j}} \\ d'_{j+1,j+1} =& d_{j+1,j+1} - l_{j+1,j} u'_{j,j+1}. \end{aligned}$$

We see that $d'_{j+1,j+1} d'_{j,j}$ equals the $2 \times 2$ principal subdeterminant of $D - L - U$ corresponding to rows and columns $j$ and $j+1$. It follows from our assumptions that this quantity (and so also, by induction, $d'_{j+1,j+1}$) is positive. This shows that the elements of $L'$ and $U'$ are non-negative.

Our original problem has now been transformed to examining the eigenvalues of a matrixproduct

$$B = \prod_{j=1}^{3n} B^{(j)},$$

where the matrices $B^{(j)}$ are of two types. Either, for all $r, s$,

$$b^{(j)}_{r,s} = 0 \text{ unless } r - s \in \{0, 1\}$$

or, for all $r, s$,

$$b^{(j)}_{r,s} = 0 \text{ unless } s - r \in \{0, 1\}.$$

For all $j, r, s$,

$$\begin{aligned} b^{(j)}_{r,r} >& 0 \\ b^{(j)}_{r,s} \le& 0 \text{ for } |r - s| = 1. \end{aligned}$$

We shall show that the principal subdeterminants of $B$ are positive. To do this, we need an expression for the subdeterminants of a matrixproduct. The formula is well known, but for the reader's convenience I shall give a proof anyway.

Let $A = \prod_{j=1}^{q} A^{(j)}$ be a product of $m \times m$ matrices. We wish to find an expression for a subdeterminant of order $p < m$. Its row and column numbers are given by vectors $\underline{r}$ and $\underline{s}$, respectively. It suffices to consider the case $q = 2$.

The usual formula for the determinant of a matrix gives in the present case

$$|A_{\underline{r},\underline{s}}| = \sum_{\sigma} sign(\sigma) \prod_{t=1}^{p} a_{r_t, \sigma(s_t)},$$

where the summation is over all permutations of the $p$ chosen column numbers relative to their original ordering in the vector $\underline{s}$.

Introducing the factors, we find

$$
\begin{aligned}
|A_{\underline{r},\underline{s}}| &= \sum_{\sigma} sign(\sigma) \prod_{t=1}^{p} \sum_{u_t=1}^{m} a^{(1)}_{r_t,u_t} a^{(2)}_{u_t,\sigma(s_t)} \\
&= \sum_{\sigma} sign(\sigma) \sum_{u_1=1}^{m} \cdots \sum_{u_p=1}^{m} \prod_{t=1}^{p} a^{(1)}_{r_t,u_t} a^{(2)}_{u_t,\sigma(s_t)} \\
&= \sum_{u_1=1}^{m} \cdots \sum_{u_p=1}^{m} \prod_{t=1}^{p} a^{(1)}_{r_t,u_t} \sum_{\sigma} sign(\sigma) \prod_{t=1}^{p} a^{(2)}_{u_t,\sigma(s_t)} \\
&= \sum_{u_1=1}^{m} \cdots \sum_{u_p=1}^{m} \prod_{t=1}^{p} a^{(1)}_{r_t,u_t} |A^{(2)}_{\underline{u},\underline{s}}|.
\end{aligned}
$$

It follows from the properties of the determinant that only terms with all $u_t$ different give a contribution. Collecting the terms where the $u_t$ are permutations of the same numbers, we find that

$$
|A_{\underline{r},\underline{s}}| = \sum_{\underline{v}} |A^{(1)}_{\underline{r},\underline{v}}||A^{(2)}_{\underline{v},\underline{s}}|,
$$

where the summation is over all subsets, consisting of $p$ numbers, chosen from the set of integers $1, 2, \ldots, m$. Since the vectors $\underline{v}$ are just meant to indicate unordered sets, we shall assume that the coordinates of these vectors are given in their natural order. The same goes for the vectors $\underline{r}$ and $\underline{s}$.

Applying these results on the matrix product $B$, we see that the determinant of $B_{\underline{r},\underline{s}}$ is a sum of products

$$
|B^{(1)}_{\underline{r},\underline{v}_1}||B^{(2)}_{\underline{v}_1,\underline{v}_2}| \ldots |B^{(3n)}_{\underline{v}_{3n-1},\underline{s}}|.
$$

We shall need the sign of a subdeterminant of order $p$ of a bilinear matrix. For definiteness we consider a matrix of the form $B = D - L$. Then

$$
|B_{\underline{r},\underline{s}}| = \sum_{\sigma} sign(\sigma) \prod_{t=1}^{p} b_{r_t,\sigma(s_t)}.
$$

Here, as noted above, we can assume

$$
\begin{aligned}
r_1 <& r_2 < \cdots < r_p \\
s_1 <& s_2 < \cdots < s_p.
\end{aligned}
$$

We only get a contribution from those terms where, for all $t$, we have $\sigma(s_t) - r_t \in \{0, -1\}$. Assume that we had a contribution from a permutation $\sigma$ different from the identical one. Then, for some $t$, we would have

$$
\sigma(s_{t+1}) < \sigma(s_t) \leq r_t \leq r_{t+1} - 1,
$$

and so the factor with index $t + 1$ would be zero, a contradiction.

The sign of factor number $t$ is $(-1)^{(r_t-s_t)}$, if non-zero. Thus the sign of the subdeterminant, if non-zero, becomes $(-1)^{\sum_{t=1}^{p}(r_t-s_t)}$.

Going back to the matrix product $B$, we see that the sign of a non-vanishing term becomes

$$(-1)^{\sum_{t=1}^{p}(r_t-v_{1,t})+\sum_{t=1}^{p}(v_{1,t}-v_{2,t})+\cdots+\sum_{t=1}^{p}(v_{3n-1,t}-s_t)},$$

which always equals $(-1)^{\sum_{t=1}^{p}(r_t-s_t)}$.

In particular, the subdeterminants $|B_{\underline{r},\underline{r}}|$ are always positive, ensuring that $B$ does not have any negative real eigenvalues.

To show that $B$ has only positive real eigenvalues we must show that $B$ does not have any non-real eigenvalues $\lambda$. Since any power of $B$ has a product representation of the same form as $B$ has, it suffices to show that a matrix of this form cannot have an eigenvalue with negative real part.

Assume that $B$ has the eigenvalue $-\alpha + i\beta$ with $\alpha > 0$ and $\beta \neq 0$. Then $|(B+\alpha I)^2+\beta^2 I| = 0$, i.e. the matrix $(B+\alpha I)^2$ has a negative eigenvalue. To exclude this possibility it suffices to show that the principal subdeterminants $|(B+\alpha I)^2_{\underline{r},\underline{r}}|$ are positive.

In the usual notation

$$|(B+\alpha I)^2_{\underline{r},\underline{r}}| = \sum_{\underline{v}} |(B+\alpha I)_{\underline{r},\underline{v}}||(B+\alpha I)_{\underline{v},\underline{r}}|.$$

Here $|(B+\alpha I)_{\underline{r},\underline{v}}|$ is a polynomial in $\alpha$ whose coefficients are sums of subdeterminants $|(B+\alpha I)_{\underline{r}',\underline{v}'}|$ whose row and column numbers are obtained from those of $\underline{r}$ and $\underline{v}$, respectively, by disregarding the same set of numbers (corresponding to diagonal elements in $B$), and so such a subdeterminant still has the sign $(-1)^{\sum_{t=1}^{p}(r_t-v_t)}$. But $|(B+\alpha I)_{\underline{v},\underline{r}}|$ has the same sign, so that all contributions to $|(B+\alpha I)^2_{\underline{r},\underline{r}}|$ are positive, q.e.d.

*Remark.*

In general, the product of more than two positive definite matrices does not have all eigenvalues positive. The result above shows that it does, if the matrices are tridiagonal.

## References

1. Gundorph K. Kristiansen, *Description of DC-2, a two-dimensional, cylindrical geometry, two-group diffusion theory code for DASK, and a discussion of the theory for such codes*, RisøReport no. 55, Danish atomic energy commission research establishment Risø, 1963.