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EXISTENCE AND UNIQUENESS THEOREMS IN INVARIANT IMBEDDING-I: CONSERVATION PRINCIPLES

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SANTA MONICA • CALIFORNIA

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PREFACE

Part of the RAND research program consists of basic supporting studies in mathematics. This Memorandum is the first in a series dealing with a number of rigorous aspects of the highly useful mathematical theory known as invariant imbedding. In this theory invariance principles are applied to handle a variety of conceptual and computational aspects of mathematical physics.

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SUMMARY

In a series of papers of which this is the first, we wish to study some of the rigorous aspects of invariant imbedding: existence and uniqueness of solution, asymptotic behavior over space and time, stability, computational stability, applications to classical boundary-value theory, and so on.

The first paper will be devoted to the use of an important conservation property, obvious on physical grounds, in establishing the existence of the solution of a matrix Riccati equation without recourse to the associated linear differential equation, and thus without any appeal to spectral theory.

CONTENTS

EXISTENCE AND UNIQUENESS THEOREMS IN INVARIANT IMBEDDING — I: CONSERVATION PRINCIPLES

1. INTRODUCTION

Invariant imbedding is a mathematical theory designed to handle a variety of conceptual, analytic, and computational aspects of mathematical physics in a unified fashion without the intervention of boundary-value problems. By means of appropriate choices of space and time variables, all problems are of initial-value type. An expository account of the application of this theory to neutron transport, radiative transfer, diffusion, and scattering will be found in [1]; application to wave propagation will be found in [2], [3].

Invariant imbedding is a systematic application and extension of the "invariance principles" introduced into the study of radiative transfer by Ambarzumian and Chandrasekhar, [4]. More generally, it utilizes the "point-of-regeneration" technique of the type used by Bellman and Harris in the study of branching processes, [5]; see also Harris, [6].

Over the last few years, frequently in collaboration with Ueno [7], we have derived a large number of functional equations describing a variety of physical processes, and carried out some large-scale numerical calculations ([8], [9]).

2. THE MATRIX RICCATI EQUATION

The equation we wish to study is

$$(1)\qquad R'(x) = B(x) + D(x)R(x) + R(x)D(x) + R(x)B(x)R(x),$$
$$R(0) = 0,$$

where B, D, and R are $N \times N$ matrices and it is assumed that

(2) (a) $d_{ij}(x) \geq 0, \quad i \neq j,$

(b) $d_{jj}(x) \leq 0,$

(c) $b_{ij}(x) \geq 0.$

Rather than tackle this equation directly, let us indicate its physical source, and then show how the simultaneous consideration of R(x) and two related functions enables us to establish existence of the solution of (1) for all $x > 0$ in a simple and painless fashion.

3. STEADY-STATE NEUTRON TRANSPORT WITH DISCRETE ENERGY LEVELS

Let us begin by describing a model of a steady-state transport process which will be the explicit or implicit source of many of the analytical ideas we shall utilize in what follows.

Consider an idealized neutron-transport process taking place in a one-dimensional, homogeneous, isotropic rod extending along an axis from $z = 0$ to $z = x$. We suppose initially that there are only a finite number, N, of different types of particles moving along the rod. These possible states can be considered to be energy levels, labelled $i = 1, 2, \cdots, N$.

It is assumed that when a particle in state i traverses a segment of the rod, it is subject to interactions with the substance composing the rod. These interactions produce two possible effects: forward or backward scattering into any of the N possible states, and absorption. However, no fission occurs, which is to say, there is no spontaneous generation of new particles.

It follows that the total number of particles in the process, taking account of those absorbed as well as of those scattered, is changed only by addition from an external source. This obvious conservation principle will be the key to the result obtained below concerning the existence of the solutions of (2.1).

In this paper, we shall exclude the possibility of collisions or interactions between neutrons themselves. This will permit us to use ordinary differential equations in our application of invariant imbedding. Subsequently, when dealing with collisions, we shall encounter hyperbolic partial differential equations.

Finally, let us note that as far as the analysis is concerned, one-dimensional transport with energy levels is equivalent to two-dimensional transport in a plane parallel slab with energy and angular dependence. We are thus treating a quite general transport process connected with a geometric figure such as sphere, cylinder, or plane-parallel region.

4. ANALYTIC PRELIMINARIES

Let us now make the model of a transport process discussed above more precise. We suppose that when a particle in state j $(j = 1,2,\cdots,N)$ enters the infinitesimal segment of length Δ contained in $[x + \Delta, x]$ from either direction (the assumption of isotropy), the following events take place:

(1) (a) The expected number leaving the segment in state j, moving in the same direction, is $1 + d_{jj}(x)\Delta + O(\Delta^2)$.

(b) The expected number leaving the segment in state i, $i \neq j$, moving in the same direction, is $d_{ij}(x)\Delta + O(\Delta^2)$. (Forward scattering.)

(c) The expected number leaving the segment, moving the opposite direction in state i, is $b_{ij}(x)\Delta + O(\Delta^2)$. (Back scattering.)

(d) The expected number absorbed by the medium is $f_{jj}(\Delta) + O(\Delta^2)$.

We call the matrices $D(x) = (d_{ij}(x))$, $B(x) = (b_{ij}(x))$, $F(x) = (f_{ii}(x)\delta_{ij})$, the <u>forward scattering</u>, <u>back scattering</u>, and <u>absorption matrices</u>, respectively.

We assume, on physical grounds, that

(2) (a) $d_{ij}(x) \geq 0, \quad i \neq j,$

(b) $b_{ij}(x) \geq 0,$

(c) $f_{ii}(x) \geq 0,$

for $x \geq 0$. The basic assumption of the conservation of matter requires that

$$(3) \qquad d_{jj}(x) = -\left[\sum_{i=1}^{N} b_{ij}(x) + \sum_{\substack{i=1 \\ i \neq j}}^{N} d_{ij}(x) + f_{jj}(x)\right], \quad j = 1,2,\ldots,N.$$

This implies that $d_{jj}(x) \leq 0$, a condition required to account for the increments to other states and for the particles absorbed.

Introducing the matrix

$$(4) \qquad M = \begin{pmatrix} 1 & 1 & \ldots & 1 \\ 0 & 0 & \ldots & 0 \\ \vdots & \vdots & & \\ 0 & 0 & \ldots & 0 \end{pmatrix},$$

the relations of (3) can be written in the simple form

$$(5) \qquad M(B(x) + D(x) + F(x)) = 0, \quad x \geq 0.$$

This is the fundamental conservation assumption which will yield a corresponding conservation relation for the matrix functions introduced below.

5. REFLECTION, TRANSMISSION AND LOSS MATRICES

Let us now introduce the following functions. For $i,j = 1,2,\ldots,N$, let

(1) $r_{ij}(x)$ = expected flux of neutrons in state i, reflected from a rod of length x, resulting from an incident flux at x of unit intensity in state j;

$t_{ij}(x)$ = expected flux of neutrons in state i, transmitted through a rod of length x resulting from an incident flux at x of unit intensity in state j;

$\ell_{ij}(x)$ = expected flux of neutrons in state i, absorbed within a rod of length x, resulting from an incident flux at x of unit intensity in state j.

Schematically,

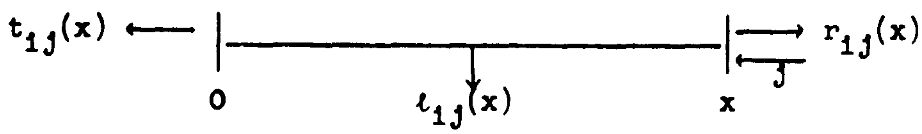

Fig. 1

When we say a rod of length x, we mean one whose ends are respectively at the fixed position 0 and the variable position x, as pictured above. As a consequence of the assumption made above concerning no interaction between neutrons, the reflections, transmissions and absorptions depend linearly upon the intensity of the incident flux. Hence we may restrict ourselves here to unit incident fluxes.

Let $R(x) = (r_{ij}(x))$, $T(x) = (t_{ij}(x))$, $L(x) = \ell_{ij}(x))$ be called respectively the reflection, transmission, and absorption matrices. Using invariant imbedding techniques, as indicated in [1], we can derive differential equations for these matrices. For the sake of completeness, let us present the derivation here.

Consider the process described above for a rod of length $x + \Delta$ and let an incident flux c be applied at $x + \Delta$. Here c is a vector flux whose j-th component represents the intensity of the incident flux in state j. By virtue of the assumptions of Sec. 4, this results in a flux of $(I + D\Delta)c$ incident at x, a flux of $Bc\Delta$ reflected from $x + \Delta$, and a flux of $Fc\Delta$ absorbed, all to terms in $O(\Delta^2)$. The flux $(I + D\Delta)c$ incident at x results in a flux $R(x)(I + D\Delta)c$ reflected at x, a flux $T(x)(I + D\Delta)c$ transmitted through the rod, and a flux $L(x)(I + D\Delta)c$ absorbed in $[x,0]$. Here B, D, and F depend upon x, as indicated above.

The flux $R(x)(I + D\Delta)c$ now enters the segment $[x,x + \Delta]$ and results in further interactions. As a result of this, we have the additional reflection $(1 + D\Delta)R(x)(I + \Delta D)c$, an additional absorption $(\Delta F)R(x)(I + D\Delta)c = \Delta FR(x)c + O(\Delta^2)$, and a quantity $\Delta BR(x)c + O(\Delta^2)$ as incident flux upon $[x,0]$. This incident flux results in a reflection from $[x,0]$ of $R(x)(\Delta BR(x)c) + O(\Delta^2)$, a transmitted flux of $T(x)(\Delta BR(x)c) + O(\Delta^2)$, and a loss of $L(x)(\Delta BR(x)c) + O(\Delta^2)$. The flux $RBR\Delta + O(\Delta^2)$ through $[x,x + \Delta]$ contributes $RBR\Delta + O(\Delta^2)$ to the total reflected flux.

Schematically, we have

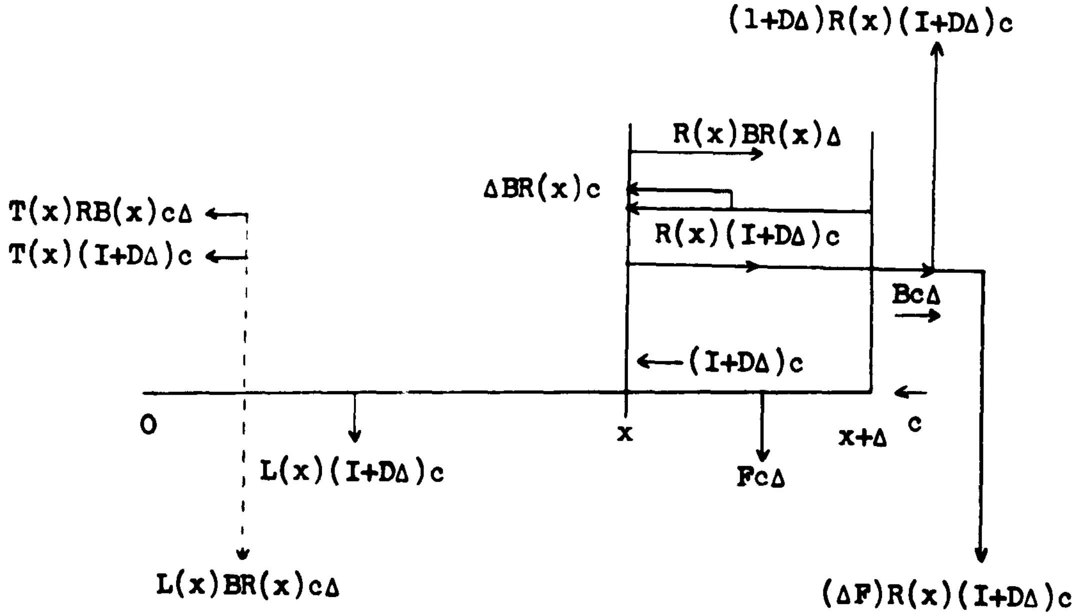

Fig. 2

Adding up these effects, we obtain the recurrence relations

$$(2)\qquad R(x+\Delta)c = Bc\Delta + (I+D\Delta)R(x)(I+D\Delta)c + R(x)BR(x)c\Delta + O(\Delta^2),$$

$$T(x+\Delta)c = T(x)(I+D\Delta)c + T(x)BR(x)c\Delta + O(\Delta^2),$$

$$L(x+\Delta)c = Fc\Delta + L(x)(I + D\Delta)c + FR(x)c\Delta + L(x)BR(x)c\Delta + O(\Delta^2).$$

Since these equations hold for arbitrary c, we can discard c. Expanding the left-hand side, and passing to the limit as $\Delta \to 0$, we obtain the Riccati differential equations

$$(3)\qquad R'(x) = B + DR(x) + R(x)D + R(x)BR(x),$$

$$T'(x) = T(x)(D + BR(x)),$$

$$L'(x) = L(x)(D + BR(x) + F(I + R(x)),$$

with the physically obvious initial conditions

$$(4)\qquad R(0) = 0,\quad T(0) = I,\quad L(0) = 0.$$

Observe that of the three functions, it is only the reflection function which occurs alone, independently of the other two. The remaining two functions have been deliberately introduced to take advantage of conservation properties.

6. EXISTENCE AND UNIQUENESS OF SOLUTIONS

The conventional existence and uniqueness theory of ordinary differential equations establishes the existence and uniqueness of a solution of (5.3) over some initial interval $[0,a]$. Since it is intuitively clear that the reflection, transmission, and loss functions must exist for all $x \geq 0$ (since no fission is allowed), the question arises as to how to establish this analytically. For the case of constant coefficients (homogeneous rod), we can reduce the equations to linear equations with constant coefficients and use the explicit solutions to help us. For inhomogeneous equations, this approach is more difficult.

To obtain an equivalent linear equation, let us first proceed formally. Consider the two first order matrix equations

$$(1) \qquad X' = EX + FY,$$

$$Y' = GX + HY,$$

where E, F, G, and H can be dependent on x. Consider the matrix $Z = XY^{-1}$. We have

$$(2) \qquad Z^1 = (XY^{-1})^1$$

$$= (EX + FY)Y^{-1} - X(Y^{-1}(GX + HY)Y^{-1})$$

$$= EZ + F - ZGZ - ZH,$$

an equation similar to that satisfied by $R(x)$. The identification is complete if we set

(3) $E = D, \quad F = B, \quad H = -D, \quad G = -B,$

so that (1) becomes

(4) $$X' = DX + BY,$$
$$Y' = -BX - DY.$$

This procedure is much more than formal, since it turns out that the equations of (4) are the transport equations obtained by applying the usual procedure to the study of the fluxes inside the rod.

As indicated above, it is not a trivial matter to study (4) when B and D are variable matrices.

To establish nonlocal existence of the solutions of (5.3), we add two ingredients: nonnegativity of the matrices $R(x)$, $T(x)$, and $L(x)$, and the conservation relation

$$M(R(x) + T(x) + L(x)) = M.$$

Both of these conditions are intuitively clear, and, as we shall see, readily established rigorously. Once we have done this, it follows that $R(x)$, $T(x)$, and $L(x)$ are uniformly bounded over any interval of existence. It follows that the solutions can be continued for all $x \geq 0$. We are going through this in some detail since the same line of reasoning can be employed for many classes of functional equations arising in mathematical physics.

7. PROOF OF CONSERVATION RELATION

To establish the conservation relation of (6.1), we consider the function

$$(1) \qquad Q(x) = M(R(x) + T(x) + L(x))$$

and differentiate it with respect to x. We have

$$\begin{aligned}(2) \qquad Q'(x) &= M(R' + T' + L') \\ &= M(R + T + L)(TR + D) + M(DR + FR + B + F) \\ &= Q(BR + D) + M(DR + FR + B + F),\end{aligned}$$

upon using the equations of (5.3).

Considered as a differential equation in Q, we observe that (2) is satisfied by $Q(x) = M$, since

$$\begin{aligned}(3) \qquad & M(BR + D) + M(DR + FR + B + F) \\ &= M(B + D + F)(R + I) = 0,\end{aligned}$$

by virtue of (4.5). Since $Q(0) = M$, we see that $Q(x) = M$ within the interval of existence of $R(x)$, $T(x)$, and $L(x)$. This argument can now be repeated from interval to interval.

It is remarkable that one has to use this sophistication to establish a relation which is so immediate from physical considerations. One would expect in place of (2) merely the relation $Q' = 0$.

8. PROOF OF NONNEGATIVITY

Local existence and nonnegativity of solutions can be established in several different ways. One way is to convert the original system of differential equations into a set of integral equations. Let us begin by writing the differential equations in the form

$$(1)\quad \frac{d}{dx}(e^{-Dx}R(x)e^{-Dx}) = e^{-Dx}[B + R(x)BR(x)]e^{-Dx},\ R(x_0) = R_0,$$

$$\frac{d}{dx}(T(x)e^{-Dx}) = T(x)BR(x)e^{-Dx},\ T(x_0) = T_0,$$

$$\frac{d}{dx}(L(x)e^{-Dx}) = [L(x)BR(x) + F + FR(x)]e^{-Dx},\ L(x_0) = L_0.$$

Thus an appropriate set of integral equations is

$$(2)\qquad R(x) = e^{D(x-x_0)}R_0e^{D(x-x_0)} + \int_{x_0}^{x} e^{D(x-x_1)}[B + R(x_1)BR(x_1)]e^{D(x-x_1)}dx_1 = \theta_1(R,T,L),$$

$$T(x) = T_0e^{D(x-x_0)} + \int_{x_0}^{x} T(x_1)BR(x_1)e^{D(x-x_1)}dx_1 = \theta_2(R,T,L),$$

$$
\begin{aligned}
L(x) &= L_0 e^{D(x-x_0)} \\
&\quad + \int_{x_0}^{x} [L(x_1)BR(x_1) + F + FR(x_1)] e^{D(x-x_1)} dx_1 \\
&= \theta_3(R,T,L).
\end{aligned}
$$

The principal result we wish to employ to establish nonnegativity is that $d_{ij} \geq 0$ implies that e^{Dx} is a nonnegative matrix for $x \geq 0$; see [10].

Consider the space S of triples of continuous matrix functions $R(x)$, $T(x)$, and $L(x)$ defined on $x_0 \leq x \leq x_0 + a$, with the initial values $R(x_0) = R_0$, $T(x_0) = T_0$, $L(x_0) = L_0$, all nonnegative matrices, satisfying the constraints

$$(3) \qquad ||R(x)|| \leq c_1, \ ||T(x)|| \leq c_1, \ ||L(x)|| \leq c_1,$$

where

$$(4) \qquad c_1 > \text{Max}\ [||R_0||, \ ||T_0||, \ ||L_0||].$$

Consider the mapping θ defined on S by means of the right-hand sides of (2). It is readily seen that T is a contractive mapping of S into itself, provided that a is sufficiently small. Thus, by virtue of the Caccioppoli fixed-point theorem, θ has a unique fixed point, the solution of (2).

Alternatively, we can construct the solutions as the limit of a sequence of successive approximations given by

(5) $$R_{n+1} = \theta_1(R_n, T_n, L_n), \quad n \geq 0,$$

$$T_{n+1} = \theta_2(R_n, T_n, L_n),$$

$$L_{n+1} = \theta_3(R_n, T_n, L_n).$$

Applying the foregoing result with $x_0 = 0$, $c_1 > N$, where N is the dimension of the system, we obtain a solution over an interval $0 \leq x \leq a$. From the conservation relation combined with the nonnegativity of $R(x)$, $T(x)$, $L(x)$ on $0 \leq x \leq a$, it follows that $R(x)$, $T(x)$, $L(x)$ are uniformly bounded. In fact,

(6) $$||R(x)||, \ ||T(x)||, \ ||L(x)|| \leq N, \quad 0 \leq x \leq a.$$

We can therefore apply the result with $x_0 = a$ and the same c_1 as before. The solution can thus be continued indefinitely.

A third approach starts with the difference equations obtained from (5.2) by neglecting the terms which are $O(\Delta^2)$. The matrices $R(x)$, $T(x)$, $L(x)$ are defined in this way for $x = 0, \Delta, 2\Delta, \cdots$, and defined by means of linear interpolation for other values of x. Since $I + D\Delta \geq 0$ for small Δ, we see that the matrices obtained in this fashion are nonnegative for $x \geq 0$. As is well known, these functions approach the solutions of the differential equation in an initial interval $0 \leq x \leq b$, thus once again establishing nonnegativity.

9. STATEMENT OF RESULT

We have thus established the following result.

Theorem. If

(1) (a) $b_{ij}(x) \geq 0$,

(b) $d_{ij}(x) \geq 0, \quad i \neq j$,

(c) $f_{jj}(x) \geq 0$,

and

$$M(B(x) + D(x) + F(x)) = 0$$

for $x \geq 0$, *where* $B = (b_{ij}(x))$, $D = (d_{ij}(x))$, $F = (f_{jj}(x)\delta_{ij})$, *and* $M = (\delta_{ij})$, *then the equations*

(2) $$R'(x) = B + DR(x) + R(x)D + R(x)BR(x), \quad R(0) = 0,$$

$$T'(x) = T(x)(D + BR(x)), \quad T(0) = I,$$

$$L'(x) = L(x)(D + BR(x)) + F(I + R(x)), \quad L(0) = 0,$$

possess a unique solution for $x \geq 0$. *This solution satisfies the conservation relation*

(3) $$M(R(x) + T(x) + L(x)) = M,$$

for $x \geq 0$.

In physical terms, this means that the reflection, transmission, and loss matrices are defined for $x \geq 0$, and satisfy the equations of invariant imbedding.

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