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by

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TRANSPORT EQUATIONS WITH APPLICATION TO POPULATION
DISPERSAL AND TISSUE BULK FLOW MODELS

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ABSTRACT

We develop techniques for estimating the coefficients, boundary data,
and initial data associated with transport equations (or more generally,
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spline approximations, for which convergence results are given. We discuss
the performance of these techniques in two investigations of biological
interest: (1) transport of labeled sucrose in brain tissue white matter
(2) insect dispersal that cannot be modeled by a random diffusion
mechanism alone.

§1 Introduction

In this paper we propose general parameter estimation techniques to
be used in modeling of transport phenomena. While the fundamental ideas
we discuss have proved quite successful in other areas of application
(elasticity, seismology, enzyme column reactors, etc.--see, for example,
[2], [3], [4], [6], [9]), our emphasis here is a class of transport equations
arising in biology. We treat models in which certain of the coefficients
to be estimated are spatially varying. The methods are valid in more
complex transport problems with coefficients that vary both temporally and
spatially (see [6],[7]), but the underlying theory is technically somewhat
different and more complicated.

We begin in section 2 by formulating an "identification" or parameter
estimation problem involving a general transport equation. Although for
convenience in exposition we treat only scalar equations, the ideas and
convergence results easily extend to vector systems. Indeed, in a number
of problems we have successfully employed the techniques for coupled systems
of equations.

In section 3, we then reformulate the estimation problem, putting it in
abstract form for concise development of our ideas. This abstract problem
is approximated by a sequence of estimation problems in section 4 where we
give convergence results for states and parameters. We also explain our use
of computational packages to solve the estimation problems. In section 5,
we apply the methods to two examples:

(1) estimation of diffusion and bulk flow parameters for the transport
of substances in tissue (specifically, for transport of sucrose in
cat brain white matter)

(ii)   estimation of spatially varying coefficients in population

diaperaal models (in this case, models of flea beetle movement

within linear arrays of collard patches).

As we shall explain in our concluding remarks, the methods we have developed

have yielded satisfactory results and insight into biological systems. We

are confident that other investigations concerning transport models in biology

could also be served by the application of our parameter estimation methods.

In our discussions in sections 3 and 4, it will be convenient to employ

notation from elementary functional analysis. Although this notation will

be quite familiar to our more mathematically trained readers, we summarize

some of it briefly for others. By $L_2(0,1)$ we shall mean the standard Hilbert

space of "functions" f defined on (0,1) with $\int_0^1 f^2 < \infty$. The inner product

in this space is $<f,g> = \int_0^1 fg$.   We denote by H^1 the usual Sobolev space

of functions f in $L_2(0,1)$ with first derivatives Df in $L_2(0,1)$; the subspace

of functions i H^1 vanishing at $x = 0$ and $x = 1$ is denoted by H_0^1. More

generally, H^j will be the Sobolev space of functions having derivatives up

to order j, with the jth derivative $D^j f$ in L_2.

The usual space of essentially bounded functions is denoted by L_∞

with the norm being given by $|g|_\infty = ess \sup|g(x)|$. The space W_∞^j is the

space of functions f having j derivatives with $D^j f$ in L_∞.

We shall use the symbol $|\cdot|$ to denote a norm in most situations.

However, in some discussions, for clarity we resort to the more cumbersome

notation of $|\cdot|_2$, $|\cdot|_\infty$ etc. representing norms in L_2, L_∞ etc.

§2 A fundamental estimation problem

We begin by considering the general transport equation (based on mass balance laws) given by

$$(1) \qquad \frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(Vu) = \frac{\partial}{\partial x}\left(\mathscr{D}\frac{\partial u}{\partial x}\right) + f(x,u) \qquad \begin{array}{l} 0 \le x \le 1, \\ t > 0. \end{array}$$

Here the term involving V represents a general "directed movement" mechanism such as convection in tissue transport models or attractive/chemotactic phenomena in population dispersal models. We shall assume that in general this "velocity" V is spatially varying, i.e., $V = V(x)$. The first term on the right in equation (1) is a result of the usual Fick's first law of diffusion and we shall assume for our presentation that the coefficient of diffusion $\mathscr{D}$ is constant. The last term in (1) represents general sink/source mechanisms (death/birth, reaction, etc.) that might be present. Of course, u represents the concentration (in tissue transport) or population density (in species dispersal) that is of primary interest.

We assume that along with (1) certain initial conditions $u(0,x) = \psi(x)$ and Dirichlet boundary conditions $u(t,0) = g_0(t)$, $u(t,1) = g_1(t)$ are given (or perhaps must be estimated--both situations arise in the situations discussed below). Using a standard transformation of variables $(\bar{u} = u-(1-x)g_0-xg_1)$, one can transform the resulting Initial-Boundary Value Problem (IBVP) for (1) into an IBVP with homogeneous boundary conditions. We assume that this has been done and furthermore we make the assumption throughout that f is linear in u. (This linearity assumption is not at all essential for the methods discussed below to be valid, but it greatly simplifies our presentation--for a discussion of estimation results concerning problems with rather general nonlinearities in f, see [5], [8].)

After a change of variables in (1) and some elementary manipulations one obtains the transformed version of the IBVP that will be central to our presentation (we drop the ~ on the transformed variable $\tilde{u}$):

$$\frac{\partial u}{\partial t} = q_1 \frac{\partial^2 u}{\partial x^2} + q_2(x)\frac{\partial u}{\partial x} + q_3(x)u + g(t,x), \qquad 0 \le x \le 1,$$

(2)
$$u(t,0) = u(t,1) = 0, \qquad t > 0,$$

$$u(0,x) = \Psi(x), \qquad 0 \le x \le 1.$$

Given observations of a general biological process that can be represented by equation (2), our task is to use observations of u to determine the positive constant q_1 and the bounded functions q_2 and q_3. More precisely, we have observations $\{y_i(x) \mid 0 \le x \le 1\}$ at times $t_i > 0$, $i = 1, \ldots, m$, and a given set $Q \subset R \times L_\infty(0,1) \times L_\infty(0,1)$ of admissible parameters (q_1, q_2, q_3), over which we wish to minimize the fit-to-data criterion function

(3)
$$J(q) = \sum_{i=1}^{m} \int_0^1 |u(t_i,x) - y_i(x)|^2 dx$$

where $u(t_i,x) = u(t_i,x;q)$ represents the solution of (2) corresponding to $q = (q_1, q_2, q_3)$.

In many practical situations, one has discrete data y_{ij} for u at points (t_i, x_j) and in applying our methods one might instead of (3) employ the alternate criterion function

(4)
$$\tilde{J}(q) = \sum_{i,j} |u(t_i,x_j) - y_{ij}|^2.$$

Indeed we did this in both the specific applications discussed below. (One could, of course, use (3) with discrete data y_{ij} by first constructing--say

by interpolation—an observed "data function" $y_i(x)$ from the discrete observations y_{ij}.) The convergence theory for use of our methods with criteria of the form $\tilde{J}$ is somewhat more delicate, requiring one to establish a pointwise in x—as opposed to L_2—convergence of approximating solutions. We therefore shall restrict our discussions of the theoretical aspects of our method to the "continuous data" experimental situation which results in a problem of minimizing (3) over Q subject to (2).

The ideas behind our methods are most succinctly discussed in the context of an abstract form of (2), which we formulate in the next section.

§3 An abstract estimation problem

We first rewrite (2) as an initial value problem in the state space $Z = L_2(0, 1)$. Letting $z(t) = u(t,\cdot)$ and $G(t) = g(t,\cdot)$ denote time varying functions with values in Z, we can formally write (2) as the system

(5)
$$\dot{z}(t) = A(q)z(t) + G(t) \qquad t > 0,$$
$$z(0) = \Psi$$

where the operator $A(q)$ is defined on $\text{Dom}(A(q)) = H^2 \cap H_0^1$ by $A(q)\phi = q_1 D^2 \phi + q_2 D\phi + q_3 \phi$. (Here and below the operator D is differentiation, i.e. $D = \frac{\partial}{\partial x}$.) The equation under consideration can thus be viewed as an ordinary differential equation in the state space Z. The analogue to the usual (in the case A is a matrix operator) solution operator e^{At} is in this case the solution semigroup (a one parameter family of operators on Z) associated with (5) which we shall denote by $S(t)$ (or $S(t;q)$ if we wish to emphasize the dependence on q). Thus solutions to (5) with $G \equiv 0$ are given by $z(t) = S(t)z(0) = S(t)\Psi$ and a corresponding "variation-of-constants" formula can be used to define solutions of (5) in the case that G is nontrivial. We summarize results for (5) in the

following lemma (for arguments see Appendix 1 and for detailed discussions on semigroups and abstract differential equations see [1], [15]).

Lemma 3.1. Suppose $q_2 \in W_\infty^1, q_3 \in L_\infty$. Then the operator $A(q)$ in (5) satisfies the dissipative inequality $\langle A(q)z,z \rangle \leq \omega \langle z,z \rangle$ where $\omega \equiv \frac{1}{2}|Dq_2|_\infty + |q_3|_\infty$. Furthermore A generates a C_0-semigroup $\{S(t)\}$ satisfying $\|S(t)\| \leq e^{\omega t}$ and (mild) solutions to (5) are given (for G integrable) by

$$(6) \qquad z(t;q) = S(t;q)\Psi + \int_0^t S(t-\sigma;q)G(\sigma)d\sigma.$$

In view of the system reformulation just presented, we recast our basic parameter estimation problem as one of minimizing over Q the functional

$$(7) \qquad J(q) = \sum_{i=1}^m |z(t_i;q) - y_i|_2^2$$

where y_i is the observation function at time t_i as introduced in discussing (3) above and $z(t_i;q)$ is defined by (6).

This problem clearly consists of minimizing a functional defined via a state equation in the infinite dimensional space $Z = L_2(0, 1)$. Any type of computational procedure must be founded on some type of approximation to the equation (6). We turn next to one class of approximation schemes which have proved both theoretically and computationally sound.

§4 Approximations of the estimation problem

We approximate the estimation problem involving (6), (7) by a sequence
of problems defined on subspaces Z^N, $N = 1, 2, \ldots$, of Z. Numerous possi-
bilities abound, but the schemes we discuss here have proved most useful in
not only the biological applications presented below, but also in a number
of other areas as indicated in the introduction. The subspaces Z^N we choose
are those generated by cubic spline elements. Full details on similar
problems are given in [5] but for the convenience of readers and the sake
of completeness, we briefly summarize the fundamentals. Let B_0^N, B_1^N, $\ldots$, B_N^N
denote the cubic B-spline elements (piecewise cubic $C^2(0,1)$ functions
corresponding to the partition $\Delta^N = \{x_j\}$, $x_j = j/N$, $j = 0,1,\ldots,N$,
of $[0, 1]$ --see [16, p. 208-209]) modified to satisfy the boundary conditions
$B_j^N(0) = B_j^N(1) = 0$. Define $Z^N = \text{span } \{B_0^N, B_1^N, \ldots B_N^N\}$. In the usual notation,
$Z^N = S_0^3(\Delta^N) = \{\phi \in S^3(\Delta^N) | \phi(0) = \phi(1) = 0\}$ where $S^3(\Delta^N) \equiv \{\phi \in C^2(0,1) | \phi$
is a cubic polynomial on each interval $[x_i, x_{i+1}]\}$. Explicit formulae for
basis elements for $S^3(\Delta^N)$ can be given ([16, p. 89], [3]) and these can be
used to give analytical expressions for the modified basis elements B_j^N (e.g.,
see [5, p. 10], [3, p. 12]).

Given the subspaces Z^N, we let P^N denote the orthogonal projection of Z
onto Z^N; that is, for any $z \in Z$, $P^N z$ is that unique element in Z^N defined by the
relationships $<P^N z-z, B_j^N> = 0$, $j = 0,1,\ldots,N$. Define approximates A^N to A by
$A^N(q) \equiv P^N A(q) P^N$; these are bounded operators in Z. Let $\{S^N(t)\}$ be the
semigroup generated by A^N, i.e. $S^N(t;q) = \exp\{A^N(q)t\}$ --in this case, this
exponential definition has its usual power series definition since A^N is
bounded.

We use these constructs to approximate (6) by

$$(8) \qquad z^N(t;q) = S^N(t;q)P^N\psi + \int_0^t S^N(t-\sigma;q)P^N G(\sigma)d\sigma,$$

or, equivalently, we approximate (5) by

$$(9) \qquad \begin{aligned} \dot{z}^N(t) &= A^N(q)z^N(t) + P^N G(t) \\ z^N(0) &= P^N\psi. \end{aligned}$$

The associated fit-to-data criterion is then taken as

$$(10) \qquad J^N(q) = \sum_{i=1}^{m} |z^N(t_i;q) - y_i|_2^2,$$

and the sequence of approximating parameter estimation problems can be simply stated: Minimize $J^N(q)$ over Q subject to (8) or (9). Before discussing convergence properties of solutions to these problems, we explain how one can easily implement these approximate estimation problems. We summarize the more complete discussions given in [5, p. 10-11; p. 22-24].

We first note that any $z^N(t) \in Z^N$ (and, in particular, any solution of (8) or (9)) can be written as $z^N(t) = \sum_{j=0}^{N} w_j^N(t;q)B_j^N$ for appropriately chosen real coefficients $w_j^N(t;q)$. It is also easily seen that (9) is equivalent to the Galerkin system of equations

$$(11) \qquad \begin{aligned} \langle \dot{z}^N(t), B_j^N \rangle &= \langle A(q)z^N(t), B_j^N \rangle + \langle G(t), B_j^N \rangle \\ \langle z^N(0), B_j^N \rangle &= \langle \psi, B_j^N \rangle, \qquad\qquad j = 0,1,\ldots,N. \end{aligned}$$

If we substitute $z^N = \sum_i w_i^N B_i^N$ into (11), then we obtain the matrix system

$$(12) \quad \begin{aligned} Q^N \dot{w}^N(t) &= K^N w^N(t) + R^N(G(t)) \\ Q^N w^N(0) &= R^N(\Psi) \end{aligned}$$

where Q^N, K^N are $(N + 1) \times (N + 1)$ matrices with elements

$$(13) \quad \begin{aligned} Q^N_{ij} &= \langle B^N_i, B^N_j \rangle \\ K^N_{ij} &= \langle B^N_i, A(q) B^N_j \rangle, \end{aligned}$$

and R^N, w^N are $N + 1$ vectors given by

$$(14) \quad \begin{aligned} R^N(\Psi)_i &= \langle \Psi, B^N_i \rangle \\ w^N &= \mathrm{col}(w^N_0, w^N_1, \ldots, w^N_N). \end{aligned}$$

Thus, to solve the approximate estimation problems, one deals with vector systems of ordinary differential equations. More precisely, for a given index N of approximation, one minimizes (10) iteratively, using (12) to compute $w^N(t;q)$ (and hence $z^N(t;q)$) for each value of q in the iterative procedure. The matrices Q^N are seven-banded and symmetric in this case while the K^N are seven-banded, in general unsymmetric, and involve the unknown parameters q_1, q_2, q_3. The iterative procedure we have used with great success when minimizing (10) is the Levenberg-Marquardt algorithm (a modified Gauss-Newton type routine) as packaged in the IMSL routine ZXSSQ. Either an IMSL package (DGEAR) employing Gear's variable order, variable step method for stiff systems or an IMSL package (DVERK) for a variable order, variable step Runge-Kutta, was used to solve (12) at each step in the Levenberg-Marquardt. (An implementation of the Cholesky algorithm is used to solve equations of the form $Q^N x = y$ for x.)

Let $\vec{q}^N = (\vec{q}_1^N, \vec{q}_2^N, \vec{q}_3^N)$ denote a solution to the problem of minimizing (10) for a given fixed N (assuming for the present that such solutions exist). Our goal, of course, is to obtain a sequence of estimates (either $\vec{q}^N$ or some subsequence) that converges as $N \to \infty$ to an estimate $\bar{q}$ that will be a solution of the minimization problem involving (7) (or equivalently (3)). We shall establish such a convergence result through a series of results below. We first argue that $z^N(t;q^N) \to z(t;q^*)$ when q^N is any sequence converging to q^* in an appropriate manner. We then, under reasonable compactness hypotheses on Q, the set of admissible parameters, argue that some subsequence of $\{\vec{q}^N\}$ (where $\vec{q}^N$ is a solution of the Nth approximate estimation problem) converges in this manner to a limit parameter $\bar{q}$ in Q that is a desired optimal estimate for the original problem for (7). We begin this program with the following fundamental convergence statement.

__Theorem 4.1.__ Suppose $q^N = (q_1^N, q_2^N, q_3^N)$ is any sequence in $Q \cap ([a,b] \times W_\infty^1 \times L_\infty)$, $0 < a < b < \infty$, satisfying $|q_2^N|_\infty, |Dq_2^N|_\infty, |q_3^N|_\infty$ are bounded with $q_1^N \to q_1^*$, $q_i^N \to q_i^*$ in L_2, $i = 2,3$. Furthermore, assume $q_2^*, q_3^* \in W_\infty^2$. Then $|z^N(t;q^N) - z(t;q^*)|_2 \to 0$ as $N \to \infty$, where z^N, z are given by (8) and (6) resp.

A convenient tool to be used in establishing this theorem is a version of the Trotter-Kato approximation theorem from linear semigroup theory. We state and use here a simple version (see [5]; in particular take $\pi^N = I$ and $\mathscr{P}^N = \mathscr{P}$ in Prop. 2.1 of that reference). For other versions see [15], [8], [5] and the references given there.

__Theorem 4.2.__ Let $\mathscr{H}$ be a Hilbert space and suppose $T^N(t)$, $T(t)$ are C_0-semigroups on $\mathscr{H}$ generated by linear operators $\mathscr{A}^N$, $\mathscr{A}$ respectively. If (i) (stability) there exist constants M and β independent of N such that

$\|T^N(t)\| \le Me^{\beta t}$,   (ii) (consistency) there exist a subset $\mathscr{D}$ of $\mathscr{X}$

dense in $\mathscr{X}$ with $\mathscr{D} \subset \text{Dom}(\mathscr{A})$ and $(\lambda_0 - \mathscr{A})\mathscr{D}$ dense in $\mathscr{X}$ for some $\lambda_0 > 0$

and for $z \in \mathscr{D}$ we have $|\mathscr{A}^N z - \mathscr{A} z| \to 0$ as $N \to \infty$,

then

$$|T^N(t)z - T(t)z| \to 0 \quad \text{as} \quad N \to \infty \quad \text{for all} \quad z \in \mathscr{X}$$

and the convergence is uniform in t on compact subsets of $(0, \infty)$.

We begin the proof of Theorem 4.1 by supposing that $\{q^N\}$ is given

as stated in that Theorem and then choosing $\mathscr{A}^N \equiv A^N(q^N)$ and $\mathscr{A} = A(q^*)$ in Theorem 4.2.

Here, of course A^N, A are as defined in section 3 and above; we thus know

that $\mathscr{A}^N$ and $\mathscr{A}$ generate semigroups $T^N(t) = S^N(t; q^N)$ and $T(t) = S(t; q^*)$

respectively. We first use Theorem 4.2 to establish that $S^N(t; q^N)z \to S(t; q^*)z$

for each $z \in Z$.

To verify the stability condition (i) of Theorem 4.2, we observe that,

since $|q_2^N|_\infty, |q_3^N|_\infty$ are bounded, one has in view of Lemma 3.1,

$$\langle A^N(q^N)z, z \rangle = \langle P^N A(q^N)P^N z, z \rangle = \langle A(q^N) P^N z, P^N z \rangle$$

$$\le \omega(q^N) \langle P^N z, P^N z \rangle \le \omega(q^N) \langle z, z \rangle$$

$$\le \beta \langle z, z \rangle$$

for β appropriately chosen, independent of N. It thus follows from standard

arguments (e.g. see the discussions in [15, p. 16 -22]) that an exponential

bound as in (i) holds.

Next we turn to condition (ii) and observing that $A(q^*)$ is the

infinitesimal generator of a C_0-semigroup, we note that $\mathscr{D} \equiv \text{Dom}(A^2(q^*))$

is dense in Z (see [15, p.8]). Clearly $\mathscr{D} \subset \text{Dom}(A(q^*))$, and

for $\lambda_0 > \omega(q^*)$, we have that the resolvent operator $R_{\lambda_0}(A(q^*)) = [\lambda_0 - A(q^*)]^{-1}$

exists. For $\psi \in \text{Dom}(A(q^*))$ we find $R_{\lambda_0}(A(q^*))\psi \in \text{Dom}(A^2(q^*)) = \mathscr{D}$. Thus

for any $\psi \in \text{Dom}(A(q^*))$ the equation $[\lambda_0 - A(q^*)]\phi = \psi$ is solvable for

$\phi \in \mathscr{D}$ (just take $\phi = R_{\lambda_0}\psi$). Hence $(\lambda_0 - A(q^*))\mathscr{D} \supset \text{Dom}(A(q^*))$ so that

$(\lambda_0 - A(q^*))\mathscr{D}$ is dense in Z. To satisfy (ii) it remains to demonstrate that $A^N(q^N)z \to A(q^*)z$ for z in the set $\mathscr{D}$ just defined. We state this as a lemma and defer detailed arguments to Appendix 2.

<u>Lemma 4.1.</u> For $z \in \mathscr{D} \equiv \text{Dom}(A^2(q^*))$, we have

$$|A^N(q^N)z - A(q^*)z|_2 \to 0 \quad \text{as} \quad N \to \infty.$$

Having verified the hypotheses of the Trotter-Kato theorem in the case of interest to us here, we thus have $S^N(t;q^N)z \to S(t;q^*)z$ for $z \in Z$, uniformly in t on compact intervals and this holds for any sequence $q^N \to q^*$ satisfying the hypotheses of Theorem 4.1.

To complete the proof of Theorem 4.1, we use (6) and (8) to write (again $|\cdot|$ denotes $|\cdot|_2$)

$$|z^N(t;q^N) - z(t;q^*)| \leq |P^N\Psi - \Psi| + \left|\int_0^t [S^N(t-\sigma)P^N G(\sigma) - S(t-\sigma)G(\sigma)]d\sigma\right|$$

where $S^N(t) = S^N(t;q^N)$, $S(t) = S(t;q^*)$. Thus we have

$$|z^N(t;q^N) - z(t;q^*)| \leq |P^N\Psi - \Psi| + \int_0^t |S^N(t-\sigma)[P^N G(\sigma) - G(\sigma)]|d\sigma$$

$$+ \int_0^t |[S^N(t-\sigma) - S(t-\sigma)]G(\sigma)|d\sigma$$

$$\leq |P^N\Psi - \Psi| + Me^{\beta t}\int_0^t |P^N G(\sigma) - G(\sigma)|d\sigma$$

$$+ \int_0^t |[S^N(t-\sigma) - S(t-\sigma)]G(\sigma)|d\sigma.$$

Each of these terms $\to 0$ as $N \to \infty$ from the convergence properties of P^N and $S^N(t)$ already established plus the dominated convergence theorem. This completes the arguments establishing Theorem 4.1.

We turn finally to explain how the convergence results of Theorem 4.1 can be used to obtain desired results for our parameter estimation problems. We first place restrictions on the admissible parameter set Q. Let $0 < a < b < \infty$, let B_2 be a bounded subset of W_∞^1 (i.e. there exists K such that $q_2 \in B_2$ implies $|q_2|_\infty \le K$ and $|Dq_2|_\infty \le K$) and B_3 be a bounded subset of L_∞. We assume

H(a) $Q \subset \{q=(q_1,q_2,q_3) \in R^1 \times W_\infty^2 \times W_\infty^2 \mid a\le q_1\le b, \; q_2 \in B_2, q_3 \in B_3\}$,

H(b) Q is compact in the $R^1 \times L_2 \times L_2$ topology.

Consider now the functional J^N defined in (10) where $z^N(t;q) = \sum_{i=0}^{N} w_i^N(t;q)B_i^N$ is defined via (12),(13),(14). Noting that $K_{ij}^N = \langle B_i^N, q_1 D^2 B_j^N + q_2 D B_j^N + q_3 B_j^N \rangle$ depends continuously on q in the $R^1 \times L_2 \times L_2$ topology, one sees that it is not difficult to argue that $q \to z^N(t;q)$, and hence $q \to J^N(q)$, are continuous in the same sense. Thus from the compactness assumption (b) on Q we see there exists $\bar{q}^N \in Q$ that is a solution to the problem of minimizing J^N over Q, $N = 1,2,\ldots$.

The sequence $\{\bar{q}^N\}$ thus obtained is in the compact set Q and hence we can extract a subsequence $\{\bar{q}^{N_k}\}$ converging to some limit parameter $\bar{q}$ in Q. We claim that $\bar{q}$ is a solution to the problem of minimizing (7) subject to (6). To see this, we first observe that by definition

(15) $J^{N_k}(\bar{q}^{N_k}) \le J^{N_k}(q)$ for all $q \in Q$.

Since $\bar{q}_2,\bar{q}_3 \in W_\infty^2$, we have by Theorem 4.1 that $z^{N_k}(t_i;\bar{q}^{N_k}) \to z(t_i;\bar{q})$ as $N_k \to \infty$. Furthermore, that same theorem with $q^N \equiv q$ for all N yields $z^{N_k}(t_i;q) \to z(t_i;q)$ for any $q \in Q$. Recalling (10) and taking the limits in the inequality (15), we obtain $J(\bar{q}) \le J(q)$ for any $q \in Q$; i.e., $\bar{q}$ is a

minimizer for J. We summarize our findings in a formal statement.

<u>Theorem 4.3.</u> Assume that Q satisfies the hypotheses H(a),H(b). Then
solutions $\overline{q}^N$ to the problem of minimizing J^N exist and there exists <u>a</u>
subsequence $\{\overline{q}^{N_k}\}$ converging in the $R^1 \times L_2 \times L_2$ topology to a solution
$\overline{q}$ of the problem of minimizing J given in (7).

We conclude this section with several remarks on the above discussions.
First note that we only obtain (theoretically) convergence of some <u>subsequence</u>
of the approximate estimates. In actual practice we almost always have found
that the sequence $\{\overline{q}^N\}$ itself converges. One can prove that this stronger
statement is true in the case that the original estimation problem (for (7))
has a unique solution - a situation unhappily rarely encountered with real
data and a sophisticated model involving a partial differential equation.

The theory developed above extends easily to the case where one wishes
to also estimate the boundary conditions (e.g., the brain transport example
below) and/or initial conditions (e.g., the insect dispersal example below).
For ease in exposition we have not treated these cases directly in our theory
sketched here; the theoretical ideas are the same in these cases (albeit
the technical arguments are slightly more involved) as the interested reader
can ascertain by consulting [5],[8].

Finally, as with most "theorems" in applied mathematics, the conclusion
of Theorem 4.3 is valid in many situations where the smoothness hypotheses
(e.g., H(a)) of the theorem are not satisfied. We have numerous computational
examples on which the methods perform well (i.e., converge) even though the
coefficients are not smooth. Indeed, in the insect dispersal example below,
we have $q_2 \notin W_\infty^2$, so strictly speaking, Theorem 4.3 is not applicable. But

as we shall see, the estimation schemes perform admirably. In this particular instance, one can, at the expense of a great increase in technical tedium, modify the arguments in this paper to actually establish convergence. However, in a number of other areas of applications, we have used our methods successfully even when we cannot establish convergence theorems for the particular class of equations under investigation.

§5. Applications to biological systems: brain transport and insect dispersal problems

In this section we apply the spline techniques to questions of biological interest. In particular, by using these techniques in conjunction with experimental data we identify convection and diffusion terms for a brain transport system and for a population of dispersing insects. Proceeding heuristically, we examine the identified parameters in order to gain insight about underlying biological mechanisms or to suggest further experimentation.

A. Testing the methods with "known" numerical data

Before applying our methods to real experimental systems, we tested their performance against "data" generated by a known diffusion and convection equation. Our intent was to investigate practical issues such as amount of data required, accuracy of method and computational hazards. In these tests we also considered a similar (in spirit) approximation method, which uses modal (eigenfunction) basis elements (see [2]). This allowed us to compare two algorithms that share a common purpose, but that may differ in their effectiveness. Since detailed discussions of our findings can be found in [20], we summarize those results only briefly below.

We consider the example

(16)
$$u_t = q_1 u_{xx} + q_2 u_x \qquad t > 0, \quad 0 \le x \le 1$$
$$u(t,0) = c_0$$
$$u(0,x) = \phi(x)$$

where $\phi(x) = -2x^2 + x + 1$. We ran tests on this example with either Dirichlet $(u(t,1) = 0)$ or Neumann $(\frac{\partial u}{\partial x}(t,1) = 0)$ boundary conditions at the right boundary $x = 1$.

"Data" for our tests were generated in the following manner:

Fixed values for q_1^*, q_2^* and c_0^* were chosen (e.g. $q_1^* = .3$, $q_2^* = 1.75$, $c_0^* = 1.0$) and an infinite series technique (independent of any of the methods being tested) was used to generate numerical solution values $\hat{u}(t_i, x_j)$ at points (t_i, x_j), $i = 1, 2, \ldots, I$, $j = 1, 2, \ldots, J$ in $(0, \infty) \times (0,1)$. Either these values alone or in some cases these values with noise added (via a packaged random noise generator) were used as data y_{ij} in the criterion function $\mathcal{J}$ of (4) and its associated approximation $\mathcal{J}^N$ with u replaced by u^N.

In general, the spline based techniques discussed in this paper proved superior to the modal techniques. For problems with homogeneous Dirichlet boundary condition at $x = 1$, we first assumed that c_o is known and attempted to estimate q_1 and q_2 in (16), given varying amounts of data. For $I = 1$, $J = 3$ (one time observation with three spatial points) the spline method produced correct converged estimates (for example, at $N = 8$, estimates $\bar{q}_1^8 = .3001$ and $\bar{q}_2^8 = 1.7486$ and residual sum of squares (RSS) $J^8(\bar{q}^8) = .69 \times 10^{-9}$ were obtained) while the modal techniques failed to produce a numerically convergence sequence of estimates. For $I = 2$ or 3 and $J = 3$ (two or three time observations, each involving three spatial points) both methods yield converged values; however, in these cases the spline based method appears to be more accurate (smaller RSS) and more efficient (computationally). Furthermore, the addition of an extra time observation ($I = 3$ vs. $I = 2$) did not improve the fit of the model. We then investigated the effects of increasing the number J of spatial points in the data sets. A general finding was that there existed a minimum number of spatial points necessary for the methods to yield good parameter estimates ($J = 3$ sufficed for the spline scheme while $J = 4$ was required for the modal method). Beyond this minimal number, extra spatial observation points did not necessarily increase the efficiency of

the methods. This means that for a given experimental system and its associated model, it may be possible to identify the number of data points required for accurate parameter identification. When the process of gathering data is expensive or time consuming, we therefore suggest that our parameter identification methods may provide guidance in deciding upon the number of time periods or spatial points that need to be sampled.

Finally, we turned to the full problem of estimating all three parameters (q_1, q_2, c_0) in (16). Our findings were quite similar to those just summarized. For the spline based scheme, one time observation with three spatial points $(I = 1, J = 3)$ were sufficient data to produce convergence to correct parameter values. Whereas taking an extra time observation $(I = 2)$ does not generally produce better estimates using the spline method, in some cases it does if one is using the modal technique.

We also examined the performance of the spline scheme with Neumann boundary conditions and equation (16). Again, the method performed well in estimating all three parameters q_1, q_2, c_0, given data sets corresponding to $I = 1, J = 3$. Slightly better parameter estimates were obtained with $I = 2$ as opposed to $I = 1$, no matter the value of J ($J = 3, 4, 5, 6$). For fixed $I = 1$ or 2, estimates based on 3 or 4 spatial points were as good as those obtained from 5 or 6 spatial points.

In summary, the tests of the cubic spline scheme we carried out on the model (16) persuade us that the method proposed can be used with a good deal of numerical confidence with regard to fitting data to models of the form (2).

B. Understanding brain fluid transport

A primary question concerning transport mechanism in brain tissue is whether diffusion alone or diffusion and convection are responsible for transport in gray and white matter ([12],[17],[18]). Mathematically, we can view this as a question of determining the magnitude and thus contribution of V (convection) and D (passive diffusion) in the equation

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = D\frac{\partial^2 u}{\partial x^2}$$

where u represents the concentration of a substance being transported in the brain. To investigate this problem we have used our spline techniques with experimental data kindly provided by Kyner, Rosenberg and associates ([17],[18]). The data consist of laboratory measurements of u values at various locations in the tissue at a fixed time. These measurements were obtained from experiments (described in [17][18]) using adult cats. Artificial cerebrospinal fluid containing labeled sucrose was perfused into each cat's lateral ventricle. At the end of the perfusion period, the animals were sacrificed and their brains were rapidly removed and frozen. Samples of gray and white matter along a direction perpendicular to the ventricular surface (which will be the x-axis in our model) were removed, serially sectioned and analyzed. From measurements of radioactivity, the average concentration of sucrose in each slice was determined, yielding data which corresponds to observation at a fixed time t_1 (t_1 = 1, 2, or 4 hrs. for the cat experiments). From this data $\{\hat{u}(t_1, x_j)\}$ for the concentration u, the transport of sucrose in gray matter can be compared with that in white matter.

To analyze these data we used the cubic spline procedures to estimate parameters representing diffusion (q_1 in (16)), convection (q_2) and the

concentration (c_o) at the boundary $x = 0$. In Table 1 we have extracted typical results of these analyses from a more detailed report by Sives and Sato [20]. To interpret these results we have examined the predicted concentrations as though they were obtained from a least-squares regression approach and then analyzed the data with F-statistics (see [22]). Of course our model is not a simple curvilinear regression equation since it is a dynamic model, but the parameters were estimated using a least-squares minimization routine. This approach then focuses on: the total variation in data (total sums of squares or TSSQ), the variation explained by the model (explained sums of squares or ESSQ), and the sum of squares error between the model's prediction and the data (the residuals or unexplained variation, denoted RSS). This application of F-statistics is not strictly appropriate because we do not know anything about the distribution of residual errors; nonetheless, it provides a quantitative measure of the performance of different parameter estimates and is couched in terms that facilitate comparisons between models (e.g., explained and unexplained variation). The degrees of freedom were selected in the following manner (following the conventions and notation set out in [22]): explained df = the number of parameters estimated by our spline technique (analogous to the number of terms used in polynomial regressions), total df = number of data points, and unexplained df = (total df) - (explained df).

From Table 1 two conclusions are striking:

1) both models (diffusion alone, or diffusion plus convection) explain an enormous portion of the variation in the data (a minimum of 97%½),

Table 1. Parameter estimates for diffusion coefficients, convection coefficients, and boundary concentrations using Kyner and Rosenberg cat-brain data (from Sives & Sato [20]). RSS = unexplained sums of squares; TSSQ = total sums of squares; ESSQ = explained variation or explained sums of squares.

Model	df	Source of Variation	F-statistic	parameter values
		Kyner/Rosenberg data set 1		
Diffusion alone	2	TSSQ = 8367 ESSQ = 8187 RSS = 180	$F_{2,5} = 180.17$ $p < .001$	$D = 5.43 \times 10^{-6}\ cm^2/sec$ $c_0 = 138.86$
Diffusion & convection	3	TSSQ = 8367 ESSQ = 8261 RSS = 106	$F_{3,4} = 103.8$ $p < .001$	$D = 2.087 \times 10^{-6}\ cm^2/sec$ $V = -17.12\ \mu m/hr$ $c_0 = 105.9$
		Kyner/Rosenberg data set 7		
Diffusion alone	2	TSSQ = 10161.8 ESSQ = 10139.1 RSS = 22.7	$F_{2,5} = 1116$ $p < .001$	$D = 2.82 \times 10^{-6}\ cm^2/sec$ $c_0 = 183.99$
Diffusion & convection	3	TSSQ = 10161.8 ESSQ = 10154.0 RSS = 7.8	$F_{3,4} = 1733$ $p < .001$	$D = 1.53 \times 10^{-6}\ cm^2/sec$ $V = -9.64\ \mu m/hr$ $c_0 = 146.71$

2) the differences between the success of the two models are negligible

(at most, improving the % of explained variation from 97% to 99%).

In Table 1 and in all of the analyses performed by Sives and Sato [20],
the "diffusion plus convection" model always explained more of the variation
than did the "diffusion alone" model. The addition of a convection term
often resulted in dramatic reductions in unexplained variation (or residual
error); for example, in Table 1 we see that for data set 7, inclusion of
convection reduced the RSS from 22.7 to 7.8. However, because both models
were consistently so successful, it is difficult to establish that one is
significantly better than the other. When we calculated F statistics for
the improvement of explained variation by moving from the 2-parameter
diffusion-alone model to the 3-parameter diffusion-and-convection model,
our F statistics never attained the $p < .05$ level, and were at the $p < .1$
level in only one instance.

Clearly, the cubic spline methods yield parameter estimates that perform
exceedingly well in describing the data. This reinforces our faith in the
methods. Unfortunately, we are not able to answer the initial question
about the relative importance of convection in brain transport. The
consistently better (albeit only slightly) performance of diffusion plus
convection models temptingly hints at the role of convection. Our inability
to resolve the issue of convection cannot be blamed on the parameter
identification methods. Instead, we argue from Table 1 and similar analyses
that it is apparent that data must be obtained for more than one time
point after perfusion. When only one concentration profile is available,
there is too much freedom for juggling combinations of D and c_o or of D,
V and c_o such that the data are "fit." Our analyses point out that the
experiments need to be modified in order to assess the importance of

convection. The addition of another time period is feasible by changing the label during the course of the experiment (Kyner and Rosenberg, pers. comm.). Indeed, as we shall see in the following section, data taken at two time periods allow us to identify the importance of "convection" terms in models for populations of dispersing insects.

C. Modeling insect movement in cultivated gardens

Since Skellam's [21] pioneering work in 1951, diffusion models have been used to model animal dispersal. Unfortunately, most of this modeling has proceeded independently of data ([13], [14]). In fact, some researchers have suggested that the paradigm of diffusive flux is inappropriate for animal movement and have advised instead a purely descriptive regression approach to quantifying dispersal ([24], [25]). One of the problems with previous diffusion models is that only the simplest process, that is pure passive diffusion, lends itself to tests with experimental data (see [14]). Recently one of the authors exhaustively applied passive diffusion models to the movement of two common flea beetles, Phyllotreta cruciferae and Phyllotreta striolata [11]. Although the models provided a good description of beetle movement in some cases, several experimental results clearly did not conform to simple passive diffusion (see [11]). We subsequently applied spline parameter identification methods to these beetle data with a model extended to include a spatially-varying convection term.

Using mark-recapture experiments, beetle movement was studied in experimental linear arrays. These arrays were 1 m x 80 m cultivated strips in the middle of dense goldenrod stands, each array containing patches of one of the beetles favored foodplants, collards. Since the goldenrod field surrounding each array contained no foodplants for the beetles,

the beetles tended to move only in one dimension -- up and down the
linear arrays along the 80 m axis. Details about the marking and
recapture procedure and experimental design are described in [11].
The important point is that marked flea beetles were recaptured anywhere
from 1 hour to 3 days after their release in the experimental arrays;
these recapture distributions represent the data that we seek to
describe with a diffusion-convection model. The model we examined is

$$(17) \qquad \frac{\partial u}{\partial t} = - \frac{\partial}{\partial x} (V(x)u) + D \frac{\partial^2 u}{\partial x^2} - \mu u \qquad 0 \leq x \leq 1, \quad t > 0$$

with u(0,x) (which represents the initial distribution of marked beetles) known
and u(t,0) = u(t,1) = 0. Here the linear arrays have been rescaled to
fit in the (0,1) interval. On this rescaled interval the cultivated strips
extended between .1 and .9 and the actual sampling points (recapture stations)
are evenly spaced between approximately .20 and .80. The center of each
experimental array thus corresponds to x = .5. The negative μu term in
(17) represents beetles that disappear from the system either because they
die or engage in long distance migration (both processes are negligible
over the short time scale of our experiments but would become important
over longer-running time periods). We have considered several different
V(x) functions and combinations of V(x) with spatially varying μ(x) terms.
In a separate report we will synthesize these analyses to dissect differences
between beetle species and to quantify the influence of crop spacing on
the movement process (Kareiva and Banks, in prep.). Our ultimate goal
is to describe the changes in density (u) of beetles through time and

space. In this paper, our more limited goal is to demonstrate the application of the spline techniques to insect dispersal data, and to point out some of the problems of such analyses. To do this we have selected a small subset of our analyses for illustrative purposes.

Technically the spline approximation scheme was successful in two ways:

1) it often identified combinations of $V(x)$ and D in equation (17) that predicted beetle distributions in close accordance to observed distributions (see Table 2, example 5.2)

2) it identified convection terms that significantly reduced RSS relative to diffusion-alone models (again see Table 2, example 5.3).

It is important to note that the addition of convection significantly reduced RSS while using only the initial data and one time period after that initial data. This is in marked contrast to the case involving brain transport, where the performance of diffusion-alone versus diffusion-and-convection models could not be distinguished. We were able to use results of the beetle dispersal experiments to examine the differences between transport processes with and without convection because the initial date in these experiments was known and fixed. Consequently, the only un-identified parameters influencing the fit of the model to data are diffusion and convection parameters. These positive statements are balanced below by some cautionary tales concerning the problems we had analyzing insect dispersal data.

One of the difficulties uncovered by our analysis was that a wide variety of different convection functions yielded low RSS's. Moreover, the convection functions that worked best represent functions that

contradicted our initial biological hypotheses. In particular, $V(x)$

functions corresponding to no convection near $x = .5$ and biased motion

out the ends of arrays (away from the center of the gardens) yielded

the lowest RSS values. This contradicts our initial hypothesis that

there should be convection near the ends of each array back towards

the central position (toward $x = .5$). At this stage, however, because

there are so many reasonable possibilities for $V(x)$ that we have not

examined, we are reluctant to draw any firm conclusions about the shape

of $V(x)$ for these beetle experiments. Note that the spline methods as we

have used them here do not magically reveal the shape of functions such as

$V(x)$ -- they only estimate the constant parameters in an assumed functional

form. We are also cautious because we feel,in retrospect,that the beetle mark-

recapture experiments are not well suited for identifying convection functions.

This unsuitability results from the release of all beetles in one position,

and the fact that subsequent recaptures tended to overrepresent the

middle regions of arrays and underrepresent the peripheral reaches of

each array. Note that the shortage of recaptures near the periphery

could be explained by either of two opposite convection processes:

i) only a few beetles are caught away from the center because convection

towards the center prevents their outward spread, or (ii) only a few

beetles are caught away from the center because whenever they enter that

region, they are rapidly transported out of the arrays due to an outward

convection. To best identify convection processes, mark-recapture

experiments should begin with a uniform distribution of marked individuals.

Changes in that uniform distribution could then be used to distinguish

among different models. The flea beetle experiments suffer because too

few individuals were observed in regions that we speculated would be characterized by high convection.

A second major limitation of our analysis concerns its assumption of constant parameters through time in spite of the biological inevitability of temporal variation in insect movement behavior. Indeed, Table 3 includes examples of what appear to be temporally varying parameters, that is parameter estimates which vary widely using recapture data from different days, but identical experiments and beetle species. Only rarely were we able to find one set of parameters that predicted several consecutive recapture distributions. Because insects are ectotherms and are very sensitive to weather, their movement behavior will vary from day-to-day as a consequence of variation in weather. We are in the process of extending our analyses to include temporal variation in D, V and μ in equation (17). This elaboration is necessary if we are to model insect dispersal in extended field situations.

A final caution involves the potential for obtaining good matches between model and data (i.e., low RSS's), yet biological nonsense. Applications of these identification approaches should always entail efforts to get independent estimates of parameters as much as possible. Otherwise, what appears to be numerical success might correspond to biological absurdity. For example, one of the sets of parameters that we sought to identify was D and μ in equation (17), holding $V(x) \equiv 0$. Doing this we occasionally obtained low RSS's, even for more than one consecutive time period. But, the decay rates or μ's that were thus identified were impossibly high -- they corresponded to decay rates five times higher than anything ever observed for flea beetles in the experimental arrays.

6. Concluding remarks

The spline techniques we describe in this paper are very effective at fitting particular transport equations to data. By itself, this parameter identification approach cannot, however, lead to correct choices about what type of transport equations are appropriate for particular biological systems. Data must be collected and experiments designed in special ways if one wants to use the parameter identification approach to distinguish between different transport models. We recommend experimenting with the spline methods before collecting experimental data. In that way an experimental design might be tailored so that it can extract the maximum information from spline identification methods. Factors such as initial data, time schedule for collecting data and the spatial sampling regime will all influence the performance of spline methods. We have found, for example, that one of the worst types of initial data is a point release of marked insects, and now we plan to modify our mark-recapture experiments hereafter. Spline identification methods will undoubtedly challenge biologists in their interpretation of data. Most importantly they allow us to address complex transport processes well beyond simple random diffusion and conventional numerical methods.

TABLE 2

Applying the spline parameter identification approach to Phyllotreta striolata
dispersal in different experimental arrays. N = number of spline basis
elements; % expl. = % TSSQ explained by model, that is, it equals
$\frac{TSSQ-RSS}{TSSQ}$ × 100; t = time period or periods at which data were collected. In
all cases the initial data are u(0,x) = 211.2 for x = .5 and 0.0 for x ≠ 0.5.
The initial spline for t = 0 was fixed to be the same for all analyses below
- it was the spline that best approximated above initial data. Note that the
results of any given identification run may depend on initial guesses.

Example 5.1   Identify D, V, and μ   in

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + \frac{\partial}{\partial x}\ (V(x-.5)u)\ -\ \mu u$$

9m interpatch spacing

N = 32

t = 1 and 3 days

We searched first for D, then D plus μ, then D,μ and V

D = 20.0 m^2/day   % expl. = 74.6%

μ = 1.9

V = +59.2 m/day $F_{3,10}$ = 9.77

                                      p < .005

Table 2 - continued

3m interpatch spacing

N = 32

t = 1 day only

D = 4.0 m^2/day   % expl. = 99.9%

μ = 1.35

V = -178.4 m/day $F_{3,5}$ = 851.0

                               p < .001

Example 5.2   Identify D and V in

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + \frac{\partial}{\partial x} (V(15(x-.5))^3 u)$$

9m interpatch spacing

N = 22   % expl. = 21%

t = 2 hrs, 3 hrs. $F_{2,11}$ = 1.45

D = 1600 m^2/day   p < .5

V = -2.4 m/day

Example 5.3

Contrast diffusion alone, to diffusion plus convection in

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} + \frac{\partial}{\partial x} (V(6.25(x-.5)^5 u)$$

Table 2 - continued

6m interpatch spacing

$$N = 22$$

$$t = 1 \text{ day}$$

Diffusion alone	Diffusion and convection

Diffusion alone

$D = 2520 \text{ m}^2/\text{day}$

% expl. = 24%

$F_{1,7} = 2.19, \; p < .25$

Diffusion and convection

$D = 240 \text{ m}^2/\text{day}, \quad V = -114 \text{ m/day}$

% expl. = 95.6%

$F_{2,6} = 65.6, \quad p < .001$

Improvement in % expl. by adding convection

$$F_{1,6} = 98.4, \quad p < .001$$

3m interpatch spacing

$$N = 22$$

$$t = 1 \text{ day}$$

Diffusion alone

$D = 2190 \text{ m}^2/\text{day}$

% expl. = 31%

$F_{1,7} = 3.12, \; p < .25$

Diffusion and convection

$D = 320 \text{ m}^2/\text{day}, \quad V = -43.7 \text{ m/day}$

% expl. = 97.3%

$F_{2,6} = 72.0 \quad p < .001$

Improvement in % expl. by adding convection

$$F_{1,6} = 98.3, \quad p < .001$$

TABLE 3

Parameter identification using data from the same experiment and beetle species, but different time period after release. As in Table 2, the initial spline was fixed to provide the best fit to $u(0,x) = 211.2$ for $x = 0.5$ and 0.0 for $x \neq 0.5$. All analyses below were run with the number of spline basis elements equal to 22. The "% expl." below refers to the % of TSSQ explained by diffusion model, that is, it equals $\frac{TSSQ-RSS}{TSSQ} \times 100$.

Example 5.4   Identify D in

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$

I. **Phyllotreta striolata** in linear array with 3m interpatch spacing

    (i) data from $t = 1$ day

        estimated $D = 2190$ m^2/day   % expl. = 31%

        $F_{1,7} = 3.12$, $p < .25$

    (ii) data from $t = 3$ days

        estimated $D = 8800$ m^2/day

        $F_{1,7} = 3.63$, $p < .25$ % expl. = 34%

II. **Phyllotreta striolata** in linear array with 6m interpatch spacing

    (i) data from $t = 1$ day

        estimated $D = 2520$ m^2/day

        $F_{1,7} = 2.19$, $p < .25$ % expl. = 24%

    (ii) data from $t = 3$ days

        estimated $D = 8900$ m^2/day

        $F_{1,7} = 2.94$, $p < .25$ % expl. = 30%

Table 3 - continued

III. _Phyllotreta_ _striolata_ in linear array with 9m interpatch spacing

    (i) data from t = 1 day

        estimated $D = 2330 \ m^2/day$

        $F_{1,5} = .66,$ $p < .5$ % expl. = 12%

    (ii) data from t = 3 days

        estimated $D = 9600 \ m^2/day$

        $F_{1,5} = 2.74,$ $p < .25$ % expl. = 35%

Note that in none of the examples, does diffusion alone provide a statistically significant description of recapture distribution. Nonetheless, the variation in D's as a function of time is striking.

Appendix 1

For the arguments to establish Lemma 3.1, we assume the reader is familiar with the theory of linear semigroups and dissipative operators on a Hilbert space (see [1],[15]). We first define $A_0(q) = q_1 D^2$ and $A_1(q) = q_2 D + q_3$ so that $A = A_0 + A_1$. Here $\text{Dom }(A_0) = \text{Dom}(A)$ and $\text{Dom}(A_1) = H_0^1$. Next we observe that $A_0(q)$ is maximal dissipative in Z and is thus the infinitesimal generator of a C_0-semigroup of contractions [15, p.17, Thm. 4.5b]. The dissipative estimate follows immediately:

$$\langle A_0(q)z,z \rangle = \langle q_1 D^2 z, z \rangle = -|q_1||Dz|_2^2 \leq 0.$$

Indeed, A_0 is self-adjoint with spectrum in $(-\infty, 0]$ so $\mathscr{R}(A_0 - \lambda I) = Z$ for $\lambda > 0$ (see [19,p.349]) and hence A_0 is maximal dissipative.

We procede by considering $A_1(q)$ and demonstrating that it is a relatively bounded dissipative perturbation of $A_0(q)$. First observe that for $\phi \in H_0^1$, an integration by parts yields

$$\int_0^1 (q_2 D\phi)\phi = -\int_0^1 \phi D(q_2 \phi) = -\int_0^1 \phi [Dq_2 + q_2 D\phi]$$

or

$$2\int (q_2 D\phi)\phi = -\int Dq_2 \phi^2.$$

Thus
$$\langle A_1(q)\phi,\phi \rangle = \int (q_2 D\phi + q_3 \phi)\phi = \int [-\tfrac{1}{2}Dq_2 + q_3]\phi^2$$

$$\leq (\tfrac{1}{2}|Dq_2|_\infty + |q_3|_\infty)|\phi|_2^2$$

and hence $A_1(q) - \omega I$ is dissipative where ω is as defined in the statement of Lemma 3.1.

Turning next to arguing relative boundedness, we suppose $\phi \in \text{Dom}(A_0) = H^2 \cap H_0^1$.

Then

(A1) $$|A_1\phi|_2 = |q_2 D\phi + q_3\phi|_2 \le |q_2 D\phi|_2 + |q_3|_\infty |\phi|_2$$

while   (again we integrate by parts)

$$\int_0^1 |D\phi|^2 = \frac{1}{q_1} \int_0^1 q_1 (D\phi)(D\phi) = \frac{1}{q_1} \int_0^1 -q_1 (D^2\phi)\phi$$

$$= \frac{1}{q_1} \int_0^1 -(A_0\phi)\phi \le \frac{1}{q_1} \int |A_0\phi| |\phi|.$$

If we consider this last term as $\frac{1}{q_1} \int (\alpha |A_0\phi|)(\frac{1}{\alpha}|\phi|)$ and use the fact that $ab \le \frac{1}{2}(a^2 + b^2)$,   we thus obtain

$$\int |D\phi|^2 \le \frac{1}{q_1} \int \{\frac{\alpha^2}{2}|A_0\phi|^2 + \frac{1}{2\alpha^2}|\phi|^2\}$$

$$= \frac{\alpha^2}{2q_1}|A_0\phi|_2^2 + \frac{1}{2q_1\alpha^2}|\phi|_2^2.$$

Hence we have

$$|D\phi|_2 \le \frac{\alpha}{\sqrt{2q_1}}|A_0\phi|_2 + \frac{1}{\alpha\sqrt{2q_1}}|\phi|_2.$$

Choosing $\alpha = \frac{1}{2}(\sqrt{2q_1})/|q_2|_\infty$,   we find

$$|q_2 D\phi|_2 \le |q_2|_\infty |D\phi|_2 \le \frac{1}{2}|A_0\phi|_2 + \frac{|q_2|_\infty^2}{q_1}|\phi|_2.$$

Combining this last estimate with (A1), we finally obtain

$$|A_1\phi|_2 \le \frac{1}{2}|A_0\phi|_2 + \{|q_2|_\infty^2/q_1 + |q_3|_\infty\}|\phi|_2,$$

so that

$$|(A_1(q)-\omega I)\phi|_2 \le \frac{1}{2}|A_0\phi|_2 + \{\omega + |q_2|_\infty^2/q_1 + |q_3|_\infty\}|\phi|_2.$$

It follows that $A_1(q) - \omega I$ is dissipative and relatively bounded with respect to A_0 and satisfies the hypothesis of [15,p.84, Thm. 3.1]. Thus $A(q) - \omega I = A_0(q) + A_1(q) - \omega I$ is the generator of a C_0-semigroup of contractions and hence $A(q) = (A_0(q) + A_1(q) - \omega I) + \omega I$ is the generator of a C_0-semigroup $\{S(t)\}$ satisfying $\|S(t)\| \leq e^{\omega t}$ (see [15, p.80, Thm.1.1]). This yields (see [15, p.16,17, Thm. 4.5(a)]) the first two claims of Lemma 3.1.

That mild solutions of (5) are given by (6) actually follows by definition from the usual theory of linear semigroups and abstract evolution equations (e.g., see [1],[15]).

Appendix 2

We establish the veracity of Lemma 4.1. First, simple arguments reveal that whenever $q_2^*, q_3^* \in W_\infty^2$, we have $\mathscr{D} \equiv \text{Dom}(A^2(q^*)) \subset H^4 \cap H_0^1$. For if $\phi \in \text{Dom}(A^2(q^*))$, then $A(q^*)\phi \in \text{Dom}(A(q^*)) = H^2 \cap H_0^1$; that is, $q_1^* D^2 \phi + q_2^* D\phi + q_3^* \phi = \gamma$ is in $H^2 \cap H_0^1$. It follows immediately that $D^2\phi = 1/q_1^* [\gamma - q_2^* D\phi - q_3^* \phi]$ is in H^2 or that $\phi \in H^4$ (we have $\phi \in H_0^1$ since $\text{Dom}(A^2(q^*)) \subset \text{Dom}(A(q^*)) = H^2 \cap H_0^1$).

To complete the arguments for Lemma 4.1, we need some estimates on the projection operators $P^N : Z \to Z^N$ as defined above. These estimates, which are themselves derivable from well-known results from the theory of spline approximations, are given in [5, Lemma 2.3] and are as follows:

There exist constants c_i such that for $z \in H^4 \cap H_0^1$,

$$|P^N z - z|_2 \leq c_0 N^{-4} |D^4 z|_2$$

$$|D(P^N z - z)|_2 \leq c_1 N^{-3} |D^4 z|_2$$

$$|D^2(P^N z - z)|_2 \leq c_2 N^{-2} |D^4 z|_2.$$

Finally, for $z \in \mathscr{D} \subset H^4 \cap H_0^1$ we consider the estimates (to facilitate notation we use $|\cdot|$ for $|\cdot|_2$ here)

$$|A^N(q^N)z - A(q^*)z| = |P^N A(q^N) P^N z - A(q^*)z|$$

$$\leq |P^N(A(q^N)P^N z - A(q^*)z| + |(P^N - I)A(q^*)z|$$

$$\leq |A(q^N)P^N z - A(q^*)z| + |(P^N - I)A(q^*)z|.$$

The second term in this last expression $\to 0$ as $N \to \infty$. This follows since

$P^N \to I$ on Z (the above estimate yields that $P^N z \to z$ for a dense set of z in Z and the $\{P^N\}$ are uniformly bounded on Z).

Consider the first term:

$$|A(q^N)P^N z - A(q^*)z| = |(q_1^N D^2 + q_2^N D + q_3^N)P^N z - (q_1^* D^2 + q_2^* D + q_3^*)z|$$

$$\leq |q_1^N D^2 (P^N z - z)| + |(q_1^N - q_1^*)D^2 z|$$

$$+ |q_2^N D(P^N z - z)| + |(q_2^N - q_2^*)Dz|$$

$$+ |q_3^N (P^N z - z)| + |(q_3^N - q_3^*)z|$$

$$\leq |q_1^N||D^2(P^N z - z)|_2 + |q_1^N - q_1^*||D^2 z|_2$$

$$+ |q_2^N|_\infty |D(P^N z - z)|_2 + |q_2^N - q_2^*|_2 |Dz|_\infty$$

$$+ |q_3^N|_\infty |P^N z - z|_2 + |q_3^N - q_3^*|_2 |z|_\infty.$$

But every term in this last sum $\to 0$ as $N \to \infty$ due to the following facts: $|q_1^N|, |q_2^N|_\infty, |q_3^N|_\infty$ are bounded, $q_1^N \to q_1^*$, $q_i^N \to q_i^*$ in L_2, $i = 2,3$, and $P^N z, DP^N z, D^2 P^N z$ converge to $z, Dz, D^2 z$, respectively.

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