MATHEMATICAL CONTROL THEORY
BANACH CENTER PUBLICATIONS, VOLUME 14
PWN – POLISH SCIENTIFIC PUBLISHERS
WARSAW 1985

IDENTIFICATION AND ESTIMATION OF PARAMETERS IN ABSTRACT CAUCHY PROBLEMS

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1. Introduction

When describing processes that evolve in time by mathematical means one commonly encounters differential—or integral equations. Let us assume that we want to model a particular system (biological, physical or otherwise) and that a priori knowledge guides us to use a certain type of equation. Suppose further that in the mathematical model of our system we were not able to fix values of certain parameters: for example we might not know the value of the diffusion coefficient in a parabolic partial differential equation, or we are uncertain whether diffusion should be taken into consideration at all. In a similar manner we might have to deal with unknown quantities in the initial data or in the forcing function of an equation. To recover the unknown quantities of the system we assume that we are given observations, possibly in a continuous manner over some time interval or only at discrete times.

Many interesting mathematical questions can be formulated and studied in the situation just described and here we shall address two: parameter identification and parameter estimation. Our particular attention is directed towards the latter. To be specific let us assume to be given the abstract Cauchy problem in $X(q)$:

$$\begin{aligned} \dot{u}(t) &= A(q)u(t), \\ u(0) &= u_0(q), \end{aligned} \tag{1.1}$$

where $A(q)$ is the infinitesimal generator of a linear C_0-semigroup $T(t; q)$ or simply $T(t)$ in a Hilbert space $X(q)$, $q \in Q \subset \boldsymbol{R}^k$, $k > 0$. The necessity to allow for the generality of a parameter dependent state space will be demonstrated in Example 3.1. We let $u(t; q) = T(t; q)u_0(q)$ for each $u_0(q) \in X(q)$ and recall that $t \to u(t; q)$ is a strong solution of (1.1) for each $u_0(q) \in \operatorname{dom} A(q)$. Let Y be the observation space and assume that observations $\hat{y}(t) \in Y$ are known for $t \in I$, where I is a finite or infinite subset of $[0, T]$. Corresponding to the set of observations $\{\hat{y}(t) \colon t \in T\}$ we define outputs of system (1.1) by

$$y(t) = y(t; q) = \tilde{\mathscr{C}}(t; q)u(t; q), \qquad t \in I,$$

where the output operator $\tilde{\mathscr{C}}(t; q) \colon X(q) \to Y$ is defined for each $(t, q) \in I \times Q$. *Identifiability* of the parameter $q \in \boldsymbol{R}^k$ is the question of injectivity of the map $\mathscr{I} \colon Q \to \mathscr{F}(I; Y)$, given by $\mathscr{I}(q) = \tilde{\mathscr{C}}(t; q)u(t; q)$, where $\mathscr{F}$ denotes some function space over I, [6], [7], [10].

The related question of parameter estimation arises if we wish to fit the observations $\hat{y}$ to the model (1.1) by an appropriate choice of $q \in Q$. In this case we define a fit-to-data criterion J involving the solutions $u(t; q)$, q and $\hat{y}(t)$, $t \in I$. The parameter estimation problem is defined next:

(P) Given observations $\hat{y} = \{\hat{y}(t), t \in I\}$, with I a subset of $[0, T]$, minimize $J\big(q, u(\cdot; q), \hat{y}\big)$ over $q \in Q$ subject to $u(\cdot; q)$ satisfying (1.1) on $[0, T]$.

It is obvious that even if identifiability is assured for a certain system, one cannot expect to be able to calculate a specific $\bar{q}$ explicitly from the output $y(t; \bar{q})$ and one will also have to resort to estimates in this situation.

We shall next describe one particular choice of fit-to-data criterion, which will be used in the numerical examples that will be discussed further below. From now on it is assumed that for each $q \in Q$, the space $X(q)$ is a function space of $\boldsymbol{R}^n$-valued functions (or one of the usual Lebesgue spaces of equivalence classes of functions) defined on $[0, 1]$. The observations $\hat{y}(t_i)$ are taken at discrete points

$$0 \leqslant t_1 \leqslant \ldots \leqslant t_r \leqslant T, \qquad \text{with} \qquad \hat{y}(t_i) \in Y \equiv \prod_{j=1}^{l} \boldsymbol{R}^\nu, \; \nu \leqslant n,$$

corresponding to measurement points

$$\{x_j\}_{j=1}^{l}, \qquad x_j \in [0, 1] \qquad \text{at time} \qquad t_i.$$

These observations $\hat{y}(t_i)$ correspond to outputs $\mathscr{C}(t_i; q)z(t_i; q)$, where

$$z(t_i; q) = \operatorname{col}\big(u(t_i, x_1; q), \ldots, u(t_i, x_l; q)\big)$$

and $\mathscr{C}(t_i; q)$ is an $(\nu l) \times (nl)$-matrix depending continuously on q for each fixed t_i. The associated quadratic fit-to-data criterion then becomes

$$(1.2)\qquad J\big(q, u(\cdot; q), \hat{y}\big) = \sum_{i=1}^{r} |\hat{y}(t_i) - \mathscr{C}(t_i; q) z(t_i; q)|^2 w_i^2.$$

The weights $w_i \in \boldsymbol{R}$ are included to compensate for certain a priori known extreme behavior of the solution; for example one might know that the solutions of (1.1) decrease exponentially for all $q \in Q$, in which case J would only try to match the model to the data for very small values of t, unless weights are used.

We point out that we have made the implicit assumption that $u(t_i, x_j; q)$ is well defined, i.e., that point evaluation is meaningful. This, of course, needs a detailed discussion for each specific example. Note also that instead of finding an estimate for the "correct" value of q by minimizing a certain fit-to-data criterion, we could have equally well employed a maximum likelihood estimator; we shall not follow this idea any further here, but refer to [1] and the references given there.

Although we have chosen to consider only linear equations in this paper, all the results that will be discussed for parameter estimation carry over to a broad class of semilinear equations of the type

$$\dot{u}(t) = A(q)u(t) + F\big(t, q, u(t)\big), \quad t > 0,$$
$$u(0) = u_0(q),$$

where $A(q)$ is as above and F is a nonlinear operator which is Lipschitz continuous in $u(t)$; we refer to [2], Section 3, for details.

If $X(q)$ is an infinite-dimensional space then (P) will be an infinite-dimensional problem. In the next section therefore we shall develop techniques to approximate (P) by a sequence of problems (P^N) in subspaces $X^N(q)$ of $X(q)$. Once $X^N(q)$ is chosen finite-dimensional for $N = 1, 2, \ldots$, the resulting optimization problems can be treated by standard numerical techniques. A forthcoming paper will contain detailed proofs as well as a discussion and comparison of the schemes that are proposed in this paper and several additional examples.

2. Parameter estimation techniques

In this section we develop the theoretical framework for approximating unknown parameters in abstract equations of type (1.1). For each q let $X^N(q)$ be a sequence of closed linear subspaces of $X(q)$ and let $P^N(q)$: $X(q) \to X^N(q)$ denote the canonical projections along $X^N(q)^\perp$. The norm of an element $x \in X(q)$ will be denoted by $|x|_q$. A number of hypotheses that will be used at various points in the sequel are summarized next. Condition (H1) will be a standing assumption throughout the paper:

(H1) The spaces $X(q)$, $q \in Q \subset \boldsymbol{R}^k$, are set theoretically equal and uniformly topologically isomorphic, so that there exists a constant $\varkappa \geq 1$ such that $|x|_{q_1} \leq \varkappa |x|_{q_2}$ for all $x \in X = X(q)$ and all $q_1, q_2 \in Q$;

(H2) For each $q \in Q$, $A(q)$ generates a linear C_0-semigroup $T(t; q)$ on $X(q)$;

(H3) Q is a compact subset of $\boldsymbol{R}^k$;

(H4) For each $q \in Q$ and $N = 1, 2, \ldots$, let $A^N(q)\colon X(q) \to X^N(q)$ generate a linear C_0-semigroup on $X(q)$ denoted by $T^N(t; q)$. Further there exist constants $M = M(N)$ and $\omega = \omega(N)$ for each N, independent of $q \in Q$, such that

$$\|T^N(t; q)\|_q \leq M e^{\omega t};$$

(H5) For each convergent sequence in Q, say $q^N \to q^0$, we have

$$\lim_{N\to\infty} |T^N(t; q^N) P^N(q^N) x - T(t; q^0) x|_{q^N} = 0$$

uniformly in $t \in [0, T]$ for each $x \in X$;

(H6) The projections $P^N(q)\colon X(q) \to X^N(q)$ are such that for any convergent sequence $q^N \to q^0$ one has

$$\lim_N |P^N(q^N) x - x|_{q^N} = 0$$

for all $x \in X$;

(H7) For each convergent sequence $q^N \to q^0$, there exist constants $\mathscr{M}$ and ω^* such that

$$\|T^N(t; q^N)\|_{q^0} \leq \mathscr{M} e^{\omega^* t}$$

uniformly in N;

(H8) Let $q^N \to q^0$ be any convergent sequence in Q and let $I^N\colon X(q^0) \to \to X(q^N)$ denote the canonical isomorphisms.

Then
$$\lim_N |I^N x|_{q^N} = |x|_{q^0}$$

for all $x \in X$.

Notice that the projections $P^N(q)$ depend on q since $X(q)$ does. The equations approximating (1.1) are defined by

$$\begin{aligned} \dot{u}^N(t) &= A^N(q) u^N(t), \qquad t > 0 \\ u^N(0) &= P^N(q) u_0(q) \end{aligned} \tag{2.1}$$

in $X(q)$. Analogously to $u(t;q)$ we define

$$u^N(t;q) = T^N(t;q)P^N(q)u_0(q).$$

Again, if $P^N(q)u_0(q) \in \operatorname{dom} A^N(q)$ then $u^N(t;q)$ is a strong solution of (2.1) and in addition, if $X^N(q)$ is finite-dimensional then $u^N(t;q)$ is a strong solution of (2.1) for each initial datum. We also remark that $t \to u^N(t;q)$ and $t \to u(t;q)$, $q \in Q$, are elements in $C(0, T; X(q))$ for all $u_0(q)$. The sequence of approximating parameter estimation problems is defined next.

(P^N) Given observations $\hat{y} = \{\hat{y}(t) | \ t \in I\}$, $I \subset [0, T]$ and the fit-to-data criterion J, minimize $J(q, u^N(\cdot; q), \hat{y})$ over $q \in Q$ subject to $u^N(\cdot; q)$ satisfying (2.1) on $[0, T]$.

THEOREM 2.1. *Assume that* (H1)–(H4) *hold and that* $J(\cdot, \cdot, \hat{y})$: $Q \times \times C(0, T; X) \to \mathbf{R}$ *is continuous. Suppose, moreover, that*

$$q \to u_0(q), \qquad q \to P^N(q)x \quad \text{and} \quad q \to T^N(t;q)x, \qquad x \in X$$

are continuous with the latter holding uniformly in $t \in [0, T]$. *Then*

(a) *for each* N *there exists a solution* q^N *of* (P^N) *and* q^N *possesses a convergent subsequence* $q^{N_k} \to \bar{q}$;

(b) *if further* (H5) *holds, then* $\bar{q}$ *is a solution of* (P).

Proof. By (H4) and the additional hypotheses of the theorem it is simple to see that $q \to u^N(t;q)$ is continuous uniformly in $t \in [0, T]$. (H3) then implies (a). Next let $q^{N_k} \to \bar{q}$. For each $q \in Q$ we have

$$J(q^{N_k}, u^{N_k}(\cdot; q^{N_k}), \hat{y}) \leqslant J(q, u^{N_k}(\cdot; q), \hat{y})$$

for all $q \in Q$. From (H1) and (H5) it follows that

$$u^{N_k}(t; q^{N_k}) \to u(t; \bar{q}) \quad \text{and} \quad u^{N_k}(t;q) \to u(t;q)$$

as $N_k \to \infty$ for each $q \in Q$ in any $|\cdot|_q$-norm and uniformly in $t \in [0, T]$. Therefore

$$J(\bar{q}, u(\cdot; \bar{q}), \hat{y}) \leqslant J(q, u(\cdot; q), \hat{y})$$

for all $q \in Q$. This proves (b).

Of course, the most stringent hypothesis in the previous theorem is (H5). We now turn to a discussion of this hypothesis. It will be convenient to study (H5) in the more precise form:

$$\lim_N |T^N(t;q^N)P^N(q^N)I^N x - I^N T(t;q^0)x|_{q^N} = 0, \tag{2.2}$$

where I^N was defined in (H8). Note that by (H1) and (H7) we get

$$|T^N(t; q^N)P^N(q^N)I^N x - I^N T(t; q^0)x|_{q^N}$$
$$\leqslant |T^N(t; q^N)P^N(q^N)I^N x - T^N(t; q^N)I^N x|_{q^N} + |T^N(t; q^N)I^N x - I^N T(t; q^0)x|_{q^N}$$
$$\leqslant \varkappa^2 \mathscr{M} e^{\omega t}|P^N(q^N)I^N x - I^N x|_{q^N} + |T^N(t; q^N)I^N x - I^N T(t; q^0)x|_{q^N}.$$

This simple estimate shows that (H1), (H6), (H7) and (H9), which is formulated below, imply (H5).

(H9) For each convergent sequence $q^N \to q^0$ in Q, one has

$$\lim_N |T^N(t; q^N)I^N x - I^N T(t; q^0)x|_{q^N} = 0$$

uniformly in $t \in [0, T]$ for all $x \in X$.

This is now the final form of the essential convergence assumption on the approximating semigroups $T^N(t; q^N)$. We also point out that the technically precise version of (H6) is given by

$$\lim_N |P^N(q^N)I^N x - I^N x|_{q^N} = 0 \qquad \text{for all } x \in X(q^0).$$

In the sequel we shall present three choices for infinitesimal generators $A^N(q)$ such that $T^N(t; q)$ satisfy (H9). Before, however, we recall a special version of the well-known Trotter–Kato theorem.

Let Z and Z^N, $N = 1, 2, \ldots$, denote Hilbert spaces with inner products $(\cdot; \cdot)$ and $(\cdot, \cdot)_N$ and norms $|\cdot|$ and $|\cdot|_N$, respectively. Moreover, let $\mathscr{I}^N$: $Z \to Z^N$ be bounded linear operators. The sequence of spaces Z^N is called *Kato-convergent to Z*, if the following two conditions hold:

(K1) $\lim_N |\mathscr{I}^N z|_N = |z|$ for all $z \in Z$;

and

(K2) there exists a constant K, independent of N, such that for each $z_N \in Z^N$ there exists a $z^{(N)} \in Z$ with $z_N = \mathscr{I}^N z^{(N)}$ and $|z^{(N)}| \leqslant K|z_N|_N$.

THEOREM 2.2. *Let Z^N be Kato-convergent to Z and let $\mathscr{T}(t)$ and $\mathscr{T}^N(t)$ be linear C_0-semigroups on Z and Z^N generated by $\mathscr{A}$ and $\mathscr{A}^N$, respectively. Then conditions* (A) *and* (B) *together are equivalent to* (C), *where*

(A) *there exists a complex number λ_0 such that*

$$\lim_N |(\lambda_0 - \mathscr{A}^N)^{-1}\mathscr{I}^N z - \mathscr{I}^N(\lambda_0 - \mathscr{A})^{-1}z|_N = 0$$

for all $z \in Z$;

(B) *there exist constants* $\tilde{M}$ *and* $\tilde{\omega}$ *such that*

$$\|\mathscr{T}^N(t)\|_N \leqslant \tilde{M}e^{\tilde{\omega}t} \quad \textit{for all } t \geqslant 0 \textit{ and } N = 1, 2, \dots,$$

(C) *for each* $T > 0$ *and* $z \in Z$,

$$\lim_N |\mathscr{T}^N(t)\mathscr{I}^N z - \mathscr{I}^N \mathscr{T}(t) z|_N = 0$$

uniformly in $t \in [0, T]$.

The proof of this theorem can be found in [12]; we note that (K2) is actually superfluous for the proof that (A) and (B) imply (C). This can be seen from a careful inspection of the proof in [12].

COROLLARY 2.1. *Assume the hypotheses of the previous theorem and let* (A) *be replaced by:*

(A′) *there exists a set* $\mathscr{D} \subset Z$ *such that* $\mathscr{D} \subset \operatorname{dom}(\mathscr{A})$, $\overline{(\lambda_0 - \mathscr{A})\mathscr{D}} = Z$ *for some* λ_0 *with* $\operatorname{Re}\lambda_0 > \tilde{\omega}$, *and for each* $z \in \mathscr{D}$ *we have*

$$\lim_N |\mathscr{A}^N \mathscr{I}^N z - \mathscr{I}^N \mathscr{A} z|_N = 0;$$

then (A′) *and* (B) *together imply* (C).

Proof. Corollary 2.1 is a slightly modified statement of Theorem 2.1 in [8]. Here we show how it follows from the previous theorem. Let y be an arbitrarily chosen element in $(\lambda_0 - \mathscr{A})\mathscr{D}$ and let $x \in \mathscr{D}$ be such that $(\lambda_0 - \mathscr{A})x = y$. From (A′) it follows that

$$\mathscr{I}^N x \in \operatorname{dom}(\mathscr{A}^N)$$

and

$$\lim_N |\mathscr{A}^N \mathscr{I}^N x - \mathscr{I}^N \mathscr{A} x|_N = 0.$$

We define

$$y^N = (\lambda_0 - \mathscr{A}^N)\mathscr{I}^N x.$$

Then

$$\begin{aligned} &|(\lambda_0 - \mathscr{A}^N)^{-1}\mathscr{I}^N y - \mathscr{I}^N(\lambda_0 - \mathscr{A})^{-1} y|_N \\ &\leqslant |(\lambda_0 - \mathscr{A}^N)^{-1}\mathscr{I}^N y - (\lambda_0 - \mathscr{A}^N)^{-1} y^N|_N + |(\lambda_0 - \mathscr{A}^N)^{-1} y^N - \mathscr{I}^N(\lambda_0 - \mathscr{A})^{-1} y|_N \\ &\leqslant \tilde{M} \operatorname{Re}(\lambda_0 - \tilde{\omega})^{-1} |\mathscr{I}^N y - y^N|_N \leqslant \tilde{M} \operatorname{Re}(\lambda_0 - \tilde{\omega})^{-1} |\lambda_0 \mathscr{I}^N x - \mathscr{I}^N \mathscr{A} x - \lambda_0 \mathscr{I}^N x \\ &\qquad + \mathscr{A}^N \mathscr{I}^N x|_N. \end{aligned}$$

This last term tends to zero as N goes to infinity. Therefore

$$\lim_N |(\lambda_0 - \mathscr{A}^N)^{-1}\mathscr{I}^N y - \mathscr{I}^N(\lambda_0 - \mathscr{A})^{-1} y|_N = 0$$

for all y in the dense set $(\lambda_0 - \mathscr{A})\mathscr{D}$. Notice now that $\{\|\mathscr{I}^N\|_N\colon N = 1, 2, \ldots\}$ is bounded. Indeed, (K1) implies that the set $\{x\colon |\mathscr{I}^N x|_N \leqslant 1\}$ is a barrel in Z and therefore a neighborhood of 0 in Z. This short argument first appeared in [12]. It is obvious that

$$\{\|(\lambda_0 - \mathscr{A}^N)^{-1}\mathscr{I}^N - \mathscr{I}^N(\lambda_0 - \mathscr{A})^{-1}\|_N\colon N = 1, 2, \ldots\}$$

is bounded and therefore by the usual density argument it follows that (A′) implies (A). Theorem 2.1 now implies the claim. Again (K2) is not necessary for this theorem to hold.

Remark 2.1. The conditions on $\mathscr{D}$ in (A′) to the effect that

$$\mathscr{D} \subset \operatorname{dom}(\mathscr{A}) \quad \text{and} \quad \overline{(\lambda_0 - \mathscr{A})\mathscr{D}} = Z$$

for some λ_0 with $\operatorname{Re}\lambda_0 > \tilde{\omega}$ imply that $\mathscr{D}$ is a core for $\mathscr{A}$, if in addition $\lambda_0 \in \varrho(\mathscr{A})$, the resolvent set of $\mathscr{A}$. Conversely, if $\mathscr{D}$ is a core for $\mathscr{A}$, then $\mathscr{D}$ satisfies the conditions on $\mathscr{D}$ in (A′).

For let

$$M = \{(x, \mathscr{A}x) \in Z \times Z\colon x \in \mathscr{D}\}$$

and let $(u, \mathscr{A}u)$ be an arbitrary element in the graph of $\mathscr{A}$. Since $(\lambda_0 - \mathscr{A})\mathscr{D}$ is dense in Z, there exists a sequence $u_n \in \mathscr{D}$ such that $\lim_n (\lambda_0 - \mathscr{A})u_n = (\lambda_0 - \mathscr{A})u$. Applying $(\lambda_0 - \mathscr{A})^{-1}$ to this last equation we find $\lim_n u_n = u$ and $\lim_n \mathscr{A}u_n = \mathscr{A}u$; therefore $\mathscr{D}$ is a core for $\mathscr{A}$. Conversely, if $\mathscr{D}$ is a core for $\mathscr{A}$ and $\lambda_0 \in \varrho(\mathscr{A})$, then $\mathscr{D}$ is also a core for $\lambda_0 - \mathscr{A}$. Therefore $(\lambda_0 - \mathscr{A})\mathscr{D}$ is dense in $(\lambda_0 - \mathscr{A})Z = Z$.

As indicated before we shall next describe various possibilities for defining $A^N(q)$. Recall that a linear operator B in Y is called *ω-dissipative* if $\operatorname{Re}(Bx, x) \leqslant \omega|x|^2$ for all $x \in \operatorname{dom}(B)$ ([9], p. 244). B is the *generator* of a C_0-semigroup $S(t)$ with $\|S(t)\| \leqslant e^{\omega t}$ if and only if B is ω-dissipative, closed, densely defined and the resolvent set of B contains (ω, ∞) ([9], p. 283).

PROPOSITION 2.1. *Let $q^N \to q^0$ be an arbitrary convergent sequence in Q and assume that* (H1), (H2), (H6), (H8) *hold and that*

$$\operatorname{Re}\big(A(q)x, x\big)_q \leqslant \overline{\omega}|x|_q^2$$

for all $x \in \operatorname{dom} A(q)$ with $\overline{\omega}$ independent of q. Further let $X^N(q) \subset \operatorname{dom} A(q)$,

$$A^N(q) = P^N(q)A(q)P^N(q), \tag{2.3}$$

and assume that

$$\lim_N |A(q^N)P^N(q^N)I^N y - I^N A(q^0)y|_N = 0 \tag{2.4}$$

for all y in a core of $A(q^0)$. Then $X(q^N)$ is a Kato-convergent sequence to $X(q^0)$; moreover, (H4), (H7), (H9) *and consequently* (H5) *hold.*

Proof. First notice that Kato-convergence of $X(q^N)$ to $X(q^0)$ is a simple consequence of (H1) and (H9). Since $P^N(q)$ is bounded and since $A(q)$ is an infinitesimal generator and therefore closed, $A^N(q)$ itself is a bounded operator. Consequently $A^N(q)$ generates a semigroup $T^N(t;q)$ for each N and q. Since for each $x \in X(q)$ we have

$$\operatorname{Re}\left(A^N(q)x, x\right)_q \leqslant \operatorname{Re}\left(A(q)P^N(q)x,\ P^N(q)x\right)_q \leqslant \overline{\omega}\,|x|_q^2,$$

it follows that (H4) and (H7) are satisfied (see e.g. [9], p. 92).

We shall evoke Corollary 2.1 with

$$Z = X(q^0), \quad Z^N = X(q^N), \quad \mathscr{A}^N = A^N(q^N), \quad \mathscr{A} = A(q^0),$$
$$\mathscr{I}^N = I^N\colon X(q^0) \to X(q^N),$$

and

$$\mathscr{T}^N(t) = T^N(t;q^N), \quad \mathscr{T}(t) = T(t;q^0).$$

Clearly (B) is satisfied. To verify (A′) we choose y in the core of $A(q^0)$ and find that

$$\begin{aligned}
&|A^N(q^N)I^N y - I^N A(q^0)y|_{q^N} \\
&\quad \leqslant |P^N(q^N)A(q^N)P^N(q^N)I^N y - P^N(q^N)I^N A(q^0)y|_{q^N} \\
&\qquad + |P^N(q^N)I^N A(q^0)y - I^N A(q^0)y|_{q^N} \\
&\quad \leqslant |A(q^N)P^N(q^N)I^N y - I^N A(q^0)y|_{q^N} + \left|\left(P^N(q^N) - I\right)I^N A(q^0)y\right|_{q^N},
\end{aligned}$$

which tends to 0 as $N \to \infty$ by (H6) and (2.4). Therefore Corollary 2.1 is applicable and implies (H9). This concludes the proof.

Remark 2.2. If $A(q)$ is a differential operator, then the condition $X^N(q) \subset \operatorname{dom} A(q)$ restricts the possibilities of choosing approximating subspaces by requiring a certain order of smoothness of the elements in $X^N(q)$. In the following two propositions we show how this hypothesis can be weakened at the expense of stronger conditions on A.

PROPOSITION 2.2. *Let $q^N \to q^0$ be an arbitrary convergent sequence in Q and assume that* (H1), (H6), (H8) *hold, that $(I^N)^{-1}BI^N$ is selfadjoint in $X(q^0)$ for every selfadjoint operator B in $X(q^N)$, and that $A(q)$ is selfadjoint and $\operatorname{Re}\left(A(q)x, x\right)_q \leqslant 0$ for all $x \in \operatorname{dom} A(q)$, $q \in Q$. Further let $X^N(q) \subset \operatorname{dom} A^{1/2}(q)$,*

$$A^N(q) = P^N(q)A^{1/2}(q)P^N(q)A^{1/2}(q)P^N(q), \tag{2.5}$$

and assume that

$$\lim_N |A^{1/2}(q^N)P^N(q^N)I^N y - I^N A^{1/2}(q^0)y|_{q^N} = 0 \tag{2.6}$$

for all y in a core of $A^{1/2}(q^0)$. Then $X(q^N)$ is a Kato-convergent sequence to $X(q^0)$; moreover, (H2), (H4), (H7), (H9) *and consequently* (H5) *hold.*

With the aid of the following lemma due to Sz.-Nagy the proof of the above proposition will be quite simple.

LEMMA 2.1 ([4], p. 1263). *If B^N are selfadjoint operators in the Hilbert space Z, for $N = 1, 2, \dots$, if $\lim_N B^N z = Bz$ for all z in a core of B and if B itself is selfadjoint, then*

$$\lim_N \big(I + (B^N)^2\big)^{-1} z = (I + B^2)^{-1} z$$

for all $z \in Z$.

Proof of Proposition 2.2. Since $A(q)$ is selfadjoint and dissipative, it is necessarily densely defined and closed ([5], p. 279). Moreover, $A(q)$ generates a contraction semigroup $T(t;q)$ for each $q \in Q$ and therefore (H2) holds. There exists a square root $A^{1/2}$ of A, such that $iA^{1/2}$ is selfadjoint and $\operatorname{dom} A$ is a core for $A^{1/2}$ ([5], p. 281). Clearly, $X(q^N)$ is Kato-convergent to $X(q^0)$ and, as before, $A^N(q)$ is a bounded operator on $X(q)$ and generator of a C_0-semigroup $T^N(t;q)$. Let x be an arbitrary element in $X(q)$; then

$$\begin{aligned} -\big(A^N(q)x, x\big)_q &= \big(iA^{1/2}(q)P^N(q)iA^{1/2}(q)P^N(q)x, P^N(q)x\big)_q \\ &= \big(P^N(q)iA^{1/2}(q)P^N(q)x, P^N(q)iA^{1/2}(q)P^N(q)x\big)_q \geqslant 0. \end{aligned}$$

Therefore $\big(A^N(q)x, x\big)_q \leqslant 0$ for all $q \in Q$ and all N, so that $T^N(t;q)$ is a contraction semigroup. This implies (H4) and (H7). As in the proof of Proposition 2.1, using (H6) and (2.6) we find that

$$\lim_N |P^N(q^N)A^{1/2}(q^N)P^N(q^N)I^N y - I^N A^{1/2}(q^0)y|_{q^N} = 0,$$

for all y in the core for $A^{1/2}(q^0)$. By (H1) this implies

$$\lim_N |(I^N)^{-1}P^N(q^N)iA^{1/2}(q^N)P^N(q^N)I^N y - iA^{1/2}(q^0)y|_{q^0} = 0$$

and by Lemma 2.1 and again (H1) we have

$$\lim_N \big|\big(I - A^N(q^N)\big)^{-1} I^N x - I^N\big(I - A(q^0)\big)^{-1} x\big|_{q^N} = 0$$

for all $x \in X(q^0)$. We can now apply Theorem 2.2 to find

$$\lim_N |T^N(t;q^N)I^N x - I^N T(t;q^0)x|_{q^N} = 0$$

uniformly in bounded subsets of $[0, \infty)$. Therefore (H9) and (H5) are satisfied.

Remark 2.3. It is well known that the square root of a selfadjoint differential operator is not a differential operator, in general, and (2.6) will then be difficult to verify. On the other hand, there are important partial differential equations where A admits an easy expression for $A^{1/2}$ (e.g. the heat equation with periodic boundary conditions, or the fourth order equation describing the small free vibrations of a beam with certain boundary conditions) and in many practical cases the requirements on the smoothness on the elements in $X^N(q)$ implicit in $X^N(q) \subset \operatorname{dom} A(q)$ will be diminished by a factor of $\frac{1}{2}$ by requiring only $X^N(q) \subset \operatorname{dom} A^{1/2}(q)$. In practical implementations of the approximation schemes arising from (2.1) and (2.3) or (2.5) the subspaces $X^N(q)$ of $X(q)$ are chosen to be finite-dimensional and the operators involved in (2.3), (2.5) will have matrix representations that can easily be calculated, compare for instance [2]. Let us now think of $X^N(q)$ as subspaces of spline functions or finite elements; then to lower the degree of smoothness of the elements in $X^N(q)$ results in a decrease of the approximation properties, but in an increase of the algebraic simplicity of the matrices that are involved. One might argue that (2.5) will involve several matrix multiplications and that the advantage of the mentioned algebraic simplicity gets lost. In specific examples, however, the number of significant computer operations can be kept quite small. This will be discussed in Example 2 below.

In the following third choice for operators A^N we shall present the essence of the approximation scheme developed in [13], [14] in a somewhat modified form. We will need some additional technicalities. For each $q \in Q$ let $X(q)$ and $\tilde{X}(q)$ be Hilbert spaces and let $C(q)$ be a densely defined linear operator from $X(q)$ into $\tilde{X}(q)$ such that for some $\delta > 0$, independent of q, we have

$$|C(q)x|_q \geqslant \delta |x|_q \tag{2.7}$$

for all $x \in \operatorname{dom} C(q)$. We will not distinguish between the norms in $X(q)$ and $\tilde{X}(q)$, the meaning always being clear from the context. The set $\operatorname{dom} C(q)$, endowed with the inner product $\langle x, y\rangle_q = \big(C(q)x, C(q)y\big)_q$ is denoted by $X_1(q)$; as a consequence of (2.7) it is a Hilbert space. Finally, we define an operator $A(q)$ in $X(q)$ by $A(q) = -C^*(q)C(q)$.

By von Neumann's theorem ([5], p. 275) $A(q)$ is selfadjoint and $\operatorname{dom} A(q)$ is a core for $C(q)$. Moreover, it follows from (2.7) that

$$\big(A(q)x, x\big)_q \leqslant -\delta^2 |x|_q^2$$

for all $x \in \operatorname{dom} A(q)$. For the subspaces $X^N(q) \subset X(q)$ we need the following additional condition:

(H10) For each N we have $X^N(q) \subset X_1(q)$.

The sets $X^N(q)$ endowed with the topology of $X_1(q)$ are denoted by $X_1^N(q)$. Note that as a consequence of (2.7) $X_1^N(q)$ will be closed in $X_1(q)$. We let

$$P^N(q)\colon X(q) \to X^N(q) \quad \text{and} \quad P_1^N(q)\colon X_1(q) \to X_1^N(q)$$

stand for the canonical projections onto $X^N(q)$ and $X_1^N(q)$ with respect to the $X(q)$ and $X_1(q)$ norm, respectively. Conditions (H1) and (H6) need to be extended to hold for $X(q)$ and $X_1(q)$:

(H1*) This is condition (H1) for $X(q)$ and for $X_1(q)$ replacing $X(q)$.

(H6*) This is condition (H6) for $P^N(q)$ and for $P_1^N(q)$ replacing $P^N(q)$.

PROPOSITION 2.3. *Let $q^N \to q^0$ be an arbitrary convergent sequence in Q and let A be defined as above. Assume that* (H1*), (H6*), (H8), (H10) *hold and that $q \to A^{-1}(q)x$ is continuous for all $x \in X$. Finally, define on $X(q^N)$ the operators*

$$A^N(q^N) = -\big(C(q^N)P^N(q^N)\big)^* C(q^N)P^N(q^N). \tag{2.8}$$

Then $X(q^N)$ is Kato-convergent to $X(q^0)$ and (H2), (H4), (H7), (H9) *and* (H5) *hold.*

Proof. First notice that in the presence of (H1*), the continuity condition of $q \to A^{-1}(q)x$ is well defined. From the conditions on $C(q)$ it follows that $A(q)$ generates a contraction semigroup $T(t;q)$ on $X(q)$ for each $q \in Q$, so that (H2) is satisfied. Similarly it is simple to see that $A^N(q)$ generates a semigroup $T^N(t;q)$ for each N and q and that (H4) and (H7) hold. To verify (H9) we would like to apply Theorem 2.2. But (A) seems to be difficult to verify directly and we therefore introduce the operators $\tilde{A}^N(q) = A^N(q)|X^N(q)$. Obviously $\tilde{A}^N(q)$ generates a semigroup on $X^N(q)$ given by $T^N(t;q)|X^N(q)$ and

$$|T^N(t;q)x|_q \leqslant e^{-\delta^2 t}|x|_q$$

for all $x \in X^N(q)$ and $q \in Q$. We will now apply Theorem 2.2 with

$$\mathscr{A}^N = \tilde{A}^N(q^N), \quad Z = X(q^0), \quad Z^N = X^N(q^N) \quad \text{and} \quad \mathscr{I}^N = P^N(q^N)I^N.$$

By (H6) and (H8) we find that $X^N(q^N)$ is a Kato-convergent sequence to $X(q^0)$. To verify (A) we show that

$$\lim_N |(\tilde{A}^N)^{-1}(q^N)P^N(q^N)I^N x - P^N(q^N)I^N A^{-1}(q^0)x|_{q^N} = 0$$

for each $x \in X$. By (H6) and continuity of $q \to A^{-1}(q)x$ it suffices to verify

$$\lim_N |(\tilde{A}^N)^{-1}(q^N)P^N(q^N)I^N x - P^N(q^N)A^{-1}(q^N)I^N x|_{q^N} = 0,$$

which follows from (H6*) with techniques similar to those used in ([12], Theorem 2.1). Theorem 2.2 implies that

$$\lim_N |P^N(q^N)I^N T(t; q^0)x - T^N(t; q^N)P^N(q^N)I^N x|_{q^N} = 0$$

for all $x \in X$, which is (H5). From the last equality it also follows that

$$\lim_N |I^N(I - A(q^0))^{-1}x - (I - A^N(q^N))^{-1}I^N x|_{q^N} = 0.$$

A second application of Theorem 2.2 with $\mathscr{A}^N = A^N(q^N)$, $Z = X(q^0)$, $Z^N = X(q^N)$ and $\mathscr{I}^N = I^N$ yields (H9). This ends the proof.

Remark 2.4. Let $A(q) = B(q) + q_i I$, for some component q_i of $q \in \mathbf{R}^k$, where $B(q)$ satisfies the conditions of $A(q)$ in Proposition 2.3, and define

$$B^N(q) = -\big(C(q)P^N(q)\big)^* C(q)P^N(q) \quad \text{with} \quad B(q) = -C^*(q)C(q).$$

Proposition 2.3 remains correct with $A^N(q) = B^N(q) + q_i P^N(q)$. This follows from a simple application of the variation of constants formula. A similar remark applies to Proposition 2.2.

3. Application and numerical results

In this section we shall discuss two applications of the theory developed in the previous section. The first example demonstrates the need to allow for the generality of q-dependent topologies of the state space. In the second example we study the Fourier problem on the ring. The approximation schemes defined in Propositions 1.2 and 1.3 with the subspaces taken as linear spline functions are used for the latter example. Since the approximation scheme (2.5) seems to be new even for state approximation we present data not only for the parameter estimation problem but we also include a short comparison of the approximation of the state given by (2.5), (2.8) and the classical Crank–Nicolson method.

EXAMPLE 3.1. We consider the one-dimensional hyperbolic equation

$$u_{tt} = q_1 u_{xx} + q_2 u_t + q_3 u, \tag{3.1}$$

with $u = u(t, x)$ and initial and boundary conditions

$$\text{(IC)} \qquad \begin{aligned} u(0, x) &= q_4 \varphi(x), \\ u_t(0, x) &= q_5 \psi(x), \quad 0 \leqslant x \leqslant 1, \end{aligned}$$

$$\text{(BC)} \qquad u(t, 0) = u(t, 1) = 0, \quad t \geqslant 0,$$

where q_i are scalars. Here $q = (q_1, \ldots, q_5)$ is restricted to the set $Q \subset \mathbf{R}^5$. To apply the results from the previous section we rewrite (3.1) in the usual manner as an abstract first order equation. Let $\Delta = \frac{\partial^2}{\partial x^2}$ in H^0 with $\operatorname{dom}\Delta = H_0^1 \cap H^2$, where we use the usual notation for Sobolev spaces H^i of $\mathbf{R}^1$-valued functions defined on $[0,1]$. Clearly Δ is a selfadjoint operator and $(\Delta u, u)_{H^0} \leqslant 0$ for all $u \in \operatorname{dom}\Delta$. We need the following additional assumption on q_1:

(HQ) There exists a positive number $\tilde{r}$ such that $\tilde{r}^{-1} \leqslant q_1 \leqslant \tilde{r}$ for all $q \in Q$.

If (HQ) holds then the sets H_0^1 endowed with the inner products $\langle u, v\rangle_{q^1} = (q_1 u_x, v_x)_{H^0}$ are Hilbert spaces, which will be denoted by $V(q_1)$. The state space $X(q)$ will be chosen to be the Hilbert space $V(q_1) \times H^0$ endowed with the obvious product topology. Suppressing the x-dependence we rewrite (3.1), (BC), (IC) in $X(q)$ as

$$\frac{d}{dt}\begin{bmatrix} u(t) \\ v(t) \end{bmatrix} = A(q)\begin{bmatrix} u(t) \\ v(t) \end{bmatrix}, \quad t > 0,$$

$u(0) = q_4\varphi$, $v(0) = q_5\psi$, $u_t = v$, where $(\varphi, \psi) \in X(q)$, $\operatorname{dom} A(q) = (H_0^1 \cap H^2) \times \times H_0^1$ and

$$A(q) = \begin{bmatrix} 0 & 1 \\ q_1\Delta + q_3 & q_2 \end{bmatrix}.$$

The operator Δ is selfadjoint in H^0 with compact resolvent and the eigenfunctions $\{\tilde{E}_j\}_{j=1}^{\infty}$ and $\{E_j\}_{j=1}^{\infty}$, where

$$\tilde{E}_j(x) = \frac{\sqrt{2}}{j\pi}\sin j\pi x \quad \text{and} \quad E_j(x) = \sqrt{2}\sin j\pi x,$$

constitute complete orthonormal sets in $V(1)$ and H^0, respectively. For this example we choose as modal subspaces $X^N(q) \subset X(q)$ the subspaces given by

$$X^N(q) = \operatorname{span}\left\{\begin{bmatrix} \tilde{E}_1 \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} \tilde{E}_N \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ E_1 \end{bmatrix}, \ldots, \begin{bmatrix} 0 \\ E_N \end{bmatrix}\right\}.$$

Note that

$$\bigcup_{j=1}^{\infty}\left\{\begin{bmatrix} \tilde{E}_j \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ E_j \end{bmatrix}\right\}$$

is a complete orthonormal set in $X(\tilde{q})$, where $\tilde{q} = (1, 0, \ldots, 0)$. For this particular choice of subspaces $X^N(q) \subset \operatorname{dom} A(q)$ is clearly satisfied and we define the modal approximations of $A(q)$ by $A^N(q) = P^N(q)A(q)P^N(q)$, where again $P^N(q)$: $X(q) \to X^N(q)$ stand for the canonical projections. In view of the above assumptions and definitions, (H1), (H2), (H4), (H6), (H7) and (H8) are satisfied; for details we refer to [2]. To verify (2.4) let $\mathscr{D} = \bigcup_{N=1}^{\infty} X^N(q^0)$. Clearly, $\bar{\mathscr{D}} = X(q^0)$ and $(\lambda - A(q^0))\mathscr{D} = \mathscr{D}$ for $\lambda \in \varrho(A(q^0))$, so that $\mathscr{D}$ is a core for $A(q^0)$. For each $z \in \mathscr{D}$ we find for $N = N(z)$ sufficiently large that

$$|A(q^N)P^N(q^N)I^N z - I^N A(q^0)z|_N = |A(q^N)I^N z - I^N A(q^0)z|_N,$$

which converges to 0 as $N \to \infty$ as a consequence of the special form of $A(q)$.

Proposition 2.1 is now applicable and yields (H5). We are thus in a position to apply Theorem 2.1 for any appropriately defined fit-to-data criterion J.

Numerical experiments were carried out to approximate q in (3.1), (IC), (BC). J was chosen as described in Section 1 with $w_i = 1$, $T = 2$, $l = r = 10$, $\nu = 1$, since only observations of the state, not of the velocity, were assumed to be known. The observation 10×20-matrix $\mathscr{C}(t; q)$ was chosen to be

$$\mathscr{C}(t; q) = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \dots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{bmatrix}.$$

For solving the finite-dimensional approximating identification problems in this and the following example a standard Levenberg–Marquardt routine [14] was used and "exact" solutions for (3.1) were generated by a simple Crank–Nicolson scheme. Some of these values were used for the "data" $\hat{y}$ in (P^N).

EXAMPLE 3.1.1. In the equation

$$u_{tt} = q_1 u_{xx} + q_2 u_t + q_3 u,$$

$$u(x, 0) = q_4 x(1 - x),$$

$$u_t(x, 0) = 0,$$

$$u(0, t) = u(1, t) = 0$$

the parameter vector $q = (q_1, \dots, q_4)$ is searched for. The true parameter values were chosen to be $\bar{q} = (1.414, -1, 1, 2)$ and for start-up values we took $q^{N,0} = (1, 0, 0, 1)$. For the sake of an easier comparsion of the data we took the same start-up value in each iteration step N. In practice, of course, one would use the "optimal" value found in iteration step N as a start-up value for iteration step $N+1$ (or $N+k$, for some k). The numerical data of Example 3.1.1 are found in Table 1.

Table 1

Start-up value	1	0	0	1
N	q_1^N	q_2^N	q_3^N	q_4^N
4	1.3743	−0.9967	0.6400	1.9981
8	1.4060	−1.0021	0.9355	2.0030
16	1.4092	−0.9996	0.9632	2.0004
32	1.4125	−0.9992	0.9959	2.0001
true value	1.414	−1	1	2

EXAMPLE 3.1.2. This is the nonlinear equation

$$u_{tt} = q_1 u_{xx} + u + \frac{u}{1+u},$$

$$u(x,0) = q_4 x(1-x),$$

$$u_t(x,0) = 0, \qquad u(0,t) = u(1,t) = 0,$$

where a search was performed for $q = (q_1, q_4)$ with the true model parameters being $\bar{q} = (1.414, 2)$ and start-up values $q^{N,0} = (1,1)$. The data for this example are given in Table 2. As pointed out before, the general theory developed in Section 2 can be extended so as to include the present example.

Many other examples besides the two presented here have been calculated at Brown University and we are grateful to J. Crowley for his efforts in developing the software packages. These two samples are characteristic for our numerical findings for the hyperbolic equation (3.1). For parabolic equations the approximating ordinary differential equation parameter identification problems turned out to be not identifiable for certain combinations of parameters when using model approximations. This difficulty could be overcome by using subspaces of spline functions.

Table 2

start-up value	1	1
N	q_1^N	q_4^N
4	1.4129	2.0006
8	1.4137	2.0004
16	1.4142	2.0000
true value	1.414	2

EXAMPLE 3.2. Here we study the one-dimensional heat equation

$$u_t = q_1 u_{xx} + q_2 u, \quad t > 0, \tag{3.2}$$

with initial and boundary conditions

(IC) $$u(0, x) = q_3 \varphi(x), \quad 0 \leqslant x \leqslant 1,$$

(BC) $$u(t, 0) = u(t, 1),$$
$$u_x(t, 0) = u_x(t, 1),$$

where $u = u(t, x)$, $q = (q_1, q_2, q_3) \in Q \subset \mathbf{R}^3$ and $\varphi \in H^0$. Again we assume (HQ) to hold. We rewrite the problem as an abstract Cauchy problem in H^0. Let

$$A(q) = q_1 \Delta + q_2 I,$$

with

$$\operatorname{dom} A(q) = \{u \in H^0 \colon \ u \in H^2, u(0) = u(1), u_x(0) = u_x(1)\}.$$

We will also use the selfadjoint and dissipative operators $B(q)$ given by $\operatorname{dom} B(q) = \operatorname{dom} A(q)$ and $B(q) = q_1 \Delta$. Notice that in this example the state space $X = H^0$ will not depend on q. Problem (3.2), (IC), (BC) can be written as an equation in H^0:

$$\frac{d}{dt} u(t) = A(q) u(t), \quad t > 0,$$
$$u(0) = q_3 \varphi, \tag{3.3}$$

for $\varphi \in H^0$. For the relationship between solutions of (3.2) and (3.3) we refer to the literature ([9], et al.). Here we only point out that as a consequence of the smoothing effect of selfadjoint dissipative operators, we have $u(t) \in \operatorname{dom} A(q)$ for each initial datum and $t > 0$. Therefore point evaluation $x \to u(t, x)$, $x \in [0, 1]$ is a well defined operation for $t > 0$ and the fit-to-data criterion (1.2) with $t_1 > 0$, $T = 2$, $\nu = n = 1$, $l = r = 10$ and $\mathscr{C}(t_i; q) = I$ can be used. The continuity assumption of Theorem 2.1 on J is not satisfied but it can be shown that the assertion of Theorem 2.1 remains correct for this example when the approximation scheme is chosen as in Proposition 2.1. For the schemes in Proposition 2.2 and 2.3 further research is required to justify convergence in the presence of *point* observations.

We choose subspaces of linear spline functions $X^N = \{e \in H^1 \colon e$ is a linear spline with knots at $t_i = i/N$, $i = 0, \ldots, N$, $e(0) = e(1)\}$, [11]. Let $\tilde{e}_i \in H^1$ be given by $\tilde{e}_i(t_j) = \delta_{ij}$ for $i, j = 0, \ldots, N$. Then $\{e_i\}_{i=1}^N$ given by $e_i = \tilde{e}_i$ for $i = 1, \ldots, N-1$ and $e_N = \tilde{e}_0 + \tilde{e}_N$ constitutes a basis for X^N. The application of the approximation schemes introduced in Propositions 2.2 and 2.3 is discussed now. It is simple to see that $B^{1/2}(q)$

defined by

$$\operatorname{dom} B^{1/2}(q) = \{u \mid u \in H^1,\ u(0) = u(1)\}, \qquad B^{1/2}(q)u = \sqrt{q_1}u_x$$

is a square root of $B(q)$ and that $iB^{1/2}(q)$ is selfadjoint. On $X = H^0$ we define the operators

$$A_R^N(q) = P^N B^{1/2}(q)P^N + B^{1/2}(q)P^N + q_2 P^N;$$

the projections P^N are independent of q in this case. Similarly define $C(q)\colon H^0 \to H^0 \times H^0$ by

$$\operatorname{dom} C(q) = \operatorname{dom} B^{1/2}(q) \quad \text{and} \quad C(q)u = (u, \sqrt{q_1}u_x).$$

A short calculation reveals that

$$\operatorname{dom} C^*(q) = \{(u, v) \in H^0 \times H^0\colon v \in H^1, v(0) = v(1)\},$$

$$C^*(u, v) = u - \sqrt{q_1}\, v_x \quad \text{and} \quad A(q) = -C^*(q)C(q) + (q_2+1)I.$$

The second sequence of approximating operators in H^0 becomes

$$A_U^N(q) = -\big(C(q)P^N\big)^* C(q)P^N + (q_2+1)P^N.$$

In view of the above remark concerning the applicability of Theorem 2.1 we want (H1), (H2) and (H4), (H5) to hold. (H1), (H2) and (H4) are trivially satisfied for the semigroups generated by $A_R^N(q)$ as well as $A_U^N(q)$. To verify (H5) we appeal to Remark 2.4 and apply Proposition 2.2 to $B^N(q)$ and Proposition 2.3 to $-\big(C(q)P^N\big)^* C(q)P^N$, respectively. The dissipativity conditions, $X^N \subset \operatorname{dom} B^{1/2}(q)$ and (H8*) are clearly satisfied and

$$|C(q)u|_{H^0 \times H^0} \geq |u|_{H^0} \quad \text{for all } u \in \operatorname{dom} C(q).$$

(H6*) is a consequence of well-known results in spline analysis. We are thus in a position to use $A_R^N(q)$ and $A_U^N(q)$ for state approximation as well as parameter estimation. Approximation by $A_R^N(q)$ is referred to as 1/2-method, whereas the Ushijima-method is used to denote approximation via $A_U^N(q)$. The software packages were developed by E. Graif at the Technical University in Graz and we are very thankful for his cooperation.

EXAMPLE 3.2.1. Here we consider the equation

$$\begin{aligned} u_t &= \pi^{-2} u_{xx} + 3u, \\ u(0, x) &= \cos 2\pi x, \end{aligned} \tag{3.2}$$

with periodic boundary conditions as above. The solution can be calculated explicitly in this case and is given by $u(t, x) = e^{-t}\cos 2\pi x$. We introduce the relative error $E(t) = 100\big(u^N(t) - u(t)\big)u^{-1}(t)$, where u denotes the exact solution and u^N an approximating solution. In this and the following example the relative error is found to be practically independent of x and we therefore suppress the x-dependence in $E(t)$. Moreover, in all our examples the relative error was found to be a monotone function of time and so we only record the relative errors close to the initial time and at the terminal time. The data for this example can be found in Table 3. The x-discretization step length due to approximation of A by A^N is given by $1/N$ and was also taken for the length of the x-discretization in the Crank–Nicolson scheme, which employed a simple three-point formula. The time discretization step length for the integration of the ordinary differential equations was taken to be $\Delta t = 0.00667$ unless specified otherwise. The "divergent" in the Ushijima-method for $N = 32$ could probably be eliminated by decreasing Δt and thus the ratio $\frac{\Delta t}{\Delta x^2}$. Concerning this point see also Example 3.2.3. In this and all the other examples we found that the error of the 1/2-method remained almost constant as t was increased. This is in contrast to the Crank–Nicolson approximation and the Ushijima method, where the error in absolute value sometimes increased drastically as t was increased. It was also observed that the 1/2-method was significantly less sensitive to the factor $\frac{\Delta t}{\Delta x^2}$ than the other two methods in the examples tested. The number of significant operations for executing the 1/2-method was almost exactly the same as for the Ushijima method, whereas for the Crank–Nicolson method only a sixth to a third as many operations were needed.

Table 3

	$E(0.2)$	$E(1)$	$E(0.2)$	$E(1)$	$E(0.2)$	$E(1)$	$E(0.2)$	$E(1)$
Crank–Nicolson	16.36	113.34	4.11	22.31	1.03	5.25	0.26	1.29
1/2-method	30.46	72.96	5.62	7.17	1.31	1.40	0.32	0.33
Ushijima-method	2.30	−48.72	0.92	−14.65	0.25	−3.81	divergent	
	$N = 4$		$N = 8$		$N = 16$		$N = 32$	

Example 3.2.2. This is the example

$$u_t = 0.1\pi^{-2}u_{xx} + 0.2u,$$

$$u(0, x) = \cos 2\pi x$$

and periodic boundary conditions. The exact solution equals $e^{-0.2t}\cos 2\pi x$ and the data are recorded in Table 4.

Table 4

	$E(0.2)$	$E(1)$	$E(0.2)$	$E(1)$	$E(0.2)$	$E(1)$	$E(0.2)$	$E(1)$
Crank–Nicolson	1.53	7.87	0.40	2.03	0.10	0.51	0.03	0.13
1/2-method	22.45	25.95	5.28	5.43	1.29	1.30	0.32	0.32
Ushijima-method	19.50	11.53	4.80	3.06	1.19	0.77	0.30	0.19
	$N = 4$		$N = 8$		$N = 16$		$N = 32$	

EXAMPLE 3.2.3. Consider the example

$$u_t = q_1 u_{xx} + q_2 u,$$
$$u(0, x) = \varphi(x)$$

with periodic boundary conditions and $\varphi(x) = 4x$ for $x \in [0, 1/4]$, $\varphi(x) = -4x+2$ for $x \in [1/4, 3/4]$ and $\varphi(x) = 4x-4$ for $x \in [3/4, 1]$. The exact solution is given by

$$u(x, t) = \frac{8}{\pi^2} \sum_{n=1}^{\infty} (-1)^{n+1} \frac{1}{(2n-1)^2} \big(\sin(2n-1)2\pi x\big) \exp\big((-4\pi^2 n^2 q_1 + q_2)t\big)$$

and numerically the "exact" solutions were determined by the requirement that three consecutive terms in the expansion were less than 10^{-15}. The relative error for this example is defined by $\bar{E}(t) = \max_x |100\big(u(t, x) - u^N(t, x)\big) u^{-1}(t, x)|$ and the numerical data can be found in Table 5.

Table 5

	$\bar{E}(0.2)$	$\bar{E}(1)$	$\bar{E}(0.2)$	$\bar{E}(1)$	$\bar{E}(0.2)$	$\bar{E}(1)$
Crank–Nicolson	10.08	28.0	2.36	6.60	0.58	1.61
1/2-method	6.89	7.23	1.34	1.40	0.33	0.33
Ushijima-method	0.99	14.6	0.26	3.8	divergent	
	$N = 8$		$N = 16$		$N = 32$	

For the data in Table 5 $\Delta t = 0.05$ was used, and when employing Ushijima's method with $N = 32$, it was necessary to decrease Δt to 0.005, before convergence could be observed.

For the same initial data with parameter values $q_1 = \pi^{-2}$, $q_2 = 0$ the Ushijima-method turned out to be very sensitive to the ratio $\frac{\Delta t}{\Delta x^2}$, for the Crank–Nicolson approximation a high relative error was observed, whereas the 1/2-method proved to be very satisfactory, with significantly smaller error than the Crank–Nicolson scheme and with $\Delta t = 0.0667$.

EXAMPLE 3.2.4. Here we summarize some data on parameter estimation using the 1/2-method in the problem

$$\begin{aligned} u_t &= q_1 u_{xx} + q_2 u, \\ u(0, x) &= q_3 \cos 2\pi x, \end{aligned} \tag{3.3}$$

with periodic boundary condition. We search for the true model parameter $\bar{q} = (0.1\pi^{-2}, 0.2, 1)$ by using 100 equally spaced observation points in $[0, 1] \times [0, 1]$. The CPU-time for the search for two parameters simultaneously ranged from 14 to 204 seconds depending on N. The data can be found in Table 6.

Table 6

search on	q_1	q_2	q_3	(q_1, q_3)	(q_2, q_3)
start-up value	0.1	0.4	4	(0.1, 2)	(0.4, 2)
$N = 8$	0.01212	0.12175	0.94932	(0.01018, 0.95022)	(0.19818, 0.95022)
$N = 16$	0.01062	0.18084	0.98719	(0.01013, 0.98725)	(0.19989, 0.98725)
$N = 32$	0.01025	0.19523	0.99679	(0.01013, 0.99679)	(0.19999, 0.99679)
true value	0.01013	0.2	1	(0.01013, 1)	(0.2, 1)

Since the explicit solutions for (3.3) are given by

$$u(t, x) = q_3 \cos(2\pi x) \exp\big((-4\pi^2 q_1 + q_2)t\big),$$

the identifiability problem is easily solved for this example. The pair (q_1, q_2) is not identifiable [6] even if the state is observed for all $t \geqslant 0$ and $x \in [0, 1]$. On the other hand, identifiability of q_1, q_2, q_3 separately is already guaranteed by observation of one point $(t^*, x^*) \in (0, 1] \times R$, where R is the open interval $(0, 1)$ minus the points 1/4, 3/4. Observation of two points (t^*, x^*) and (τ^*, x^*) in $(0, 1] \times R$ guarantees identifiability of the pairs (q_1, q_3) and (q_2, q_3), where $q_3 \neq 0$ and $t^* \neq \tau^*$. It appears that a general theory of identifiability of parameters in the presence of point observations as employed in (1.2) is not available in the literature.

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