APPROXIMATING SEMIGROUPS
BY USING PSEUDOSPECTRA

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1 Introduction

Let $A$ be the generator of a one-parameter semigroup $T_t$ acting in a Hilbert space $\mathcal{H}$. We discuss the numerical computation of $T_t f$, or equivalently the solution of the initial value problem

$$f'(t) = Af(t)$$

(1)

given $f(0) = f$. This involves several problems. The first is that the spectral mapping property may fail; that is one may have

$$\text{Spec}(T_t) \backslash \{0\} \neq \{e^{\lambda t} : \lambda \in \text{Spec}(A)\}.$$

In particular $\|T_t\|$ may grow faster than $e^{st}$ as $t$ increases, where

$$s = \sup \{\text{Re} (\lambda) : \lambda \in \text{Spec}(A)\}.$$

This problem is well known and has been studied from many points of view, but it remains a difficulty, even if $A$ has discrete spectrum, $[2, 5, 10, 12, 13, 14, 17]$.

The second problem arises for differential operators, particularly in several space dimensions, when the matrix approximations have very high dimensions. Even if $A$ has a sparse matrix, $T_t$ generally has a full matrix, so storing the matrix entries is not feasible. The obvious solution is to find a subspace of relatively small dimension which contains most information of interest. One might try to do this by taking the linear span of a finite number of eigenvectors, those for which the real parts of the eigenvalues are largest. Unfortunately experience shows that for many non-self-adjoint operators $A$, the eigenvectors do not form a basis; indeed the norms of the spectral projections often increase exponentially fast according to natural orderings of the eigenvalues. This forces one to be very cautious about assuming that a spectral expansion of some given $f$ will yield useful results.

This phenomenon is linked to the appearance of non-trivial pseudospectra. When this happens the determination of more than a small number of eigenvalues may
become numerically impossible. Even if theorems about the convergence of the
eigenfunction expansion of a general $f \in \mathcal{B}$ subject to a resummation method can
be proved, they have limited use if most of the eigenvalues and eigenvectors cannot
be determined.

Many recent papers about pseudospectra have drawn attention to possible instabil-
ity problems which are not revealed by looking at the spectrum alone, [15, 16, 7, 19,
18, 20]. Our goal in this paper is more positive: we use pseudospectral methods to
solve the evolution equation above for highly non-self-adjoint operators. The exist-
ence of a large number of approximate eigenvalues is regarded as a resource rather
than an embarrassment. We develop an ‘approximate spectral expansion’ which
may have little to do with the true eigenvalues and eigenvectors of the operator.
In spite of this our main result, Theorem 5, may be used to solve the evolution
equation to a high degree of accuracy. In the examples studied numerically we
demonstrate that it is far more accurate than the normal spectral expansion.

Our method is particularly useful if one wishes to solve the initial value problem
(1) for a large number of different choices of the initial data. The approximate
eigenvalues and eigenvectors only need to be produced once, and the computa-
tions needed for each choice of the initial data are fairly easy.

The examples which we consider in this paper are convection-diffusion operators.
There are arguments in favour of studying the associated semigroups $T_t = e^{At}$ in
$L^1$ rather than $L^2$. Diffusion is a probabilistic phenomenon, and the conserva-
tion of probability is not easy to study in an $L^2$ context. It is shown in [2, 5, 9, 21]
that the ‘same’ semigroup may have different growth properties when studied in
$L^1$ or in $L^2$. Nevertheless we will focus on the $L^2$ theory, for the same reason as in
classical Fourier theory: the theorems are much simpler to state and apply.

2 The Abstract Setting

We start with several assumptions. The first is the choice of numbers $M, \gamma$ such that
\[ \|T_t\| \leq Me^{\gamma t} \]  
for all $t \geq 0$. The second is the existence of a set $S$ equipped with a $\sigma$-field of
subsets and a finite measure $\mu$. We assume that we are given measurable families
of unit vectors $u_s \in \mathcal{H}$ and of complex numbers $\lambda_s$ parametrized by $s \in S$ and
satisfying
\[ \inf\{\|u_s - w\| + \|Aw - \lambda_s w\| : w \in \text{Dom}(A)\} < \epsilon. \]  
Throughout this paper $\epsilon$ is a given ‘acceptable’ error satisfying $0 < \epsilon < 1/2$. From
a purely theoretical point of view the assumption
\[ \|Au_s - \lambda_s u_s\| < \epsilon \]  

\[ \text{(4)} \]
for all \( s \in S \) would be simpler. We prefer (3) because it permits simpler expressions for the vectors \( u_s \) in applications. Clearly \( \lambda_s \) are approximate eigenvalues of \( A \), up to the error \( \varepsilon > 0 \). The assumption (3) implies that

\[
\lambda_s \in \text{Spec}_{2\varepsilon}(A) := \{ z : \| (zI - A)^{-1} \| \geq (2\varepsilon)^{-1} \}
\]

in the language of pseudospectral theory.

If \( A \) is highly non-self-adjoint, the fact that \( \lambda_s \) are approximate eigenvalues of \( A \) does not imply that they are close to the spectrum of \( A \). This allows us to go far beyond what is possible by means of conventional spectral methods. In numerical applications we will take \( S \) to be finite, but the above setting allows a better understanding of the general theory.

We define a bounded, linear ‘pseudospectral’ transform \( \mathcal{G} \) from \( L^1(S) \) to \( \mathcal{H} \) by

\[
\mathcal{G}\phi = \int_S \phi(s)u_s \, ds.
\]

We restrict \( \mathcal{G} \) to \( L^2(S) \) and note that it is then bounded with \( \| \mathcal{G} \| \leq |S|^{1/2} \), where \( |S| \) is the measure of \( S \). The adjoint operator \( \mathcal{G}^* : \mathcal{H} \to L^2(S) \) is given by

\[
(\mathcal{G}^* f)(s) = \langle f, u_s \rangle
\]

and \( B = \mathcal{G}^* \mathcal{G} : L^2(S) \to L^2(S) \) is given by

\[
(B\phi)(s) = \int_S b(s,t)\phi(t) \, dt
\]

where

\[
b(s,t) = \langle u_t, u_s \rangle.
\]

Since \( b \) is a bounded measurable function, \( B \) is a Hilbert-Schmidt operator on \( L^2(S) \).

It is immediate from the definitions that \( B\phi = 0 \) if and only if \( \mathcal{G}\phi = 0 \). We assume throughout the paper that \( B \) is invertible, a matter which needs to be confirmed in any application.

The following theorem describes how best to approximate \( f \in \mathcal{H} \) by expressions of the form \( \mathcal{G}\phi \) where \( \phi \in L^2(S) \). We will frequently refer to the algebraic sum \( \mathcal{M} = \mathcal{L} + \mathcal{L}^\perp \), where \( \mathcal{L} \) is the range of \( \mathcal{G} \) in \( \mathcal{H} \). This is a dense linear subspace of \( \mathcal{H} \). If \( S \) is finite, as in all numerical applications, then \( \mathcal{L} \) is closed and \( \mathcal{M} = \mathcal{H} \).

**Theorem 1** If \( P \) is the orthogonal projection on \( \mathcal{H} \) with range \( \mathcal{L} \), then

\[
P f = \mathcal{G}B^{-1}\mathcal{G}^* f
\]

for all \( f \in \mathcal{M} \). For such \( f \) the quantity \( \| \mathcal{G}\phi - f \| \), where \( \phi \in L^2(S) \), is minimized by \( \phi = B^{-1}\mathcal{G}^* f \). We also write \( \phi = \mathcal{G} \setminus f \), as in Matlab.
Proof If \( f \in L^\perp \) then \( G^*f = 0 \), so \( GB^{-1}G^*f = 0 \). If \( f = G\phi \) then
\[
GB^{-1}G^*f = G(B^{-1}G^*)\phi = G\phi = f.
\]
This proves the first statement. If \( f = G\psi + g \) where \( \psi \in L^2(S) \) and \( g \in L^\perp \) then
\[
\|f - G\phi\|^2 = \|G(\phi - \psi)\|^2 + \|g\|^2.
\]
This is clearly minimized for \( \phi = \psi \) and, under our standing hypothesis that \( G \) is one-one, this is the unique minimum. We also have
\[
B^{-1}G^*f = B^{-1}G^*(G\psi + g) = \psi.
\]

The above method of approximation should be contrasted with the following alternative. Suppose that \( A \) has a complete set of eigenvectors \( u_n, n = 1, 2, \ldots \) and that \( u_n^* \) are corresponding eigenvectors of \( A^* \), so that the two sets form a biorthogonal system in the sense that \( \langle u_n, u_m^* \rangle = \delta_{m,n} \). The standard spectral expansion with respect to this system is
\[
f = \lim_{N \to \infty} Q_Nf \tag{5}
\]
where
\[
Q_Nf = \sum_{n=1}^{N} \langle f, u_n^* \rangle u_n. \tag{6}
\]
If the identity (5) holds for all \( f \in \mathcal{H} \) one says that \( u_n \) form a basis in \( \mathcal{H} \). Unfortunately this is rarely true for highly non-self-adjoint operators. Indeed \( \|Q_N\| \) frequently diverges at an exponential rate in applications. One might modify the above formula by assuming Cesaro or Abel summability, but convergence would still have to be verified and is not always true.

One the other hand if the set \( \{u_n\}_{n=1}^{\infty} \) is complete we always have
\[
f = \lim_{N \to \infty} P_Nf
\]
where \( P_N \) is the orthogonal projection of \( \mathcal{H} \) onto \( \operatorname{lin}\{u_n : 1 \leq n \leq N\} \), and this is indeed the optimal approximation sequence to \( f \). Putting \( S = \{1, \ldots, N\} \) the theorem above enables one to compute \( P_N \). The main disadvantage of the projections \( P_N \) is that they do not commute with \( A \).

Returning to the general context at the start of this section, we use the operators defined above to solve the evolution equation approximately. We start by obtaining a bound on the real parts of approximate eigenvalues.

Lemma 2 If \( \|u\| = 1 \) and
\[
\|u - w\| + \|Aw - \lambda w\| < \varepsilon
\]
then \( \operatorname{Re}(\lambda) \leq \gamma + 2M\varepsilon \).
Proof. We first observe that $0 < \varepsilon < 1/2$ implies $1/2 \leq \|w\| \leq 3/2$. Putting $\mu = \text{Re} (\lambda)$, the identity

$$\frac{d}{ds}\left\{ T_{t-s}e^{\lambda s}w \right\} = T_{t-s}e^{\lambda s}(\lambda w - Aw)$$

implies that

$$\|T_t w - e^{\lambda t}w\| = \left\| \int_0^t T_{t-s}e^{\lambda s}(\lambda w - Aw) \, ds \right\|$$

$$\leq \int_0^t Me^{-\gamma(t-s) + \mu s \varepsilon} \, ds$$

$$= M\varepsilon \frac{e^{\mu t} - e^{\gamma t}}{\mu - \gamma}$$

It follows that

$$e^{\mu t}/2 \leq 2Me^{\gamma t} + M\varepsilon \frac{e^{\mu t} - e^{\gamma t}}{\mu - \gamma}.$$ 

If $\mu > \gamma$ then letting $t \to +\infty$, we deduce that

$$1 \leq \frac{2M\varepsilon}{\mu - \gamma}$$

which is equivalent to the statement of the lemma.

It follows immediately from the lemma that if $\text{Re} (\lambda) > \gamma$ and we put $\tilde{\lambda} = \gamma + i \text{Im} (\lambda)$ then $|\lambda - \tilde{\lambda}| \leq 2M\varepsilon$. Therefore

$$\|u - w\| + \|Aw - \tilde{\lambda}w\| < \varepsilon(3M + 1).$$

In the rest of the paper we assume that these changes in the approximate eigenvalues have been made, so that $\text{Re} (\lambda_s) \leq \gamma$ for all $s \in S$, and that $\varepsilon$ has been increased correspondingly.

The main theorem of this paper is best formulated in terms of certain approximating semigroups $R_t$.

**Theorem 3** Let $e^{\lambda t}$ be the multiplication operator on $L^2(S)$ defined by

$$(e^{\lambda t}\phi)(s) = e^{\lambda s}t_0(s).$$

and define $R_t$ on $\mathcal{M}$ for $t \geq 0$ by

$$R_t = Ge^{\lambda t}B^{-1}G^*$$

Then $R_0 = P$, $R_t(\mathcal{L}^\perp) = 0$ and $R_t(\mathcal{L}) \subseteq \mathcal{L}$ for all $t \geq 0$. We also have

$$R_t R_u f = R_{t+u} f$$

for all $t, u \geq 0$ and $f \in \mathcal{M}$. 


Proof If \( f \in L^\perp \) then \( G^* f = 0 \) so \( R_t f = 0 \). If \( f = G \phi \) where \( \phi \in L^2(S) \) then
\[
R_t f = Ge^{\lambda t}B^{-1}G^*G\phi = G(e^{\lambda t} \phi) \in L.
\]
Finally, if \( f = G \phi \) then
\[
R_t R_u f = R_t G(e^{\lambda u} \phi) = G(e^{\lambda u} e^{\lambda t}\phi) = R_{t+u} f.
\]

**Theorem 4** Suppose that \( S \) is finite and \( \mathcal{H} = L^2(X, dx) \), and rewrite \( u_\epsilon(x) = u(x,s) \). Then
\[
(R_t f)(x) = \int_X K_t(x,y)f(y) \, dy
\]
for all \( f \in \mathcal{H} \), where
\[
K_t(x,y) = \sum_{r,s} u(x,s)e^{\lambda t}(B^{-1})_{s,r}u(y,r)
\]

Proof Since \( S \) is finite, \( L \) is a finite-dimensional subspace of \( \mathcal{H} \), and \( L + L^\perp = \mathcal{H} \). We deduce that \( R_t \) has domain \( \mathcal{H} \). The formulae of the theorem are the result of rewriting (7) in integral operator form.

One might conjecture that the integral kernel of \( R_t \) is uniformly close to that of \( T_t \) under suitable conditions, but we do not have any such results.

The following is our main theorem. It is only numerically efficient if \( \epsilon > 0 \) and \( \delta = \|f - Pf\| \) are both small. We discuss this further in the next section.

**Theorem 5** If \( f \in M \) then
\[
\|T_t f - R_t f\| < \|f - Pf\|Me^{\gamma t} + \epsilon(1 + M + Mt)\|G\|_1 e^{\gamma t}
\]
for all \( t \geq 0 \).

Proof If we put \( \phi = G\setminus f = B^{-1}G^* f \) then the estimate can be rewritten in the form
\[
\|T_t f - G\phi_t\| < \|f - G\phi\|Me^{\gamma t} + \epsilon(1 + M + Mt)\|f\|_1 e^{\gamma t}
\]
where \( \phi_t = e^{\lambda t}\phi \). We follow the argument of Lemma 2 up to
\[
\|T_t w - e^{\lambda t} w\| \leq \int_0^t Me^{\gamma(t-s)+\mu s}\epsilon \, ds
\]
\[
\leq \int_0^t Me^{\gamma t}\epsilon \, ds
\]
\[
= \epsilon Mt e^{\gamma t}.
\]
Hence
\[
\|T_t u - e^{\lambda t} u\| \leq \|e^{\lambda t}(w - u)\| + \|T_t(u - w)\| + \|T_t w - e^{\lambda t} w\|
\]
\[
= \epsilon(1 + M + Mt)e^{\gamma t}.
\]
Applying this to each $u_s$ in the expansion

$$G\phi = \int_S \phi(s)u_s \, ds$$

yields

$$\|T_t G\phi - G\phi_t\| \leq \varepsilon (1 + M + Mt)\|\phi\|_1 e^{\gamma t}. $$

The theorem follows by combining this with the bound

$$\|T_t f - T_t G\phi\| \leq Me^{\gamma t}\|f - G\phi\|. $$

The above theorem is only useful as long as the right hand side of (8) is much smaller than $\|R_t f\|$. Since

$$\|R_t f\| = \|G\phi_t\| \leq \|\phi\|_1 e^{\mu t}$$

where

$$\mu = \sup\{\Re (\lambda_s) : s \in S\},$$

the estimates are only useful for a short time if $\mu \ll \gamma$. The point here is that $\mu$ may be substantially larger than $\sup\{\Re (z) : z \in \Spec (A)\}$, so pseudospectral methods may be correspondingly more accurate than spectral methods.

### 3 Numerical implementation

In numerical applications we take $S$ to be a finite set, possibly containing fewer than a hundred points. This implies that $\mathcal{M} = \mathcal{H}$. The main task is the choice of the vectors $u_s \in \mathcal{H}$. Once this has been done, there are three possible methods of computing $\phi = B^{-1}G^*f$ given $f \in \mathcal{H}$. The vectors $u_s$ determine $G^*$, and also the operator $B$ via the kernel $b(s, t)$. One might compute $B^{-1}$ and then apply the above formula to obtain $\phi$. Since the operator $B^{-1}$ is highly singular it is better to evaluate $B^{-1}\psi$ for $\psi = G^*f$ without computing $B^{-1}$; Matlab uses the command $B\backslash\psi$ for this purpose. One may finally avoid any reference to $G^*$ or $B$, by using Matlab to compute $\phi = G\backslash f$ directly. Since $G$ is a rectangular matrix, Matlab actually finds the ‘solution’ with least squares error. We tried all three methods, and found, as expected, that the third is by far the most accurate. Once $\phi$ has been determined we do not use Theorem 5 as stated, but the reformulation in (9).

The choice of a suitably small $\varepsilon > 0$ is made before starting the computation. On the other hand the verification that $\|f - G\phi\|$ is small is done on a posterior basis. Since $\phi$ and $G$ have to be computed in any case, this poses no problems.

There are two obvious ways of choosing the unit vectors $u_s$. One may use one’s physical intuition, as in the examples of this paper, to select certain vectors, and then show that they satisfy the fundamental inequality (3) for a suitably small $\varepsilon > 0$. This method has been used successfully in the semiclassical context, [3, 4, 6, 22].
The second method depends upon numerical, pseudospectral calculations, and will be described in more detail in a later publication. The first stage is the replacement of the differential operator $A$ by a sparse matrix approximation, possibly in a space of very high dimension. This may involve finite element methods or wavelets, and is not the focus of this article. There is now a well-developed technology for calculating pseudospectra, and it may be applied to very large sparse matrices. Given $\varepsilon > 0$, we next have to choose a finite set of numbers from the set $\text{Spec}_\varepsilon(A)$. If $t > 0$ is known, there is no need to consider points in $\lambda \in \text{Spec}_\varepsilon(A)$ for which $e^{\lambda t}$ is extremely small, because the contributions of the corresponding terms of $G\phi_t$ will be negligible. This applies in particular to any eigenvalues of $A$ whose real parts are much less than $\gamma$. For each $\lambda_s$ we finally choose a unit vector $u_s$ for which $\|Au_s - \lambda u_s\| < \varepsilon$.

In some cases it might be advisable to chose several vectors $u_s$ corresponding to each $\lambda_s$, providing each vector with a different label $s$. The choice depends upon how many eigenvalues of order $\varepsilon^2$ the operator $D_s = (\lambda_s I - A)^*(\lambda_s I - A)$ possesses. For rotationally invariant problems in dimension two, for example, one would treat each angular momentum sector independently, and include that parameter in the labelling of $S$. The $\varepsilon$-pseudospectra for different sectors may well overlap.

4 A Pure Convection Operator

The theory above has applications to convection-diffusion operators, but the simplest example is given by the pure convection operator

$$(Af)(x) = f'(x)$$

acting in $L^2(0,a)$ subject to the boundary condition $f(a) = 0$. This is the generator of the one-parameter semigroup $T_t$ given by

$$(T_t f)(x) = \begin{cases} f(x+t) & \text{if } x+t < a \\ 0 & \text{otherwise.} \end{cases}$$

Since $T_t = 0$ for all $t \geq a$, $\gamma$ can take any value in the estimate (2). Nevertheless, since we are interested primarily in the case of large $a$, we take $\gamma = 0$ and $M = 1$. The fact that $\text{Spec}(A) = \emptyset$ implies that one cannot hope to use spectral expansions to evaluate $T_t$, but pseudospectral expansions are still possible. Since this example is exactly soluble, we only analyze it by our method in order to understand how well the method works. We will see in the next section that the pseudospectral expansion of this operator is an asymptotic form of the corresponding expansion for a simple convection-diffusion operator.
The following constructions depend upon the choice of positive constants \( c \) and \( \alpha \). In many cases an appropriate value of \( c \) may be found in the range \( 5 \leq c \leq 10 \). The value \( c = 0 \) leads to a Fourier series expansion, which is not appropriate for this problem. One could put \( \alpha = 1 \), but for asymptotic theorems it might be more appropriate to make it proportional to \( a \) and/or inversely proportional to \( c \). Let \( v : [0,1] \to [0,1] \) be the function

\[
v(x) = \begin{cases} 
1 & \text{if } 0 \leq x \leq a - \alpha \\
(a - x)/\alpha & \text{if } a - \alpha \leq x \leq a.
\end{cases}
\]

(Many other choices would be equally suitable, for example \( v(x) = 1 - e^{(x-a)/\alpha} \).)

Given \( s \in \mathbb{Z} \) we define \( u_s \in L^2(0,a) \) by

\[
u_s(x) = ke^{-cx/a+2\pi isx/a}
\]

where

\[
k^{-2} = \frac{a}{2c} \left\{ 1 - e^{-2c} \right\}.
\]

This choice implies the identity \( \|u_s\| = 1 \). We also see that \( ak^2/2c \to 1 \) at an exponential rate as \( c \) increases. If we define \( w_s \in \text{Dom}(A) \) by

\[
w_s(x) = u_s(x)v(x)
\]

then

\[
\|u_s - w_s\|^2 = k^2 \int_0^a e^{-2cx/a}(1 - v(x))^2 \, dx \\
\leq \frac{ak^2}{2c} e^{-2c(1-\alpha/a)}.
\]

If we put \( \lambda_s = -c/a + 2\pi is/a \) then

\[
\|Aw_s - \lambda_s w_s\|^2 = k^2 \int_0^a e^{-2cx/a}v'(x)^2 \, dx \\
\leq \frac{ak^2}{2c\alpha^2} e^{-2c(1-\alpha/a)}.
\]

This indicates that the bound (3) holds with \( \varepsilon = O(e^{-c(1-\alpha/a)}) \) as \( c \to \infty \).

Having chosen a sufficiently large \( N > 0 \), we then put

\[
S = \{ s \in \mathbb{Z} : -N \leq s \leq N \}.
\]

The integral kernel of \( B = \mathcal{G}^* \mathcal{G} \) is

\[
b(s, t) = \langle u_t, u_s \rangle \\
= k^2 \int_0^a e^{-2cx/a+2\pi i(t-s)x/a} \, dx \\
= k^2 \frac{1}{2c/a - 2\pi i(t - s)/a} \\
\sim \frac{1}{1 - \pi i(t - s)/c}
\]
if \( c \) is sufficiently large.

If \( f \in L^2(0, a) \) and \( g = G^* f \) then

\[
g(s) = k \int_0^a f(x) e^{-cx/a - 2\pi isx/a} \, dx
\]

and

\[
(Pf)(x) = ke^{-cx/a} \sum_{s=-N}^{N} (B^{-1} g)(s) e^{2\pi isx/a}.
\]  \tag{11}

If \( Pf \) is approximately equal to \( f \) then we have shown that

\[
(T_tf)(x) \sim ke^{-cx/a} \sum_{s=-N}^{N} (B^{-1} g)(s) e^{2\pi isx/a + (-c/a + 2\pi isx/a)t}
\]  \tag{12}

for \( t > 0 \). In numerical implementations one actually uses the equivalent formula

\[
(T_tf)(x) \sim ke^{-cx/a} \sum_{s=-N}^{N} \phi(s) e^{2\pi isx/a + (-c/a + 2\pi isx/a)t}
\]  \tag{13}

where \( \phi = G \setminus f \), in the notation of Matlab.

Let us compare this with what one gets by using ordinary Fourier series, by making the choices \( c = 0 \) and \( N = \infty \) in the above formulae. We then have \( k = a^{-1/2} \) and

\[
u_a(x) = a^{-1/2} e^{2\pi isx/a}
\]

for all \( s \in \mathbb{Z} \). We also have

\[
g(s) = a^{-1/2} \int_0^a f(x) e^{-2\pi isx/a} \, dx
\]

so \( g \) is the sequence of Fourier coefficients of \( f \), assuming periodic boundary conditions. Since

\[
b(s,t) = \begin{cases} 1 & \text{if } s = t \\ 0 & \text{otherwise,} \end{cases}
\]

\( B \) is the identity operator on \( l^2(\mathbb{Z}) \), and (11) is replaced by

\[
f(x) = a^{-1/2} \sum_{s=-\infty}^{\infty} g(s) e^{2\pi isx/a},
\]

while (12) is replaced by

\[
(\tilde{T}_tf)(x) = a^{-1/2} \sum_{s=-\infty}^{\infty} g(s) e^{2\pi isx/a + 2\pi ist/a}
= f(x + t),
\]

subject to periodic boundary conditions on \([0, a]\). The use of Fourier series therefore solves a different problem from that in which we are interested.
We implemented the above ideas numerically for two choices of the initial function. We put $a = 20$ and divided each unit interval into 50 equally spaced points, so that functions on $[0, a]$ are approximated by sequences with 1000 terms. We chose the initial function to be

$$f(x) = 2e^{-10(x-5)^2} - e^{(x-5)^2/10}.$$  

We defined $f_t$ to be the right-hand side of (12) and computed

$$p = \|f - f_0\|_\infty \quad q = \|T_tf - f_t\|_\infty$$

for various values of $c, N$, putting $t = 5$. (Similar results are obtained using the $L^2$ norm.) The results are presented in Table 1. Our conclusion from the data is

| $c$ | $N$ | $p$  | $q$  |
|-----|-----|------|------|
| 5   | 30  | 0.056| 0.056|
| 10  | 30  | 0.049| 0.049|
| 5   | 40  | 0.0075| 0.0075|
| 10  | 40  | 0.0063| 0.0063|
| 3   | 50  | 0.0040| 0.050 |
| 5   | 50  | 0.00063| 0.0067|
| 10  | 50  | 0.00051| 0.00051|

Table 1

that the errors depend more upon the number of terms $2N + 1$ in the expansion than upon the value of $c$. However, in the best case, $N = 50$, we see that $c$ needs to be substantially bigger than 5 for accurate results.

We also considered the initial function $f = 1$, for which $T_tf$ is the characteristic function of $(0, a-t)$. We made the same choices $a = 20$, $N = 50$, $c = 10$ and $t = 5$ as above. This case is highly singular, since neither $f$ nor $T_tf$ are close to being in the domain of $A$. Although the computed values of $f_t$ are close to 1 for $x < 15$ and close to 0 for $x > 15$, there is a Gibbs-type phenomenon near $x = 15$, the maximum value of $f_t$ being about 1.21. As expected, the maximum is unchanged for $N = 100$.

The example of this section may be described in terms of a global approximating semigroup, to be contrasted with the local approximating semigroups of Theorem 9.

We introduce the operator

$$(A_c f)(x) = f'(x)$$

acting in $L^2(0, a)$ subject to the boundary conditions $f(a) = e^{-c}f(0)$. If $c \geq 0$ this is the generator of a one-parameter semigroup $T_{c,t}$ acting on $L^2(0, a)$. One sees immediately that $u_s, \lambda_s$ are the eigenvectors and eigenvalues respectively of $A_c$. Section 2 provides estimates of how closely solutions of $f'(t) = Af(t)$ are
approximated by solutions of $f'(t) = A_c f(t)$ which involve only a finite number of eigenvectors of $A_c$. However, the right-hand side of (12) is not simply a spectral expansion of $T_{c,t}$. The similarity between $T_t$ and $T_{c,t}$ explains why we should expect steadily better approximations as $c$ increases, provided the computations remain feasible.

5 A Convection-Diffusion Operator

The difference between the $L^1$ and $L^2$ behaviour of semigroups is well illustrated by the pure convection operator

$$(Af)(x) = -2xf'(x)$$

which generates the semigroup

$$(T_t f)(x) = f(e^{-2t}x).$$

This is a positivity preserving contraction semigroup on $C_0(\mathbb{R})$, but on $L^2(\mathbb{R})$ we have $\|T_t\| = e^t$ for all $t \geq 0$. The semigroup has the same behaviour when acting on $L^2(-a,a)$, and if $b > 0$ is large enough one would expect similar behaviour for the convection-diffusion operator

$$(Af)(x) = b^{-1}f''(x) - 2xf'(x)$$

acting in $L^2(-a,a)$ subject to Dirichlet boundary conditions at $\pm a$.

We consider the somewhat simpler operator

$$(Af)(x) = b^{-1}f''(x) + f'(x)$$

acting in $L^2(0,a)$ in more detail. The first term produces a diffusion effect while the second cause a drift to the left at speed 1. If we impose Dirichlet boundary conditions then $T_t = e^{At}$ is a positivity preserving contraction semigroup on $L^p(0,a)$ for all $1 \leq p < \infty$. If $b$ is large then the norm of $T_t$ remains close to 1 for $t$ up to about $a$ and then decreases rapidly towards 0. We put $M = 1$ and $\gamma = 0$ in our theorems.

The following results are well-known. The eigenvectors and eigenvalues of $A$ are given by $e_n(x) = k_n e^{-bx/2} \sin(\pi nx/a)$ and $\lambda_n = -b/4 - \pi^2 n^2/ba^2$ respectively for $n = 1, 2, \ldots$. We have $\|e_n\| = 1$ for all $n$ if

$$k_n^{-2} = \frac{1}{4} \int_0^a e^{-bx} \left| e^{\pi i nx/a} - e^{-\pi i nx/a} \right|^2 \, dx$$

$$= \frac{2\pi^2 n^2 (1 - e^{-ba})}{b(b^2a^2 + 4\pi^2 n^2)}.$$

We see that

$$k_n^2 \sim \frac{b^3 a^2}{2\pi^2 n^2}$$

(14)
as \( b \to \infty \) for fixed \( n, a \). The spectrum of \( A \) is asymptotically empty as \( b \to \infty \) for fixed \( a \). It converges to \((-\infty, -b/4]\) as \( a \to \infty \), but this is not the spectrum of \( A \) considered either in \( L^2(0, \infty) \) or in \( L^2(\mathbb{R}) \). The normalized eigenvectors of \( A^* \) are \( e^*_n = k_ne^{b(x-a)/2} \sin(\pi nx/a) \).

**Lemma 6** The two sets of eigenvectors \( \{e_n\} \) and \( \{e^*_m\} \) satisfy \( \langle e_n, e^*_m \rangle = 0 \) if \( m \neq n \). The corresponding spectral projections \( P_n \) of \( A \) satisfy

\[
\|P_n\| \sim \frac{2\pi^2 n^2}{b^3 a^3} e^{ba/2}
\]
as \( b \to \infty \) for each \( n, a \).

**Proof** The first statement can be verified directly, but it is a consequence of the fact that the two sets are eigenvectors of \( A \) and \( A^* \) respectively. A direct calculation shows that

\[
\langle e_n, e^*_n \rangle = \frac{k_n^2 a}{2e^{ba/2}}.
\]

The second statement now follows by substituting (14) and (15) into

\[
\|P_n\| = |\langle e_n, e^*_n \rangle|^{-1}.
\]

All of the above facts suggest that one should not use spectral expansions for large \( b \).

In order to test this we computed \( P_N f \) as defined by Theorem 1 with \( \mathcal{L} = \text{lin}\{e_1, \ldots, e_N\} \) and \( Q_N f \) as defined by (6). We chose \( a = 20 \) and discretized using 10 points per unit interval, so that \([0, a]\) was replaced by a set of 201 points, including the endpoints. We took the function \( f \) to be

\[
f(x) = e^{-(x-a/2)^2}.
\]

Table 2 shows the sizes of \( p = \|f - P_N f\| \) and \( q = \|f - Q_N f\| \) for a range of choices of \( N \) when \( b = 2.5 \) and when \( b = 5.0 \). We see that both methods have comparable accuracy for \( N = 100 \). However, the method using \( P_N \) attains this accuracy far more rapidly as \( N \) increases than the pure spectral method using \( Q_N \). As \( b \) increases the convergence of both methods deteriorates, and for \( b = 7.5 \) neither method gives useful results for any value of \( N \) up to 100.

Our goal in the remainder of this section is to demonstrate that pseudospectral expansions are useful for much larger values of \( b \). For any choice of \( b \) the pseudospectra behave in an interesting way as \( a \) increases. For every \( z \) inside the parabola \( \sigma \in \mathbb{R} \to -b^{-1}\sigma^2 + i\sigma \) one has

\[
\lim_{a \to \infty} \|(zI - A)^{-1}\| = +\infty
\]

and one can construct approximate eigenfunctions for all such \( z \) by the following method. Given \( \delta \) satisfying \( 0 < \delta < 1/2 \) and \( \sigma \in \mathbb{R} \), we put

\[
u_\sigma(x) = k \left( e^{(-b/2 + b\delta + i\sigma)x} - e^{(-b/2 - b\delta - i\sigma)x} \right)
\]

(16)
Clearly \( k \), where \( 0 < c < ab/2 \), is given by

\[
k^{-2} = \int_0^\alpha \left| e^{(-b/2 + b\delta + i\sigma)x} - e^{(-b/2 - b\delta - i\sigma)x} \right|^2 \, dx.
\]

Clearly \( \| u_\sigma \| = 1 \). We make \( \delta \) depend upon \( a \) according to the formula

\[
\delta = 1/2 - c/(ab)
\]

where \( 0 < c < ab/2 \). (As before one might choose \( c \) in the range \( 5 \leq c \leq 10 \).) This choice of \( \delta \) ensures that \( k^{-2} \sim a(1 - e^{-2c})/2c \), \( |u_\sigma(a)| \sim ke^{-c} \), \( u_\sigma(0) = 0 \) and \( u'_\sigma(0) \sim k(b + 2i\sigma) \) as \( a \to \infty \). We also put

\[
w_\sigma(x) = u_\sigma(x)v(x)
\]

where \( v(x) = 1 - e^{(x-a)/\alpha} \), and \( \alpha \) is a constant such as \( \alpha = 1 \). Finally we put

\[
\mu_\sigma = b^{-1}(-b/2 + b\delta + i\sigma)^2 + (-b/2 + b\delta + i\sigma)
\]

\[
= \left( b\delta^2 - b/4 \right) - b^{-1}\sigma^2 + 2i\delta\sigma
\]

\[
= -b^{-1}\sigma^2 + i\sigma - c/a + c^2/(a^2b) - 2i\sigma c/(ab)
\]

\[
\to -b^{-1}\sigma^2 + i\sigma
\]

as \( a \to \infty \).

There is no reason to expect that taking a large value of \( b \) should cause problems. Indeed, as \( b \to \infty \), the functions \( u_\sigma \) defined by \( \mu_\sigma \) converge to the corresponding functions \( u_s \) defined for the pure convection operator of Section 4. In both cases the size of the constant \( c \) controls the degree of accuracy of the fundamental estimate \( \sigma \). As we have seen before, this has to be weighed against the increased difficulty of performing the computations for large \( c \).

\[
\begin{array}{cccccc}
N & p & q & N & p & q \\
10 & 3.9 \times 10^{-1} & 1.8 \times 10^{3} & 10 & 7.3 \times 10^{-1} & 3.3 \times 10^{9} \\
20 & 4.6 \times 10^{-2} & 1.3 \times 10^{3} & 20 & 1.1 \times 10^{-1} & 1.4 \times 10^{7} \\
30 & 1.7 \times 10^{-3} & 5.7 \times 10^{1} & 30 & 4.8 \times 10^{-3} & 3.3 \times 10^{7} \\
40 & 1.8 \times 10^{-5} & 1.4 \times 10^{-1} & 40 & 1.4 \times 10^{-4} & 2.8 \times 10^{5} \\
50 & 5.3 \times 10^{-8} & 2.0 \times 10^{-3} & 50 & 1.9 \times 10^{-4} & 8.3 \times 10^{2} \\
60 & 4.1 \times 10^{-11} & 2.9 \times 10^{-6} & 60 & 3.4 \times 10^{-5} & 1.7 \times 10^{0} \\
70 & 1.7 \times 10^{-11} & 4.4 \times 10^{-10} & 70 & 4.8 \times 10^{-4} & 6.0 \times 10^{-5} \\
80 & 9.0 \times 10^{-12} & 1.4 \times 10^{-10} & 80 & 2.4 \times 10^{-5} & 5.9 \times 10^{-5} \\
90 & 1.2 \times 10^{-11} & 2.0 \times 10^{-10} & 90 & 1.4 \times 10^{-5} & 9.5 \times 10^{-5} \\
100 & 9.3 \times 10^{-12} & 3.4 \times 10^{-10} & 100 & 1.0 \times 10^{-4} & 2.1 \times 10^{-4} \\
\end{array}
\]

Table 2

\[\sigma(0) = 0\]
Theorem 7 Under the above conditions there exists a constant $K_{\alpha,b,\sigma}$ such that

$$\|u_\sigma - w_\sigma\| + \|Aw_\sigma - \mu_\sigma w_\sigma\| \leq K_{\alpha,b,\sigma} a^{-1/2} \left\{ \frac{2c}{e^{2c} - 1} \right\}^{1/2}$$

for large enough $a > 0$.

Proof We have

$$\|u_\sigma - w_\sigma\|^2 = k^2 \int_0^a \left| e^{(-b/2+b\delta+i\sigma)x} - e^{(-b/2-b\delta-i\sigma)x} \right|^2 e^{2(x-a)/\alpha} \, dx$$

$$\leq 4k^2 \int_0^a e^{(-b+2b\delta)x+2(x-a)/\alpha} \, dx$$

$$= \frac{2k^2}{\alpha - c/a} \left( e^{-2c} - e^{-2a/\alpha} \right)$$

$$\leq 3k^2 \alpha e^{-2c}$$

for large enough $a > 0$.

Since $b^{-1}u''_\sigma + u'_\sigma = \mu_\sigma u_\sigma$ and $w_\sigma \in \text{Dom}(A)$, we have

$$Aw_\sigma - \mu_\sigma w_\sigma = 2b^{-1}u'_\sigma v' + b^{-1}u_\sigma v'' + u_\sigma v'.$$

Therefore

$$\|Aw_\sigma - \mu_\sigma w_\sigma\| \leq 2b^{-1}\|u'_\sigma v'\| + b^{-1}\|u_\sigma v''\| + \|u_\sigma v'\|.$$

Each of the terms on the right-hand side is estimated in the same way as above. For example

$$\|u_\sigma v'\|^2 = k^2 \alpha^{-2} \int_0^a \left| e^{(-b/2+b\delta+i\sigma)x} - e^{(-b/2-b\delta-i\sigma)x} \right|^2 e^{2(x-a)/\alpha} \, dx$$

$$\leq \frac{2k^2}{\alpha^2(1 - c/a)} \left( e^{-2c} - e^{-2a/\alpha} \right)$$

$$\leq 3k^2 \alpha^{-1} e^{-2c}$$

for large enough $a > 0$. Combining all these estimates yields the statement of the theorem.

For general values of $\sigma \in \mathbb{R}$ the functions $u_\sigma$ do not satisfy any set of linear boundary conditions. However, if we put $\sigma = 2\pi s/a$ where $s \in \mathbb{Z}$ then there exist non-zero constants $c_i$ such that $u_\sigma(0) = 0$, $u'_\sigma(0) = c_1 + c_2 \sigma$, $u_\sigma(a) = c_3$ and $u'_\sigma(a) = c_4 + c_5 \sigma$. Therefore the functions $u_\sigma$ all satisfy boundary conditions of the form $u(0) = 0$ and

$$c_5 u'(0) - c_2 u'(a) = c_6 u(a).$$

We tested the above ideas numerically. We re-parametrized by means of the substitution $\sigma = 2\pi s/a$ where $s \in \mathbb{Z}$ and $-N \leq s \leq N$. We put $a = 20$, each unit
interval in $[0, a]$ being represented by 10 equally spaced points. We put $\alpha = 1$, $b = 20$ and $c = 5$. We took the same function $f$ as before, that is

$$f(x) = e^{-(x-a/2)^2}.$$ 

Table 3 shows the values of $p = \|f - P_N f\|$ for various values of $N$. The dimension of the subspace $\mathcal{L}$ is $2N + 1$.

| $2N + 1$ | $p$         |
|----------|-------------|
| 11       | $3.3 \times 10^{-1}$ |
| 21       | $3.4 \times 10^{-2}$ |
| 31       | $1.1 \times 10^{-3}$ |
| 41       | $1.1 \times 10^{-5}$ |
| 51       | $3.4 \times 10^{-8}$ |
| 61       | $2.9 \times 10^{-11}$ |
| 71       | $1.3 \times 10^{-14}$ |

The superiority of this method of expansion over both of the previous ones is immediately clear. Further computations show that the pseudo-spectral method works just as well for all values of $b$ from 5 to 100 (and probably beyond that).

We finally computed the approximation $f_t = G \phi_t$ to $T_t f$ given by the formula (8) of Theorem 5. We chose the parameters and initial value of $f$ as above but put $N = 15$; the choice $N = 30$ gave the same results up to the accuracy displayed. We discovered, as expected, that $f_t$ is approximately non-negative; in fact

$$-3 \times 10^{-4} \leq \min \{f_t(x) : 0 \leq x \leq a\} \leq 0$$

for all $0 \leq t \leq 16$, at which point we stopped the computation. The shape of $f_t$ remained approximately gaussian as $t$ increased, with the centre moving to the left and the width slowly increasing. The maximum of $f_t$ decreases slowly up to $t \sim 10$, when the centre of the peak approaches the origin, after which it decreases rapidly. The graphs of $f$, $f_4$, $f_8$, $f_{12}$ are plotted in Figure 1.
Figure 1. Graphs of $f$, $f_8$ (dotted) and $f_4$, $f_{12}$ (solid)
The detailed behaviour of the maximum $m$ is presented in Table 4 for $c = 10$. The values are the same for $c = 5$ up to $t = 14$ after which they decrease more slowly. We compare $m$ with $m_\infty = (1 + 4t/b)^{-1/2}$. This is the ‘same’ constant calculated using Fourier transforms when $a = \infty$, i.e. for the semigroup on $L^2(\mathbb{R})$ when the initial function is $f(x) = e^{-x^2}$. The two agree up to $t = 10$, which is all that one could expect. All of the results confirm that the pseudospectral approximation to the semigroup is highly reliable for the stated values of $a$ and $b$, at least for this choice of the initial function $f$.

| $t$ | $m$     | $m_\infty$ |
|-----|---------|------------|
| 0   | 1.0000  | 1.0000     |
| 2   | 0.8451  | 0.8452     |
| 4   | 0.7454  | 0.7454     |
| 6   | 0.6742  | 0.6742     |
| 8   | 0.6202  | 0.6202     |
| 10  | 0.5593  | 0.5774     |
| 12  | 0.1268  | 0.5423     |
| 14  | 0.0049  | 0.5130     |
| 16  | 0.0000  | 0.4880     |

Table 4

We repeated the calculations leading to Figure 1, but with the initial function $g(x) = 1$ for all $x \in [0, a]$. This is a much more serious test of the method since $g$ does not satisfy the boundary conditions even approximately. With $N = 15$ and $c = 5$ we obtained the results shown in Figure 2. One sees that $g_t$ is close to the characteristic function of $[0, a - t]$, but smoothed out because of the diffusion term in $A$. By contrast with the similar calculation in Section 4, there is no Gibbs phenomenon, presumably again because of the diffusion term. For smaller values of $b$, such as $b = 5$, the fact that $g_t(0) = 0$ for all $t > 0$ is much more obvious.
Figure 2. Graphs of $g$, $g_8$ (dotted) and $g_4$, $g_{12}$ (solid)
Table 5 lists the first few eigenvalues $\lambda_n$ and approximate eigenvalues $\mu_s$ of $A$ in decreasing order of their real parts, where $a = 20$, $b = 20$ and $c = 5$. The largest eigenvalue $-5.001$ controls the asymptotic decay of the semigroup as $t \to \infty$, but it has little influence on the size of $\|T_t f\|$ for $t = 10$. One of the main reasons for the accuracy of the pseudospectral expansion is the fact that there are so many approximate eigenvalues whose real parts are close to zero. For $c = 10$ the real parts of these $\mu_s$ decrease from $-0.488$ to $-0.729$.

| $\lambda_n$ | $\mu_s$          |
|-------------|------------------|
| $-5.001$    | $-0.247$         |
| $-5.005$    | $-0.252 \pm 0.306i$ |
| $-5.011$    | $-0.252 \pm 0.306i$ |
| $-5.020$    | $-0.267 \pm 0.613i$ |
| $-5.031$    | $-0.291 \pm 0.919i$ |
| $-5.044$    | $-0.326 \pm 1.225i$ |
| $-5.060$    | $-0.370 \pm 1.532i$ |
| $-5.079$    | $-0.425 \pm 1.838i$ |

Table 5

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