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Spectral Approximation of Time Windows in Waveform Relaxation

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Abstract. We establish a relationship between the spectral parameter arising in Laplace transform of the solution of a linear differential system and the time window in which this system is solved.

Keywords: Linear differential systems, time window, spectral approximation, waveform relaxation iterations
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INTRODUCTION

Consider the differential system

$$\begin{cases} x'(t) + Ax(t) = g(t), & t \in [0,T], \\ x(0) = 0, \end{cases} \tag{1}$$

and its equivalent in the spectral domain

$$(sI + A)X(s) = G(s), \quad s \geq 0, \tag{2}$$

where the terms $X(s)$ and $G(s)$ denote the Laplace transforms $\mathscr{L}\{x(t)\}$ and $\mathscr{L}\{g(t)\}$ of x and g, respectively. Steady state solutions are obtained by letting $T \to \infty$ in (1) or $s = 0$ in (2). On the other hand, only high frequency components of $X(s)$ affect the solution on short time windows, i.e., large values of s "correspond" to values of T close to 0. The question then arises whether a relationship between s and T can be derived for finite but nonzero time windows.

For given T we fix $s = s^*$ in the matrix $sI + A$. From (2) we then obtain

$$(s^*I + A)X(s) \approx G(s), \quad s \geq 0, \tag{3}$$

i.e.,

$$(s^*I + A)x(t) \approx g(t), \quad t \in [0,T],$$

back in the temporal domain. The idea behind (3) is to substitute a "representative" frequency s^* for all frequencies s associated with the differentiation process in the temporal domain. Define $y = y(t)$ by

$$(s^*I + A)y(t) = g(t), \quad t \in [0,T]. \tag{4}$$

When s^* is chosen appropriately we may expect $y(t) \approx x(t)$ for a range of t values. Thus, we define s^* by requiring that $\|x - y\|$ be minimal. Here, $\|\cdot\|$ is some norm or seminorm.

A CONSTANT RIGHT-HAND SIDE

Assume that $g(t) = g$ is constant and that $\|x\| = \|x(T)\|_2$. The solution $x(t)$ to (1) then becomes

$$x(t) = A^{-1}(I - e^{-tA})g, \quad t \in [0,T].$$

Let $A = U\Sigma V^T$ denote the singular value decomposition of the matrix A with Σ defined by

$$\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n), \quad 0 < \sigma_n \leq \cdots \leq \sigma_1.$$

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Then

$$\begin{aligned} \|x-y\|^2 &= \|A^{-1}(I-e^{-TA})g-(s^*I+A)^{-1}g\|_2^2 \\ &= \|\Sigma^{-1}(I-e^{-T\Sigma})g-(s^*I+\Sigma)^{-1}g\|_2^2 \\ &= \sum_{i=1}^{n}|f(\sigma_i,T,s^*|^2|b_i|^2, \end{aligned}$$

with

$$f(\sigma,t,s)=\frac{1-e^{-t\sigma}}{\sigma}-\frac{1}{s+\sigma} \quad \text{and} \quad b=Ug.$$

We have the following result.

Theorem 1 *Given $T>0$, there exists a value $\sigma^*>0$ such that $\sigma_n \le \sigma^* \le \sigma_1$ and $\|x(T)-y(T)\|^2$ is minimal for*

$$s^*=\frac{\sigma^*}{e^{T\sigma^*}-1}. \tag{5}$$

Proof: Let $T>0$. Then the function $F(s)$ given by

$$F(s)=\sum_{i=1}^{n}|f(\sigma_i,T,s)|^2|b_i|^2$$

is defined and continuously differentiable for all $s>0$. Since

$$f(\sigma,T,0)=-\frac{e^{-T\sigma}}{\sigma}<0 \quad \text{and} \quad f(\sigma,T,\infty)=\frac{1-e^{-T\sigma}}{\sigma}\ge 0,$$

the function

$$F'(s)=2\sum_{i=1}^{n}\frac{f(\sigma_i,T,s^*)}{(s+\sigma_i)^2}|b_i|^2=2\sum_{i=1}^{n}\left(\frac{1-e^{-T\sigma_i}}{\sigma_i}-\frac{1}{s+\sigma_i}\right)\frac{|b_i|^2}{(s+\sigma_i)^2}$$

admits at least one zero $s=s^*>0$. The relation $F'(s^*)=0$ can be written in the form

$$\sum_{i=1}^{n}\left(\frac{s^*}{\sigma_i(s^*+\sigma_i)}-\frac{e^{-T\sigma_i}}{\sigma_i}\right)\frac{|b_i|^2}{(s^*+\sigma_i)^2}=\sum_{i=1}^{n}\alpha_i\left(s^*-\frac{\sigma_i}{e^{T\sigma_i}-1}\right)=0$$

with

$$\alpha_i=\frac{1-e^{-T\sigma_i}}{\sigma_i(s^*+\sigma_i)^2}|b_i|^2.$$

Observe that if $b_i\neq 0$ then $\alpha_i>0$ so that $b\neq 0$ imples that $\sum_{j=1}^{n}\alpha_j\neq 0$. Since the function $h(\sigma)$ defined by

$$h(\sigma)=\frac{\sigma}{e^{T\sigma}-1}$$

is decreasing, the critical point s^* of $F(s)$ satisfies the inequalities

$$\frac{\sigma_1}{e^{T\sigma_1}-1}\le s^*=\sum_{i=1}^{n}\left(\frac{\alpha_i}{\sum_{j=1}^{n}\alpha_j}\right)\frac{\sigma_i}{e^{T\sigma_i}-1}\le\frac{\sigma_n}{e^{T\sigma_n}-1}, \tag{6}$$

and therefore (5) holds. The fact that the function $F(s)$ reaches its minimum at s^* follows from $F'(0)<0$ and $F'(\infty)=0^+$.

For small time windows T, expanding $e^{T\sigma^*}$ into Taylor series around $T=0$, the value s^* given by (5) becomes

$$s^*\approx\frac{1}{T}. \tag{7}$$

The formula (7) was first proposed by Leimkuhler [6] for estimating window of convergence of waveform relaxation iterations applied to (1). He based his analysis on the size of spectral radius of the matrix $sI+A$ for $\mathrm{Re}(s)>s^*$. He noted that (7) is a simplification, a fact later confirmed, especially for larger time windows, by extensive numerical experiments conducted by Burrage et al. [2], [3]. Jackiewicz et al. [5] proposed instead an estimate of the form

$$s^* = \frac{C}{T}$$

for some constant C. They related the size of C to the ε-contour of the pseudospectrum [7] of the matrix A, namely $C = -\ln(\varepsilon)$, but determined the appropriate values of ε only numerically by comparing the pseudospectra of a discrete version of the integral operator

$$x(t) = \int_0^t e^{-(t-s)A} g(s) ds$$

corresponding to (1), and of the Laplace transform $(sI + A)^{-1}$ of its kernel e^{-tA}.

The relationship between the size of the time window and spectral parameter s^* lays at the center of a recent strategy developed by Burrage et al. [1] for accelerating the convergence of waveform relaxation iterations. Therefere, it is important to make this relation more precise, and in particular to find out whether such relation between these parameters can be established for larger time windows. For large time windows T, for example if $T\sigma_n \gg 1$, such a relationship can be obtained from (5). In this case, the coeffcients α_i appearing in (6) reduce to

$$\alpha_i \approx \frac{|b_i|^2}{\sigma_i(s^* + \sigma_i)} \ll \alpha_n.$$

Consequently, $\sigma^* \approx \sigma_n$ and the relation (5) becomes

$$s^* \approx \sigma_n e^{-T\sigma_n}. \tag{8}$$

We consider next the seminorm $\|\cdot\|$ defined by

$$\|x\| = \|(s^* I + A)x(T)\|_2.$$

Then

$$\begin{aligned} \|x-y\|^2 &= \|(s^* I + A)x(T) - (s^* I + A)y(T)\|_2^2 \\ &= \|(s^* I + A)A^{-1}(I - e^{-TA})g - g\|_2^2 \\ &= \|s^* A^{-1}(I - e^{-TA})g - e^{-TA}g\|_2^2 \\ &= \sum_{i=1}^{n} \left(s^* \frac{1 - e^{-T\sigma_i}}{\sigma_i} - e^{-T\sigma_i} \right) |b_i|^2. \end{aligned}$$

Thus $\|x-y\|$ is a convex quadratic function with respect to s^* which attains its minimum when

$$s^* = \sum_{i=1}^{n} \left(\frac{\beta_i}{\sum_{j=1}^{n} \beta_j} \right) \frac{\sigma_i}{e^{T\sigma_i} - 1}, \quad \text{where} \quad \beta_i = \left(\frac{1 - e^{-T\sigma_i}}{\sigma_i} \right)^2 |b_i|^2 \geq 0.$$

As a result, Theorem 1 also holds for this choice of the seminorm. Moreover, since

$$\|x-y\| = \|(s^* I + A)x(T) - g\|_2 = \|s^* x(T) - x'(T)\|_2,$$

this choice of the seminorm provides a best fit of the derivative $x'(t)$ by a multiple of the solution $x(t)$ to the differential system (1).

THE CASE OF AN INTEGRAL SEMINORM

In this section we consider the integral seminorm $\|\cdot\|$ defined by

$$\|x\| = \left\| \int_0^T x(t) dt \right\|_2. \tag{9}$$

This choice yields

$$
\begin{aligned}
\|x-y\|^2 &= \left\| \int_0^T x(t)dt - \int_0^T y(t)dt \right\|_2^2 \\
&= \left\| \int_0^T A^{-1}(I-e^{-TA})gdt - T(s^*I+A)^{-1}g \right\|_2^2 \\
&= \left\| A^{-1}\big(TI - A^{-1}(I-e^{-TA})\big)g - T(s^*I+A)^{-1}g \right\|_2^2 \\
&= \left\| \Sigma^{-1}\big(TI - \Sigma^{-1}(I-e^{-T\Sigma})\big)b - T(s^*I+\Sigma)^{-1}b \right\|_2^2 \\
&= \sum_{i=1}^{n} \left| \frac{T}{\sigma_i} - \frac{1-e^{-T\sigma_i}}{\sigma_i^2} - \frac{T}{s^*+\sigma_i} \right|^2 |b_i|^2.
\end{aligned}
$$

Similarly as in the Theorem 1 the optimal valuee of s^* is given in the following result.

Theorem 2 *Given $T > 0$, there exists a value σ^* such that $\sigma_n \le \sigma^* \le \sigma_1$, and $\|x-y\| = \|\int_0^T (x(t)-y(t))dt\|_2$ given by (9) is minimal for*

$$
s^* = \frac{1-e^{-T\sigma^*}}{T - \frac{1-e^{-T\sigma^*}}{\sigma^*}}. \tag{10}
$$

Proof: Procceding similarly as in the proof of Theorem 1 one arrives at the expression

$$
s^* = \sum_{i=1}^{n} \left(\frac{\gamma_i}{\sum_{j=1}^{n} \gamma_j} \right) \frac{1-e^{-T\sigma_i}}{T - \frac{1-e^{-T\sigma_i}}{\sigma_i}} \quad \text{with} \quad \gamma_i = \frac{T - \frac{1-e^{-T\sigma_i}}{\sigma_i}}{\sigma_i(s^*+\sigma_i)^3} |b_i|^2 \ge 0.
$$

Now, (10) follows from the monotonicity of the function $h(\sigma)$ defined by

$$
h(\sigma) = \frac{1-e^{-T\sigma}}{T - \frac{1-e^{-T\sigma}}{\sigma}}.
$$

For small time windows a Taylor series expansion of $e^{-T\sigma^*}$ in (10) around $T = 0$ yields

$$
s^* \approx \frac{2}{T}.
$$

On the other hand, for long time windows one easily obtains

$$
s^* \approx \frac{1}{T}
$$

which is markedly different from the behaviour of s^* given by (8).

The estimation of the spectral parameter s^* for the monomial, exponential, and the general right hand side $g(t)$ in (1) is considered in [4].

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