Approximation of the diffusive representation by decreasing exponential functions

Emilie Blanc*

Abstract

Diffusive representation of pseudo-differential operators is a theory that has attracted interest during the last years, and the discretization of the diffusive representation allows significant simplifications for numerical integration encountered in many physical models. The feasibility of such integration relies on efficient determination of the coefficients involved in the representation. In this report a novel way to determine such coefficients is proposed based on non-linear optimization. Compared to the typical method using Gaussian quadrature, our new approach is shown to lead to more accurate approximation in a particular case with application to computational biology.

Key-words: diffusive representation, exponential sum, nonlinear optimization

1 Introduction

The diffusive representation $\mu(s)$ of a pseudo-differential operator $H(p)$ has been introduced by Desch and Miller in 1988 [5] and by Staffans in 1994 [15] under the name *completely monotone kernel*. The diffusive representation was also developed independently by Audounet, Matignon and Montseny [13, 12]. It is intrinsically related to the existence of a continuous spectrum of $H(p)$ on the negative real axis. The diffusive representation corresponds to a decomposition of a function into a continuum of decreasing Mittag-Leffler exponentials, with weights obtained by the inverse Laplace transform of the impulse response $h(t)$ related to the operator $H(p)$. It offers a unified and useful mathematical framework in which efficient numerical integration can be implemented. The diffusive approximation of fractional operators has been applied to various physical models, for instance in musical acoustics [8, 7], in viscoelasticity [1], in poroelasticity [10, 2, 3] ; whereas the diffusive approximation of the function $\frac{1}{t^{\alpha+1}}$ has been used in cellular biology [11, 4]. We focus on the latter case in this report. To our best knowledge, only one approach to this problem have been proposed so far in the literature, based on a Gaussian quadrature [11]. In the example proposed in [11], 16 quadrature nodes are used, making large-scale simulations out of reach. The aim of the present study is therefore to develop a new diffusive approximation method in which this drawback does not arise.

*Division of Scientific Computing, Department of Information Technology, Uppsala University, P.O. Box 337, SE-75105 Uppsala, Sweden. Electronic mail: emilie.blanc@it.uu.se

2 The diffusive representation

We denote by $\mathcal{L}$ the Laplace transform of a function f defined by

$$(\mathcal{L}\, f)(s) = \int_0^\infty f(t)\, e^{-s\, t}\, dt. \tag{2.1}$$

We consider a causal function $\mu : \mathbb{R} \to \mathbb{C}$, and the impulse reponse h, defined as the Laplace transform of μ, $h = \mathcal{L}\, \mu$

$$h(t) = \int_0^\infty \mu(s)\, e^{-s\, t}\, ds. \tag{2.2}$$

The function μ defined by (2.2) is called the diffusive representation of the operator $u \to h \star u$, with symbol $H = \mathcal{L}\, h$ [13, 12]. The diffusive representation is then a Laplace transform, but in which t plays the role of the Laplace variable:

$$\begin{array}{ccccc} \text{diffusive representation} & \xrightarrow{\mathcal{L}} & \text{convolutive response} & \xrightarrow{\mathcal{L}} & \text{symbol} \\ \mu(s) & & h(t) & & H(p) \end{array} \tag{2.3}$$

For the particular impulse response $h(t) = \frac{1}{t^{\alpha+1}}$, the diffusive representation is given by $\mu(s) = \frac{s^\alpha}{\Gamma(1+\alpha)}$, i.e.

$$\frac{1}{t^{\alpha+1}} = \frac{1}{\Gamma(1+\alpha)} \int_0^\infty s^\alpha\, e^{-s\, t}\, ds. \tag{2.4}$$

3 Diffusive approximation

The aim of this section is to approximate the function $\frac{1}{t^{\alpha+1}}$ by a finite number of decreasing exponential, using a numerically tractable approach. For this purpose, we use a diffusive representation, initially proposed in [11]. Using a quadrature formula on N points, with weights a_ℓ and abcissa $s_\ell > 0$, (2.4) can be approximated by

$$\frac{1}{t^{1+\alpha}} = \frac{1}{\Gamma(1+\alpha)} \int_0^\infty s^\alpha\, e^{-s\, t}\, ds \simeq \sum_{\ell=1}^N a_\ell\, e^{-s_\ell\, t}. \tag{3.1}$$

Two approaches can be employed for this purpose. While the most commonly used one is based on orthogonal polynomials, the second approach is associated with an optimization procedure.

3.1 Gauss-Legendre quadrature

The Gauss-Legendre quadrature is written

$$\int_0^{s_{max}} f(x)\, dx \simeq \sum_{\ell=1}^N w_\ell\, f(x_\ell). \tag{3.2}$$

To approximate the integral (3.1) it is first restricted to a finite interval, then Gauss-Legendre quadrature is used:

$$\begin{aligned} \frac{1}{\Gamma(1+\alpha)} \int_0^{\infty} x^{\alpha}\, e^{-x\,t}\, dx &\simeq \frac{1}{\Gamma(1+\alpha)} \int_0^{s_{max}} x^{\alpha}\, e^{-x\,t}\, dx, \\ &\simeq \frac{1}{\Gamma(1+\alpha)} \sum_{\ell=1}^{N} w_\ell\, x_\ell^{\alpha}\, e^{-x_\ell\, t}. \end{aligned} \tag{3.3}$$

The abscissae x_ℓ, which are the zeros of the Gauss-Legendre polynomials, and the weights w_ℓ can be computed by standard routines [6]. The coefficients s_ℓ and a_ℓ involved in (3.1) are therefore related to the coefficients x_ℓ and w_ℓ by

$$s_\ell = x_\ell, \qquad a_\ell = \frac{x_\ell^{\alpha}\, w_\ell}{\Gamma(1+\alpha)}. \tag{3.4}$$

3.2 Nonlinear constrained optimization

Our objective in this approach is to approximate the function $F_{ex}(t) = \frac{1}{t^{1+\alpha}}$ by $F_{approx}(t) = \sum_{\ell=1}^{N} a_\ell\, e^{-s_\ell\, t}$ in a time range of interest $[t_{min}, t_{max}]$. This leads to the minimization of the quantity χ^2 with respect to the abcissae s_ℓ and to the weights a_ℓ

$$\chi^2 = \sum_{k=1}^{K} \left| \frac{F_{approx}(t_k)}{F_{ex}(t_k)} - 1 \right|^2 = \sum_{k=1}^{K} \left| t_k^{-(1+\alpha)} \sum_{\ell=1}^{N} a_\ell\, e^{-s_\ell\, t_k} - 1 \right|^2, \tag{3.5}$$

where the times t_k are distributed linearly in $[t_{min}, t_{max}]$ on a logarithmic scale of K points

$$t_k = t_{min} \left(\frac{t_{max}}{t_{min}} \right)^{\frac{k-1}{K-1}}, \quad k = 1, \cdots, K. \tag{3.6}$$

The coefficients s_ℓ and a_ℓ are constrained to be positive. A nonlinear constrained optimization is developed, where both the abcissae and the weights are optimized. The constrained minimization problem is nonlinear and non-quadratic with respect to abscissae s_ℓ. To solve it, we implement the program SolvOpt [9, 14]. Since this Shor's algorithm is iterative, it requires an initial estimate s_ℓ^0, a_ℓ^0 of the coefficients which satisfies the positivity constraints. For this purpose, s_ℓ^0 and a_ℓ^0 are initialized with the method based on the Gauss-Legendre quadrature formula (3.4).

In what follows, we always use the parameter $K = 10\, N$.

3.3 Discussion

To compare the quadrature methods presented in sections 3.1 and 3.2, we define the error of model ε_{mod} as

$$\varepsilon_{mod} = \left\| \frac{F_{approx}(t)}{F_{ex}(t)} - 1 \right\|_{L_2} = \left(\frac{1}{t_{max} - t_{min}} \int_{t_{min}}^{t_{max}} \left| \frac{F_{approx}(t)}{F_{ex}(t)} - 1 \right|^2 dt \right)^{1/2}. \tag{3.7}$$

The variation of ε_{mod} in terms of the number of N of internal states is represented in Figure 3.1-(a) for $\alpha = 0.5$, $t_{min} = 10^{-4}$ and $t_{max} = 0.05$, and in Figure 3.1-(b) for $\alpha = 0.5$, $t_{min} = 10^{-3}$ and $t_{max} = 1$. In both cases, the Gauss-Legendre quadrature converges very slowly. Moreover,

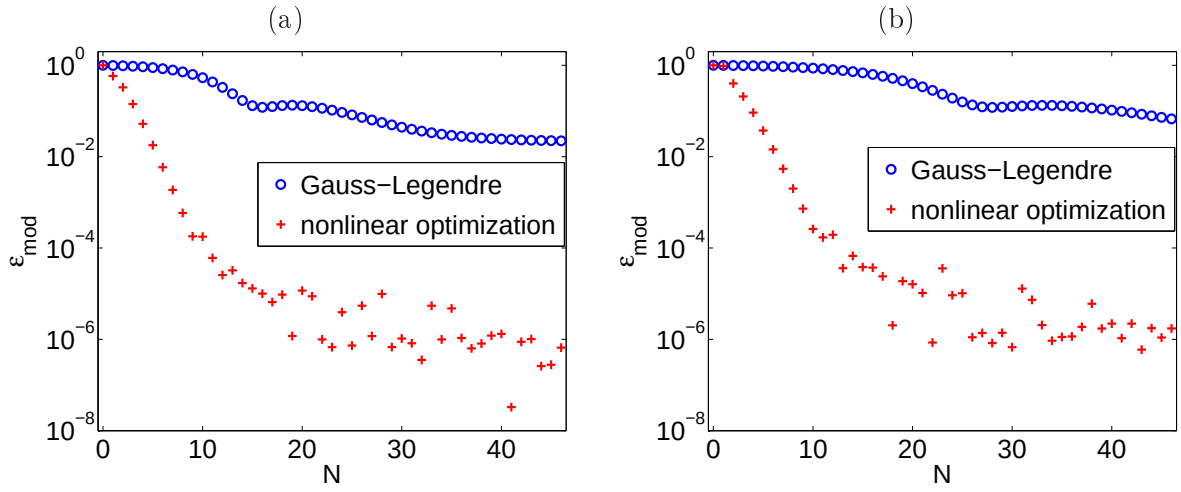

Figure 3.1: relative error ε_{mod} in terms of N for both the Gauss-Legendre quadrature and the nonlinear constrained optimization. (a): $\alpha = 0.5$, $t_{min} = 10^{-4}$ s and $t_{max} = 5\,10^{-2}$ s, (b): $\alpha = 0.5$, $t_{min} = 10^{-3}$ s and $t_{max} = 1.5$ s.

in Figure 3.1-(b), the error is always larger than 0.7. For the nonlinear optimization, the error decreases rapidly with N. In Figure 3.1-(b) for $N = 8$ for instance, the relative error of the nonlinear optimization ($\varepsilon_{mod} \simeq 2.5 \cdot 10^{-3}$) is 448 times smaller than the error of the Gauss-Legendre quadrature ($\varepsilon_{mod} \simeq 1.12$). For large values of N, typically $N > 10$, the system is poorly conditioned and the order of convergence deteriorates. This is not a problem in practice since large values of N are not used. Based on these results, the nonlinear optimization is therefore considered as the better way to determine the coefficients of the approximation.

4 Conclusion

Using the concept of diffusive representation, a pseudo-differential operator is approximated by a finite number of decreasing exponentials. In this note we have demonstrated that quadrature based on orthogonal polynomials is not an efficient way to obtain the parameters of the exponentials. Instead, we have proposed a superior method based on an optimization procedure (Fig. 3.1). The number $N = 4$, used in this note, is to be compared with the number $N = 16$ used in [11] based on Gauss-Legendre quadrature.

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