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BOOSTING THE INVERSE INTERPOLATION PROBLEM BY A SUM OF DECAYING EXPONENTIALS USING AN ALGEBRAIC APPROACH*

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Dedicated to Víctor Pereyra on the occasion of his 70th birthday

Abstract. An algebraic method is proposed to solve the inverse interpolation problem for data fitting by a linear combination of decaying exponentials. The method transforms the interpolation question into a problem of finding the roots of a single polynomial. The method is validated by numerical simulations using noiseless synthetic data with excellent results. The method is applied to medical data coming from magnetic resonance images of tumoral lesions in brain to obtain relaxation rate distribution functions, with results that are trustworthy and fast when compared with inverse Laplace methods.

Key words. de Prony's method, continuation methods, Gröbner bases, exponential equations, polynomial equations, nonlinear algebraic equations.

AMS subject classifications. 15A15, 15A09, 15A23

1. Introduction and preliminaries. The idea of using a linear combination of n exponentials to interpolate a sequence of points sampled at equally spaced intervals of time was introduced in 1795 (though practical use of this method awaited the digital computer) by Baron Gaspard Riche de Prony [13], and is usually known as de Prony's method. It has a variety of applications in physics and engineering. Many papers have been written about its applications; among these, we would like to point to the papers of Ruhe [14], Martin et al. [8], and Osborne and Smyth [12]. An application in the field of tissue segmentation from NMR brain data was considered in [9].

In this paper, we introduce algebraic manipulations that simplify the interpolation or approximation of k points using linear combinations of exponentials. Given $2n$ real numbers C_i and λ_i, $i = 1, \ldots, n$, we consider the function

$$y(t) = C_1 e^{-\lambda_1 t} + \cdots + C_n e^{-\lambda_n t}. \tag{1.1}$$

If we take $2n$ evenly spaced samples of time $j\Delta t$, for $j = 1, \ldots, k$, we get that the points $p_j = y(j\Delta t)$ are given in terms of polynomial expressions

$$\begin{cases} p_1 = C_1 e^{-\lambda_1 \Delta t} & + \cdots + \quad C_n e^{-\lambda_n \Delta t} \\ p_2 = C_1 e^{-2\lambda_1 \Delta t} & + \cdots + \quad C_n e^{-2\lambda_n \Delta t} \\ \qquad \vdots & \qquad \vdots \qquad\qquad \vdots \\ p_k = C_1 e^{-k\lambda_1 \Delta t} & + \cdots + \quad C_n e^{-k\lambda_n \Delta t}, \end{cases} \tag{1.2}$$

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Defining $x_1 = e^{-\lambda_1 \Delta t}, x_2 = e^{-\lambda_2 \Delta t}, \ldots, x_n = e^{-\lambda_n \Delta t}$, for $j = 1, \ldots, n$ in (1.2) yields

$$\begin{cases} p_1 = C_1 x_1 & + \cdots + & C_n x_n \\ p_2 = C_1 x_1^2 & + \cdots + & C_n x_n^2 \\ \quad \vdots & \vdots & \vdots \\ p_k = C_1 x_1^k & + \cdots + & C_n x_n^k, \end{cases} \tag{1.3}$$

and transforms the exponential system (1.2) into the polynomial system (1.3), where our unknowns are the C_i and the x_i for $i = 1, \ldots, n$.

The problem of de Prony is the inverse question: given k evenly spaced measurements $p_1, p_2, \ldots, p_k$, for a given n, we want to find real numbers C_i and λ_i, $i = 1, \ldots, n$, such that

$$p_j = C_1 e^{-j\lambda_1 \Delta t} + C_2 e^{-j\lambda_2 \Delta t} + \cdots + C_n e^{-j\lambda_n \Delta t}$$

for $j = 1, \ldots, k$. This is equivalent to solving (1.2) for the C_i and λ_i, $i = 1, \ldots, n$, in terms of the measurements $p_1, p_2, \ldots, p_k$. Clearly, this problem does not have a unique solution unless there is a constraint relationship between k and n (so that a rank condition might be satisfied).

In the special case that $k = 2n$, an iterative method is presented in [8], which we review in Section 2. Our goal in this paper is to propose an algebraic numerical scheme that reduces the problem to finding roots and solving a linear equation or performing a standard least squares process. This is discussed in Section 3. It should be pointed out that it is also possible to deal with problem (1.3) in terms of Gröbner bases, but this becomes rather computationally expensive for $n > 4$.

2. Homotopy continuation method. Intuitively speaking, two functions are homotopic if one can be deformed continuously into the other. Formally, a homotopy between two continuous function f and g from a topological space X to a topological space Y is defined to be a continuous function $H : X \times [0, 1] \to Y$ such that, for all points x in X, $H(x, 0) = f(x)$ and $H(x, 1) = g(x)$. We will not go into details about homotopic continuation beyond a few lines that provide a quick look within the context of the approximation problem in this paper; for further details, see [8] or [7].

Let us start by rewriting (1.3) as

$$\begin{cases} f_1 = C_1 x_1 & + \cdots + & C_n x_n - p_1 \\ f_2 = C_1 x_1^2 & + \cdots + & C_n x_n^2 - p_2 \\ \quad \vdots & \vdots & \vdots \\ f_k = C_1 x_1^k & + \cdots + & C_n x_n^k - p_k, \end{cases} \tag{2.1}$$

where each f_i is a function of the variables $(C_1, \ldots, C_n, x_1, \ldots, x_n)$. Expression (2.1) gives the components of a function $F : R^{2n} \to R^k$. Whenever $f_i \equiv 0$ for all $i = 1, \ldots, k$ we get a solution of system (2.1). Now, suppose that we have a "good" $2n$-dimensional initial estimate b to a zero of F, i.e., $F(b)$ will be small in some sense when b is close to the root being sought. The next step is to compute a curve $s(t) = (s_1(t), \ldots, s_{2n}(t))$ satisfying

$$F(s(t)) = (1 - t)F(b) \tag{2.2}$$

for $0 \leq t \leq 1$, such that $F(s(0)) = F(b)$ and $F(s(1)) = 0$. Upon differentiation of (2.2), the curve $s(t)$ has to satisfy

$$F'(s(t))\frac{ds}{dt} = -F(b) \tag{2.3}$$

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with initial condition $s(0) = b$, where F' is the Jacobian of F. In this procedure, each iteration for $0 \leq t \leq 1$ requires the solution of a linear system of equations; hence, it is computationally expensive.

3. Algebraic–numerical scheme. Our idea is to introduce nonlinear changes of variables in expression (1.3) that reduce the computation of the x_i to the solution of a Toeplitz linear system. This decouples the problem into a linear part in terms of the symmetric functions of the x_i, and finding the roots of a polynomial. We will focus our attention on the case $n = 4$ and various k because of its relevance in the tumor segmentation NMR application; see [9].

If $k = 2n+1$ and $n = 4$, the system (1.3) takes the form

$$\begin{array}{l} p_1 = C_1x_1 \;+\; C_2x_2 \;+\; C_3x_3 \;+\; C_4x_4 \\ p_2 = C_1x_1^2 \;+\; C_2x_2^2 \;+\; C_3x_3^2 \;+\; C_4x_4^2 \\ \quad\vdots \qquad\quad \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\ p_9 = C_1x_1^9 \;+\; C_2x_2^9 \;+\; C_3x_3^9 \;+\; C_4x_4^9, \end{array} \tag{3.1}$$

and we proceed as follows. First, we reduce the number of equations in (3.1) with the transformation $q_j = p_j - p_{j+1}$ for $j = 1, \ldots, 8$; and for $i = 1, \ldots, 4$, we define new variables $u_i = C_i\,(1 - x_i)$, getting

$$\begin{array}{l} q_1 = u_1x_1 \;+\; u_2x_2 \;+\; u_3x_3 \;+\; u_4x_4 \\ q_2 = u_1x_1^2 \;+\; u_2x_2^2 \;+\; u_3x_3^2 \;+\; u_4x_4^2 \\ \quad\vdots \qquad\quad \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\ q_8 = u_1x_1^8 \;+\; u_2x_2^8 \;+\; u_3x_3^8 \;+\; u_4x_4^8. \end{array} \tag{3.2}$$

By taking the differences $q_{j+1} - q_jx_1$, together with the change of variables $v_i = u_i(x_i - x_1)$, equation (3.2) gets transformed into

$$\begin{array}{l} q_2 = q_1x_1 \;+\; v_2x_2 \;+\; v_3x_3 \;+\; v_4x_4 \\ q_3 = q_2x_1 \;+\; v_2x_2^2 \;+\; v_3x_3^2 \;+\; v_4x_4^2 \\ \quad\vdots \qquad\quad \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\ q_8 = q_7x_1 \;+\; v_2x_2^7 \;+\; v_3x_3^7 \;+\; v_4x_4^7. \end{array} \tag{3.3}$$

Next, eliminate v_2 by computing $q_{j+1} - q_jx_2$ for $j = 2, \ldots, 7$ to obtain

$$\begin{array}{l} q_3 = q_2\,(x_1 + x_2) \;-\; q_1x_1x_2 \;+\; w_3x_3 \;+\; w_4x_4 \\ q_4 = q_3\,(x_1 + x_2) \;-\; q_2x_1x_2 \;+\; w_3x_3^2 \;+\; w_4x_4^2 \\ \quad\vdots \qquad\qquad\quad \vdots \qquad\qquad\quad \vdots \qquad\qquad \vdots \\ q_8 = q_7\,(x_1 + x_2) \;-\; q_6x_1x_2 \;+\; w_3x_3^6 \;+\; w_4x_4^6, \end{array} \tag{3.4}$$

where $w_j = v_j(x_j - x_2)$ for $j = 3, 4$. Now, eliminate w_3 from (3.4) by calculating $q_{j+1} - q_jx_3$ for $j = 3, \ldots, 7$, which yields

$$\begin{array}{l} q_4 = q_3\,(x_1 + x_2 + x_3) \;-\; q_2\,(x_1x_2 + x_1x_3 + x_2x_3) \;+\; q_1x_1x_2x_3 \;+\; t_4x_4 \\ q_5 = q_4\,(x_1 + x_2 + x_3) \;-\; q_3\,(x_1x_2 + x_1x_3 + x_2x_3) \;+\; q_2x_1x_2x_3 \;+\; t_4x_4^2 \\ \quad\vdots \qquad\qquad\qquad \vdots \qquad\qquad\qquad\qquad\qquad\qquad \vdots \qquad\qquad\quad \vdots \\ q_8 = q_7\,(x_1 + x_2 + x_3) \;-\; q_6\,(x_1x_2 + x_1x_3 + x_2x_3) \;+\; q_5x_1x_2x_3 \;+\; t_4x_4^5, \end{array} \tag{3.5}$$

where $t_4 = w_4(x_4 - x_3)$. Finally, we eliminate t_4 from (3.5) by calculating $q_{j+1} - q_jx_4$ for $j = 4, \cdots, 7$, which yields

$$Q = MZ, \tag{3.6}$$

where

$$Q = \begin{bmatrix} q_5 \\ q_6 \\ q_7 \\ q_8 \end{bmatrix}, \qquad M = \begin{bmatrix} q_4 & -q_3 & q_2 & -q_1 \\ q_5 & -q_4 & q_3 & -q_2 \\ q_6 & -q_5 & q_4 & -q_3 \\ q_7 & -q_6 & q_5 & -q_4 \end{bmatrix}. \tag{3.7}$$

Hence, we have obtained a linear modified Toeplitz system[1] in the symmetric functions of the variables x_1, x_2, x_3, and x_4, namely

$$\begin{aligned} Z_1 &= x_1 + x_2 + x_3 + x_4 \\ Z_2 &= x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 + x_2x_4 + x_3x_4 \\ Z_3 &= x_1x_2x_3 + x_1x_2x_4 + x_1x_3x_4 + x_2x_3x_4 \\ Z_4 &= x_1x_2x_3x_4. \end{aligned} \tag{3.8}$$

It is easy to check that x_1, x_2, x_3, x_4 are the roots of the quartic equation

$$x^4 - Z_1x^3 + Z_2x^2 - Z_3x + Z_4 = 0. \tag{3.9}$$

We tested the above technique within the framework of our application: recovering the exponents λ_i and the coefficients c_i for data sets of eight and nine points. Namely, we considered the exponential fitting problem (1.2) for $n = 4$ and $k = 2n + 1$ at the points $t_i = 44i/1000$ for $i = 1, ..., 9$. We take the p_i as given by (1.3) with positive coefficients c_i, for $i = 1, 2, 3, 4$, chosen randomly and normalized so that $\sum c_i = 1$ and λ_i, for $i = 1, 2, 3, 4$, random between 0 and 20. Then the returned values for $e^{-t_i\lambda_i}$ and c_i lie within 10^{-5} of the exact values unless the condition number of the Toeplitz matrix M given in (3.7) is of order greater than 10^9. The tests were run with standard MATLAB routines. This unstable numerical behavior can be traced back to nearly coincident (within 3%) values of the exponents, which collides with the assumption that the number of different tissues is four. Consequently, the occurrence of a large condition number for the 4×4 Toeplitz matrix is a pointer to the possibility that the data set might be better approximated by fewer than four exponentials. This will be explored in detail in the context of our application in a forthcoming paper; see also [9].

At a recent conference, the II International Congress on Numerical and Computational Simulations, the authors became aware that the problem can also be solved using the VARPRO system developed in the classical work of Gene Golub and Victor Pereyra [6] of 1973[2]. In fact, under the change of variables $u_i = C_i(1 - x_i)x_i$ for $i = 1, \ldots, 4$, and taking $y_j = p_j - p_{j+1}$ for $j = 1, \ldots, 8$, our system (2.1) takes the Vandermonde form, which for $n = 4$ is

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ x_1^2 & x_2^2 & x_3^2 & x_4^2 \\ x_1^3 & x_2^3 & x_3^3 & x_4^3 \\ x_1^4 & x_2^4 & x_3^4 & x_4^4 \\ x_1^5 & x_2^5 & x_3^5 & x_4^5 \\ x_1^6 & x_2^6 & x_3^6 & x_4^6 \\ x_1^7 & x_2^7 & x_3^7 & x_4^7 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}, \tag{3.10}$$

[1] The modified Toeplitz system is exactly Toeplitz in the variables $Z_1, -Z_2, Z_3$ and $-Z_4$.

[2] See [5] for an interesting review of the history of the development of the idea of separable nonlinear least squares and its applications.

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and hence it can be solved using VARPRO. See [2] and [3] for further examples in the area of Lattice Quantum Chromodynamics.

4. The rectangular Toeplitz cases. If the number of measurements k is not equal to $2n+1$ where n is the number of variables, our Toeplitz system is not square. If $k < 2n+1$, the Toeplitz system is underdetermined. In terms of the NMR brain tissue segmentation problem, this means that we could fix arbitrarily one type of tissue (or more, depending on the rank of the Toeplitz matrix). If $k > 2n+1$, the Toeplitz system is overdetermined, and hence there is no interpolatory solution, but an approximate solution may be determined using least squares. In the case that $n = 4$ and the number of equations is 10, the resulting Toeplitz system is $Q = MZ$, where Z is computed by minimizing $\|Q - MZ\|_2$, and

$$Q = \begin{bmatrix} q_5 \\ q_6 \\ q_7 \\ q_8 \\ q_9 \end{bmatrix}, \qquad M = \begin{bmatrix} q_4 & -q_3 & q_2 & -q_1 \\ q_5 & -q_4 & q_3 & -q_2 \\ q_6 & -q_5 & q_4 & -q_3 \\ q_7 & -q_6 & q_5 & -q_4 \\ q_8 & -q_7 & q_6 & -q_5 \end{bmatrix}.$$

The solution x_1, x_2, x_3, and x_4 can be retrieved from (3.8). In the case of noisy data, we can supplement the original data with additional data points, and this leads naturally to overdetermined Toeplitz systems.

In order to evaluate the overall performance of the method, a synthetic image data set was constructed using the BrainWeb Simulated Brain Database [1] as a template for different tissue types. It was assumed that only four different types of tissues were present, including cerebrospinal fluid, gray and white matter, and connective tissue. Synthetic data were constructed as follows. For each tissue, the relaxation rate was assumed to be normally distributed around a mean value dependent on the tissue characteristics; these mean values were 2 s^{-1} for cerebrospinal fluid, 10 s^{-1} for gray matter, 12 s^{-1} for white matter, and 20 s^{-1} for connective tissue. The resulting relaxation rate distribution function is shown in Figure 4.1 (top right). The baseline for data points was assumed to be distributed according to a Rice-Rayleigh distribution, also shown in Figure 4.1 (bottom right). To consider the effect of noise, fluctuations distributed according to normal distributions were added to data points. In doing so, data sets for standard deviations ranging from 10 to 0.0001 were constructed. The results are shown in Figure 4.1 for the region of interest delimited in the figure.

5. Conclusions. It is clear that the method is fast and easy to implement. Also, it is a reasonable alternative in the undetermined cases. We conducted experiments with noiseless synthetic data that were numerically stable unless the condition number of the Toeplitz matrix was very large. The problem of segmenting tumor tissue in the brain from NMR relaxation data has been tackled successfully in [10]; see also [11] and [4]. In [10] and [11], the authors use the Inverse Laplace Transform, which is rather slow. The present method improves the computation time roughly by a factor of one thousand.

Figure 5.1 (a) and (b) compare the relative frequencies of the relaxation times of the pixels in the shown regions of interest as computed with the Inverse Laplace Transform and the technique proposed in this paper, respectively. The computed relaxation time is the average of the exponents λ_i weighted by the coefficients c_i. In this particular example, there are eight measurements and one of the four exponents is set to one, i.e., there is a baseline; see [9].

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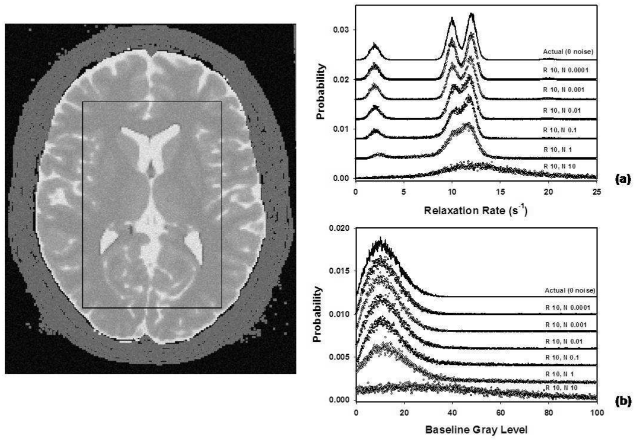

FIGURE 4.1. *The effect of noise on the distribution of relaxation rates.*

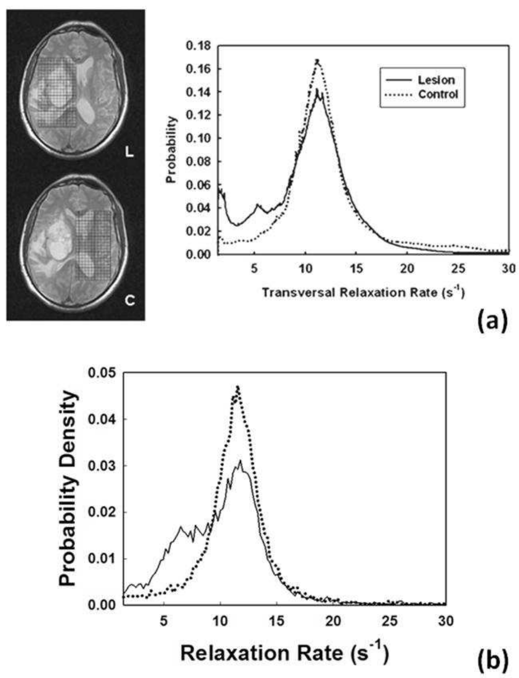

FIGURE 5.1. *Comparison between the proposed method and the Inverse Laplace Transform (ILT) algorithm of [10]. (a) Corresponds to Figure 11 of [10], showing the comparison between tumoral lesion and control (contralateral region). (b) Illustrates results obtained by the proposed method for regions similar to those of (a).*

present this article in the II International Congress on Numerical and Computational Simulations Cumaná 2007. We also dedicate this paper to the memory of Gene Golub.

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