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Yunkang Liu

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Department of Applied Mathematics and Theoretical Physics
Silver Street
Cambridge
England CB3 9EW

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Yunkang Liu

Gonville and Caius College, Cambridge University, Cambridge CB2 1TA, U.K

Abstract: Müntz theorems from classical approximation theory are used to lay the mathematical foundation for the discrete spectral representations of the relaxation modulus and creep compliance. Algorithms that can automatically generate nonnegative discrete relaxation and retardation strength are formulated by using the nonnegative least square method.

Key words: Relaxation modulus; creep compliance; Müntz Theorems; Dirichlet series; nonnegative least square method

1 Introduction

The discrete spectral representations of the relaxation modulus and creep compliance in rheology are associated with the problem of approximating given real functions over $[0, \infty)$ by linear combinations of exponentials. In the case of relaxation modulus, it is of theoretical importance to know whether a continuous relaxation modulus G can be approximated arbitrarily closely by a Dirichlet (or Prony) series of the form

$$G_0 + \sum_{k=1}^{n} G_k \mathrm{e}^{-t/\lambda_k} \tag{1.1}$$

where $G_0, G_1, G_2, \ldots$ are nonnegative constants and $\lambda_1, \lambda_2, \ldots$ are distinct positive constants. Typical assumptions on G include (Joseph [12, p. 542])

$$G(t) > 0, \quad G'(t) < 0 \quad \text{and} \quad G''(t) > 0. \tag{1.2}$$

In the case of creep compliance, one would like to known whether a continuous creep compliance J can be approximated arbitrarily closely by a Dirichlet series of the form

$$J_0 - \sum_{k=1}^{n} J_k \mathrm{e}^{-t/\tau_k} \tag{1.3}$$

where $J_0, J_1, J_2, \ldots$ are nonnegative constants and $\tau_1, \tau_2, \ldots$ are distinct positive constants. The usual assumptions on J are

$$J(t) > 0, \quad J'(t) > 0 \quad \text{and} \quad J''(t) < 0. \tag{1.4}$$

The relaxation strength $G_0, G_1, \ldots$, and the retardation strength $J_0, J_1, \ldots$ are required to be nonnegative, since (1.1) and (1.3) are supposed to be the corresponding relaxation modulus and creep compliance of a generalized Maxwell model and a generalized Kelvin (Voigt) model, respectively.

In practice, the relaxation modulus, creep compliance or dynamical moduli (storage and loss functions) are measured at some discrete points over certain ranges only. Various algorithms for fitting the discrete relaxation modulus and creep compliance to experimental or simulated data are proposed in [1, 6, 9, 10, 11, 13, 18], to name just a few recent papers. Some methods developed before 1989 are reviewed in Tschoegl [17].

The first problem one may encounter in obtaining accurate discrete relaxation modulus and creep compliance is how to choose the discrete relaxation times λ_k and the retardation times τ_k, $k = 1, 2, \ldots, n$. These two sets of quantities can not be measured experimentally. The *Doi and Edwards molecular theory for polymer melts* [8, p. 228] suggests

$$\lambda_k = \lambda_0/(2k+1)^2, \qquad k = 1, 2, \ldots \tag{1.5}$$

while the *Rouse molecular theory for dilute polymer solutions* (see, e.g., Doi and Edwards [8, p. 226]) gives

$$\lambda_k = \lambda_0/k^2, \qquad k = 1, 2, \ldots \tag{1.6}$$

with λ_0 being a positive constant in both cases. In general, λ_k's and τ_k's do not necessarily have any physical meaning. They are usually chosen so that with a finite n, (1.1) and (1.3) can give good approximation to G and J, respectively. In theory, the Prony's method and the method of differential approximation can be used, in conjunction with least square procedures, to calculate the relaxation/retardation times. The Prony's method can be found in Prony [16] or Bellman and Roth [4], while the method of differential approximation is described in Bellman [3] and is used by Haddad [11] in the context of rheology. However, both approaches are likely to generate complex or negative relaxation/retardation times even with small n. In many recent papers such as [4, 6, 10, 13, 18], the relaxation and retardation times are simply chosen to be logarithmic equidistant spaced:

$$\lambda_k = \rho^k \lambda_0, \qquad \tau_k = \rho^k \tau_0, \qquad k = 1, 2, \ldots \tag{1.7}$$

where $\rho \neq 1$, λ_0 and τ_0 are positive constant.

However, there is at present no discussion in rheology on the choice of relaxation/retardation times in a mathematical setting. The fundamental question here is whether a smooth function, satisfying all or part of the assumptions listed in (1.2) or (1.4), can be approximated arbitrarily closely by Dirichlet series, giving a particular choice of relaxation/retardation times such as (1.7). One purpose of this paper is to use Müntz theorems from approximation theory to demonstrate that the relaxation times $\{\lambda_k\}$ and retardation times $\{\tau_k\}$ must satisfy, respectively,

$$\sum_{k=1}^{\infty} \frac{\lambda_k}{1+\lambda_k^2} = \infty \tag{1.8}$$

and

$$\sum_{k=1}^{\infty} \frac{\tau_k}{1+\tau_k^2} = \infty \tag{1.9}$$

It will be shown in the next section that there are functions satisfying all the assumptions listed in (1.2) (or (1.4)), but yet can not be approximated arbitrarily closely by functions of the form (1.1) (or (1.3)) if (1.8) (or (1.9)) fails to hold.

Another purpose of this paper is to formulate algorithms for calculating the relaxation strength $G_0, G_1, \ldots$ and the retardation strength $J_0, J_1, \ldots$, assuming that the relaxation modulus G and creep compliance J are known at some discrete points in $[0,\infty)$. Earlier methods such as procedure X, collocation method and multidata method (see, e.g., Tschoegl [17]) may generate negative relaxation and retardation strength. The algorithms to be given in Section 3 of this paper are based on the nonnegative least square method. They produce nonnegative relaxation and retardation strength automatically. Compared with the method of Emri and Tschoegl [10], they have better global minimization property and are much easier to implement. Numerical experiment with simulated data are presented to show the accuracy of our algorithms with different sets of relaxation/retardation times.

It is worthwhile to mention that this paper is motivated by the question raised in Joseph [12, p. 569] and it is strongly influenced by the paper of Baxter and Iserles [2] on Dirichlet series of the form $\sum_{k=1}^{\infty} d_n \mathrm{e}^{-ap^n t}$ with $a > 0$ and $p \in (0,1)$.

2 Approximation by Dirichlet series

First, we introduce some notation. The Hilbert space $\mathrm{L}^2(a,b)$ consists of all (real) functions defined on the interval (a,b) that are measurable and square-integrable in the sense that

$$\int_a^b |f(t)|^2 \,\mathrm{d}t < \infty, \qquad \forall f \in \mathrm{L}^2(a,b).$$

The inner product of $\mathrm{L}^2(a,b)$ is defined by

$$(f,g) = \int_a^b f(t)g(t)\,\mathrm{d}t$$

and the corresponding norm by

$$\|f\|_2 = (f,f)^{1/2}. \tag{2.1}$$

The Banach space $\mathrm{C}_R[0,\infty)$ consists of all functions in $\mathrm{C}[0,\infty)$ that obey

$$\lim_{t\to\infty} f(t) = 0. \tag{2.2}$$

The norm of $\mathrm{C}_R[0,\infty)$ is the usual supremum norm defined by

$$\|f\|_\infty = \sup_{t\in[0,\infty)} |f(t)|.$$

For a sequence $\{x_k\}$ in a normed linear space X, the linear subspace of all linear combinations of the elements of $\{x_k\}$ is denoted by $\mathrm{Span}\{x_k\}$. This subspace is said to be *dense* in X if every element in X can be approximated arbitrarily closely by elements in $\mathrm{Span}\{x_k\}$.

We consider the problem of approximating functions in $\mathrm{L}^2(0,\infty)$ and in $\mathrm{C}_R[0,\infty)$ by Dirichlet series of the form

$$f_n(t) = \sum_{k=1}^{n} a_k \mathrm{e}^{-\alpha_k t}, \tag{2.3}$$

where $1 \le n \le \infty$, $a_1, a_2 \ldots$ are real constants and $\alpha_1, \alpha_2, \ldots$ are distinct positive constants. We are particularly interested in for what $\{\alpha_k\}$ can the linear space $\mathrm{Span}\{\mathrm{e}^{-\alpha_1 t}, \mathrm{e}^{-\alpha_2 t}, \ldots\}$ be *dense* in $\mathrm{L}^2(0,\infty)$ and/or in $\mathrm{C}_R[0,\infty)$. The relevance of this to the discrete representations of the relaxation modulus and creep compliance is obvious.

At this stage our discussion is not restricted to the case of $a_1, a_2 \ldots$ being nonnegative for two reasons. First, the available mathematical theory allows us to give a complete answer to the question of approximating functions in $\mathrm{L}^2(0,\infty)$ and in $\mathrm{C}_R[0,\infty)$ by Dirichlet series. Second, it can be proven rigourously that with bad choice of $\{\alpha_k\}$ there are functions that can not be approximated arbitrarily closely by Dirichlet series even without imposing the restriction that $a_1, a_2, \ldots$ be nonnegative.

Corresponding to the function space $\mathrm{L}^2(0,\infty)$, the following two approximation results hold.

Theorem 1 (Müntz Theorem in $\mathrm{L}^2(0,\infty)$) *Let $\{\alpha_k\}$ be an infinite sequence of distinct positive numbers. Then $\mathrm{Span}\{\mathrm{e}^{-\alpha_1 t}, \mathrm{e}^{-\alpha_2 t}, \ldots\}$ is dense in $\mathrm{L}^2(0,\infty)$ if and only if*

$$\sum_{k=1}^{\infty} \frac{\alpha_k}{1+\alpha_k^2} = \infty. \tag{2.4}$$

Theorem 2 *The function $\mathrm{e}^{-\alpha t}$, $\alpha > 0$ and $\alpha \notin \{\alpha_k\}$, which satisfies all the conditions listed in (1.2), can not be approximated arbitrarily closely by functions of the form (2.3) in $\mathrm{L}^2(0,\infty)$, unless (2.4) is satisfied.*

Remark 1. Related to the case of creep compliance, it can be said that the function $J_0 - \mathrm{e}^{-\alpha t}$, $J_0 > 1$, $\alpha > 0$ and $\alpha \notin \{\alpha_k\}$, which satisfies all the conditions listed in (1.3), can not be approximated arbitrarily closely in terms of the norm (2.1) by functions of the form $a_0 + \sum_{k=1}^{n} a_k \mathrm{e}^{-\alpha_k t}$, unless (2.4) is satisfied.

Theorem 1 follows trivially from the Müntz Theorem in $\mathrm{L}^2(0,1)$ (see Appendix). To prove Theorem 2, we consider the function $\mathrm{e}^{-\alpha t}$, $\alpha > 0$. Let

$$\mathrm{E}_n(\alpha) = \min_{a_k} \left\| \mathrm{e}^{-\alpha t} - \sum_{k=1}^{n} a_k \mathrm{e}^{-\alpha_k t} \right\|_2, \qquad \mathrm{E}(\alpha) = \inf_{n \ge 1} \mathrm{E}_n(\alpha).$$

It follows from Lemma 11.3.2 in [7] that

$$\mathrm{E}_n(\alpha) = \frac{1}{\sqrt{2\alpha}} \prod_{k=1}^{n} \frac{|\alpha_k - \alpha|}{\alpha_k + \alpha}, \qquad \mathrm{E}(\alpha) = \frac{1}{\sqrt{2\alpha}} \prod_{k=1}^{\infty} \frac{|\alpha_k - \alpha|}{\alpha_k + \alpha}. \tag{2.5}$$

If (2.4) is not satisfied then $\mathrm{E}(\alpha) > 0$ for every $\alpha \notin \{\alpha_k\}$. This completes the proof of Theorem 2.

Corresponding to the function space $\mathrm{C}_R[0,\infty)$, the following two approximation results hold.

Theorem 3 (Müntz Theorem in $\mathrm{C}_R[0,\infty)$) *Let $\{\alpha_k\}$ be an infinite sequence of distinct positive numbers. Then $\mathrm{Span}\{\mathrm{e}^{-\alpha_1 t}, \mathrm{e}^{-\alpha_2 t}, \ldots\}$ is dense in $\mathrm{C}_R[0,\infty)$ if and only if (2.4) holds.*

Theorem 4 *The function $\mathrm{e}^{-\alpha t}$, $\alpha > 0$ and $\alpha \notin \{\alpha_k\}$, which satisfies all the conditions listed in (1.2), can not be approximated arbitrarily closely by functions of the form (1.1) in $\mathrm{C}_R[0,\infty)$ if*

$$\sum_{k=1}^{\infty} 1/\alpha_k < \infty \tag{2.6}$$

or

$$\sum_{k=1}^{\infty} \alpha_k < \infty, \quad \alpha > 11(1+\eta). \tag{2.7}$$

Remark 2. As in Remark 1, we may say that the function $J_0 - \mathrm{e}^{-\alpha t}$, $J_0 > 1$, $\alpha > 0$ and $\alpha \notin \{\alpha_k\}$, can not be approximated arbitrarily closely in terms of the norm (2.1) by functions of the form $a_0 + \sum_{k=1}^{n} a_k \mathrm{e}^{-\alpha_k t}$, if (2.6) or (2.7) is the case.

Proof of the preceding two theorems will be given in the Appendix. To demonstrate the magnitude of the error function $\mathrm{E}(\alpha)$, we plot it in Figures 1–4 for the following cases:

1. $\alpha_k = 10^{k-1}$;
2. $\alpha_k = 2^{k-1}$;
3. $\alpha_k = k^2$;
4. $\alpha_k = (2k-1)^2$.

The first two correspond to (1.7) with $\rho = 1/10$ and $1/2$, the last two correspond to (1.5) and (1.6) respectively. Apart from showing that $\mathrm{E}(\alpha) \not\equiv 0$ for the above four choices of $\{\alpha_k\}$, these four figures also demonstrate that $\mathrm{E}(\alpha)$ is large for small α.

According to the above four theorems, one should alway choose the discrete relaxation and retardation times such that (1.8) and (1.9) hold, respectively. A surprising fact is that (1.5) and (1.6) do not satisfy (1.8). In the case of (1.7), (1.8) and (1.9) are violated as well if ρ is fixed.

A particularly suitable choice is

$$\alpha_k = \rho k + \gamma, \qquad k = 1, 2, \ldots, \tag{2.8}$$

where $\rho > 0$ and $\gamma > -\rho$ are parameters. It is easy to see that (2.4) holds for any fixed ρ and γ.

3 Algorithms

In this section we formulate algorithms for calculating the relaxation strength $G_0, G_1, \dots$ and the retardation strength $J_0, J_1, \dots$, assuming that the relaxation modulus G and the creep compliance J are known at certain points in $[0, \infty)$ and that the relaxation and retardation times have already been chosen.

We describe briefly the least square method and the nonnegative least square method. Given a $m \times (n+1)$ matrix $A = (a_{ij})$ and an m-dimensional vector $b = (b_1, b_2, \dots, b_m)^T$, the least square method finds $x = (x_0, x_1, \dots, x_n)^T$ such that

$$\sum_{i=1}^{m} \left(\sum_{j=0}^{n} a_{ij} x_j - b_i \right)^2 = \min_{-\infty < y_j < \infty} \sum_{i=1}^{m} \left(\sum_{j=0}^{n} a_{ij} y_j - b_i \right)^2 .$$

By contrast, the nonnegative least square method finds $x = (x_0, x_1, \dots, x_n)^T$ such that

$$x_j \geq 0, \qquad j = 0, 1, \dots, n$$

and

$$\sum_{i=1}^{m} \left(\sum_{j=0}^{n} a_{ij} x_j - b_i \right)^2 = \min_{y_j \geq 0} \sum_{i=1}^{m} \left(\sum_{j=0}^{n} a_{ij} y_j - b_i \right)^2 . \tag{3.1}$$

Detail of the least square method and the nonnegative least square method can be found in Lawson and Hanson [14].

Since nonnegative relaxation and retardation strength are required, we use the nonnegative least square method in algorithms to be formulated in the following two subsections.

3.1 Relaxation modulus

Given a set of data points $\{t_i\}_{i=1}^m$ in the interval $[0, \infty)$ and the corresponding relaxation modulus $G(t_i)$, one can find the nonnegative relaxation strength $G_0, G_1, \dots, G_n$ by minimize the quadratic function

$$F(g_0, g_1, \dots, g_n) = \sum_{i=1}^{m} w_i (G^*(t_i, n) - G(t_i))^2,$$

where $w_1, w_2, \dots, w_m$ are nonnegative weights and

$$G^*(t, n) = g_0 + \sum_{j=1}^{n} g_j \mathrm{e}^{-t/\lambda_j},$$

namely,

$$F(G_0, G_1, \dots, G_n) = \min_{g_0, g_1, \dots, g_n \geq 0} F(g_0, g_1, \dots, g_n).$$

A typical choice of weights is

$$w_i = \begin{cases} (t_2 - t_1)/2, & i = 1 \\ (t_{i+1} - t_{i-1})/2, & 1 < i < m \\ (t_m - t_{m-1})/2, & i = m \end{cases} \tag{3.2}$$

which means that $F(g_0, g_1, \ldots, g_n)$ is the discretization (by trapezoidal rule) of the integral

$$\int_{t_0}^{t_m} (G^*(t,n) - G(t))^2 \, \mathrm{d}t.$$

Alternatively, one may choose

$$w_i = \begin{cases} (t_2 - t_1)/(2G(t_1)^2), & i = 1 \\ (t_{i+1} - t_{i-1})/(2G(t_i)^2), & 1 < i < m \\ (t_m - t_{m-1})/(2G(t_m)^2), & i = m. \end{cases} \tag{3.3}$$

In this case, $F(g_0, g_1, \ldots, g_n)$ is the discretization of

$$\int_{t_0}^{t_m} (G^*(t,n)/G(t) - 1)^2 \, \mathrm{d}t.$$

Corresponding to the formulation (3.1) of the nonnegative least square method, we have

$$a_{ij} = \begin{cases} \sqrt{w_i}, & j = 0 \\ \sqrt{w_i}\mathrm{e}^{-t_i/\lambda_j}, & j = 1, 2, \ldots, n \end{cases} \qquad b_i = \sqrt{w_i}G(t_i), \qquad i = 1, 2, \ldots, m.$$

3.2 Creep compliance

Consider the case of given creep compliance $J(t_i)$ at the set of data points $\{t_i\}_{i=1}^m$ in the interval $[0, \infty)$. One can find the nonnegative retardation strength $J_0, J_1, \ldots, J_n$ so that

$$F(J_0, J_1, \ldots, J_n) = \min_{j_0, j_1, \ldots, j_n \geq 0} F(j_0, j_1, \ldots, j_n)),$$

where

$$F(j_0, j_1, \ldots, j_n) := \sum_{i=1}^{m} w_i (J^*(t_i, n) - J(t_i))^2$$

with $w_1, w_2, \ldots, w_m$ being nonnegative weights and

$$J^*(t,n) = j_0 - \sum_{k=1}^{n} j_k \mathrm{e}^{-t/\tau_k}.$$

For the weights, one may choose either (3.2) or

$$w_i = \begin{cases} (t_2 - t_1)/(2J(t_1)^2), & i = 1 \\ (t_{i+1} - t_{i-1})/(2J(t_i)^2), & 1 < i < m \\ (t_m - t_{m-1})/(2J(t_m)^2), & i = m. \end{cases} \tag{3.4}$$

Corresponding to the formulation (3.1) of the nonnegative least square method, we have

$$a_{ij} = \begin{cases} \sqrt{w_i}, & j = 0 \\ -\sqrt{w_i}\mathrm{e}^{-t_i/\tau_j}, & j = 1, 2, \ldots, n \end{cases} \qquad b_i = \sqrt{w_i} J(t_i), \qquad i = 1, 2, \ldots, m$$

3.3 Numerical examples

A Fortran subroutine for the nonnegative least square method is provided in Lawson and Hanson [14]. Moreover, any programs, subroutines or software packages that are designed for handling quadratic optimization with (linear) inequality constraints are also capable of solving nonnegative least square problem. We use the software package MATLAB to conduct the numerical experiment in this subsection. The MATLAB **nnls** function implements the nonnegative least square method with the algorithm provided in [14].

We shall concentrate on the case of relaxation modulus since the algorithm for the case of creep compliance is not different mathematically. The weights in the quadratic function $F(g_0, g_1, \ldots, g_n)$ shall be chosen as (3.2). This is because the result obtained from using (3.3) is either similar (when $G_0 \not\approx 0$) or worse (when $G_0 \approx 0$).

The theory in Section 2 indicates that one should choose the set of relaxation times according to (1.8). However, (1.8) can never be satisfied as only a finite number of relaxation modes is used. Therefore, experimenting with giving data is very important for achieving good accuracy. In fact, Baumgaertel and Winter [1] has pointed out that the number of relaxation modes and the relaxation times should be freely adjustable. We shall experiment with the following sets of relaxation times:

$$\lambda_k = \lambda/k, \qquad k = 1, 2, \ldots, \tag{3.5}$$

$$\lambda_k = \lambda/k^2, \qquad k = 1, 2, \ldots, \tag{3.6}$$

$$\lambda_k = \lambda/\rho^k, \qquad k = 1, 2, \ldots, \tag{3.7}$$

where ρ and γ are positive parameters.

The following two quantities shall be used to measure the accuracy of our algorithm:

$$\Phi_\infty = \max_{1 \le i \le m} |G^*(t_i, n) - G(t_i)|, \qquad \Phi_2 = \sum_{i=1}^{m} \left(G^*(t_i, n) - G(t_i)\right)^2.$$

In addition, we let $Z(n)$ be the number of nonzero (positive) relaxation strength in $G_0, G_1, \ldots, G_n$, as it is $Z(n)$, not n itself, that is meaningful.

For simulated data $\{G(m/10)\}_{m=1}^{100}$ generated from the continuous relaxation modulus

$$G(t) = 1 + \mathrm{e}^{-0.2\pi t} + \frac{1}{1000}\sum_{k=1}^{1000} \mathrm{e}^{-kt} + \mathrm{e}^{-400\pi t} \tag{3.8}$$

The following three tables give Φ_∞, Φ_2 and $Z(n)$ for a number of choices of relaxation times (with the same λ_1 in each table).

Table 1.

$\lambda_j,\ 1 \le j \le 40$	Φ_∞	Φ_2	$Z(40)$
$10/j$	2.8×10^{-4}	6.4×10^{-4}	3
$10/j^2$	1.1×10^{-2}	2.2×10^{-2}	3
$10/2^{j-1}$	6.8×10^{-3}	1.5×10^{-2}	3
$10/10^{j-1}$	4.6×10^{-2}	9.4×10^{-2}	3

Table 2.

$\lambda_j,\ 1 \le j \le 40$	Φ_∞	Φ_2	$Z(40)$
$50/j$	1.1×10^{-5}	2.2×10^{-5}	4
$50/j^2$	1.9×10^{-3}	4.3×10^{-3}	3
$50/2^{j-1}$	8.8×10^{-4}	1.6×10^{-3}	3
$50/10^{j-1}$	8.8×10^{-2}	1.4×10^{-1}	3

Table 3.

$\lambda_j,\ 1 \le j \le 40$	Φ_∞	Φ_2	$Z(40)$
$250/j$	3.0×10^{-1}	3.7×10^{-1}	2
$250/j^2$	3.7×10^{-4}	8.3×10^{-4}	3
$250/2^{j-1}$	6.6×10^{-3}	1.3×10^{-2}	3
$250/10^{j-1}$	3.9×10^{-2}	6.9×10^{-2}	3

The next three tables give Φ_∞, Φ_2 and $Z(n)$ for a number of choices of relaxation times when $\{G(m/10)\}_{m=1}^{100}$ are generated from the function

$$G(t) = 1 + \mathrm{e}^{-0.2*\pi t} + \frac{1}{1000}\sum_{k=1}^{1000} \mathrm{e}^{-t/k} + \mathrm{e}^{-\pi t}. \tag{3.9}$$

Table 4.

$\lambda_j,\ 1 \le j \le 40$	Φ_∞	Φ_2	$Z(40)$
$10/j$	7.9×10^{-2}	4.3×10^{-1}	4
$10/j^2$	7.9×10^{-2}	4.3×10^{-1}	4
$10/2^{j-1}$	7.9×10^{-2}	4.3×10^{-1}	4
$10/10^{j-1}$	7.9×10^{-2}	4.3×10^{-1}	4

Table 5.

$\lambda_j,\ 1 \le j \le 40$	Φ_∞	Φ_2	$Z(40)$
$50/j$	2.0×10^{-2}	8.7×10^{-2}	4
$50/j^2$	2.0×10^{-2}	8.7×10^{-2}	4
$50/2^{j-1}$	2.0×10^{-2}	8.9×10^{-2}	4
$50/10^{j-1}$	8.7×10^{-2}	1.7×10^{-1}	4

Table 6.

$\lambda_j,\ 1 \le j \le 40$	Φ_∞	Φ_2	$Z(40)$
$250/j$	3.1×10^{-1}	3.7×10^{-1}	3
$250/j^2$	2.5×10^{-5}	5.4×10^{-5}	9
$250/2^{j-1}$	1.9×10^{-3}	3.7×10^{-3}	7
$250/10^{j-1}$	2.9×10^{-2}	5.4×10^{-2}	5

For simulated data generated from the continuous relaxation modulus (3.8) the best result is achieved in Table 2 using (3.5) with $\lambda = 50$. However, for data generated from (3.9), the best result is obtained in Table 6 using (3.6) with $\lambda = 250$. Our numerical experiment with different sets of relaxation times indicate that one should always use the relaxation times as free adjustable parameters in order to achieve best result.

In the case of creep compliance, almost identical results as in the above six tables are observed for simulated data generated from

$$J(t) = 4 - \mathrm{e}^{-0.2\pi t} - \frac{1}{1000}\sum_{k=1}^{1000} \mathrm{e}^{-kt} - \mathrm{e}^{-400\pi t}$$

and from

$$J(t) = 4 - \mathrm{e}^{-0.2\pi t} - \frac{1}{1000}\sum_{k=1}^{1000} \mathrm{e}^{-t/k} - \mathrm{e}^{-\pi t}.$$

4 Conclusion

The approximation theory in Section 2 provides a rigourous mathematical justification for the discrete spectral representations of the relaxation modulus and creep compliance in rheology. It also tells us that discrete relaxation and retardation times do not necessarily have any physical meaning since the continuous relaxation modulus and creep compliance can be approximated arbitrarily closely by discrete ones with different sets of relaxation and retardation times, as long as (1.8) and (1.9) are satisfied by the corresponding relaxation and retardation times, respectively.

On the practical side, the nonnegative least square method is used in Section 3 to formulate algorithms that can yield nonnegative relaxation and retardation strength automatically. The numerical experiment demonstrate not only the efficiency of our algorithms but also the importance of keeping the relaxation and retardation times as free adjustable parameters.

We have not addressed the case of given experimentally determined data of the storage and loss functions

$$G'(\omega) = G_0 + \sum_{j=1}^{n} G_j \frac{(\omega\lambda_j)^2}{1 + (\omega\lambda_j)^2}, \qquad G''(\omega) = \sum_{j=1}^{n} G_j \frac{\omega\lambda_j}{1 + (\omega\lambda_j)^2}.$$

Algorithms for obtaining nonnegative weights from given data of the storage and loss functions can be formulated using nonnegative least square method. On the theoretical side, Theorem 2 and Theorem 4 apply to this case to certain extend. But Theorem 1 and Theorem 3 do not. We wish to discuss this case in detail in a forthcoming paper.

Appendix

This appendix provides rigourous proof of Theorems 1, 3 and 4 given in Section 2. Theorem 1 is follows easily from the following Müntz theorem in $\mathrm{L}^2(0,1)$ (see, e.g., Borwein and Erdélyi [5] or Davis [7]).

Müntz theorem in $\mathrm{L}^2(0,1)$: *Let* $\{\alpha_k\}$ *be an infinite sequence of distinct positive numbers. Then* $\mathrm{Span}\{x^{\alpha_1}, x^{\alpha_2}, \ldots\}$ *is dense in* $\mathrm{L}^2(0,1)$ *if and only if*

$$\sum_{k=1}^{\infty} \frac{\alpha_k + 1/2}{1 + (\alpha_k + 1/2)^2} = \infty.$$

The connection between Müntz Theorem in $\mathrm{L}^2(0,\infty)$, i.e., Theorem 1 and the Müntz theorem in $\mathrm{L}^2(0,1)$ is through the change of variable $x = \mathrm{e}^{-t}$, noting that

$$\left\| f(t) - \sum_{k=1}^{n} a_k \mathrm{e}^{-\alpha_k t} \right\|_2^2 = \int_0^1 \left| f(-\ln x) x^{-1/2} - \sum_{k=1}^{n} a_k x^{\alpha_k - 1/2} \right|^2 \mathrm{d}x \qquad (4.1)$$

for $f \in \mathrm{L}^2(0,\infty)$.

Proof of Theorem 3. Suppose that (2.4) holds. For any fixed $\alpha > 0$ and $n > 0$, let $\{a_k^*\}$ be such that

$$\left\| \mathrm{e}^{-\alpha t} - \sum_{k=1}^{n} a_k^* \mathrm{e}^{-\alpha_k t} \right\|_2 = \min_{a_k} \left\| \mathrm{e}^{-\alpha t} - \sum_{k=1}^{n} a_k \mathrm{e}^{-\alpha_k t} \right\|_2 .$$

Using Cauchy-Schwartz inequality, we obtain

$$\begin{aligned} & \left| \mathrm{e}^{-\alpha t} - \textstyle\sum_{k=1}^{n} \frac{\alpha+1/2}{\alpha_k+1/2} a_k^* \mathrm{e}^{-\alpha_k t} \right| \\ = \; & (\alpha + 1/2) \left| \mathrm{e}^{-t/2} \textstyle\int_t^\infty \mathrm{e}^{-\tau/2} \left(\mathrm{e}^{-\alpha\tau} - \sum_{k=1}^{n} a_k^* \mathrm{e}^{-\alpha_k \tau} \right) \mathrm{d}\tau \right| \\ \le \; & (\alpha + 1/2) \left\| \mathrm{e}^{-\alpha t} - \textstyle\sum_{k=1}^{n} a_k^* \mathrm{e}^{-\alpha_k t} \right\|_2 \end{aligned}$$

It follows from the above estimate and (2.5) that that

$$\min_{a_k} \left\| \mathrm{e}^{-\alpha t} - \sum_{k=1}^{n} a_k \mathrm{e}^{-\alpha_k t} \right\|_\infty \le \frac{\alpha + 1/2}{\sqrt{2\alpha}} \prod_{k=1}^{n} \frac{|\alpha_k - \alpha|}{\alpha_k + \alpha}. \qquad (4.2)$$

Since the right side of (4.2) tends to zero as $n \to \infty$, we deduce that $\mathrm{e}^{-\alpha t}$ can be approximated arbitrarily closely by functions in $\mathrm{Span}\{\mathrm{e}^{-\alpha_1 t}, \mathrm{e}^{-\alpha_2 t}, \ldots\}$. According to Bernstein's proof of the Weistrass theorem (see, e.g., Davis [7, Theorem 6.2.2]), any function $g(x) \in \mathrm{C}[0,1]$ can be approximated arbitrarily closely by polynomials of the form

$$\sum_{k=0}^{n} g(k/n) \begin{pmatrix} n \\ k \end{pmatrix} x^k (1-x)^{n-k}.$$

Therefore, if $g(0) = 0$ then g can be approximated arbitrarily closely by functions in $\mathrm{Span}\{x, x^2, \ldots\}$. Equivalently, $\mathrm{Span}\left\{\mathrm{e}^{-t}, \mathrm{e}^{-2t}, \ldots\right\}$ is dense in $\mathrm{C}_R(0,\infty)$. Since it has already been shown that $\mathrm{e}^{-\alpha t}$ can be approximated arbitrarily closely by functions in Span $\{\mathrm{e}^{-\alpha_1 t}, \mathrm{e}^{-\alpha_2 t}, \ldots\}$, we conclude that Span $\{\mathrm{e}^{-\alpha_1 t}, \mathrm{e}^{-\alpha_2 t}, \ldots\}$ is dense in $\mathrm{C}_R(0,\infty)$.

The 'only if' part follows easily from the following Müntz theorem in $\mathrm{C}[0,1]$ obtained by Borwein and Erdélyi [5]. $\square$

Müntz Theorem in $\mathrm{C}[0,1]$: *Let* $\{\alpha_k\}$ *be an infinite sequence of distinct positive numbers. Then* $\mathrm{Span}\{1, x^{\alpha_1}, x^{\alpha_2}, \ldots\}$ *is dense in* $\mathrm{C}[0,1]$ *if and only if (2.4) holds.*

Proof of Theorem 4. First, we consider the case $\sum_{k=1}^{\infty} 1/\alpha_k < \infty$. Let

$$d_n := \left\| \mathrm{e}^{-\alpha t} - \sum_{k=1}^{n} a_k^* \mathrm{e}^{-\alpha_k t} \right\|_\infty = \min_{a_k} \left\| \mathrm{e}^{-\alpha t} - \sum_{k=1}^{n} a_k \mathrm{e}^{-\alpha_k t} \right\|_\infty .$$

We have

$$\left\| \mathrm{e}^{-(\alpha+1/2)t} - \sum_{k=1}^{n} a_k^* \mathrm{e}^{-(\alpha_k+1/2)t} \right\|_2 \le d_n \left(\int_0^\infty \mathrm{e}^{-t}\, \mathrm{d}t \right)^{1/2} = d_n$$

and

$$\begin{aligned} & \left\| \mathrm{e}^{-(\alpha+1/2)t} - \textstyle\sum_{k=1}^{n} a_k^* \mathrm{e}^{-(\alpha_k+1/2)t} \right\|_2 \\ \ge\ & \min_{a_k} \left\| \mathrm{e}^{-(\alpha+1/2)t} - \textstyle\sum_{k=1}^{n} a_k \mathrm{e}^{-(\alpha_k+1/2)t} \right\|_2 = \tfrac{1}{\sqrt{2\alpha+1}} \textstyle\prod_{k=1}^{n} \tfrac{|\alpha_k-\alpha|}{\alpha_k+\alpha+1} \end{aligned}$$

If $\alpha \notin \{\alpha_k\}$ and $\sum_{k=1}^{\infty} 1/\alpha_k < \infty$ then

$$d_n > \frac{1}{\sqrt{2\alpha+1}} \prod_{k=1}^{\infty} \frac{|\alpha_k - \alpha|}{\alpha_k + \alpha + 1} > 0$$

which means that the function $\mathrm{e}^{-\alpha t}$ can not be approximated arbitrarily closely by functions of the form (2.3) in $\mathrm{C}_R[0,\infty)$.

For the case $\eta := \sum_{k=1}^{\infty} \alpha_k < \infty$, we need the inequality

$$\|p'(t)\|_\infty \le 11(1+\eta)\|p(t)\|_\infty \quad \forall p \in \mathrm{Span}\{\mathrm{e}^{-\alpha_1 t}, \mathrm{e}^{-\alpha_2 t}, \ldots\}, \tag{4.3}$$

which follows trivially from Newman's inequality [15]. Using the Mean Value Theorem and (4.3), it can be shown by contradiction that the function $\mathrm{e}^{-\alpha t}$, $\alpha > 11(1+\eta)$ and $\alpha \notin \{\alpha_k\}$, can not be approximated arbitrarily closely by functions of the form (2.3) in $\mathrm{C}_R[0,\infty)$. $\square$

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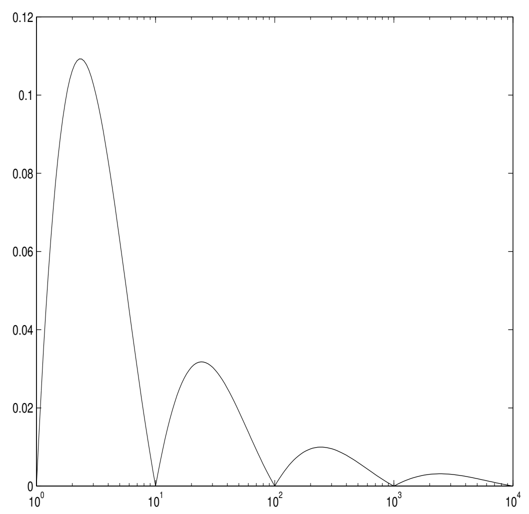

Figure 1.

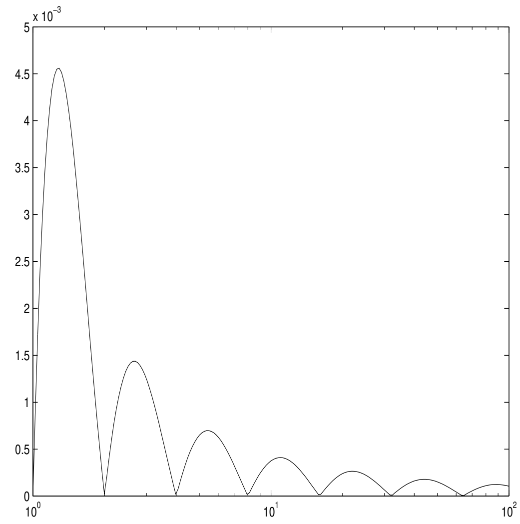

Figure 2.

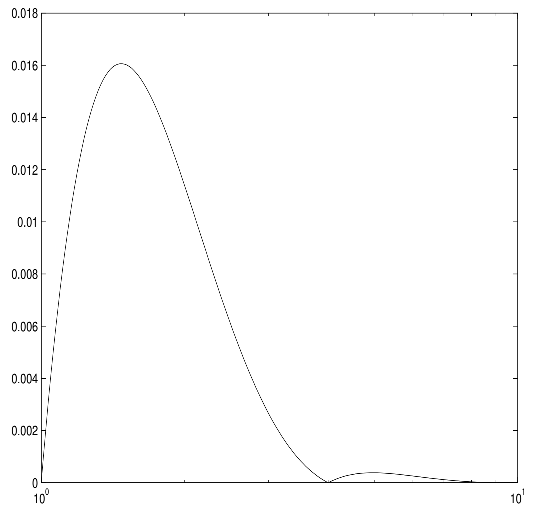

Figure 3.

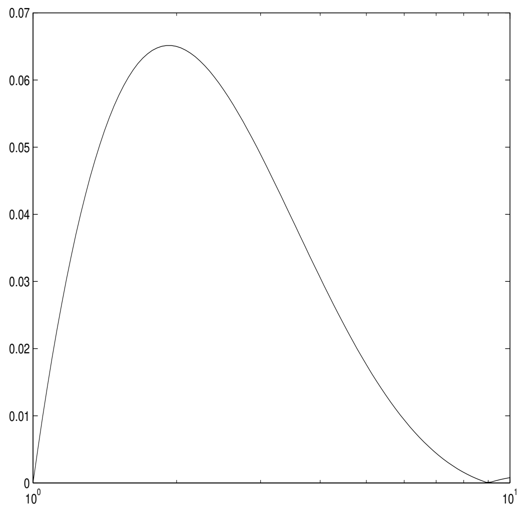

Figure 4.