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A spectral measure estimation problem in rheology

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HIGHLIGHTS

- The determination of a spectral measure is a standard inverse problem with convex constraints.
- The convex constraints come in from the experimental measurement errors.
- The method of maximum entropy in the mean handles this class of problems in a natural way.

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ABSTRACT

In this paper we consider an inverse problem appearing in rheology, consisting of determining a spectral measure over the set of relaxation times, that yields an observed collection of loss and storage moduli. Mathematically speaking, the problem consists of solving a system of Fredholm equations. To solve it, we propose an extended version of the maximum entropy method in the mean which is flexible enough to incorporate potential measurement errors.

1. Introduction and preliminaries

To describe the tensile strength of synthetic fibers, or to be more precise, of polymer melts, some standard experimental tests are carried on. The rheological measurements include linear viscoelastic shear oscillations, as well as linear elongations. The idea behind the measurements is to determine the relationship between the force (stress) and strain (deformation) in the material. When a material is deformed, part of the work exerted is stored as in the deformation, and part is spent as heat. These are known as storage modulus and storage loss respectively.

In his thesis, Berger [1], and in a report based on it, Berger and Meissner [2], described the results of the experiments. Different viscoelastic mixtures are subjected to torsional oscillations, and the storage and loss moduli are measured at different frequencies ω and different temperatures. We will follow their notation to denote as $G'(\omega)$ and $G''(\omega)$, the storage and the loss modulus respectively.

Their interest consists of determining the discrete relaxation spectrum $\{(g_n, \tau_n)|n \geq 1\}$ such that

$$G'(\omega) = \sum_n g_n \frac{\omega^2 \tau_n^2}{1 + \omega^2 \tau_n^2} \tag{1}$$

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as well as

$$G''(\omega) = \sum_n g_n \frac{\omega\tau_n}{1+\omega^2\tau_n^2}. \tag{2}$$

They select the relaxation times arbitrarily within the range $\tau_{max} = 1/\omega_{min}$ and $\tau_{min} = 1/\omega_{max}$, and then determine the (discrete) spectral measure g_n by a mean square error minimization procedure for each of the proportions of the polymer mixture.

Berger [1] states these equations as a discrete version of the set

$$G'(\omega) = \int H(\ln\tau)\frac{\omega^2\tau^2}{1+\omega^2\tau^2}\mathrm{d}\ln\tau \tag{3}$$

and correspondingly

$$G''(\omega) = \int H(\ln\tau)\frac{\omega\tau}{1+\omega^2\tau^2}\mathrm{d}\ln\tau \tag{4}$$

and he sets $H(\ln\tau) = g(\tau)\tau$ and $\mathrm{d}\ln\tau = \mathrm{d}\tau$ from which the discretization is apparent.

More recently, Wolpert, Ickstad and Hansen [3] and Wolpert and Ickstad [4] considered the original problem, in which the relaxation time τ is allowed to vary continuously in the interval $[\tau_{min}, \tau_{max}]$ and, instead of looking for a discrete spectrum, they propose determining a spectral measure (that is, a positive measurable function) $h(\tau)$ defined on $[\tau_{min}, \tau_{max}]$, such that

$$G'(\omega) = \int h(\tau)\frac{\omega^2\tau}{1+\omega^2\tau^2}\mathrm{d}\tau \tag{5}$$

and correspondingly

$$G''(\omega) = \int h(\tau)\frac{\omega}{1+\omega^2\tau^2}\mathrm{d}\tau \tag{6}$$

where the available information are the values of $G'(\omega_k)$ and $G''(\omega_k)$ at a collection and the connection between their $h(\tau)$ and Berger's H and g is given by $H(\ln\tau) = h(\tau)$ and $g(\tau)\tau = h(\tau)$.

In the last two mentioned papers, the authors use a Bayesian methodology to determine $g(\tau)$. Here we propose the use of the extended method of maximum entropy in the mean (MEM) to deal with a discretized version (5)–(6) augmented to take into account the measurement errors. To implement such methodology, we transform the problem into a problem consisting of solving a linear system of equations subject to non-linear, convex constrains, which is then transformed into a problem consisting of determining a probability distribution on an appropriate space and satisfying some constraints. The idea behind this procedure can be traced back to Navaza [5]. A more detailed description of the methodology, and further references, can be seen in Gzyl and Velásquez [6]. The remainder of the paper is organized as follows. In Section 2we consider the discretized version of (5)–(6) with the inclusion of measurement noise. In Section 3we recall the basics of MEM and how they relate to this type of problem, and in Section 4we present the results of applying MEM to solve (5)–(6).

2. Discretization and augmentation of (5)–(6)

Before discretizing (5)–(6) we integrate them into one single system of Fredholm equations. For that we consider a $2M$-dimensional (column) vector $G = \left(G'(\omega_1), \ldots, G'(\omega_M), G''(\omega_1), \ldots, G''(\omega_M)\right)^t$, where as usual we denote by x^t the transpose of the vector x. Here $\{\omega_1, \omega_2, \ldots, \omega_M\}$ is the collection of frequencies at which both $G'(\omega)$ and $G''(\omega)$ were measured.

Even though the output of the discretization process is similar to (1)–(2), the inner logic is different. Here we choose a uniform partition of $[\tau_{min}, \tau_{max}]$ into a number N of equal parts and denote the left-hand value of $h(\tau)$ at the left end point of each interval each by h_n. The N parts (subintervals) have end points $[\tau_n, \tau_{n+1}]$ with $\tau_n = \tau_{min} + \frac{n-1}{N}(\tau_{max} - \tau_{min})$, for $n = 1, \ldots, N+1$. There the partition is dictated by the experimental setup.

To obtain the discretized integral kernel, we define a $2M \times N$-matrix $K_{i,n}$, the entries of which are given by

$$K_{k,n} = \begin{cases} K_{k,n} = \dfrac{1}{N}\dfrac{\omega_k^2\tau_n}{1+\omega_k^2\tau_n^2} & 1 \le k \le M,\ n = 1, \ldots, N. \\ K_{k,n} = \dfrac{1}{N}\dfrac{\omega_k}{1+\omega_k^2\tau_n^2} & M+1 \le k \le 2M,\ n = 1, \ldots, N. \end{cases}$$

The factor $1/N$ in front of the K's comes from the discretization of the integral. We end up having to solve the following algebraic problem: Find h such that

$$Kh = G. \tag{7}$$

In our case we will have $N \gg K$, this algebraic problem, besides being ill conditioned has another difficulty built in: The experimental data is collected with measurement error, and since there are positivity constraints imposed on h, we shall transform the problem a bit.