IDENTIFICATION OF THE RELAXATION AND RETARDATION SPECTRA OF PLANT VISCOELASTIC MATERIALS USING CHEBYSHEV FUNCTIONS
PART I: IDENTIFICATION ALGORITHM

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Summary. The paper deals with the problem of recovery of continuous relaxation and retardation spectra of linear viscoelastic materials from discrete-time noise corrupted measurements of relaxation modulus and creep compliance obtained in stress relaxation and creep tests, respectively. In this part of the paper the optimal scheme of the least squares approximation of the relaxation spectrum by the finite series of orthogonal Chebyshev functions is presented. The problem of relaxation spectrum identification is the practical ill-posed problem of reconstructing solution of Fredholm integral equation of the first kind from the measured data. Thus, Tikhonov regularization is used to guarantee the stability of the scheme. Generalized cross validation (GCV) is adopted for the optimal choice of the regularization parameter. The numerical realization of the scheme by using the singular value decomposition (SVD) is discussed and the resulting computer algorithm is outlined. Identification of retardation spectrum and theoretical analysis of the model properties are presented in the second part of the paper. The numerical studies are the subject of the third part of the paper, where an example of the relaxation spectrum of a sample of the beet sugar root determination by applying the scheme proposed is also presented.

Keywords: Viscoelasticity, relaxation spectrum, identification, regularization, Chebyshev functions

INTRODUCTION

The need for detailed knowledge of mechanical material functions has been growing with the increased use of accurate engineering methods for rigorous predictions of the plant materials behavior, such as the finite element method (FEM), the boundary element method (BEM) and the finite difference method (FDM) [Lemaître 2001, Owens and Phillips 2002]. The soft biological materials as fruits and vegetables are often modeled in a time-domain viscoelastic regime, which is good for characterizing strain-stress dependence, creep and stress relaxation within a small deformation [De Baere et al., 1976, Rao 1999, Gohidki et al., 1998, Finores and Dejmek 2003]. Although for viscoelastic materials a multiplicity of constitutive theories exists, essentially only linear viscoelasticity is considered for which the Boltzmann superposition principle applies.

The mechanical properties of linear viscoelastic materials are characterized by relaxation or retardation spectra [Christensen 1971, Syed Mustapha and Phillips 2000, Malkin and Masalova]...
From the relaxation and retardation spectra other material functions such as the relaxation modulus or the creep compliance can be calculated without difficulty, and next both constant as well as the time-variable bulk or shear modulus or Poisson's ratio can be determined. Thus, the spectra are vital not only for constitutive models but also for the insight into the properties of a viscoelastic material [Szed Mtaym and Phillips 2000, Stankiewicz 2007].

However, the two spectra are not measurable directly, they must be determined from the appropriate response function, measured either in time or frequency-domain. These calculations require solution of an inverse problem, which happens to be ill-posed [Hansen 1997]. There are a few papers e.g., [Fujihara et al. 1995, ZI and Bažant 2002] as well as [Stankiewicz 2002, 2007] and the other previous papers by the present author cited therein, that deal with the spectra determination from time-measurement data, but the computationally efficient methods to determine the spectra are still desirable and it is the purpose of this study.

In this paper an optimal orthogonal schemes of the least-squares approximation of relaxation and retardation spectra by the linear combination of Chebyshev orthogonal functions are proposed.

RELAXATION SPECTRUM

The uniaxial and isotropic stress-strain equation for a linear viscoelastic material can be represented by a Boltzmann superposition integral [Derjaguin and Zienba 1968, Christensen 1971]:

\[ \sigma(t) = \int_0^t g(t - \tau) \varepsilon(\tau) d\tau. \]  

Here \( \sigma(t) \) denotes the stress corresponding to the given strain rate \( \dot{\varepsilon}(t) \) and \( g(t) \) is the linear relaxation modulus. Modulus \( g(t), t \geq 0 \), is given by:

\[ g(t) = \int_0^\infty H(\nu) \nu^\alpha e^{-\nu} d\nu. \]  

where: the relaxation spectrum \( H(\nu) \) characterizes the distribution of relaxation frequencies \( \nu \) in the range \( [\nu, \nu + d\nu] \).

The problem of relaxation spectrum determination is the numerical problem of reconstructing solution of Fredholm integral equation of the first kind (2) of convolution type from time-measured discrete relaxation modulus data. This problem is known to be severely Hadamard ill-posed [Hansen 1997, Stankiewicz 2007]. This means, that in particular, small changes in measured relaxation modulus can lead to arbitrarily large changes in the relaxation spectrum. In remedy, some reduction of the admissible solutions set or respective regularization of the original problem can be used. In this paper we use both the techniques simultaneously. A finite-dimensional approximation of the spectrum by the linear combination of orthogonal Chebyshev functions will be combined with Tikhonov regularization.

MODELS

Assume that \( H(\nu) \in L^2(0, \infty) \), where \( L^2(0, \infty) \) is the space of square-integrable functions on the interval \((0, \infty)\). Let \( h_k(\nu), k = 0, 1, \ldots \), be the Chebyshev functions [Szabó 1982]:

\[ h_k(\nu) = \sqrt{2\nu} \cos\left(\frac{k\pi}{\nu}\right). \]
\begin{equation}
\forall k \geq 1, \frac{1}{\sqrt{\pi}} \frac{\Gamma(k)}{\Gamma(k + 1/2)} (1 + 2a^2 \nu^2), \quad k = 1, 2, \ldots
\end{equation}

where: \( T_k \) are Chebyshev polynomials of the first kind and a time-scaling factor \( a > 0 \). The Chebyshev polynomials are given by the recursive formula [Szabat 1982]:

\begin{equation}
T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x), \quad k = 3, 4, \ldots
\end{equation}

starting with:

\begin{align}
T_0(x) &= 1, \\
T_1(x) &= x,
\end{align}

\begin{equation}
\text{and } T_2(x) = x^2 - \frac{1}{2}.
\end{equation}

The functions \( h_k(\nu) \) form an orthonormal basis of the Hilbert space \( L_2(0, \infty) \) with the weight \( e^{-2a^2 \nu^2} \) [Szabat 1982]. Thus the relaxation spectrum can be expressed as:

\begin{equation}
H(\nu) = \sum_{k=0}^{\infty} g_k \left( e^{2a^2 \nu^2} - 1 \right)^{1/2} h_k(\nu) \sum_{k=0}^{\infty} g_k \tilde{h}_k(\nu),
\end{equation}

where the normalized Chebyshev functions:

\begin{equation}
\tilde{h}_k(\nu) \left( e^{2a^2 \nu^2} - 1 \right)^{1/2} h_k(\nu),
\end{equation}

and \( g_k \) are constants. In order to reduce the set of admissible solutions, it is convenient to consider the partial sum:

\begin{equation}
H_k(\nu) = \sum_{k=0}^{K} g_k \left( e^{2a^2 \nu^2} - 1 \right)^{1/2} h_k(\nu) \sum_{k=0}^{K} g_k \tilde{h}_k(\nu).
\end{equation}

Then, the respective model of the relaxation modulus, is described by:

\begin{equation}
G_k(t) = \int_0^\infty H_k(\nu) e^{-\nu t} d\nu = \sum_{k=0}^{K} g_k \phi_k(t),
\end{equation}

where according to (2), the functions \( \phi_k(t) \) are defined as:

\begin{equation}
\phi_k(t) = \left( e^{2a^2 \nu^2} - 1 \right)^{1/2} h_k(\nu) e^{\nu t} d\nu.
\end{equation}

The useful recursive form of the basis functions \( \phi_k(t) \) is given by the following theorem, the proof is given in Appendix A.

**Theorem 1.** Let \( a > 0 \) and \( t \geq 0 \). Then the basis functions \( \phi_k(t) \) are given by the recursive formula:

\begin{equation}
\phi_0(t) = \phi_1(t) = \phi_2(t) = \phi_{2k+1}(t + 2a), \quad k = 1, 2, \ldots
\end{equation}

starting with:

\begin{align}
\phi_0(t) &= \frac{1}{2a} \frac{\Gamma \left( \frac{1}{2a} + 1 \right)}{\Gamma \left( \frac{1}{2a} + \frac{3}{2} \right)}, \\
\phi_1(t) &= \frac{1}{2a} \frac{\Gamma \left( \frac{1}{2a} + 1 \right)}{\Gamma \left( \frac{1}{2a} + \frac{3}{2} \right)} [a \ t].
\end{align}
\[ \phi_1(t) = \frac{1}{\sqrt{2\pi}} \frac{\Gamma(\frac{3}{4}) \Gamma\left(\frac{2\alpha}{4}\right)}{4\alpha^2 \Gamma\left(\frac{4\alpha}{4} + 3\right)} \left(2 + 2\alpha^2 \right) \]  

(14)

where \( \Gamma() \) is the Euler's gamma function, which is a generalization of \( n! \) for noninteger \( n \).

A few first basis functions \( f_k(\nu) \) are shown in Figure 1 for two different values of the time-scaling factor \( \alpha \); the corresponding functions \( \phi(\nu) \) are plotted in Figure 2. From the figure, it is evident that the basic functions for relaxation modulus model are in good agreement with the real relaxation modulus obtained in experiment.

![Figure 1. The Chebyshev basic functions \( f_k(\nu) \) for parameter \( \alpha = 1.5 \) and \( \alpha = 1 \), \( k = 0, 1, 2, 3, 4 \)](image)

![Figure 2. Functions \( \phi(\nu) \) of Chebyshev algorithm, the parameters \( \alpha = 1.5 \) and \( \alpha = 1 \), \( k = 0, 1, 2, 3, 4 \)](image)

**AUGMENTED MODEL**

It is well-known that for plant materials usually \( G_\infty G(\nu) = G_\infty > 0 \) [Jakubczyk and Lewicki 2003, Stankiewicz 2007], where \( G_\infty \) is the long-term modulus. It is also the case of the best root sample which is considered in the third part of the paper. Thus, instead of the classical model(9), it is convenient to consider the following augmented model of the form:
Then, the relaxation spectrum model takes the form

\[
\overline{\mathcal{R}}_{\nu}(\tau)^{-\frac{1}{2}} \mathcal{H}_x(\nu)^{\ast} \ast \Delta_{\nu} + \mathcal{G}_{\nu}(\nu) + \mathcal{G}_{w}(\nu) \quad (15)
\]

where \( \mathcal{H}_x(\nu) \) is a linear combination of Chebyshev functions (3) and \( \mathcal{G}(\nu) \) denotes the Dirac delta function. Unbounded component \( \mathcal{G}_{w}(\nu) \) of the relaxation spectrum \( \overline{\mathcal{R}}_{\nu}(\nu) \) (15) corresponds with the relaxation frequency equal to zero, or equivalently, to infinite relaxation time.

IDENTIFICATION PROBLEM

Identification consists of selecting within the given class of models defined by (9), (15) such a model, which ensures the best fit to the measurement results. Suppose, a certain identification experiment (stress relaxation test) performed on the specimen of the material under investigation resulted in a set of measurements of the relaxation modulus \( \overline{\mathcal{G}}(\xi) \), \( \mathcal{G}(\xi_i) + \varepsilon(\xi_i) \) at the sampling instants \( i \geq 0, i = 1, \ldots, N \) where \( \varepsilon(\xi) \) is additive measurement noise. As a measure of the model (9), (15) accuracy the square index is taken

\[
Q_{\nu}(\xi_i^o) = \sum_{i=1}^{N} \left[ \overline{\mathcal{G}(\xi_i)} - \overline{\mathcal{G}_{\nu}(\xi_i)} \right]^2 \| \mathcal{G}_{\nu} - \mathcal{G}_{w} \| \quad (17)
\]

where \( \| \cdot \| \) denotes the square norm in the real Euclidean space, \( \mathcal{G}_{\nu} = [\mathcal{G}_{\nu}(0) \cdots \mathcal{G}_{\nu}(K+1)]^T \) is an \((K+1)\)-element vector of unknown coefficients of the model (9). The \( N \times (K+1) \) element matrix \( \mathcal{G}_{\nu} \) and the vector \( \mathcal{G}_{w} \) are defined as follows:

\[
\mathcal{G}_{\nu} = \begin{bmatrix}
\phi_{\nu}(\xi_1) \\
\vdots \\
\phi_{\nu}(\xi_i) \\
\vdots \\
\phi_{\nu}(\xi_N)
\end{bmatrix}, \quad \mathcal{G}_{w} = \begin{bmatrix}
\overline{\mathcal{G}(\xi_1)} \\
\vdots \\
\overline{\mathcal{G}(\xi_i)} \\
\vdots \\
\overline{\mathcal{G}(\xi_N)}
\end{bmatrix} \quad (18)
\]

Then, the identification problem consists of determining the model parameter \( \hat{\mathcal{G}}_{\nu} \) minimizing the index (17). The matrix \( \mathcal{G}_{\nu} \) is usually ill-conditioned. Then, the minimum of (17) is not unique and even the normal (minimum Euclidean norm) solution \( \hat{\mathcal{G}}_{\nu}^N \) of the linear-quadratic problem (17)-(18) is non-continuous and unbounded function of the data vector \( \mathcal{G}_{w} \). i.e. when the data are noisy even small changes in \( \mathcal{G}_{w} \) would lead to arbitrarily large artefact in \( \hat{\mathcal{G}}_{\nu} \). Therefore, the numerical solution of finite dimensional problem (17)-(18) is fraught with the same difficulties that the original continuous ill-posed problem. To deal with the ill-posedness, the Tikhonov regularization method is used and presented in the subsequent section.

REGULARIZATION

Regularization aims to replace the ill-posed problem by a nearby well-posed problem. Tikhonov regularization [Tikhonov and Arsenin 1977] strives to stabilize the computation of the least-squares solution by minimizing a modified square functional of the form:
\begin{equation}
\min_{\Phi_{\lambda}} \| \mathbf{G}_\lambda \mathbf{\Phi}_{\lambda} \mathbf{G}_\lambda \|^2 + \lambda \| \mathbf{G}_\lambda \|^2
\end{equation}

where \( \lambda > 0 \) is a regularization parameter. The above problem is well-posed, that is the solution always exists, is unique, and continuously depends on both the matrix \( \Phi_{\lambda} \) as well as on the measurement data \( \mathbf{G}_\lambda \). The model parameter vector minimizing (19) is given by:
\begin{equation}
\mathbf{G}_\lambda = ( \Phi_{\lambda}^T \Phi_{\lambda} + \lambda \mathbf{I}_{(K+1)\times(K+1)})^{-1} \Phi_{\lambda}^T \mathbf{G}_\lambda
\end{equation}

where \( \mathbf{I}_{(K+1)\times(K+1)} \) is the identity matrix.

The choice of regularization parameter \( \lambda \) is crucial to identify the best model parameters. Here we apply the generalized cross-validation GCV [Golub et al. 1979, Nguyen et al. 2001], which does not depend on \textit{a priori} knowledge about the noise variance. The effectiveness of this approach in the context of relaxation spectrum identification has been verified by the early authors works see [Stankevicius 2007]. The GCV technique is based on choosing as regularization parameter that \( \lambda_{\text{GCV}} \) which minimizes the GCV functional defined by:
\begin{equation}
\mathbf{V}_{\text{GCV}}(\lambda) = \| \mathbf{r}(\lambda) \|^2 / \text{tr}(\mathbf{M}(\lambda)^2),
\end{equation}

where the matrix \( \mathbf{M}(\lambda) = \mathbf{I}_{K} - \Phi_{\lambda} \Phi_{\lambda}^T \Phi_{\lambda}^T \Phi_{\lambda} + \lambda \mathbf{I}_{(K+1)\times(K+1)} \) and \( \mathbf{r}(\lambda) = \mathbf{M}(\lambda) \mathbf{G}_\lambda \) is the residual vector for the regularized solution (20), \( \text{tr}(\mathbf{M}(\lambda)^2) \) denotes the trace of \( \mathbf{M}(\lambda)^2 \).

ALGEBRAIC BACKGROUND

For the computational purposes the elegant formula (20) is generally unsuitable. For numerical computation of regularized solution, the singular value decomposition (SVD) technique will be used. Let SVD of the \((K+1)\times(K+1)\) dimensional matrix \( \Phi_{\lambda}^T \mathbf{G}_\lambda \mathbf{G}_{\lambda} \) takes the form:
\begin{equation}
\Phi_{\lambda}^T \mathbf{G}_\lambda \mathbf{G}_{\lambda} = V \Sigma V^T,
\end{equation}

where \( V \in \mathbb{R}^{(K+1)\times(K+1)} \) is orthogonal matrix and \( \Sigma = \text{diag}(\sigma_0, \sigma_1, ..., \sigma_{K+1}) \) is \((K+1)\times(K+1)\) diagonal matrix containing the non-zero singular values \( \sigma_0, ..., \sigma_{K+1} \) of the matrix \( \Phi_{\lambda}^T \mathbf{G}_\lambda \mathbf{G}_{\lambda} \) with \( v = \text{rank}(\Phi_{\lambda}^T \mathbf{G}_\lambda) \) [Kiełbasiński and Schütte 1994]. Taking advantage of the diagonal structure of \( \Sigma \) and the matrix \( V \) orthogonality, it may be simply proved that [Stankevicius 2007]:
\begin{equation}
\mathbf{G}_\lambda = V \Omega \Sigma^2 \mathbf{G}_{\lambda} V^T.
\end{equation}

where the diagonal structure matrix \( \Omega \) is as follows:
\begin{equation}
\Omega = \text{diag}(1(\sigma_0 + \lambda), 1(\sigma_1 + \lambda), ..., 1(\sigma_{K+1} + \lambda)).
\end{equation}

Using SVD (23) also the GCV function (21) can be expressed by a convenient formula:
\begin{equation}
\mathbf{V}_{\text{GCV}}(\lambda) = \mathbf{G}_\lambda^T \Sigma^2 \mathbf{G}_\lambda \sum_{n=0}^{K+1} \frac{\sigma_n^2 + 2\lambda}{(\sigma_n + \lambda)^2} \left( \sigma_n + \lambda \right)^{-1},
\end{equation}

as a function of singular values \( \sigma_0, ..., \sigma_{K+1} \), and elements \( y \), of the vector \( V \). Using this function, the GCV minimization task can be implemented to solve the GCV minimization task.
IDENTIFICATION SCHEME

Allowing the above, the calculation of the relaxation model involves the following steps:
1. Perform the experiment - stress relaxation test [Rao 1996, Golecki 1993] - and record the measurements $G_i(t_i)$, $i = 1, \ldots, n$, of the relaxation modulus at times $t_i \geq 0$.
2. Compute the matrices $\varphi_{kk}$ (18), $\varphi_{kk}$ (23) and next determine SVD (23) of $F_{kk}$.
3. Determine GCV function $V_{gcv}(\lambda)$ (26), and next compute the optimal regularization parameter $\lambda_{gcv}$ minimizing $V_{gcv}(\lambda)$.
4. Compute the regularized solution $g_{gcv}$ according to (24) and (23) for $\lambda = \lambda_{gcv}$.
5. Determine the spectrum of relaxation frequencies $\tilde{H}_k(\nu)$ according to (cf. (8)):

$$
\tilde{H}_k(\nu) = \sum_{k=1}^{K} \tilde{g}_{kk}(\nu)$$

(27)

Obviously, $\tilde{H}_k(\nu) = \tilde{F}_k(\nu) + \tilde{\sigma}_k^2 \tilde{S}(\nu)$ is the relaxation spectrum of the form (16).

**Remark 1.** Only the SVD of the matrix $F_{kk}$ is space and time consuming task of the scheme. The SVD is accessible in the form of optimized numerical procedures in most commonly used contemporary computational packages (e.g., svd(A) in Matlab 7.0, [U,S,V]=svd(A) in Matlab 6.5, Matrix Singular Values Decomposition (USV) in Statistica 5.5).

**Remark 2.** It is easy to note that the matrix $F_{kk}$ depends on the choice of the basic functions as well as the measurement points $(t_i)$, however does not depend on the experiment results. Thus, when the identification scheme is applied for successive samples of the material, the step 2 have not to be multiple repeated while the same measurement points $(t_i)$ are kept.

**Remark 3.** Normalized Chebyshev functions $T_{k}(\nu)$ defined by the formula (3), (4) and (7) can be determined using Chebyshev polynomials $T_{k}(\nu)$. Polynomials $T_{k}(\nu)$ are accessible in some computational packages, they may be also computed according to simple recursive formula (5)-(6).

**Remark 4.** In the scheme proposed the parameter $\alpha > 0$ is the time-scaling factor. The following rule holds: the lower the parameter $\alpha$ is, the shorter the relaxation times are, i.e. the greater are the relaxation frequencies. The above is illustrated by figures 1 and 2. By the optimal choice of the scaling factor the best fit of the model to the experimental data can be achieved. However, in practice a simple rough rule for choosing the scaling factor $\alpha$, based on the comparison of a few first functions from the sequence $(\varphi_{kk}(\nu))$ for different values of $\alpha$ with the experimentally obtained function $G(t)$ is quite enough. In the same manner, the number $K$ of the series (9) elements can be initially evaluated. Thus, the choice both of the number $K$ as well as the parameter $\alpha$ must be done a posteriori, after the preliminary experimental data analysis.

CONCLUSIONS

An algorithm has been found for the calculation of relaxation frequencies spectrum from the measurement data of the relaxation modulus in discrete time measurements. The approach proposed is based on the approximation of the spectrum by finite linear combination of the Chebyshev functions. An analysis of the identification scheme and resulted model properties is the subject of the second part of the paper. The numerical experimental studies will be also conducted and the effectiveness of the method will be demonstrated through the computation of the relaxation spectrum of the beet sugar root sample in the third part of the paper.
APPENDIX A

Proof of Theorem 1. Suppose $a > 0$. Let us first derive the formulas (12), (13) and (14). Since $T_a(x) = T_a(x)$, substituting $x^{2a} = v$ in $\phi_v(t)$ after simple manipulations we obtain:

$$\phi_v(t) = \frac{1}{\sqrt{2\pi a}} \int_0^{\infty} \left( x^{2a} \right)^{-1/2} e^{-x^{2a} t} \, dx$$

whence, using the well-known Euler-Poisson integral $\int_0^{\infty} x^{s-1} e^{-x} \, dx = \Gamma(s)$, where $\Gamma(s)$ is the Euler's gamma function, we finally obtain eq. (12).

For $k = 1$, the Chebyshev polynomial $T_1(x) = x$ and the integral $\phi_v(t)$ can be expressed as a sum:

$$\phi_v(t) = 2 \frac{1}{\sqrt{\pi}} \int_0^{\infty} \left( x^{2a} - 1 \right) 0^a e^{-x^{2a} t} \, dx$$

or according to (A.1) as follows $\phi_v(t) = 2\phi_v(t) - 4\phi_v(t + 2a)$. Then, from eq. (12) we obtain

$$\phi_v(t) = 2 \frac{1}{\sqrt{\pi}} \int_0^{\infty} \left( x^{2a} - 1 \right) 0^a e^{-x^{2a} t} \, dx$$

and whence, using the well-known properties of the Gamma function $\Gamma(s+1) = s\Gamma(s)$, after simple algebraic manipulations we obtain finally eq. (13).

For $k = 2$ the Chebyshev polynomial $T_2(x) = x^2 - 1/2$, thus according to (4), (10) and taking account of (A.1) the integral $\phi_v(t)$ can be written as $\phi_v(t) = 2\phi_v(t) - 4\phi_v(t + 2a)$, and hence, on the basis of (12) we obtain the (14).

Now, it remains to show that (11) hold for any $k \geq 3$. Recalling the identity (5) and using (4) and (7) we obtain:

$$\phi_v(t) = 2 \frac{1}{\sqrt{\pi}} \int_0^{\infty} \left( x^{2a} - 1 \right) 0^a e^{-x^{2a} t} \, dx$$

whence, in view of the definition (10) we obtain finally (11), which concludes the proof.

REFERENCES


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IDENTYFIKACJA SPEKTRA RELAKSACJI I RETARDACJI LEPOKOSPŁYNĘTYCH MATERIAŁÓW ROŚLINNYCH Z WYKORZYSTANIEM FUNKCJI CZEBYSZEWA

ČĘŚĆ I. ALCORYTM IDENTYFIKACJI


Słowa kluczowe: lepkospłynność, spektrum relaksacji, identyfikacja, regularyzacja, funkcja Czbyšewa