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Viscoelasticity and Spectral Analysis with Tikhonov Regularization

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Abstract

The focus of this independent study is an in-depth study of viscoelasticity and the mechanisms to obtaining a viscoelastic spectrum from stress data. The independent study begins with a study of simple models such as the Maxwell, Kelvin, and Zener models. It then proceeds to biphasic models associated with Biot theory, as expounded upon by Mow and co-workers. The paper culminates with a study of spectral methods and Tikhonov regularization for the spectral analysis of material behavior, including noise sensitivity and signal-noise information.

Introduction

Viscoelasticity is the study of materials which have a time-dependence. It is of great importance in the study of mechanical properties of materials, especially in biological tissues. These materials exhibit both viscous and elastic characteristics when undergoing deformation. A viscoelastic material remembers its loading. Applying a stress quickly makes the material return to its previous state quickly, but slowly applying stress or holding a stress makes the material relax slower. Most viscoelastic materials resist quick changes because of their viscous aspect, while at the same time maintaining elastic solid properties. Most biological systems have some degree of viscoelasticity in them. It is important to understand the mechanics behind the body to better be able to treat it [1].

The test of preference to characterize linear viscoelasticity is rotational rheometry, in which a specimen is oscillated over a range of loading rates and the spectrum of responses over these loading rates is acquired directly [2-4]. However, this is often not useful for materials that are anisotropic or that cannot be gripped easily [2-4].

The motivation in studying viscoelasticity for this purpose is to understand how cells and tissues interact with each other through time dependent processes. A broad range of tissue engineered systems has been developed for this purpose [5,6]. In most cases, the objective is to infer material behavior from either natural tissues or these tissue engineered systems by assaying it using one of the following two tests [2-4,7-10]. The first is a creep test, in which a static load is applied and deformation is recorded over time; the second is a relaxation test, in which a rapid stretch is applied and the force necessary for isometric stretching is recorded over time. These tests must be performed with care because small errors in applying the ramp loading associated with them can lead to substantial errors in interpretation [11]. Other techniques that thwart this are periodic oscillation and slow cyclic loading [12-13].

An additional challenge with tissues is that they are typically nonlinear in their strain response, even if they follow linear viscoelasticity in their relaxation responses [14-16]. A common model used to account for these effects in biomechanics is the Fung quasilinear viscoelasticity (QLV) model [17-19]. However, a great number of studies show that the Fung QLV model is overly restrictive and fails to capture the behavior of tissues due to the nature of the form that temporal relaxation must take [14-16, 20-22]. A number of alternative approaches have been proposed [10,14-16,23-25], including discrete spectral approaches [26-27].

Maxwell, Kelvin, and Zener Models

Researchers have tried to model viscoelastic materials by having a representation of both the viscous and elastic parts.

The Maxwell model has a spring and dash-pot in series. The spring has an instantaneous response to stress. The strain and stress are directly related by the modulus of the spring.

$$\varepsilon = \frac{1}{E}\sigma \tag{1}$$

The spring undergoes an instantaneous elastic strain when it is loaded, holds the strain as long as the load is applied, and the strain instantaneously goes back down to zero once the stress is gone [1].

E_e

[28]
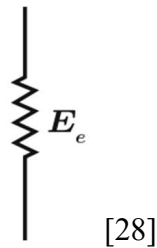
The viscous part is represented by a dash-pot. It is a piston cylinder arrangement which is filled with a viscous fluid. The piston is slowed by the viscous fluid as it is pulled through the piston. In this case the strain rate is proportional to the stress. The first derivative of the strain is proportional to the stress [1].

$$\dot{\varepsilon} = \frac{1}{\eta}\sigma \tag{2}$$

τ_1

[28]
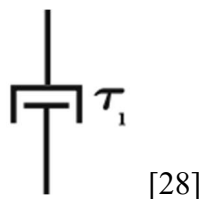
The larger the stress, the bigger the strain rate change. η is the viscosity. The Maxwell model is a sum of those two parts in series.

$$\varepsilon = \varepsilon_1 + \varepsilon_2 \tag{3}$$

If we integrate equation 1 and 3 and then plug in equations 1 and 2 into the integrated form of equation 3, we get the standard form of the constitutive equation for the Maxwell model. Note that since the spring and dashpot are in series the stress is equal in both parts, but the strain is not equal in both parts [1].

$$\sigma + \frac{\eta}{E}\dot{\sigma} = \eta\dot{\varepsilon} \tag{4}$$

[2]
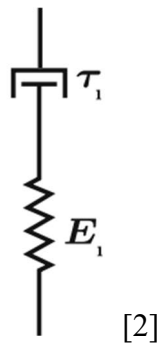
The Kevin Voight model is similar to the Maxwell model in that it includes the spring and dashpot, but here they are in parallel. The strain is equal in both the spring and the dashpot.

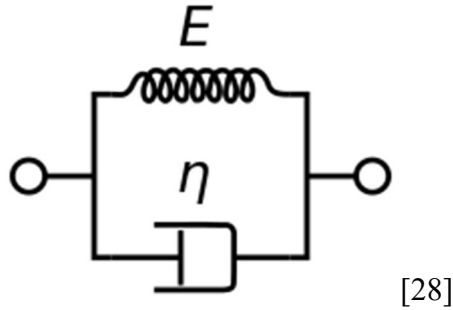$$\sigma = \sigma_1 + \sigma_2 \tag{5}$$

$$\varepsilon = \frac{1}{E}\sigma_1 \tag{6}$$

$$\dot{\varepsilon} = \frac{1}{\eta}\sigma_2 \tag{7}$$

This simplifies down to the constitutive law.

$$\sigma = E\varepsilon + \eta\dot{\varepsilon} \tag{8}$$

[28]

A creep test requires applying instantaneous stress to a viscoelastic material in equilibrium and measuring the strain over time. The material has a large strain reaction to the stress at first which becomes less over time, but viscoelastic materials keep elongating over long periods of time. A recovery/relaxation test would come next. After holding the material at a certain stress for a long time, until there looks to be equilibrium, the stress is then removed and how the material returns to its original state (relaxes) is the recovery test [1].

The Zener model or the standard linear solid is a combination of both Maxwell and kelvin models. The Maxwell model does not describe creep while the kelvin model does not describe relaxation. Thus, combining them makes a more accurate model. Usually viscoelastic models for real systems use a couple Maxwell elements in series which allows for a more accurate description of the actual mechanics. For all the parts in series the stress has to be the same, while all the parts in parallel the strain has to be the same [1].

Generalizations of the models enable large numbers of these elements to be fit to estimate the spectrum of behaviors that a material presents over a broad range of loading rates and loading times [29]. Fitting of these spectra with confidence is an ongoing challenge. This will be discussed in the final section.

Poroelasticity biphasic models associated with Biot theory

Biphasic models are based on poroelasticity. Many biological tissues are made of porous solid matrices with fluid in the pores, so as stress is applied to the material, the mechanical behavior not only depends on the solid matrix deformation but also on the movement of the fluid in and out of the pores. This type of material is very similar to viscoelastic material, so viscoelastic materials can be modeled in this way since we know the mechanical properties of the solid matrix as well as the fluid movement. It is biphasic because the solid matrix reacts immediately in one phase and the fluid is time dependent and reacts in a different phase [30], [31].

We start with some governing equations

$$\text{div}\left(\varphi^s \mathbf{v}^s + \varphi^f \mathbf{v}^f\right) = 0 \qquad \text{continuity of mass} \qquad (9)$$

$$\text{div } \boldsymbol{\sigma}^s + \boldsymbol{\pi} = \mathbf{0} \qquad \text{linear momentum for solid phase} \qquad (10)$$

$$\text{div } \boldsymbol{\sigma}^f - \boldsymbol{\pi} = \mathbf{0} \qquad \text{linear momentum for fluid phase} \qquad (11)$$

Where φ is the volume fraction and the s and f denote solid phase and fluid phase, respectively. $\mathbf{v}$ is the velocity, $\boldsymbol{\sigma}$ is the stress, and $\boldsymbol{\pi}$ is the momentum exchange [31].

$$\boldsymbol{\sigma}^s = -\varphi^s p \mathbf{I} + \boldsymbol{\sigma}^e \qquad (12)$$

$$\boldsymbol{\sigma}^f = -\varphi^s p \mathbf{I} + \boldsymbol{\sigma}^v \qquad (13)$$

Where $\mathbf{I}$ is the identity tensor, p is the fluid pressure, $\boldsymbol{\sigma}^e$ is the elastic stress of the solid phase, and $\boldsymbol{\sigma}^e$ is the viscous stress of the fluid phase. We then add the constitutive equations to get a well-posed problem.

$$\boldsymbol{\sigma}^e = \lambda_s(\text{tr}\mathbf{E})\mathbf{I} + 2\mu_s\mathbf{E} \qquad (14)$$

Where $\mathbf{E}$ is the infinitesimal strain tensor

$$E = \frac{1}{2}(\text{grad } \mathbf{u} + \text{grad}^T \mathbf{u}) \tag{15}$$

Where λ_s, μ_s are the Lamé constants of the solid matrix. The momentum exchange between the

solid and fluid phases is far greater than the momentum exchange between fluid phase molecules

alone, because of small pores which show a high resistance to fluid flow. We can assume that the

viscous stress is negligible [31].

$$\boldsymbol{\sigma}^v = 0 \tag{16}$$

The momentum exchange between the fluid and solid phases is linearly proportional to the

diffusivity drag coefficient, K, and the relative velocity between the phases

$$\boldsymbol{\pi} = K(\mathbf{v}^f - \mathbf{v}^s) \tag{17}$$

We can substitute equations 14-17 into 9-11 to get the Navier form of the governing equations

$$\text{div}(\varphi^s \mathbf{v}^s + \boldsymbol{\varphi}^f \mathbf{v}^f) = 0 \tag{18}$$

$$-\varphi^s \text{grad } p + (\lambda_s + \mu_s)\text{grad}(\text{div}\mathbf{u}) + \mu_s \nabla^2 \mathbf{u} + K(\mathbf{v}^f - \mathbf{v}^s) = \mathbf{0} \tag{19}$$

$$-\varphi^f \text{grad } p - K(\mathbf{v}^f - \mathbf{v}^s) = \mathbf{0} \tag{20}$$

Boundary conditions are needed at the interface of the biphasic mixture to be able to solve the

problem. These boundary conditions are defined with a unit outward normal vector $\mathbf{n}$. The jump

conditions across the boundary are indicated by $[[f]]$, which would be the difference of the

variable f on the positive and negative side of the interface [31].

$$[[\mathbf{v}^s]] \cdot \mathbf{n} = 0 \tag{21}$$

Solid movement at the interface must be continuous.

$$\left[[\varphi^s \mathbf{v}^s + \varphi^f \mathbf{v}^f]\right] \cdot \mathbf{n} = 0 \tag{22}$$

Mass is conserved across the boundary.

$$\left[[\boldsymbol{\sigma}^s + \boldsymbol{\sigma}^f]\right]\mathbf{n} = 0 \tag{23}$$

Traction forces are continuous across the boundary.

$$[[p]] = 0 \tag{24}$$

The fluid pressure is the same across the boundary. So basically, the boundary conditions indicate that everything is continuous across the boundary [31].

Ongoing challenges include the difficulty of fitting these models in the presence of anything other than idealized uniaxial or confined compression cases and handling the fact that biological tissues actively change cellular structure and cellular handling of fluid when stressed [32-35]. A long-term goal is to be able to learn how plant and animal cells adapt to loading through analysis of their poroelastic properties.

Spectral Methods and Tikhonov regularization

Often data can be taken discretely by measuring the stress relaxation response of a viscoelastic material. This means that researchers have the stress data but want to know the material constants such as the time spectrum and the associated young's modulus with each time constant. This requires solving the model backwards. Babaei and Rowe show how to derive the equations so that the model can input the stresses along with time stamps to solve for a spectrum of time constants and the associated modulus for each point [28], [33].

Stress response $\sigma(t)$ can be modeled using the Boltzmann superposition principal as an integral of a material response function, $\zeta(t, u)$ time the strain history. Since our material has time dependence, $\zeta(t, u) = \varphi(t - u)$. We can also assume the history starts at time 0 [28].

$$\sigma(t) = \int_0^t \varphi(t - u)\dot{\varepsilon}(u)du \tag{25}$$

We can escribe the equation in 24 as a convolution and since convolutions are commutative, we can rewrite it. Now, since most experiments are done with a constant strain rate, we can rewrite equation 24 as

$$\sigma(t) = \dot{\varepsilon} \int_0^t \varphi(u)du \tag{26}$$

If we assume that viscoelastic relaxation can be modeled as decaying exponentials the relaxation function can be modeled as

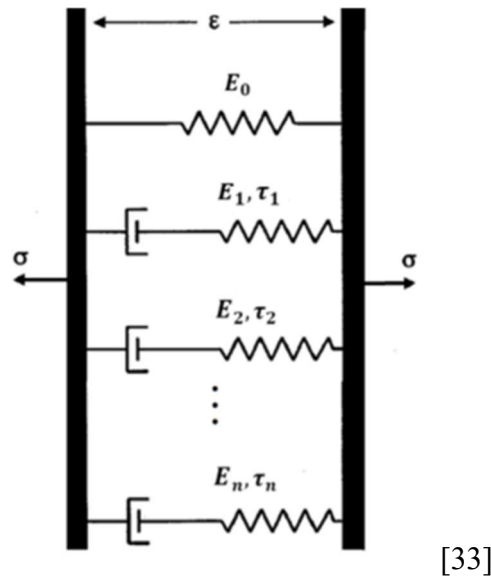$$\sigma(t) = \dot{\varepsilon} \int_0^t \left(\varphi_e + \int_0^\infty \frac{H(\tau)}{\tau} \exp\left(-\frac{t}{\tau}\right) d\tau \right) du \tag{27}$$

Unfortunately, experiments do not gather data in continuous spectra but in discreet data points. We can approximate the relaxation function using discrete Maxwell-Weichert elements

$$\varphi_e(t) \approx E(t) = E_e + \sum_{i=1}^{m} E_i \exp\left(-\frac{t}{\tau_i}\right). \tag{28}$$

Where m is the number of Maxwell elements. The following figure shows a visual representation of the equation.

[33]

When starting to solve this equation, usually there is not a clear idea of how many elements are needed. There are a couple ways of thinking about this. With the Ad hoc method, the amount of springs is specified and solved for backwards for the time constants and E, which are found by minimizing the mean squared error. This is faster, but there can be false peaks or missing information. This is better at getting the weightier time constants, but not the time constants that are really quick. This method is best if the number of peaks for the time constant are known [28].

With the discrete spectral method, τ_i is picked beforehand so that it is approximately continuous on a logarithmic scale over the full range expected. Then E is fitted to the relaxation data.

Equation 27 can be substituted in for our continuous relaxation function [28]

$$\sigma(t) = \dot{\varepsilon} \int_0^t \left(E_e + \sum_{i=1}^m E_i \exp\left(-\frac{u}{\tau_i}\right) \right) du \tag{29}$$

Usually there is a period 0 to t_p where strain is increased and then a time period where the strain

is held t_p to t_f. If we separate into two separate integrals for these time periods, we get

$$\sigma(t_j) = \begin{cases} E_0 \dot{\varepsilon} t_j + \sum_{i=1}^M E_i \tau_i \dot{\varepsilon}\left(1 - e^{-t_j/\tau_i}\right) & j = 1,2, \dots, p \\ E_0 \dot{\varepsilon} t_p + \sum_{i=1}^M E_i \tau_i \dot{\varepsilon}\left(1 - e^{-t_j/\tau_i}\right)\left(e^{-(t_j - t_p)/\tau_i}\right) & j = p, p+1, \dots, f \end{cases} \tag{30}$$

We can put this into a system of equations

$$\begin{bmatrix} \sigma_1 \\ \vdots \\ \sigma_{h-1} \\ \sigma_h \\ \vdots \\ \sigma_f \end{bmatrix} = \begin{bmatrix} \dot{\varepsilon} t_1 & a_{11} & \cdots & a_{11} \\ \vdots & \vdots & & \vdots \\ \dot{\varepsilon} t_{h-1} & a_{1(h-1)} & \cdots & a_{m(h-1)} \\ \dot{\varepsilon} t_h & b_{1h} & \cdots & b_{mh} \\ \vdots & \vdots & & \vdots \\ \dot{\varepsilon} t_f & b_{1f} & \cdots & b_{mf} \end{bmatrix} \begin{bmatrix} E_e \\ E_1 \\ \vdots \\ E_m \end{bmatrix} \tag{31}$$

where $a_{ij} = \tau_i \dot{\varepsilon}\left(1 - e^{-t_j/\tau_i}\right)$ for $i = 1,2 \dots, m$ and for $j = 1,2, \dots, h-1$; and $b_{ij} =$

$\tau_i \dot{\varepsilon}\left(1 - e^{-t_j/\tau_i}\right)\left(e^{-(t_j - t_p)/\tau_i}\right)$ for $i = 1,2 \dots, m$ and for $j = h, h+1, \dots, f$.

This means that the system of equations is of the form $\sigma \approx AE$. They are not exactly equal

because there is some error between them. To ensure finding a solution, least squares is used

[28].

$$\min_E \|AE - \sigma\|_2^2 \tag{32}$$

Our equations are continuous and discrete Fredholm integral equations of the first kind. In the

presence of noise on the left side (which all experimental data will have) a direct inversion of

this integral type leads to unbounded errors in the solution. Inverse problems are often ill-posed,

and in this case, the solution is highly sensitive to noise. The solution is not very stable.

Tikhonov regularization provides improved efficiency in parameter estimation problems in exchange for some bias. Zeroth order Tikhonov regularization can be used to penalize the length of the estimated spectra. Since we know that modulus is not limitless, we can bias our regularization parameter towards lower E [28]. The above equation is reformulated as

$$\min_{E}\{\|AE - \sigma\|_2^2 + \lambda^2\|E\|_2^2\} \tag{33}$$

where λ is the regularization parameter and controls the weighting of the penalty placed on E. The L-curve method selects a regularization parameter which balances the norm of the solution and the norm of the residuals.

Now we arrange the problem using linear algebra to allow for simple computation.

$$\min_{E}\|BE - d\|_2^2 \tag{34}$$

Where $\boldsymbol{B} = [\boldsymbol{A} \quad \lambda\boldsymbol{I}]^\mathsf{T}$ and $d = [\sigma \quad 0]^\mathsf{T}$ where $\boldsymbol{I}$ is the identity matrix.

$$d \approx \boldsymbol{B}E. \tag{35}$$

Where we use QR factorization to calculate E [28].

Conclusion

Viscoelastic responses show up in many materials. It is important to model these responses in order to better predict how materials will react to certain loads as well as learn the mechanics behind reactions.

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