

Optimization of Parameter Estimates for Nonlinear Viscoelastic Models

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Introduction: Viscoelastic Solids-Materials with Memory

- We consider the relationships between the following properties of viscoelastic solids:
 - ε -denotes strain [%].
 - σ -denotes load stress [MPa].
 - t -denotes elapsed time [hours].

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- In particular, these solids have memory in the sense that load stress applied in the past manifests as present load stress.
- For example, metals under increased temperature, composite materials such as fiberglass put under constant stress, will exhibit *creep*, that is, the strain will grow with time until the material fractures.

Graphical progression of strain with time for fixed load stress

To get an idea of how strain typically grows over time, we consider the graphs $\varepsilon \sim t$ for three fixed levels of stress:

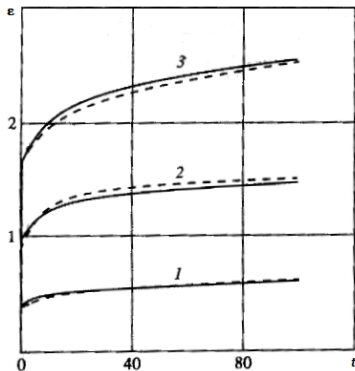


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- In practice, this models the relations between time, stress and strain successfully for a wide range of materials such as polymers, metals, and composites.

Isochronic creep diagrams $\varphi(\varepsilon(t))$

- Figure 2 gives the graphs for $\varphi(\varepsilon(t))$ for fixed t values.

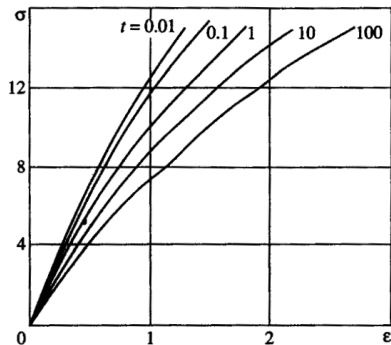


Figure: Isochronic creep diagrams

- Now, we turn to finding a suitable kernel $K(t)$.
- The most suitable kernel $K(t)$ is based on the exponential of arbitrary order function and for our purposes takes form

$$K(t) = \lambda \sum_{n=0}^{\infty} \frac{\beta^n t^{n(1-\alpha)}}{\Gamma[(1-\alpha)(n+1)]} \quad (2)$$

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- Initially, the goal of our work is to find the best way to estimate the kernel parameters $P = \{\lambda, \alpha, \beta\}$ that most accurately models the relation between stress, strain, and time with the use of (1) repeated here.

$$\varphi(\varepsilon(t)) = \sigma(t) + \int_0^t K(t-\tau)\sigma(\tau)d\tau$$

Relationship between stress, strain and time

- With the above kernel, the integral in equation (1) can be evaluated, and so (1)

$$\varphi(\varepsilon(t)) = \sigma(t) + \int_0^t K(t - \tau)\sigma(t)(\tau)d\tau$$

becomes

$$\varphi(\varepsilon(t)) = \sigma(t) \left[1 + \lambda \sum_{n=0}^{\infty} \frac{(-\beta)^n t^{(1-\alpha)(n+1)}}{\Gamma[(1-\alpha)(n+1) + 1]} \right] \quad (3)$$

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- α can be determined readily from the first term of the above infinite series (3). given as

$$\varphi(\varepsilon(t)) = \sigma(t) \left[1 + \frac{\lambda t^{(1-\alpha)}}{\Gamma[(1-\alpha) + 1]} \right] \quad (4)$$

- Using (4) and the isochronic creep diagrams given in Figure 2,

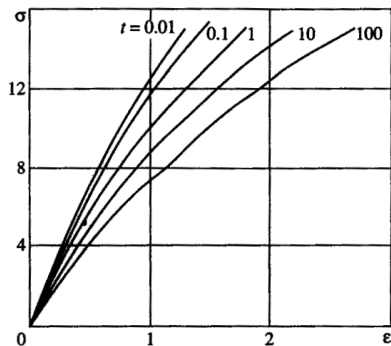


Figure: Isochronic creep diagrams

a value of $\alpha = 0.85$ is obtained in [1].

Strategy for obtaining other parameter values

Now we turn to finding the other parameters.

- We consider finding parameters for equation (3)

$$\varphi(\varepsilon) = \sigma \left[1 + \lambda \sum_{n=0}^{\infty} \frac{(-\beta)^n t^{(1-\alpha)(n+1)}}{\Gamma[(1-\alpha)(n+1) + 1]} \right]$$

that fit observed data as closely as possible.

Strategy for obtaining other parameter values

- We start by restricting to the low loading level of $\sigma = 5\text{MPa}$. (This corresponds to curve #1 in Figure 1.)

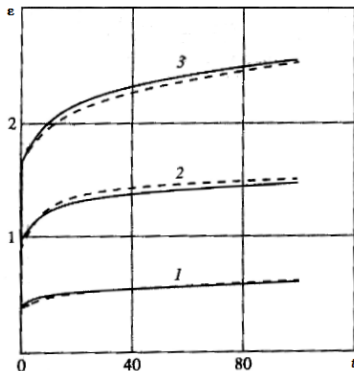


Figure: Progression of strain for three fixed levels of σ .

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- In turn, for this same loading level, ε as a function of t can be well-approximated form $\varepsilon(t) = at^b$ (Numerical results obtained: $a = 0.42$, $b = 0.079$.)
- Thus, substituting for $\varphi(\varepsilon) = E\varepsilon$, $\varepsilon = ab^t$, and $\sigma = E\varepsilon_0$, we rewrite equation (3) to get

$$at^b = \varepsilon_0 \left[1 + \lambda \sum_{n=0}^{\infty} \frac{(-\beta)^n t^{(1-\alpha)(n+1)}}{\Gamma[(1-\alpha)(n+1) + 1]} \right]$$

Strategy for obtaining other parameter values

- Now we apply the Laplace-Carson transformation to both sides of the above equation and get

$$a \frac{\Gamma(1+b)}{s^b} = \varepsilon_0 \left[1 + \frac{\lambda}{s^{1-\alpha} + \beta} \right] \quad (5)$$

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- Thus, now the question becomes one of determining parameters ε_0, λ , and β in the integral transform domain (we know α).
- The values $p = \{\varepsilon_0, \lambda, \beta\}$ obtained from (5) depend on the choice of $\Delta s = \{s_1, s_2, s_3\}$ where s_1, s_2, s_3 are non-zero complex numbers.

- For each choice of $\Delta s = \{s_1, s_2, s_3\}$, we obtain three equations of form (5) with s_i substituted for s for $i = 1, 2, 3$.

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- When s_1 , s_2 , and s_3 are fixed, these three equations can be solved for closed-form expressions for ε_0 , λ , β with a , b , and α treated as known constants.

Evaluating the choice of parameters p

- Thus, since the parameters $p = \{\varepsilon_0, \lambda, \beta\}$ depend on our choice of $\Delta s = \{s_1, s_2, s_3\}$, the optimal choice of p becomes a question of optimal choice of Δs .

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- Now, denote the most perfect model transformed from (3) by $\varepsilon[t_i, p^*]$ where the parameters p^* are the hypothetical best parameters.
- Then we can formulate our search for the optimal parameters p as the minimization of the following functional

$$F(p(\Delta s)) = \sum_{i=1}^n \left[\frac{\varepsilon[t_i, p(\Delta s)] - \varepsilon[t_i, p^*]}{\varepsilon[t_i, p^*]} \right]^2$$

over $\Delta s \in \mathbb{R}^3$ for $s_1, s_2, s_3 > 0$ and $s_1, s_2,$ and s_3 distinct. The values $\varepsilon[t_i, p^*]$ will be approximated with experimental data.

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 - With these n data points, we compare the output for the corresponding (t_i, σ_i) values obtained by substituting the parameters $p = \{\varepsilon_0, \lambda, \beta\}$ into the model

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- From (6) we obtain values for $\varepsilon[t_i, p(\Delta s)]$. With these values, we can evaluate the functional to get an idea of how well $p = \{\varepsilon_0, \lambda, \beta\}$ was chosen.

Example

- In [1], we see an example of where some value of Δs gives us $\lambda = 1.47$, $\beta = 0.13$, and $\varepsilon_0 = 0.2$. Now consider the diagrams again from Figure 1. The wellness of fit for the model with obtained parameters is shown.

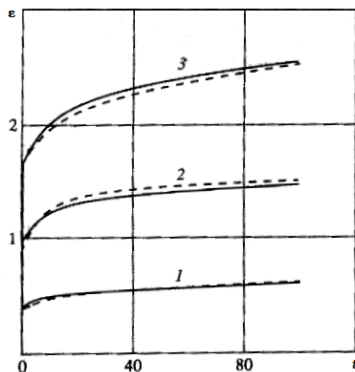


Figure: Solid lines experimental, dashed lines numerical.

Summarizing the Task of Minimization

- 1 This is constrained minimization problem over Δs .
 - 1 The only restriction is given by $\Delta s = \{s_1, s_2, s_3\} \in \mathbb{R}_{>0}^3$.
 - 2 For values Δs where any of the components approach zero, at least one of the parameters will also approach infinity, which is unrealistic.
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- 2 Even though we have closed-form expressions for $p = \{\varepsilon_0, \lambda, \beta\}$, the functional to be minimized involves an expression that is not closed form (it is an infinite sum).
- 3 Thus, we cannot simply enumerate stationary points with use of the gradient to find a global minimum. The use of an iterative algorithm is thus required.

Questions for Considerations of Optimization: Differentiability and Convexity

- Do we have gradient information for the functional

$$F(p(\Delta s)) = \sum_{i=1}^n \left[\frac{\varepsilon[t_i, p(\Delta s)] - \varepsilon[t_i, p^*]}{\varepsilon[t_i, p^*]} \right]^2$$

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- Also, is this functional that we are to minimize convex?

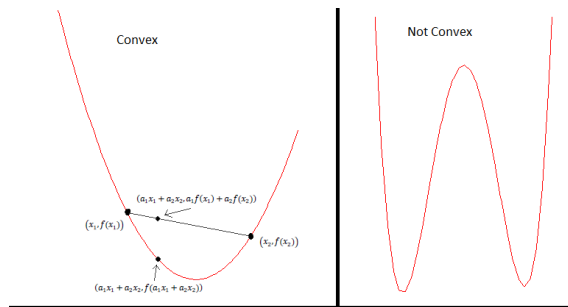
- A function f is convex if for all x in the domain, we have

$$f(a_1x_1 + a_2x_2) \leq a_1f(x_1) + a_2f(x_2) \text{ for } a_1 + a_2 = 1, a_1, a_2 \geq 0$$

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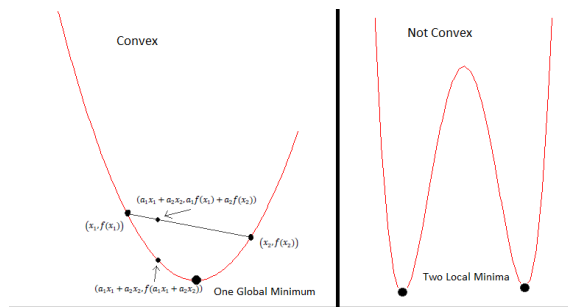
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- For functions that are convex, unconstrained minima are global, while functions that are not convex can have local unconstrained minima, not all of which are global.

- So the question becomes: Is the functional $F(\Delta s)$ that we minimize a convex function?
- Convexity theory allows us to turn this into the equivalent question: Is $\varepsilon[t_i, p(\Delta s)]$ a convex function of Δs ?

Closed form solutions for β , λ , and ϵ

$$\beta = \frac{(-s_3^{b+\alpha} s_2^{1+b} + s_3^{1+b} s_2^{b+\alpha}) s_1 + (s_3^{b+\alpha} s_1^{1+b} - s_3^{1+b} s_1^{b+\alpha}) s_2 + (-s_2^{b+\alpha} s_1^{1+b} + s_2^{1+b} s_1^{b+\alpha}) s_3}{s_3^{b+\alpha} s_2^{1+b} s_1^{\alpha} + s_2^{b+\alpha} s_1^{1+b} s_3^{\alpha} - s_2^{1+b} s_1^{b+\alpha} s_3^{\alpha} - s_3^{b+\alpha} s_1^{1+b} s_2^{\alpha} - s_3^{1+b} s_2^{b+\alpha} s_1^{\alpha} + s_3^{1+b} s_1^{b+\alpha} s_2^{\alpha}}$$

$$\lambda = -\frac{N}{M}$$

where

$$N = -s_3^{2\alpha+b} s_2^{\alpha+1} s_1^{2+2b} + s_3^{\alpha+1+b} s_2^{2+2b} s_1^{2\alpha} + s_3^{2+b} s_2^{2\alpha+2b} s_1^{\alpha+1} - s_3^{2\alpha} s_2^{\alpha+1+2b} s_1^{2+b} + \dots,$$

and

$$M = \left((s_2^{b+\alpha} s_1^{\alpha} - s_1^{b+\alpha} s_2^{\alpha}) s_3 + (s_1^{b+\alpha} s_3^{\alpha} - s_3^{b+\alpha} s_1^{\alpha}) s_2 + (s_3^{b+\alpha} s_2^{\alpha} - s_2^{b+\alpha} s_3^{\alpha}) s_1 \right) \\ \left(s_3^{b+\alpha} s_2^{1+b} s_1^{\alpha} + s_2^{b+\alpha} s_1^{1+b} s_3^{\alpha} - s_2^{1+b} s_1^{b+\alpha} s_3^{\alpha} - s_3^{b+\alpha} s_1^{1+b} s_2^{\alpha} - s_3^{1+b} s_2^{b+\alpha} s_1^{\alpha} + s_3^{1+b} s_1^{b+\alpha} s_2^{\alpha} \right)$$

$$\epsilon_0 = \frac{-a\Gamma(1+b) \left[(s_3^{b+\alpha} s_2^{\alpha} - s_2^{b+\alpha} s_3^{\alpha}) s_1 + (s_1^{b+\alpha} s_3^{\alpha} - s_3^{b+\alpha} s_1^{\alpha}) s_2 + (s_2^{b+\alpha} s_1^{\alpha} - s_1^{b+\alpha} s_2^{\alpha}) s_3 \right]}{s_3^{b+\alpha} s_2^{1+b} s_1^{\alpha} + s_2^{b+\alpha} s_1^{1+b} s_3^{\alpha} - s_2^{1+b} s_1^{b+\alpha} s_3^{\alpha} - s_3^{b+\alpha} s_1^{1+b} s_2^{\alpha} - s_3^{1+b} s_2^{b+\alpha} s_1^{\alpha} + s_3^{1+b} s_1^{b+\alpha} s_2^{\alpha}}$$

- We are especially interested in where the denominators are zero. For example, at $\{s_1, s_2, s_3\} = \{0, 0, 0\}$ or $\{s_1, s_2, s_3\} = \{1, 1, 1\}$ this would happen. (We do not allow these values anyway.)

Potential denominator zeros

- Assuming that the s_1 , s_2 , and s_3 are positive and distinct, the only possible values that can cause the above denominators to be zero are given by Maple as

$$\text{RootOf} \left(\begin{array}{l} e^{-Z+\ln(s_2)b+\ln(s_3)b+\ln(s_3)\alpha} s_2 - e^{-Z+\ln(s_3)b+\ln(s_2)b+\ln(s_2)\alpha} s_3 \\ + e^{\frac{\ln(s_3)\alpha^2 + -Z + -Z b + \ln(s_2)b\alpha + \ln(s_2)\alpha^2}{\alpha}} - e^{\frac{\ln(s_3)\alpha^2 + \ln(s_2)\alpha + \ln(s_2)b\alpha + -Z b + -Z \alpha}{\alpha}} \\ - e^{\frac{\ln(s_2)\alpha^2 + -Z + -Z b + \ln(s_3)\alpha b + \ln(s_3)\alpha^2}{\alpha}} + e^{\frac{\ln(s_2)\alpha^2 + \ln(s_3)\alpha + \ln(s_3)\alpha b + -Z b + -Z \alpha}{\alpha}} \end{array} \right) \alpha^{-1},$$

$[s_1 = e$
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and,

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- It seems possible that there will be hypersurfaces in the set of allowable $\{s_1, s_2, s_3\}$ for which at least one of the parameters is not defined, and these same places are where the gradients would not exist.

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- The (possibly two) hypersurfaces where the parameters p are not defined will for the above reason suggest that the functional $F(\Delta s)$ to be minimized is not convex.

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 - Otherwise, if we cannot see "how badly" the functional lacks convexity, a metaheuristic approach is needed such as simulated annealing or genetic algorithm.

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Thank You!