Tutorial Machine Learning in Solid Mechanics (Winter term 2022–2023)

TECHNISCHE UNIVERSITÄT DARMSTADT

Cyber-Physical Simulation TU Darmstadt

Task 4: Viscoelasticity

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In Task 2 + 3 of this tutorial, neural networks were used to model hyperelastic material behavior. In the framework of hyperelasticity, energy is conserved, i.e., no energy is dissipated. This is a strong assumption, as inelastic effects are not considered in this framework. A very important class of inelasticity is viscoelasticity, which is used, e.g., in rubber dampers, and includes time-dependence of the stress-strain relation [4].

In the last task of this tutorial, viscoelastic material behavior is modelled. While in the previous task we described material behavior in three dimensions, here the model is restricted to 1D. This last task gives an outlook on another class of neural networks, namely: Recurrent Neural Networks (RNNs) [1], as well as their usage for the modeling of inelastic material behavior.

1 Theory

1.1 Second law of thermodynamics

The second law of thermodynamics is one of the most important physical conditions that a constitutive model should fulfill. It is also referred to as Clausius-Duhem inequality. In the one-dimensional, purely mechanical case, the Clausius-Duhem inequality is given by

$$\sigma\,\dot{\varepsilon} - \dot{e} \geq 0 \tag{1}$$

with the strain ε, the stress σ and the internal energy e. Here, $\dot{a} = \frac{\partial a}{\partial t}$ denotes the time derivative of a. Eq. (1) states that the energy dissipation is always non-negative. In the following, we consider energy functions $e = e(\varepsilon, \gamma)$, which depend on the strain ε, as well as on an internal variable γ, which will be further specified in Sec. 1.2. Then, the Clausius-Duhem inequality is given by

$$\begin{aligned} &\sigma\,\dot{\varepsilon} - \frac{\partial e(\varepsilon,\,\gamma)}{\partial \varepsilon}\dot{\varepsilon} - \frac{\partial e(\varepsilon,\,\gamma)}{\partial \gamma}\dot{\gamma} \geq 0 \\ &\qquad\qquad \Leftrightarrow \\ &\left(\sigma - \frac{\partial e(\varepsilon,\,\gamma)}{\partial \varepsilon}\right)\dot{\varepsilon} - \frac{\partial e(\varepsilon,\,\gamma)}{\partial \gamma}\dot{\gamma} \geq 0\,. \end{aligned} \tag{2}$$

From the left bracket in Eq. (2) follows the constitutive equation for the stress

$$\sigma = \frac{\partial e(\varepsilon,\,\gamma)}{\partial \varepsilon}\,, \tag{3}$$

while the right bracket yields the dissipation inequality

$$\mathcal{D} = -\frac{\partial e(\varepsilon,\,\gamma)}{\partial \gamma}\dot{\gamma} \geq 0\,. \tag{4}$$

In the case of purely elastic material behavior, the energy only depends on ε. Then, there is no energy dissipation, i.e., $\mathcal{D} = 0$, and the stress is given as the gradient of the energy e w.r.t. the strain ε, cf. Eq. (3). Generalizing this approach to three dimensions, the stress relation for hyperelasticity can be derived.

1.2 Maxwell model

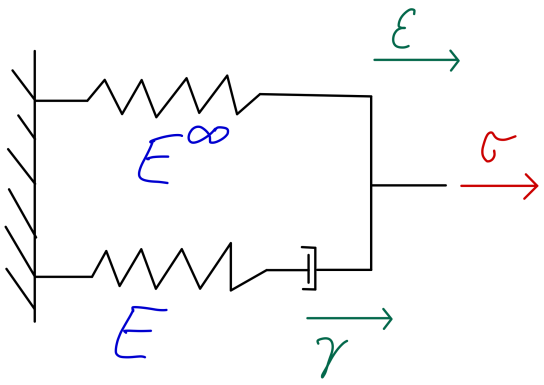

Figure 1: Generalized Maxwell model

The choice of the internal variable γ and the functional relationship of e in (ε, γ) depends on the class of inelasticity that is considered. In the case of viscoelasticity, both can be motivated by the *generalized Maxwell model*, see Fig. 1. Here, an *equilibrium spring* with stiffness $E^\infty > 0$ is in parallel to a series connection of a *non-equilibrium spring* with stiffness $E > 0$ in series with a *damper*. Here, ε denotes the overall strain acting on the system, while the internal variable γ denotes the strain acting on the damper. Consequently, the strain $(\varepsilon - \gamma)$ acts on the non-equilibrium spring. The overall stress σ is composed of both the stress acting in the equilibrium spring and the stress acting in the series connection of spring and damper. Energy is stored in both the equilibrium and the non-equilibrium spring, leading to the overall energy

$$e = \frac{1}{2} E^\infty \varepsilon^2 + \frac{1}{2} E (\varepsilon - \gamma)^2 \,. \tag{5}$$

With Eq. (3), the stress follows as

$$\sigma = E^\infty \varepsilon + E(\varepsilon - \gamma) \,, \tag{6}$$

while Eq. (4) yields the dissipation inequality as

$$\mathcal{D} = E(\varepsilon - \gamma)\dot{\gamma} \geq 0 \,. \tag{7}$$

Up to this point the system of constitutive equations is not closed, as the behavior of the internal variable γ is not yet specified. More explicit, we require the additional evolution equation

$$\dot{\gamma} = f(\varepsilon, \gamma, \dot{\gamma}) \,. \tag{8}$$

This evolution equation has to be chosen in such a way that the it complies with the dissipation inequality Eq. (7). Two different approaches to close the equations derived by the Maxwell model are now discussed.

1.2.1 Define the stress behavior of the damper

Assuming that the damper behaves like a Newtonian fluid, its stress is given by

$$\sigma^{\text{damper}} = \eta \, \dot{\gamma} \,, \tag{9}$$

where $\eta > 0$ is an additional material parameter which we call viscosity. From the series connection of the non-equilibrium spring and the damper we conclude that $\sigma^{\text{damper}} = \sigma^{\text{non-equilibrium}}$, which yields

$$\begin{aligned} \eta \, \dot{\gamma} &= E(\varepsilon - \gamma) \\ &\Leftrightarrow \\ \dot{\gamma} &= \frac{E}{\eta}(\varepsilon - \gamma) \,, \end{aligned} \tag{10}$$

where $\sigma^{\text{non-equilibrium}}$ directly follows from Eq. (6). Note that in this case, the model only depends on the material parameters (E^∞, E, η). This choice clearly fulfills the dissipation inequality as

$$\mathcal{D} = \frac{E^2}{\eta}(\varepsilon - \gamma)^2 \geq 0 \,. \tag{11}$$

1.2.2 Define an evolution equation

In Sec. 1.2.1, the evolution equation is a linear and increasing function in $(\varepsilon - \gamma)$. Generalizing Eq. (10) to nonlinear functional relationships yields the evolution equation

$$\dot{\gamma} = \tilde{f}(\varepsilon, \gamma)(\varepsilon - \gamma), \qquad \tilde{f}(\varepsilon, \gamma) > 0\,. \tag{12}$$

Inserting this evolution equation in the dissipation inequality Eq. (7) yields

$$\mathcal{D} = \tilde{f}(\varepsilon, \gamma)(\varepsilon - \gamma)^2 E \geq 0\,, \tag{13}$$

which is clearly fulfilled. Note that we dismissed the dependency of f in $\dot{\gamma}$, see Eq. (8), in order to arrive at an explicit formulation for the evolution equation. From this, we can receive the first approach of Sec. 1.2.1 by setting

$$\tilde{f}(\varepsilon, \gamma) = \frac{E}{\eta} = \text{const}\,. \tag{14}$$

1.3 Generalized standard materials

Now, the constitutive model is no longer motivated by the generalized Maxwell model, but is derived from the more general framework of *Generalized Standard Materials* (GSM), see [2] for an introduction. Here, we consider the energy in its most general form $e = e(\varepsilon, \gamma)$, without making any further assumption on its functional relationship. Again, the stress is given by Eq. (3). Here, we choose the evolution equation for the internal variable as

$$\dot{\gamma} = -g(\varepsilon, \gamma)\frac{\partial e(\varepsilon, \gamma)}{\partial \gamma}, \qquad g(\varepsilon, \gamma) > 0\,, \tag{15}$$

with which the Clausius-Duhem inequality is fulfilled by construction. We can again receive the first approach of Sec. 1.2 by setting e as in Eq. (5), which yields

$$\frac{\partial e(\varepsilon, \gamma)}{\partial \gamma} = -E(\varepsilon - \gamma)\,, \tag{16}$$

and setting $g := \eta^{-1} = \text{const}$. In the following tasks, consider g as this constant.

Proof. The GSM framework is based on the energy potential $e = e(\varepsilon, \gamma)$ in addition with a so-called dissipation potential $\phi = \phi(\varepsilon, \gamma, \dot{\gamma})$ [2]. Here, we use the dissipation potential

$$\phi(\varepsilon, \gamma, \dot{\gamma}) = \frac{1}{2g(\varepsilon, \gamma)}\dot{\gamma}^2, \quad g(\varepsilon, \gamma) > 0\,. \tag{17}$$

For GSM models, the additional constitutive relation

$$\frac{\partial e(\varepsilon, \gamma)}{\partial \gamma} + \frac{\partial \phi(\varepsilon, \gamma, \dot{\gamma})}{\partial \dot{\gamma}} = 0\,, \tag{18}$$

is introduced, with which the Clausius-Duhem inequality is fulfilled, see Eq. (4). In particular, for the explicit choice of ϕ as in Eq. (17), it holds that

$$\mathcal{D} = -\frac{\partial e(\varepsilon, \gamma)}{\partial \gamma}\dot{\gamma} = \frac{\partial \phi(\varepsilon, \gamma, \dot{\gamma})}{\partial \dot{\gamma}}\dot{\gamma} = \frac{1}{g(\varepsilon, \gamma)}\dot{\gamma}^2 \geq 0\,, \tag{19}$$

Furthermore, Eq. (18) also implies the evolution equation for γ as

$$\frac{\partial e(\varepsilon, \gamma)}{\partial \gamma} + \frac{1}{g(\varepsilon, \gamma)}\dot{\gamma} = 0 \qquad \Leftrightarrow \qquad \dot{\gamma} = -g(\varepsilon, \gamma)\frac{\partial e(\varepsilon, \gamma)}{\partial \gamma}\,. \tag{20}$$

□

2 Tasks

For the following tasks, data was generated by applying the harmonic oscillation

$$\begin{aligned} \varepsilon(t) &= A\sin(\omega t) \\ \dot{\varepsilon}(t) &= A\,\omega\cos(\omega t) \end{aligned} \tag{21}$$

for $t \in [0, 2\pi]$ on a Maxwell element as described in Sec. 1.2.1, where the parameters are set to $\{E^\infty, E, \eta\} = \{0.5, 2, 1\}$ [3, Table 1], see Fig. 2. In addition, relaxation tests with different amplitudes are applied. For the relaxation tests, the strain as in Eq. (21) is applied until the first maximum of ε is reached, and is then fixed, see Fig. 3.

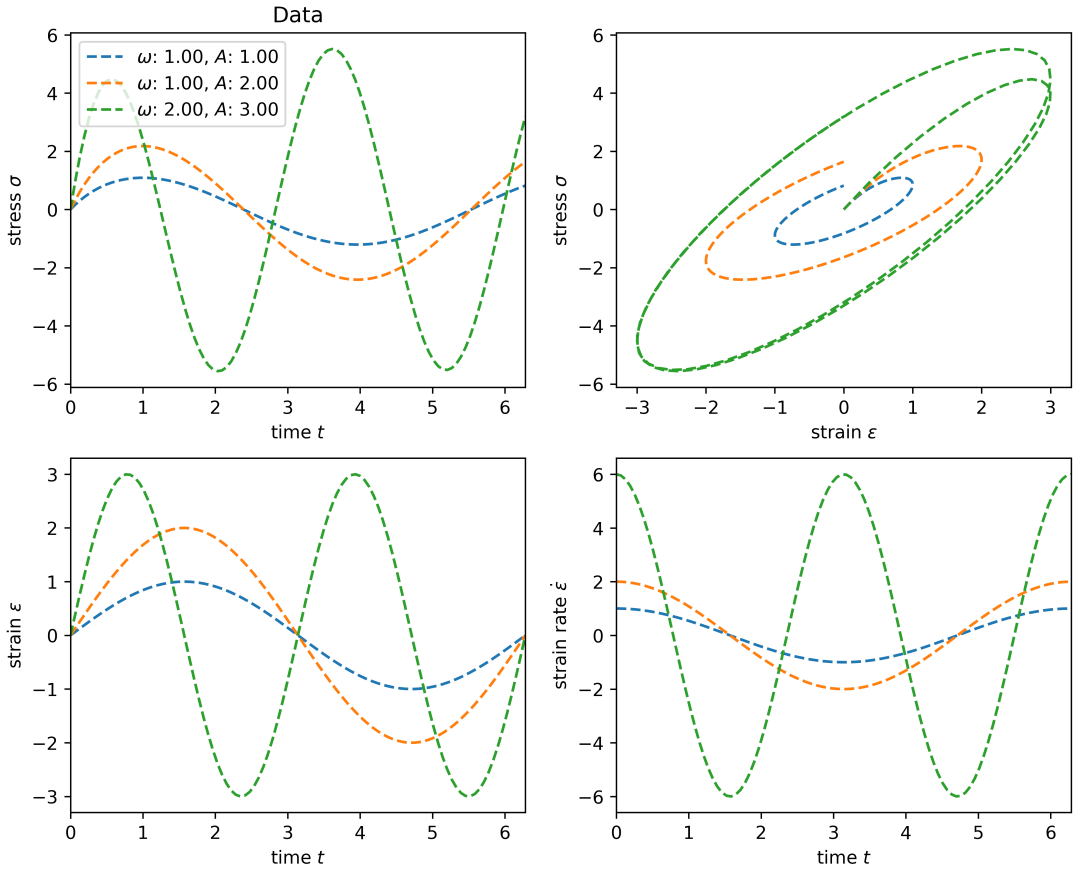

Figure 2: Data for harmonic oscillations.

After solving the following tasks, answer these questions:

- Which of the models are able to interpolate / extrapolate to the given data?
- Which load paths do you have to use for a good model generalization?
- What is the difference between the different models?
- What happens if you use other values for (A, ω) for calibration / test of the models?
- In what way is physics included in the models?

2.1 Simple RNN

Visit the GitHub repository CPShub/TutorialMLinSolidMechanics and go to the folder "04_viscoelasticity". Run the main file. This imports and visualizes the data generated with the harmonic oscillation, see Eq. (21), for arbitrary (A, ω). For the following investigations, set $(A, \omega) \in \{(1,1),(1,2),(2,3)\}$. For each of the following model calibrations, use different load paths for the calibration dataset and the rest for the test dataset.

Furthermore, running the main file imports and calibrates a "naive" RNN which does not include any physical information. Investigate the code of this RNN. Is the model able to interpolate / extrapolate the different cases?

2.2 Maxwell model – prescribed evolution equation

Implement the Maxwell model described in Sec. 1.2.1, using the parameters introduced above. This model is not trainable, as all functional relationships and parameters are fixed. For the solution of the evolution equation, see Eq. (10), use an explicit Euler scheme:

$$\gamma_{n+1} = \gamma_n + h_n \, \dot{\gamma}_n = \gamma_n + h_n \, \frac{E}{\eta} (\varepsilon_n - \gamma_n) \, . \tag{22}$$

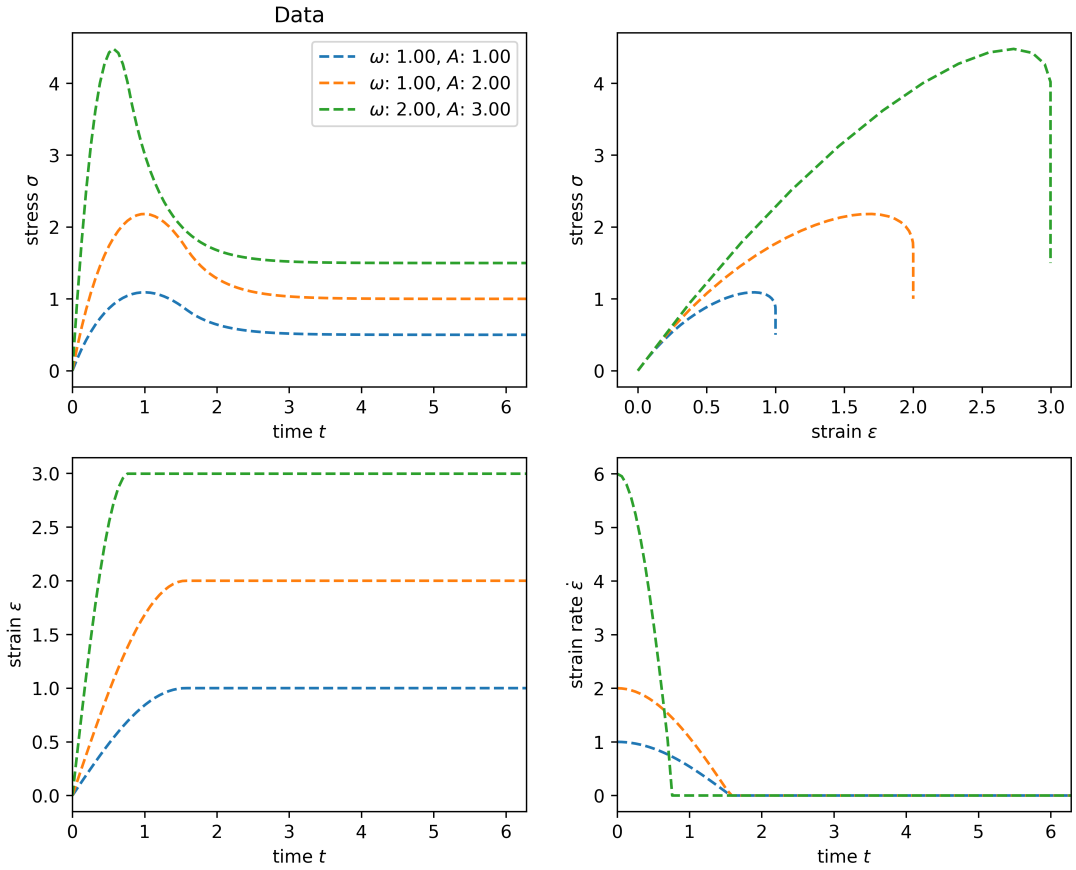

Figure 3: Relaxation data.

Here, $\gamma_n = \gamma(t_n)$, $t_{n+1} = t_n + h$, and the initial value is given by $\gamma_0 = 0$. Implement this model in TensorFlow by adapting the RNN from Sec. 2.1. Check your implementation with the data provided in the GitHub repository.

2.3 Maxwell model – evolution equation is modelled as a FFNN

Implement the Maxwell model discussed in Sec. 1.2.2. Now, the evolution equation is not fixed but a function, see Eq. (12). Model the evolution equation by using a feed-forward neural network (FFNN). Calibrate the model by using different combinations of load paths as calibration data, and use the remaining load paths as test data.

2.4 GSM model

Implement the GSM model as described in Sec. 1.3. For this, set $g := \eta^{-1} = \text{const}$, with the value for η as introduced above. Use a FFNN to represent the energy function $e = e(\varepsilon, \gamma)$, and calculate the derivatives by using "GradientTape".

References

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[2] A. Kumar and O. Lopez-Pamies. "On the two-potential constitutive modeling of rubber viscoelastic materials". In: *Comptes Rendus Mécanique* 344.2 (2016), pp. 102–112. DOI: 10.1016/j.crme.2015.11.004.

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