Formulation of the Neural Network for Implicit Constitutive Model (I) : Application to Implicit Viscoelastic Model

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Abstract

Up to now, a number of models have been proposed and discussed to describe a wide range of inelastic behaviors of materials. The fatal problem of using such models is however the existence of model errors, and the problem remains inevitably as far as a material model is written explicitly. In this paper, the authors define the implicit constitutive model and propose an implicit viscoplastic constitutive model using neural networks. In their modeling, inelastic material behaviors are generalized in a state space representation and the state space form is constructed by a neural network using input-output data sets. A technique to extract the input-output data from experimental data is also described. The proposed model was first generated from pseudo-experimental data created by one of the widely used constitutive models and was found to replace the model well. Then, having been tested with the actual experimental data, the proposed model resulted in a negligible amount of model errors indicating its superiority to all the existing explicit models in accuracy.

Key Words : Viscoplasticity, Implicit Constitutive Model, Inelastic Behaviors, Multilayer Neural Network, Explicit Model

1. Introduction

There has been an accelerating rate at which various solids and structures were developed to assist the objective of industrial designers. Because of the complexity of material behavior, a great number of inelastic constitutive models have been developed accordingly[1-3]. Inelastic material models proposed so far can be classified into two types[4]. In the first type, the model is expressed only in terms of observable variables, although it is limited in its descriptive ability[5]. The second type of model has not only observable variables but also variables representing material internal behaviors[6-8].

The significant problem involved with such models is however that the models contain errors inevitably, as they are based on simple phenomenological investigations of material properties while real behaviors of material are very complex. Up to now, researchers rather have attempted to overcome this problem by either introducing higher-performance models or better parameter identification techniques [9-11]. However, they do not tackle the substance of the problem since any model is limited by the capability of their mathematical description, i.e., the model is written explicitly.

Therefore, in this paper, the authors first define the implicit constitutive model in contrast to all conventional constitutive models, and then propose an implicit viscoplastic model using neural networks based on the state space method.

The state space representation of the proposed technique enables the description of dynamical or viscoplastic behaviors of materials, and the use of neural networks as a universal function approximator allows us to simulate the behaviors accurately.

2. Multilayer Neural Network

The multilayer feedforward neural network has been proven rigorously to be a universal function approximator for any bounded square integral function of many variables[12]. Mathematically consider a function $\psi : X \subseteq \mathbb{R}^n \rightarrow Y \subseteq \mathbb{R}^m$, from a bounded subset of $\mathbb{R}^n$ to a bounded subset, $\psi(X)$ of $\mathbb{R}^m$ where the function is unknown but is assumed to be in $L^2$. Given sufficient input-output data $[x_j, \psi(x_j)]$, often called as training patterns or training data, the neural network, as an approximation function, is determined by the well-known backpropagation algorithm as if the objective function

$$\min \sum \left\| \psi (x_j) - \Phi (x_j) \right\|^2$$

was achieved where $x_j \in \mathbb{R}^n$ is the input to the function. The network is then used for feedforward computation with various inputs. Such training of the network is normally depicted by the block diagram shown in Fig. 1.

The schematic diagram of the internal structure of the neural network is shown in Fig. 2. The network consists of the input layer, hidden layers and output layer, each having a number of units, depicted as circles. Each unit is connected to units in the neighboring layer with a weight, shown as a line in the figure. The actual neural network is thus parameterized by a set of weights $W$, and in conventional backpropagation training, the objective substantially turns out to be:
\[
\min \sum \left| \Psi(X^0, W) - \Psi(X^k) \right|^2.
\]

(2)

Where \( X^0 = X_i \) is the input to the network while \( \Psi(X^k, W) = X^k = Y_i \in \mathbb{R}^n \) is the output, represented by a K layer network.

Plastic deformations can occur only when certain combinations of stresses defined by the yield condition are reached. The coefficients appearing with the stress and strain components in the constitutive equations for plastic materials are not material constants; they depend upon the instantaneous state of stress or strain. The plastic deformations accumulate during the loading process. They are path-dependent, but do not depend on time.

Viscous deformations can occur at any level of stress. The coefficients appearing with the stress and strain components in the constitutive equations of viscous materials are material constants: they do not depend upon the instantaneous state of stress or strain. The development of viscous deformation is a function of time; hence, viscous materials are time-dependent. An important phenomenon of viscous materials is that they display greater resistance against deformations with higher rates. In addition, viscous deformations development at a constant state of stress and the stresses change at a constant state of strain. In both cases, the time variation is strains and stresses are uniquely defined by the viscous constitutive equations.

In the unified theory capable of describing cyclic loading and viscous behavior[3], the time-dependent effect is unified with the plastic deformations as a viscoplastic term, i.e.,

\[
\varepsilon = \varepsilon^p + \varepsilon^v = \varepsilon^p + \varepsilon^{vp},
\]

(1)

where \( \varepsilon^p \) and \( \varepsilon^{vp} \) represent the viscous and viscoplastic strains respectively.

Chaboche's model [2], a popular viscoplastic model, uses this flow rule and, under stationary temperature condition, has the form together with the kinematic and isotropic hardening rules:

\[
\varepsilon^v = \left(\frac{\sigma - Z}{K}\right) \text{sgn}(\sigma - Z),
\]

(2a)

\[
\dot{\varepsilon} = H\varepsilon^p - D\varepsilon^{vp},
\]

(2b)

\[
\dot{\varepsilon}^p = \frac{d\varepsilon^p}{dt} - d\varepsilon^{vp},
\]

(2c)

where \( K, n, H, D, h, d \) are material parameters and the notation \( \langle \rangle \) becomes zero if the value inside is negative. The dynamics of the equations can be uniquely specified by giving the initial conditions of the variables:

\[
\varepsilon^v \bigg|_{t=0} = \varepsilon^0_v,
\]

(3a)

\[
A_n = \dot{\varepsilon}_n,
\]

(3b)

\[
R_{t=0} = R_0.
\]

(3c)

In the case of reverse cyclic loading with constant strain limits and rates as shown in Fig. 3(a), which is of concern in the paper, we know the initial condition of strain

\[
\varepsilon^v \bigg|_{t=0} = \varepsilon_0^v.
\]

(4)

and the strain rate

\[
\dot{\varepsilon} = \begin{cases} 
\varepsilon_0^v & \text{for } 2(n+1)t \leq \langle (2n+1)\rangle \\
-\varepsilon_0^v & \text{for } (2n+1)t \leq \langle (2n+1)\rangle, \quad n=0,1,....
\end{cases}
\]

(5)

These first allow us to know the time history of strain \( \varepsilon \) iteratively

\[
\varepsilon_{k+1} = \varepsilon_k + \Delta t \cdot \dot{\varepsilon}_k.
\]

(6)

The initial stress is thus derived from Eqs. (3) and (4)

\[
\sigma \bigg|_{t=0} = E \left( \varepsilon_k - \varepsilon_0^{vp} \right).
\]

(7)

The next states of the viscoplastic strain, back stress and drag stress, and their next state can be then derived after their rate of change has been computed by Eqs. (8):

\[
\dot{\varepsilon}^{vp}_{k+1} = \dot{\varepsilon}^{vp}_k + \Delta t \cdot \dot{\varepsilon}^{vp}_k
\]

(8a)

\[
\dot{X}_k + 1 = \dot{X}_k + \Delta t \cdot \dot{X}_k
\]

(8b)

\[
\dot{R}_k + 1 = \dot{R}_k + \Delta t \cdot \dot{R}_k
\]

(8c)
We can also derive the next state of stress $\sigma_{k+1}$ through Eqs. (6) and (8a):

$$\sigma_{k+1} = E(e_{k+1} - e_{k+1}^{vp})$$  \hspace{1cm} (9)

and the repetition of Eqs. (8) and (9) enables us to carry out the whole computer simulation. The stress-strain curve, general input-output data used to show the performance of material constitutive models is shown in Fig. 3(b).

Chaboche’s model explained here is suited for inelastic material characteristics in a wide range as one of the best models although is not very appropriate to describe the tensile behavior.

### 4. Neural Constitutive Modeling

#### 4.1 Explicit and Implicit Constitutive Models

Having a look at conventional constitutive models described in the last section, we can define explicit and implicit constitutive models as follows:

**Definition - Explicit constitutive models**

Let $x$ and $a$ be a set of variables and material parameters respectively and $\varphi$ the model equations. Note here that $x$ includes both the input and output variables. In the case of material models, input variables are viscoplastic strain $e^{vp}$ and material internal variables $\xi$, and the output variable is $\sigma$. Explicit constitutive models are then given by

$$\dot{x}(x; a) = 0$$  \hspace{1cm} (10)

where $\Phi^T = [e^{vp} \xi^T]$ has an explicit expression.

In implicit constitutive models, model equations $\varphi$ ideally has no explicit expressions:

$$\Phi(x) = 0,$$  \hspace{1cm} (11)

thus containing no material parameters. Implicit constitutive models are henceforth constructed only from the input-output data without any analytical investigations.

Conclusively, the advantage of explicit constitutive models is that they can be easily developed if their mechanics are clear. On the other hand, implicit constitutive models have their potential if their mechanics are unknown but input-output data are obtainable.

#### 4.2 State Space Representation of Viscoplastic Models

The idea of state space comes from the state-variable method of describing differential equations. In this method, dynamical systems are described by a set of first-order differential equations in variables called the "state", and the solution may be visualized as a trajectory in space. The method is particularly well suited to performing calculations by computer.

Use of the state-space approach has often been referred to as modern control theory[13], whereas use of transfer-function based methods such as root locus and frequency response have been referred to as classical control design. Advantage of state-space design are especially apparent when engineers design controllers for systems with more than one control input or more than one sensed output. A further advantage of state-space design is that the system representation provides a complete internal description of the system, including possible internal oscillations or instabilities that might be hidden by inappropriate cancellations in the transfer-function (input/output) description.

The motion of any finite dynamic system can be expressed as a set of first-order ordinary differential equations. This is often referred to as the state-variable representation. In general, a nonlinear dynamic system is given by

$$\dot{x} = \psi(x, u; a)$$  \hspace{1cm} (12a)

with initial conditions:

$$x|_{t=0} = x_0$$  \hspace{1cm} (12b)

where $x \in \mathbb{R}^n$ is a set of $n$ state variables and $u \in \mathbb{R}^r$, known for all $r$ is a set of $r$ control inputs. $\psi: \mathbb{R}^n \times \mathbb{R}^r \rightarrow \mathbb{R}^n$ is assumed to be continuously differentiable with respect to each of its arguments.

In sanction with the state space method, so as to describe dynamics or viscoplasticity in constitutive models, explicit models are thus defined with the explicit equations $\Psi$:

$$\dot{x} = \psi(x, u; a)$$  \hspace{1cm} (13)

Meanwhile, implicit viscoplastic constitutive models are expressed with implicit mapping $\Psi$:

$$\dot{x} = \psi(x, u)$$  \hspace{1cm} (14)
4.3 Generalization of Viscoplastic Constitutive Models and Neural Network Constitutive Models

The state space representation of viscoplastic models described in the last section renders us possible to construct the viscoplastic constitutive models in a general fashion. Let the viscoplastic strain, internal variables, stress and material parameters be $\varepsilon_V$, $\xi$, $\sigma$ and $a$ respectively, the generalized form of explicit constitutive model may be written as

\begin{align}
\dot{\varepsilon}_V &= \dot{\varepsilon}_V (\varepsilon_V, \xi, \sigma, a), \\
\dot{\xi} &= \dot{\xi} (\varepsilon_V, \xi, \sigma, a).
\end{align}

(15a)

(15b)

It can be seen that a number of existing explicit models have similar representations. The generalized implicit constitutive model can thus have the form:

\begin{align}
\sigma &= \sigma (\varepsilon_V, \xi, \sigma), \\
\xi &= \xi (\varepsilon_V, \xi, \sigma).
\end{align}

(16a)

(16b)

Note here that internal variables can be the back and drag stresses or anything else, depending on material behavior to be described.

Considering the state space method, we can find that the viscoplastic strain and internal material variables correspond to the state variables whereas the stress acts as a control input. The dynamics of the models can be hence uniquely specified by giving the initial conditions of the state variables:

\begin{align}
\varepsilon_V |_{t=0} &= \varepsilon^{0}_V, \\
\xi |_{t=0} &= \xi^0,
\end{align}

and the control input $\sigma$, for all $t$. The viscoplastic strain and internal variables can be simulated through the discretised integration scheme:

\begin{align}
\varepsilon^{k+1}_V &= \varepsilon^{k}_V + \Delta t \cdot \dot{\varepsilon}_V^k, \\
\dot{\xi}^{k+1} &= \dot{\xi}^{k} + \Delta t \cdot \dot{\xi}^k.
\end{align}

(18a)

(18b)

Control inputs of dynamical systems should be known for all $t \ a \ priori$, normally being independent of the state variables, but the control input of the viscoplastic material is the stress and is therefore derived from the state variables iteratively, i.e., the next state of stress $\sigma_{k+1}$ can be derived from the current stress $\sigma_k$, first computing the initial stress:

\begin{align}
\sigma |_{t=0} &= \sigma^0, \\
\sigma_{k+1} &= \sigma_k + \Phi(\sigma_k).
\end{align}

(19a)

(19b)

The derivation of $\sigma_{k+1}$ is explained in Section 3.2. In accordance to the fact that state space forms in various applications have been successfully learned by neural networks, we propose a neural network constitutive model where the neural network learns the mapping $\dot{\varepsilon}$ and $\dot{\xi}$. The architecture of the proposed model is shown in Fig. 4. The model inputs the current viscoplastic strain, internal variables and stress, outputting the current rate of change of viscoplastic strain and internal variables. As an example, if two internal variables of back and drag stresses are chosen as in Chaboche’s model, the proposed model is composed of four inputs and three outputs. The block for training the model is illustrated in Fig. 5.

5. Examples

The performance of the proposed neural network is investigated using pseudo-experimental data created by computer. As an example, the neural network was determined to use tow internal variables, the back stress $Y$ and the isotropic hardening variable $R$, which are used in Chaboche’s model. The network hence is composed of four inputs and three outputs as depicted in Fig. 6.
Chaboche’s model as well. Hence the same internal variables were used, and thus we can directly investigate the performance of the network to learn each model equation.

Material parameters used to create training and validation data are listed in Table 1. The number of training were 307, and they were regularly taken from the first five cycles of a reverse cyclic loading test with a constant strain rate, parameters of which are listed in Table 2. Each validation data was plotted in the center of two neighboring training data. The stress-strain representation of the training data and validation data is indicated in Fig. 7, while Figs. 8 and 9 show the strain and stress training data with respect to time respectively. Two hidden layers each with six units were placed between the input and output layers.

Table 1. Material parameters to create training and validation data

<table>
<thead>
<tr>
<th>K</th>
<th>n</th>
<th>H</th>
<th>D</th>
<th>h</th>
<th>R0</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>3</td>
<td>5,000</td>
<td>100</td>
<td>300</td>
<td>50</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Table 2. Parameters of the reverse cyclic loading test

<table>
<thead>
<tr>
<th>εmax %</th>
<th></th>
<th>No. of training sets</th>
<th>No. of validation sets</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.036</td>
<td>5,000</td>
<td>307</td>
<td>306</td>
</tr>
</tbody>
</table>

Fig. 7 Stress-strain curve of training and validation data for the constitutive neural network

Fig. 8 Strain data for training the constitutive neural network

Fig. 9 Stress data for training the constitutive neural network

The error development of the training and validation sets until 10,000 trainings is shown in Fig. 10. Clearly, the error is approaching to zero, indicating that the neural network is learning the material law.

Fig. 10 Error development of training and validation data

Now that we found the proposed network could reproduce the training data, we will investigate the interpolative and extrapolative of the network. Also, with strain range ±0.025%, we found that the neural network have a good agreement with the exact curve in the previous study[14].

A similar material behavior to the exact curve by Chavoche’s model is also obtained ±0.040%, as shown in Figs. 11-13, though the range exceeds that of the training data. This result indicates that the neural network can create a curve similar to the exact curve extrapolatively is the extrapolation is adjacent. However, the peak of the second cycle of back stress shows large errors, indicating that there is no guarantee in extrapolation.
6. Conclusions

The implicit constitutive model has been defined and an implicit viscoplastic model using neural networks has been proposed in this paper. The proposed model, based on the state space method, has the inputs of the current viscoplastic strain, internal variables and stress and the outputs of the current rates of change of the viscoplastic strain and material internal variables.

The proposed model was trained using input-output data generated from Chaboche's model, and could reproduce the original stress-strain curve. In addition, the model demonstrated the ability of interpolation by generating untrained curves. It was also found that the model can extrapolate in close proximity to the training data although it is not extrapolatively precise to a large extent. Therefore, the proposed model can replace Chaboche's model completely by its interpolative capability if a variety of training data with different conditions are used.

References


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