Innovative approaches for modelling of inelastic material behaviours (applications of neural networks and evolutionary algorithms)

G. Yagawa, S. Yoshimura, H. Okuda, T. Furukawa
School of Engineering, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan

Abstract

This paper presents two approaches for the modelling of inelastic constitutive properties, each using a neural network or an evolutionary algorithm. In the first approach, two techniques are proposed to identify the parameter set of an existing constitutive model. One is to use evolutionary algorithms as an optimization method to minimize errors between the measured data and the corresponding data computed. In the other technique, a neural network is used as a parameter estimator given measured data as input. In the second approach, two neural networks are used as a mapping for the inelastic behavior of materials. These approaches were tested with the actual experimental data under uniaxial loading and stationary temperature and the results of the test show the effectiveness of the approaches.

1 Introduction

In many industrial fields, materials are often used under severe operating conditions such as cyclic loading, high temperature, high pressure and high irradiation, for example, if they are used as pressure vessels and pipes of a nuclear plant. For the reliable evaluation of deformation behaviors of these materials, thermo-inelastic analysis is indispensable. A variety of theoretical models to describe a wide range of viscoplastic behaviors of metallic materials have been proposed and discussed in the referenced literature\textsuperscript{1-5}. Viscoplastic constitutive equations derived from these theories are written explicitly involve many parameters, which significantly influence the behaviors of the constitutive equations. Appropriate parameters must be determined accordingly such that the accurate behaviors of materials can be expressed. Problems involved with such models
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are that:

(i) It is difficult to determine the parameters if the model of concern is complex.

(ii) The models are simply based on the phenomenological investigation of material properties. Therefore, the model contains errors inevitably.

This paper describes two approaches for the modelling of inelastic constitutive properties, each using a neural network (NN) or an evolutionary algorithm (EA). In the first approach, two techniques are proposed to identify the parameter set of an existing constitutive model. One is to use EAs as an optimization method to minimize errors between the measured data and the corresponding data computed\(^6\). The advantage of the technique is that the stable solution can be obtained even if the model is not accurate and the measurement data are subject to errors. An EA, which can search for a potential solution efficiently, is used\(^7\). In the other technique, an NN is used as a parameter estimator given measured data as input\(^8\). The NN is first trained by a set of data prepared by a number of computer simulations. The parameter set is then estimated by inputting the measured data to the trained network.

In the second approach, two NNs are used as a mapping for the inelastic behavior of materials\(^9\). First, experimental stress-strain data are decomposed to data of the drag and back stresses, and these data are each used to train and NN. The trained NNs then create the experimental stress-strain curve. This approach can significantly reduce the model errors, compared to conventional inelastic constitutive models.

In the next section, the inelastic constitutive equation is described in a general form and Chaboche’s model\(^4\) is introduced as an example for an inelastic material law. The third section deals with fundamentals of NNs and EAs. The fourth section refers to the parameter identification using an NN, whereas Section 5 describes an EA parameter identification technique. In the sixth section, neural-based constitutive laws are described. Conclusions of the paper are summarized in the final section.

2. Inelastic constitutive equations

In general, constitutive relations are given in state space form for the strain \(\varepsilon\) and a set of \(\zeta\) internal variables \(\xi \in \mathbb{R}^q\) and, typically, have the following form:

\[
\dot{\varepsilon} = \hat{\varepsilon}(\varepsilon, \xi, \theta, \sigma, \kappa),
\]

(1a)

\[
\dot{\xi} = \hat{\xi}(\varepsilon, \xi, \theta, \sigma, \kappa),
\]

(1b)

where \(\theta\) and \(\sigma\) are the temperature and stress respectively and \(\kappa \in \mathbb{R}^r\) represents a vector of \(\tau\) material parameters. The following initial conditions are given for their direct analysis:

\[
\varepsilon^i_{t=0} = \varepsilon_0,
\]

(1c)
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Chaboche's viscoplastic model, for instance, is capable of describing cyclic hardening and softening behaviors with the yielding surface and appears to model a wide range of inelastic material behavior characteristics. Its formation under the uniaxial loading and stationary temperature conditions is given by

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

\[ \sigma = E\varepsilon^e, \]  

\[ \dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^p, \]  

\[ \dot{\varepsilon}^p = \left( \left| \frac{\sigma - Y - R}{K} \right|^n \right) \text{sgn}(\sigma - Y), \]  

\[ \dot{Y} = H\dot{\varepsilon}^p - DY|\dot{\varepsilon}^p|, \]  

\[ \dot{R} = h|\dot{\varepsilon}^p| - dR|\dot{\varepsilon}^p|, \]

where variables \( \sigma, \varepsilon^e, \varepsilon^p, Y \) and \( R \) are the uniaxial stress, the uniaxial elastic strain, the uniaxial inelastic strain, the uniaxial back stress and the isotropic hardening variable respectively, and the vector \( \varphi = [K,n,H,D,h,d,E] \) represents the material parameters. The notation \( \langle \rangle \) in Eq. (2c) is zero if the value inside is negative. Initial conditions for the direct analysis of the model are given by

\[ \varepsilon |_{t=0} = \varepsilon_0, \]  

\[ Y |_{t=0} = Y_0, \]  

\[ R |_{t=0} = R_0. \]

In the cyclic loading test no external force is provided initially (\( \varepsilon |_{t=0} = 0, Y |_{t=0} = 0 \)), and thus parameters \( K, n, H, D, h, d \) and \( R \) must be determined to describe the performance of a specific material. For computer simulation, a time integration algorithm such as the mid-point rule is used to discretize the equations.

A number of tests are performed to evaluate the behavior of materials. In this paper we deal with a cyclic loading test and the subsequent strain-holding test under uniaxial loading and stationary temperature conditions.

3. Neural Networks and Evolutionary Algorithms

3.1 Neural networks

Multilayer neural networks are universal function approximators based on natural information-processing tasks. The relation between the input and output data of a processing unit is formulated as follows:
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\[ O_j = f(u_j) = \frac{1}{1 + \exp(-2U_j / U_0)}, \]  
\[ U_j = \sum_{i=1}^{I} W_{ji} \cdot I_i - \theta_j, \]  

where \( O_j \) is the output of the \( j \)th unit, \( U_j \) the weighted input to the \( j \)th unit, \( f \) the activation function, i.e., the sigmoid function here, \( U_0 \) the temperature constant, \( W_{ji} \) the connection weight between the \( i \)th and the \( j \)th units, \( I_i \) the input from the \( i \)th unit, \( \theta_j \) the bias of the \( j \)th unit, and \( I \) the number of input data.

The multilayer neural network consists of multiple layers, each of which possesses a number of processing units. To train the network, at first, the following error \( E \) is defined:

\[ E = E_p = 1/(2n) \sum_{k=1}^{n} \left( T_{pk} - O_{pk} \right)^2, \]

where \( E_p \) is the error for the \( p \)th learning pattern, \( T_{pk} \) the teaching data corresponding to the \( k \)th unit for the \( p \)th learning pattern, and \( n \) the number of training patterns. In the training process, the connection weights \( W_{ji} \) and the bias values \( \theta_j \) are modified iteratively based on the steepest gradient method to minimize the above error. Through the training, the network attains the ability of outputting the similar data to the teaching data. This training algorithm is called the back propagation.

It is theoretically proven that the multilayer neural network can approximate any kinds of continuous mapping. However, the method has some limitation in reality as the number of available units is limited from a computational viewpoint.

3.2 Evolutionary algorithms

EAs are probabilistic optimization algorithms based on the model of natural evolution, and the algorithms have clearly demonstrated their capability to create good approximate solutions in complex optimization problems.

First, a population of individuals, each represented by a vector, is initially (generation \( t = 0 \)) generated at random, i.e.,

\[ P^0 = \{ \mathbf{u}_1^0, ..., \mathbf{u}_\lambda^0 \} \subset \mathcal{I}^\lambda \]

where \( \lambda \in \mathbb{N} \) and \( \mathcal{I} \) represent the population size of parental individuals and the space of individual respectively. The population then evolves towards better regions of the search space by means of randomized processes of recombination, mutation and selection though either recombination or mutation operator is not implemented in some algorithms. These reproductive operations form one generation of the evolutionary process, which corresponds to one iteration in the algorithm, and the iteration is repeated until a given terminal criterion is satisfied.

EAs, in general, are rather formulated to comprise a broad range of optimi-
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zation problems although the problems of interest, as described in Section 2, are characterized only with continuous search space. In this section we present the EA proposed by the authors, which was specifically formulated for the optimization with continuous search space. The reproductive operations of the proposed algorithm is intended to be similar to those of GAs such that it can take the advantage of probabilistic features in GAs. The major difference of the proposed algorithm from GAs is that the representation of the individual is given by a search point itself; i.e., a real continuous vector. This formulation was made with an assumption that the direct use of the search point may search more efficiently than the representation decoded into a binary string as used in GAs. In this case, the population at generation $t$ is given by

$$P^t = \{x_1^t, \ldots, x_\lambda^t\} \subseteq X^\lambda.$$  

(7)

This representation makes us grasp the concept of the individual in a different manner. While the binary string in GAs represents a DNA chromosome, a microscopic or genetic representation of human being, the continuous vector representation corresponds to a set of macroscopic or phenomenological information of human being.

The definition of the recombination and mutation becomes the probabilistic distribution of the phenomenological measures accordingly. If the two offspring individuals are formulated to be created from a pair of randomly-selected parental individuals as in GAs, $r^{\nu} : I^2 \rightarrow I$, the recombination operation may be defined as

$$r^{\nu} (x^t_\alpha, x^t_\beta) = (1 - \mu^t_\alpha) \cdot x^t_\alpha + \mu^t_\beta \cdot x^t_\beta$$

and

$$r^{\nu} (x^t_\beta, x^t_\alpha) = \mu^t_\alpha \cdot x^t_\alpha + (1 - \mu^t_\beta) \cdot x^t_\beta,$$

where $x^t_\alpha$ and $x^t_\beta$ are parental individuals at generation $t$ and the coefficient $\mu^t_\nu$, $\forall \nu \in \{\alpha, \beta\}$, is defined by the normal distribution with mean 0 and standard deviation $\eta^t_\nu$:

$$\mu^t_\nu = N(0, \eta^t_\nu^2).$$

(9)

The standard deviation can adopt a self-adaptive strategy (variable with respect to $t$) or be simply constant. The self-adaptive strategy makes the convergence rate required for each generation faster at the expense of the computation time and vice versa. Note that the mutation is not embedded in this operator since it can allow individuals to alter largely with small possibility, when the coefficient $\mu^t_\nu$ is large.

The evaluation of the fitness can be conducted with a linear scaling, which takes into account the best individual of the population:

$$\Phi(x^t_\nu) = \max\{\psi(x^t_\nu) | x^t_\nu \in P^t\} - \psi(x^t_\nu), \forall \nu \in \{1, \ldots, \lambda\}$$

(10)

as in GAs. Proportional selection, which is the most popular selection opera-
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tion in GAs, can also be directly used in the proposed algorithm. In this selection, the reproduction probabilities of individuals \( p_x : X \rightarrow [0, 1] \) are given by their relative fitness,

\[
p_x(x'_i) = \frac{\Phi(x'_i)}{\sum_{j=1}^\infty \Phi(x'_j)}.
\]  \tag{11}

Optionally, ranking selection\(^1\) can be implemented in the algorithm.

4. Parameter Identification Using a Neural Network

4.1 Formulation and Training Procedure

The first approach is to determine parameters from a set of experimental data using a network. In this approach, the simulation program of the Chaboche’s viscoplastic model, which can calculates material behaviors for a given parameter set of \((K, n, H, D, h, d\) and \(R_p\)). By changing the combination of the seven parameters, we computed material behaviors of the tensile, cyclic hysteresis, cyclic strain hardening and stress relaxation tests. The data set of the parameter set and the computed material behaviors form a training pattern. We train the neural network to learn a number of patterns. After the error of Eq. (5) becomes sufficiently small, it is expected that the trained network approximates well the continuous relationship between the parameter set and the material behaviors. In the training process, the parameter set is given to the network as teaching data, while the material behaviors are given to it as input values as shown in Fig. 1. If real material behaviors such as cyclic hysteresis curve and stress relaxation curve are given to the trained network as input data, the network outputs the corresponding parameter set.

![Figure 1 Architecture of the neural network](image-url)
The input data employed here are as follows:

1. Stress values at every strain interval of 0.01% from the yielding point on the tensile curve (8 values).

2. Stress values at every strain interval of 0.02% from the minimum hysteresis tip to the maximum hysteresis tip on the 60th cyclic curve (21 values).

3. Maximum stress values at the hysteresis tip of the 1st, 2nd, 3rd, 6th, 10th, 20th, 30th and 60th cycles on the cyclic strain hardening curve (7 values). It should be noted that the value of the 60th cycle is already taken into account in (2).

4. Stress values at 0, 1, 2, 3, 4, 5, 10, 20, 30, 60 seconds in the stress relaxation curve (10 values).

The original values of the input data are sometimes not so sensitive to the variation of parameters to be identified. This situation may result in less accuracy of parameter identification. To improve accuracy of the method, the original values of the input data are modified so as to be more sensitive to the variation of the parameters. All the input data are taken to be the deviation of the original values from those corresponding to the parameter set of \( K = 1.00 \times 10^1, n = 3.5, H = 1.50 \times 10^5, D = 1.50 \times 10^3, h' = 1.20 \times 10^2, k = 3.5, R_n = 8.00 \times 10, \) which is taken from the center point of the training ranges of parameters. The values of the input data are transformed into the range from -0.5 to +0.5 in this paper.

Table 1 shows the training range and the number of sampling points of the seven parameters. These ranges are roughly determined based on a conventional curve fitting method. In the table, \( h' \) is defined to be \((h/d - k)\) for the purpose of convenience of training. Each training range is set to include possible parameter values. Sampling points are usually chosen inside the training ranges at the regular interval. If sampling points are not chosen properly, the neural network would not learn well throughout the training ranges. The more sampling points are chosen, the more accurate results can be obtained, while the longer training time is required. In this paper, seven sampling points are chosen in each training range. The number of all the combinations of the seven parameters with seven sampling points becomes \( 7^7 = 823,544. \) This is too many to prepare learning patterns and to train the networks. To shorten these processes, 98 combinations are carefully selected considering the close relations between some parameters. that is, \( K \) and \( n \) are related to the flow law, \( H \) and \( D \) are related to the kinematic hardening behavior, and \( d \) and \( h \) are related to the isotropic hardening.

In general, it would take much calculation time for the preparation of the

<table>
<thead>
<tr>
<th>Parameter</th>
<th>(K \times 10^3)</th>
<th>(n)</th>
<th>(H \times 10^3)</th>
<th>(D \times 10^3)</th>
<th>(h' \times 10^2)</th>
<th>(d)</th>
<th>(R_n \times 10^2)</th>
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</thead>
<tbody>
<tr>
<td>Max</td>
<td>1.5</td>
<td>6.0</td>
<td>2.5</td>
<td>2.5</td>
<td>1.7</td>
<td>6.0</td>
<td>1.2</td>
</tr>
<tr>
<td>Min</td>
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<td>1.0</td>
<td>0.5</td>
<td>0.5</td>
<td>0.7</td>
<td>1.0</td>
<td>0.4</td>
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<tr>
<td>Samples</td>
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<td>7</td>
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training patterns for all the combinations of the seven parameters. However, one can reduce significantly the effort on the preparation process because of the feature of generalization of the neural network.

4.2 Results and Discussions

Table 2 tabulates the parameter sets obtained with the present method. Table 3 also summarizes the configuration of the network used and the training conditions.

Figure 2 shows the comparison of experimental and estimated curves of cyclic hysteresis behaviors. It is clearly shown that the created curve correlated well with the experimental data. Figures 3-5 show the resultant tensile curves, that of cyclic strain hardening curves, and that of stress relaxation curves, respectively. All the curves are along the experimental data. It is expected that this method will become a powerful tool for fair comparison among different inelastic constitutive equations.

5. Parameter Identification Using an Evolutionary Algorithm

5.1 Parameter Identification of Inelastic Constitutive Equations

There have been seven parameters to be determined for Chaboche’s model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$K(\times10^5)$</th>
<th>$n$</th>
<th>$H(\times10^5)$</th>
<th>$D(\times10^5)$</th>
<th>$d' (\times10^5)$</th>
<th>$d$</th>
<th>$R_p (\times10^5)$</th>
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<td>1.02</td>
<td>3.76</td>
<td>1.34</td>
<td>1.39</td>
<td>1.85</td>
<td>1.38</td>
<td>1.22</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>No. of patterns</th>
<th>No. of units</th>
<th>No. of iterations</th>
</tr>
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<tbody>
<tr>
<td>98</td>
<td>46</td>
<td>60</td>
</tr>
</tbody>
</table>

Figure 2 Experimental and estimated cyclic hysteresis behaviors
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Figure 3  Experimental and estimated tensile behaviors

Figure 4  Experimental and estimated strain hardening hysteresis behaviors

Figure 5  Experimental and estimated relaxation behaviors
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described in Section 2. Let the parameter set \( \mathbf{x}^T = [K, n, H, D, h, d, R_0] \), and represent the constitutive equations (2) with strain \( \varepsilon \) as the input variable with respect to time and stress \( \sigma \) as the output variable in the following form:

\[
\sigma = \psi(\mathbf{x}, \varepsilon),
\]

(12)

where \( \psi: \mathbb{R}^7 \times \mathbb{R} \rightarrow \mathbb{R} \). If \( m \) pairs of stress-strain data \( \{[\sigma_1^*, \varepsilon_1^*], \ldots, [\sigma_m^*, \varepsilon_m^*]\} \) are used to determine the parameter set, then the optimization problem to be formulated according to Section 3 is:

\[
\min_{\mathbf{x}} \sum_{i=1}^{m} k_i \|\sigma_i^* - \psi(\mathbf{x}_i^*)\|^2, \tag{13}
\]

where \( k_i \) represents a weighting factor. Providing different strain rates, the solution can be uniquely determined.

5.2 Identification with Actual Experimental Data

In this section, the actual experimental data of 2 1/4Cr-1Mo Steel under a temperature of 673K, obtained from a benchmark project by the Society of Material Science, Japan, were used to investigate the capability of the proposed method. Experimental stress-strain data used for the parameter identification included information on material behaviors with different cycles and strain rates.

Parameters were identified with two other methods for comparison: one is a conventional stepwise technique and the other is a technique where a gradient-based optimization method was used to minimize the objective function (13). In the former’s technique, parameters \( K, n, H \) and \( D \) are first determined by means of the least square method after the constitutive law is simplified by letting the yield stress \( R \) be constant. Parameters \( h, d \) and \( R_0 \) are then determined in the second step.

Table 4 lists the resultant objective function value by each technique together with the values of their initial parameter set. Note here that the initial parameter set for the proposed technique is not described in the table as the initial parameter set has little influence on the performance of the algorithm, by the fact that the algorithm starts with many randomly-selected parameter sets. As shown in the table, the parameter set identified with the gradient-based technique from the initial parameter set \( \mathbf{x}^T = [200, 5, 20000, 300, 100, 5, 0] \) was almost identical to that with the proposed method. However, the cost functional by the gradient-

<table>
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<th>Table 4 Parameters identified under measurement errors</th>
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<tr>
<td>Initial parameter set</td>
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<tr>
<td>------------------------</td>
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<tr>
<td>Proposed method</td>
</tr>
<tr>
<td>Gradient-based technique</td>
</tr>
<tr>
<td>Stepwise method</td>
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</tbody>
</table>
Figure 6 Computed material curves vs experimental data

based technique diverged when the initial parameter set was $\mathbf{x}^T = [50, 5, 20000, 300, 100, 5, 0]$ though only the value of $K$ differed. Clearly this indicates that the successful performance of the technique largely depends on the initial parameter set chosen. The stepwise technique could successfully find a stable parameter set even when a different initial parameter set was selected. However, the technique created a larger cost functional value than did the proposed method.

Curves with different strain rates, created from the proposed method, are shown in Fig. 6 together with the experimental data used for the parameter iden-
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tification. Experimental data with strain rate 0.001 %/s, which were not used for the identification, and their corresponding curve created are also shown in the figure to show the appropriateness of the parameter set identified. First, we can see that there exist model errors to some degree, which cannot be removed unless we change the model used. However, the curves created are reasonably close to the experimental data, indicating that the proposed technique is adequate for finding a parameter set which describes good approximate material behaviors.

6. Neural-Based Material Modelling

6.1 Formulation

This section deals with the neural network modelling of inelastic responses, which was previously proposed and successfully demonstrated the modelling ability. The model consists of two neural networks, each of which is used to learn the back stress or the drag stress. Figure 7 illustrates the basic strategy for each neural network to learn the stress curve, which are decomposed from the original stress-strain curve. In the present approach, three historical points are used to estimate the extrapolative gradient of the curve.

Both the neural networks have the identical hardware architecture. Figure 8 shows the proposed structure of the neural networks for modelling the above inelastic laws. As is depicted in the figure, there is one hidden layer composed of 14 units between the input and output layers. The numbers of units in the input layer and in the output layer are six and unity, respectively. Table 6 lists input and output variables used in the network. Here \( v \) stands for either the back stress or the yield stress, while \( u \) indicates \( \int [\delta \varepsilon']_{n-1} \) for drag stress curve and \( \varepsilon'' \) for back stress curve.

6.2 Determination of internal stresses from experiment

A procedure to derive the back and drag stresses, given stress-strain curves of cyclic loading tests under different strain rates, is described in this section. The procedures of obtaining these stresses are as follows:

1. Identify the Young's modulus from the gradient of a curve within the elastic
range. Then remove the elastic part from the original curve and obtain tensile data from cyclic behaviors curves whose x and y axes are the values of the inelastic strain and the stress, respectively. These processes are illustrated in Fig. 9.

2. Let the back stress be the curve of the inelastic tensile behavior of the first cyclic test.

3. Draw a curve with x axis the total equivalent strain \(\int |\delta \varepsilon|\) and y axis the equivalent stress from Fig. 9. This graph then substantially represent the yield stress.

This procedure makes us possible to obtain both the back and drag stresses. This allows neural networks to learn curves separately.

### 6.3 Implementation to an FEM Program

The proposed method was implemented in a commercially available FEM general purpose code, MARC. In MARC, the user subroutine feature constitutes one of the real strength of the program, allowing the user to substitute their own subroutines for several existing ones in the program. This feature provides the user with a wide latitude for solving nonstandard problems. All the external features of the FEM system, such as pre- and post-processors can be used.

### 6.4 Numerical Example

The experimental data used to test the performance of the developed system
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were obtained by the uniaxial cyclic test under the strain control. First, the neural network was trained to trace the experimental data. Then, the performance of the FEM code into which the neural modeler is incorporated was investigated by comparing its response to the original experimental data. The test specimen described in Section 4 was used as a numerical example.

The teaching data of the back stress were converted to a logarithmic scale due to its characteristics. The training of each neural network was terminated when the mean square error of unlearned data began to increase. The back and drag stresses, which were decomposed from the original stress-strain curve, were estimated by the trained networks. These results are shown in Fig. 10. In order to demonstrate that the present FEM system can produce the material behavior close to the actual experimental data, the model simulation under identical conditions to those for the experiment was conducted.

The finite element model and the analysis conditions are shown in Fig. 11. The left-hand edge of the model is movable only to the vertical direction. The model is axisymmetric and assumed to represent the behavior of the central part of the specimen. The finite element type employed here was 8-node biquadratic.

Figure 10  Curves estimated by the neural networks
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Element type: 8-node biquadratic
Number of element: 60  Number of node: 219
Strain rate: 0.5%/s  Maximum strain: 0.5%
Strain increment: 0.02%  Minimum strain: -0.5%

Figure 11  Axisymmetric FE model

Figure 12  Equivalent stress data vs. cycles of both the computed and experimental data.

and the number of elements and nodes for the whole model were 60 and 219, respectively. The displacement increment per step for the dynamical analysis was 0.05%. The computed stress data at the maximum strain were compared to the equivalent experimental data. Figure 12 shows the stress data vs cycles of both the computed and experimental data. The figure shows that the error of the curve created to the experimental data are well less than 3.0%.
7. Conclusions

Several approaches for modelling inelastic material behaviors based on NNs and EAs have been presented. The results of the numerical examples show that the approaches are feasible for practical use. Although the parameter identification using NNs is upon an assumption that a constitutive equation used correctly represents the material behavior, it output a reasonable parameter set instantaneously. On the other hand, the EA-based parameter identification technique is used to the best-fit parameters of a constitutive equation used. The neural-based material modelling is rather to be used for material behaviors that cannot be described by the present constitutive equations.

References