The Machine Learning Embedded Method of Parameters Determination in the Constitutive Models and Potential Applications for Hydrogels

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Abstract

We propose a machine learning embedded method of parameters determination in the constitutional models of hydrogels. It is found that the developed logistic regression liked algorithm for hydrogel swelling allows us to determine the fitting parameters based on known swelling ratio and chemical potential. We also put forward the neural networks liked algorithm, which, by its own property, can converge faster as the layer deepens. We then develop neural networks liked algorithm for hydrogel under uniaxial load for experimental application purpose. Finally, we propose several machine learning embedded potential applications for hydrogels, which would provide directions for machine learning based hydrogel research.

Keywords: Machine learning; hydrogel; logistic regression; neural networks; potential application.

1. Introduction

Currently we are experiencing an influence of huge and increasing volumes of data as well as quick advances in computational hardware and reduced costs for computation, data storage and transfer. These unprecedented advances have, in turn, fueled renewed interest and progress in the field of machine learning. Machine learning algorithms are rapidly making inroads in countless important applications, including web search, email anti-spam, speech recognition, product

recommendations, and more (Brunton et al., 2019). Machine learning also shows great potential in Mechanical Engineering. For example, we have done work such as indentation test for characterization of materials (Swaddiwudhipong et al., 2008; Tho et al., 2004) and material characterization via least squares support vector machines (Swaddiwudhipong et al., 2005). Machine learning provides a modular and agile modeling framework that can be tailored to address many challenges in academic research as well, including hydrogel research.

Owning remarkable properties of imbibing water molecules and large swelling ratios, hydrogels demonstrate the great potential of emerging as one of the next-generation smart materials in future applications (Liu et al., 2015). Hydrogel superiority can also be discovered in properties such as high stretchability (Sun et al., 2012), reversible swelling (Liu and Cheng, 2018; Xu et al., 2016b), flexibility (Xu et al., 2016a), biocompatibility (Wei et al., 2015), and toughness (Bouklas et al., 2015; Gong, 2010). Due to these advantages, hydrogels have been widely applied in drug delivery (Qiu and Park, 2001; Zheng and Cheng, 2020), tissue engineering (Drury and Mooney, 2003; Nguyen and West, 2002), actuators (Liu and Calvert, 2000; Zhang et al., 2014), and matrices for biological studies (Augst et al., 2006). The list is still growing, only limited by our imagination. However, most of the hydrogel research has not exploited the great potential of machine learning. The machine learning embedded hydrogel research is still waiting to be done.

So, in this paper, we proposed a machine learning embedded method of parameters determination in the constitutional models of hydrogels, which can demonstrate the effectiveness of machine learning in hydrogel research. First by replacing the logistic function with the nonlinear constitutional models of hydrogels, we develop a logistic regression liked algorithm for hydrogel swelling, which allows us to determine the fitting parameters based on known

swelling ratio and chemical potential. Likewise, inspired by the neural networks, we then proposed the neural networks liked algorithm, which, by its own property, can be divided into neural networks liked algorithm with one hidden layer and multi-layer fully-connected neural networks liked algorithm. The fitting parameters of the neural networks liked algorithm with one hidden layer still process physical meaning. However, due to the influence of the deeper layers, which are real neural networks, the fitting parameters of multi-layer fully-connected neural networks liked algorithm don't own physical meaning anymore. Finally, for experimental application purpose, we develop neural networks liked algorithm for hydrogel under uniaxial load, which can determine all the fitting parameters with one loading experiment.

Moreover, we then proposed several machine learning embedded potential applications for hydrogels. Parameters determination for hydrogel theory, standards setting for hydrogel adhesion experiments, noise reduction of hydrogel ionic conductors, multisource underwater gel eavesdropper, reinforcement learning of motion modes for magnetic sensitive hydrogel soft robot, and recurrent neural networks embedded hydrogel structural genome are discussed in detail.

The paper is organized as follows. In Section 2 we develop logistic Regression liked algorithm for hydrogel swelling. Section 3 covers the neural networks liked algorithm, which can be divided into neural networks liked algorithm with one hidden layer and multi-layer fully-connected neural networks liked algorithm. The neural networks liked algorithm for hydrogel under uniaxial load is presented in Section 4. Section 5 discusses potential applications of machine learning in hydrogel research. Finally, concluding remarks are given in Section 6.

2. Logistic regression liked algorithm for hydrogel swelling

In this section, we develop a convergence algorithm based on the logistic regression and the large deformation theory of hydrogel. Logistic regression is a statistical model that in its basic

form uses a logistic function to model a binary dependent variable, as shown in Fig. 1. Logistic regression can also be thought as the simplest neural networks with only one neuron and one layer. As shown in Fig. 1, logistic regression algorithm is used to try to predict y given x. y is the output of the algorithm while x is the input of the algorithm. First, we assume

$$z = wx + b, \tag{1}$$

where z is the assumed value of linear hypothesis of x; w and b are the parameters of the hypothesis.

Then, logistic regression algorithm chooses:

$$\sigma(z) = \frac{1}{1+e^{-z}}, \tag{2}$$

which is called the logistic function or the sigmoid function. It should be noted that $\sigma(z)$ tends towards 1 as $z \to \infty$, and $\sigma(z)$ tends towards 0 as $z \to -\infty$. Moreover, $\sigma(z)$ is always bounded between 0 and 1. We define activation function, $a=\sigma(z)$, which is equal to the hypothesis of y, $\hat{y}$.

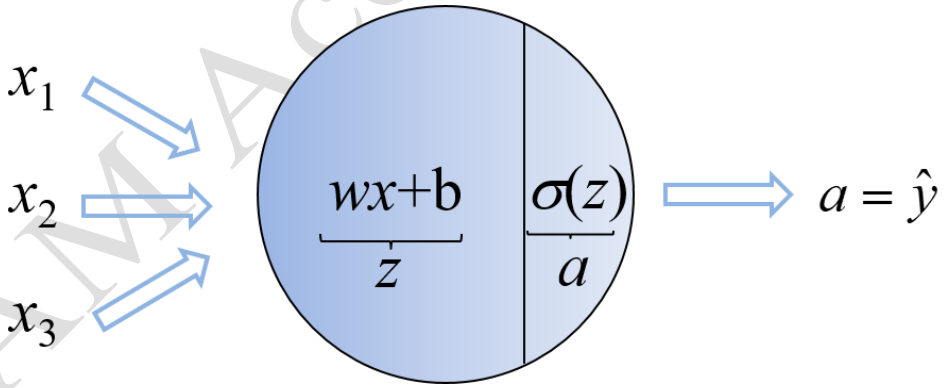


Fig. 1. The schematics of logistic regression.

Here, we develop our algorithm for hydrogel swelling based on the logistic regression. On the other hand, the large deformation theory explicitly defines the chemical potential and stretch relationship of hydrogel by considering the mixing and stretch free energy density (Hong et al., 2009):

$$\mu/kT = N\nu\left(\frac{1}{\lambda}-\frac{1}{\lambda^3}\right)+\log\left(1-\frac{1}{\lambda^3}\right)+\frac{1}{\lambda^3}+\frac{\chi}{\lambda^6}, \tag{3}$$

where μ is the chemical potential, N is the crosslink density in the reference state, kT is the temperature in the unit of energy; $k = 1.3806488\times10^{-23}\,\mathrm{m^2\cdot kg\cdot s^{-2}\cdot K^{-1}}$ the Boltzman constant; and T the absolute temperature; ν is the nominal volume of a solvent molecule and χ the interaction parameter.

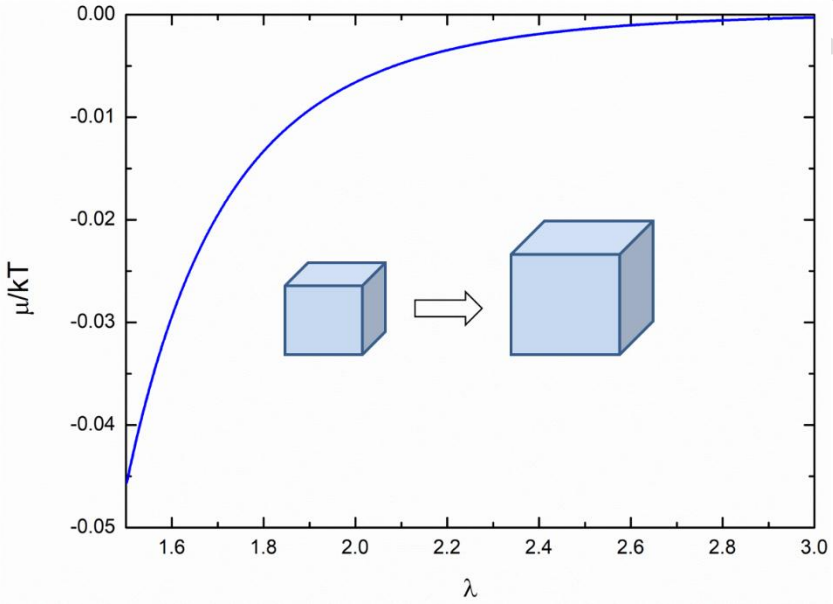


Fig. 2. The chemical potential of the solvent is plotted as a function of the stretch of a free-swelling hydrogel.

Based on Eq. (3), by setting $N\nu$ and χ are 0.001 and 0.1 respectively, we can draw μ/kT as a function of λ (Fig. 2). In Fig. 2, we can notice the nonlinearity between μ/kT and λ. Inspired by the fact that logistic function also shows the nonlinearity between z and a, we propose the logistic regression liked algorithm for hydrogel swelling, as shown in Fig. 3. With known μ/kT and λ and unknown $N\nu$ and χ, we use the logistic regression liked algorithm to determine the

fitting parameter $N\nu$ and χ through iteration. The algorithm can be described as follows. First, we define $f(\lambda)= \hat{\mu}/kT$, the hypothesis of μ/kT, as:

$$f(\lambda)=\hat{\mu}/kT=N\nu\left(\frac{1}{\lambda}-\frac{1}{\lambda^3}\right)+\log\left(1-\frac{1}{\lambda^3}\right)+\frac{1}{\lambda^3}+\frac{\chi}{\lambda^6}. \quad (4)$$

With given λ and randomly initialized $N\nu$ and χ, we calculated $\hat{\mu}/kT$ through $f(\lambda)$. Then we can calculate the loss function L using $\hat{\mu}/kT$ and μ/kT:

$$L(\hat{\mu}/kT,\mu/kT)=\frac{1}{2}(\mu/kT-\hat{\mu}/kT)^2. \quad (5)$$

For simplicity, we also refer loss function as loss. It should be noted that we do not use the cross entropy loss function as did in the logistic regression for the reason that the value of $\hat{\mu}/kT$ is not limited between 0 and 1.

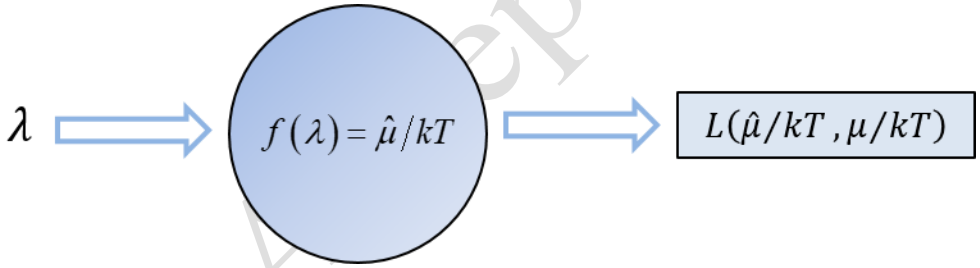


Fig. 3. The schematics of the logistic regression liked algorithm for hydrogel swelling.

In comparison, λ and μ/kT in the logistic regression liked algorithm is like x and y in the logistic regression. More importantly, we replace the logistic function with $f(\lambda)$ due to the fact that both functions have strong nonlinearity. So $N\nu$ and χ in the logistic regression liked algorithm is like w and b in the logistic regression.

Above is the forward propagation of the algorithm. We then develop the backpropagation to finish the loop of one iteration. For simplicity and common practice in machine learning, we use

da to represent the differentiation of *a*, any given parameter, with respect to *L*, the loss function. First, the differentiation $\hat{\mu}/kT$ of with respect to *L* is:

$$d\left(\hat{\mu}/kT\right)=\hat{\mu}/kT-\mu/kT. \tag{6}$$

Using the chain rule of differentiation, we can get

$$dN\nu=d\left(\hat{\mu}/kT\right)\frac{\partial f\left(\lambda\right)}{\partial N\nu}=d\left(\hat{\mu}/kT\right)\left(\frac{1}{\lambda}-\frac{1}{\lambda^3}\right), \tag{7}$$

$$d\chi=d\left(\hat{\mu}/kT\right)\frac{\partial f\left(\lambda\right)}{\partial \chi}=d\left(\hat{\mu}/kT\right)\frac{1}{\lambda^6}. \tag{8}$$

Finally, we update $N\nu$ and χ to iterate:

$$N\nu:=N\nu-\alpha dN\nu, \tag{9}$$

$$\chi:=\chi-\alpha d\chi, \tag{10}$$

where α is the learning rate.

We implement the logistic regression liked algorithm into Python and the results can be seen in Fig. 4. We input 1000 sets of (λ, μ/kT). The actual values of $N\nu$ and χ are 0.001 and 0.1, reasonable values taken in many studies (Hong et al., 2008; Huang et al., 2020b). After 2000 iterations, the algorithm output the value of $N\nu$ and χ as 0.00419828 and 0.03771538. After 10000 iterations, the algorithm output the value of $N\nu$ and χ as 0.00172635 and 0.08585473. After 20000 iterations, the algorithm output the value of $N\nu$ and χ as 0.00111388 and 0.09778232. It can be found that as the algorithm converges, the predicted $N\nu$ and χ is approaching the real $N\nu$ and χ.

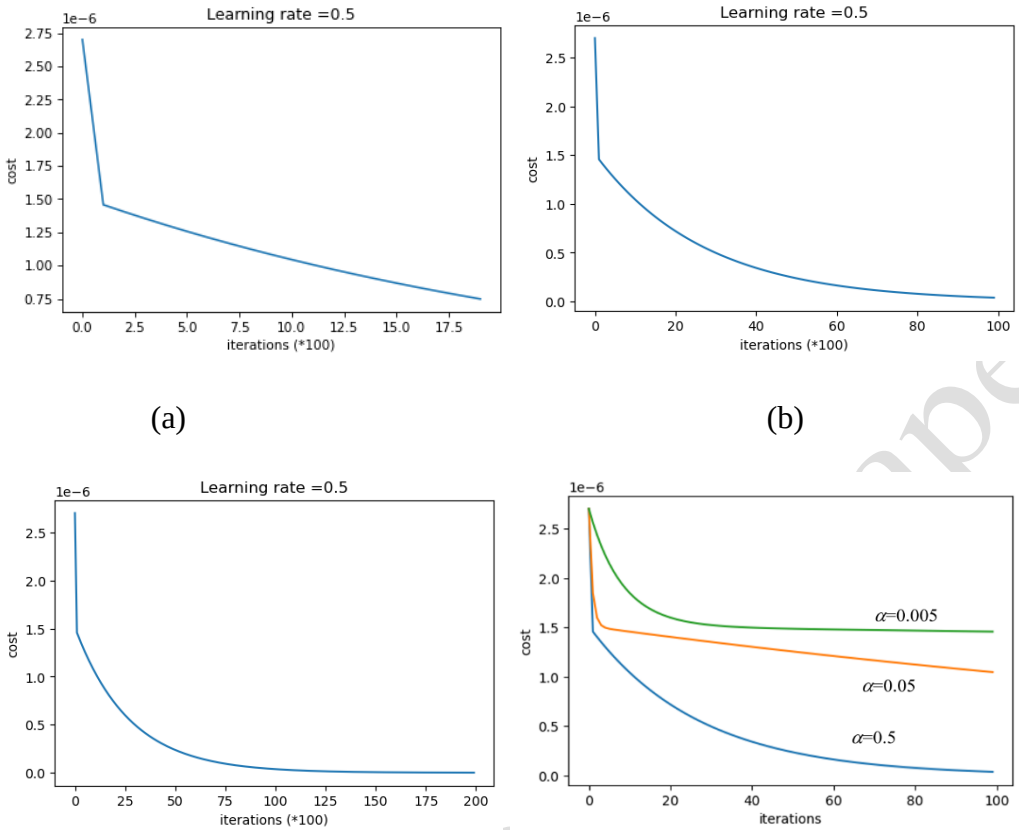


Fig. 4. The cost of the logistic regression liked algorithm is plotted as a function of iterations: (a) 2000 iterations; (b) 10000 iterations; (c) 20000 iterations; (d) 10000 iterations with the learning rate=0.5, 0.05; 0.005 respectively.

We can also found in Fig. 4d that with increased learning rate, the logistic regression liked algorithm is converged more quickly. Here we demonstrate the logistic regression liked algorithm for hydrogel swelling. With known μ/kT and λ, we use the logistic regression liked algorithm to determine the fitting parameter $N\nu$ and χ through iteration. Instead of determining $N\nu$ and χ one at a time or randomly choosing their values, we now can determine their value at the same time through iteration.

The ideology of the logistic regression liked algorithm can be applied to other constitutional models of large deformation as long as the nonlinearity exists. For example, the logistic regression liked algorithm can also be applied the large deformation theory of temperature sensitive hydrogel (Zheng and Liu, 2018), salt concentration sensitive hydrogel (Zheng and Liu, 2019) and so on (Zheng et al., 2018, 2019). Likewise, in the next section, we expanded the algorithm into the neural networks liked algorithm using the similar approach.

3. Neural Networks liked algorithm

Neural networks refer to broad type of non-linear models/parametrizations that involve combinations of matrix multiplications and other entry-wise non-linear operations. Logistic regression discussed above can be thought as the simplest neural networks with only one neuron and one layer. As shown in Fig. 5, a circular region represents for a single neuron of the neural networks. A more complex neural network may take the single neuron described above and "stack" them together such that one neuron passes its output as input into the next neuron, resulting in a more complex function:

$$z^{[1]} = W^{[1]}x + b^{[1]}, \tag{11}$$

$$a^{[1]} = \sigma\left(z^{[1]}\right), \tag{12}$$

$$z^{[2]} = W^{[2]}x + b^{[2]}, \tag{13}$$

$$a^{[2]} = \sigma\left(z^{[2]}\right). \tag{14}$$

The superscripts indices $^{[1]}$ and $^{[2]}$ are used to distinguish two sets of parameters in the first and second layers. As the name suggests, artificial neural networks were inspired by biological neural networks. The hidden units correspond to the neurons in a biological neural network, and the parameters correspond to the synapses. However, it's unclear how similar the

modern deep artificial neural networks are to the biological ones. For example, perhaps not many neuroscientists think biological neural networks could have 1000 layers, while some modern artificial neural networks do. Moreover, it's an open question whether human brains update their neural networks in a way similar to the way that computer scientists learn artificial neural networks (using backpropagation).

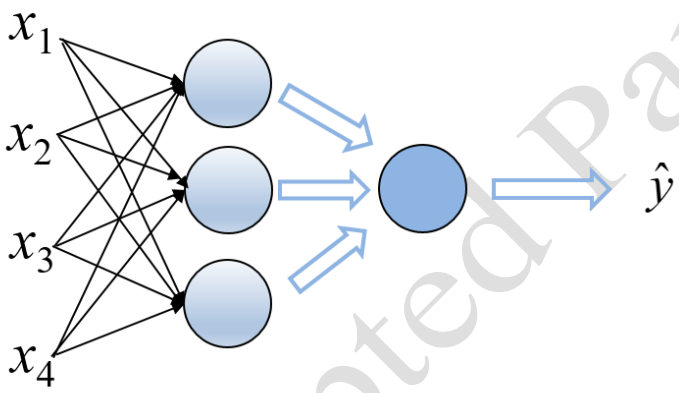


Fig. 5. The schematics of the neural networks.

Here, inspired by the structure of neural networks, we propose the neural networks liked algorithm, which, by its nature, can be divided into the neural networks liked algorithm with one hidden layer and multi-layer fully-connected neural networks liked algorithm, which can be used for solving hydrogel problems.

3.1. Neural Networks liked algorithm with one hidden layer

Based on the logistic regression liked algorithm, we can take the single neuron described above and "stack" them together in the same layer, shown in Fig. 6. We constructed the neural networks using Eq. 3. The forward propagation and the backpropagation is the same as those of the logistic regression liked algorithm.

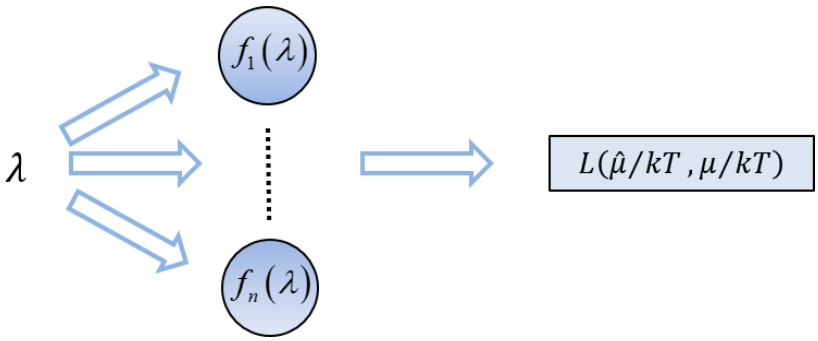


Fig. 6. The schematics of the neural networks with one hidden layer liked algorithm.

The effect of adding more neurons to the structure are discussed in detail in Section 3.2. It should be noted that the parameters $N\nu$ and χ we finally get in the neural networks liked algorithm with one hidden layer has physical meaning. $N\nu$ represents the crosslink density while χ is the interaction parameter. However, in the real neural networks algorithm, the trained parameters *w* and *b* don't share any physical meaning. They are just fitting parameters.

Next, we develop the neural networks liked algorithm with two layers or more layers based on the structure of the neural networks liked algorithm with only one layer.

3.2. Multi-layer fully-connected neural networks liked algorithm

$W^{[1]}$, $W^{[2]}$ are often referred to as the weight matrices and $b^{[1]}$, $b^{[2]}$ are referred to as the biases. The collection of $W^{[1]}$, $b^{[1]}$ is referred to as the first layer, and $W^{[2]}$, $b^{[2]}$ the second layer. The activation *a* is referred to as the hidden layer. With these succinct notations, we can stack more layers to get deeper fully-connected neural networks, as shown in Fig. 7.

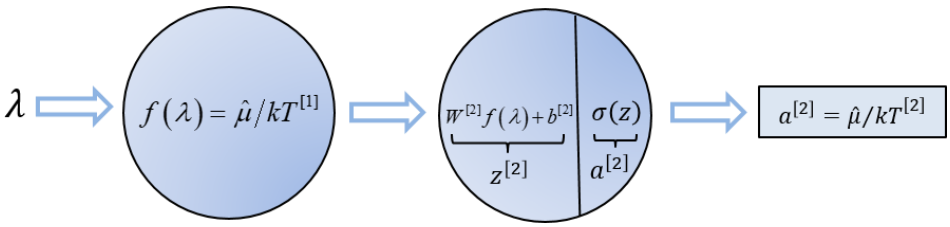


Fig. 7. The schematics of multi-layer fully-connected neural networks liked algorithm (two layers).

Inspired by the neural networks, we proposed the multi-layer fully-connected neural networks liked algorithm for hydrogel swelling. Similar to the logistic regression liked algorithm, with known μ/kT and λ and unknown $N\nu$ and χ, we first use the logistic regression liked algorithm to determine the fitting parameter $N\nu$ and χ through in the first layer. Then the calculated $\hat{\mu}/kT$ passes its output as input into the next layer of the real neural networks. In Fig. 7, we only draw two layers of the multi-layer fully-connected neural networks liked algorithm. In fact, we can stack more layers to get a deeper fully-connected neural networks liked algorithm.

The algorithm can be described as follows. First, with given λ and randomly initialized $N\nu$ and χ, we can calculated $\hat{\mu}/kT$ through $f(\lambda)$ in the first layer. Then the calculated $\hat{\mu}/kT$ passes its output as input into the next layer of the real neural networks to get $a^{[2]}$. Then we can calculate the loss function L using $\hat{\mu}/kT^{[2]}$ and μ/kT:

$$L\left(\hat{\mu}/kT^{[2]},\mu/kT\right)=-\mu/kT\log\left(\hat{\mu}/kT^{[2]}\right)-\left(1-\mu/kT\right)\log\left(1-\hat{\mu}/kT^{[2]}\right). \tag{15}$$

It should be noted that we use the cross entropy loss function as did in the real neural networks for the reason that second layer uses the logistic function to limit the value of $\hat{\mu}/kT^{[2]}$ to 0-1.

We should also notice that only replace the logistic function with $f(\lambda)$ in the first layer. The rest of the layers use the real neural networks. So $N\nu$ and χ in the multi-layer fully-connected neural networks liked algorithm don't share concrete physical meaning as it did in neural networks liked algorithm with one hidden layer.

Above is the forward propagation of the multi-layer fully-connected neural networks liked algorithm. We then develop the backpropagation to finish the loop of one iteration. First, the differentiation $\hat{\mu}/kT^{[2]}$ of with respect to L is:

$$d\left(\hat{\mu}/kT^{[2]}\right) = -\frac{\mu/kT}{\hat{\mu}/kT^{[2]}} + \frac{1-\mu/kT}{1-\hat{\mu}/kT^{[2]}}. \tag{16}$$

Using the chain rule of differentiation, we can get:

$$dz^{[2]} = \hat{\mu}/kT^{[2]} - \mu/kT, \tag{17}$$

$$dW^{[2]} = dz^{[2]}\,\hat{\mu}/kT^{[1]T}, \tag{18}$$

$$db^{[2]} = dz^{[2]}, \tag{19}$$

$$d\,\hat{\mu}/kT^{[1]} = W^{[2]}dz^{[2]}, \tag{20}$$

$$dN\nu = d\left(\hat{\mu}/kT^{[1]}\right)\frac{\partial f(\lambda)}{\partial N\nu} = d\left(\hat{\mu}/kT^{[1]}\right)\left(\frac{1}{\lambda} - \frac{1}{\lambda^3}\right), \tag{21}$$

$$d\chi = d\left(\hat{\mu}/kT^{[1]}\right)\frac{\partial f(\lambda)}{\partial \chi} = d\left(\hat{\mu}/kT^{[1]}\right)\frac{1}{\lambda^6}. \tag{22}$$

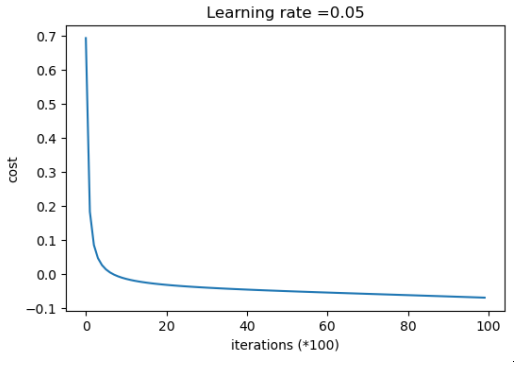
Finally, we update $N\nu$ and χ to iterate:

$$N\nu := N\nu - \alpha dN\nu, \tag{23}$$

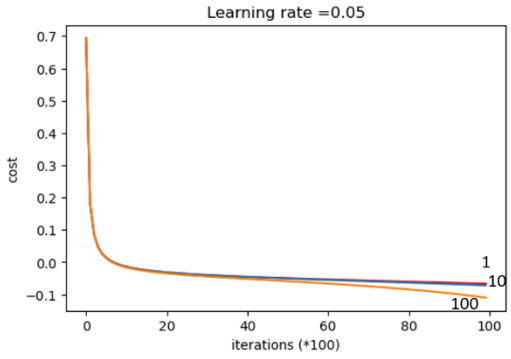
$$\chi := \chi - \alpha d\chi. \tag{24}$$

We implement the multi-layer fully-connected neural networks liked algorithm into Python and the results can be seen in Fig. 8. The first layer has 4 neurons and the second layer has one neurons. We use the same sets of (λ, μ/kT) as in Section 2. The actual values of $N\nu$ and χ are also 0.001 and 0.1. The results can be seen in Fig. 8a after 10000 iterations. Compared with the results in Section 2, it can be found that as the multi-layer fully-connected neural networks liked

algorithm converges way much faster than the logistic regression liked algorithm.



(a)



(b)

Fig. 8. The cost of the multi-layer fully-connected neural networks liked algorithm is plotted as a function of iterations: (a) 10000 iterations; (b) 10000 iterations with 1, 10, and 100 neurons in the first layer respectively.

Next, we change the neurons in the first layer to 1, 10, and 100 respectively. The results are shown in Fig. 8b. We can find that the increase of the neurons has limited influence on the convergence speed. So we can conclude that the significant improvement of the convergence speed compared to that of the logistic regression liked algorithm is due to the deeper layer of the multi-layer fully-connected neural networks liked algorithm.

However, the deeper layer causes the parameter $N\nu$ and χ lose their actual physical meaning due to the influence of the second layer. So the future work can focus on design a multi-layer fully-connected neural networks liked algorithm which has both deep layers and parameters with actual physical meanings. For example, the output of the first layer is the input of the second layer, which is constructed based on the second nonlinear mechanical models.

The ideology of the multi-layer fully-connected neural networks liked algorithm can also be applied to other constitutional models of large deformation as long as the nonlinearity exists. In

the next section, we will apply the neural networks liked algorithm into hydrogel under uniaxial load, which has a potential to be applied to the experimental study of hydrogel.

4. Neural networks liked algorithm for hydrogel under uniaxial load

In this Section, we use the neural networks liked algorithm developed in Section 3 to determine the fitting parameters for hydrogel under uniaxial load. The large deformation theory can define the stress and stretch relationship of hydrogel by giving differentiation of the mixing and stretch free energy density (Hong et al., 2009):

$$s\nu/kT = N\nu\left(\lambda_1 - \frac{1}{\lambda_1}\right) + \left[\lambda_1\lambda_2^2 \log\left(1 - \frac{1}{\lambda_1\lambda_2^2}\right) + 1 + \frac{\chi}{\lambda_1\lambda_2^2} - \frac{\mu}{kT}\lambda_1\lambda_2^2\right]\frac{1}{\lambda_1}, \tag{25}$$

where s is the nominal stress, λ_1 and λ_2 is the stretch in the pulling direction and transverse direction respectively. Its relation is reflected in Fig. 9.

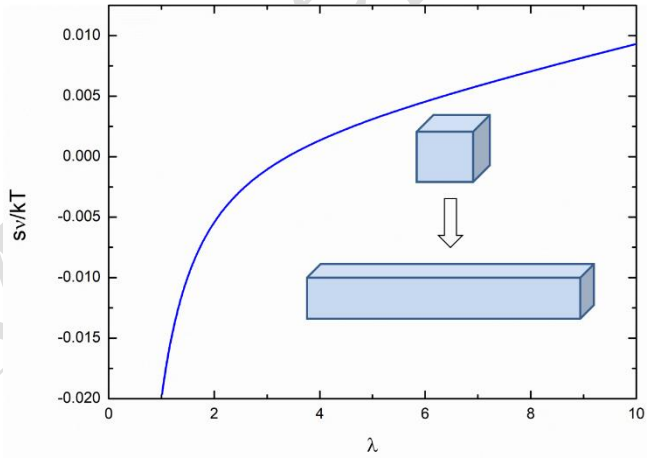


Fig. 9. A rod of a gel is subject to a uniaxial stress, and is in contact with a solvent of a given chemical potential. The applied stress is plotted as a function of the stretch, while the solvent is held at a fixed the chemical potential.

Likewise, we develop neural networks liked algorithm for hydrogel under uniaxial load, as shown in Fig. 10. With known $s\nu/kT$, λ_1 and λ_2 and unknown $N\nu$, χ, and μ/kT, we used neural

networks liked algorithm to determine the fitting parameter $N\nu$ and χ through iteration. The algorithm can be described as follows. First, we defined

$$f\left(\lambda_1,\lambda_2\right)=\hat{s}\nu/kT=N\nu\left(\lambda_1-\frac{1}{\lambda_1}\right)+\left[\lambda_1\lambda_2^2\log\left(1-\frac{1}{\lambda_1\lambda_2^2}\right)+1+\frac{\chi}{\lambda_1\lambda_2^2}-\frac{\mu}{kT}\lambda_1\lambda_2^2\right]\frac{1}{\lambda_1}. \tag{26}$$

With given λ_1 and λ_2 and randomly initialized $N\nu$, χ, and μ/kT, we calculated $\hat{s}\nu/kT$ through $f(\lambda)$. Then we can calculate the loss function L using $\hat{s}\nu/kT$ and $s\nu/kT$:

$$L\left(\hat{s}\nu/kT,s\nu/kT\right)=\frac{1}{2}\left(s\nu/kT-\hat{s}\nu/kT\right)^2. \tag{27}$$

It should be noted that we don't use the cross entropy loss function as did in the logistic regression for the reason that the value of $\hat{s}\nu/kT$ is not limited between 0 and 1.

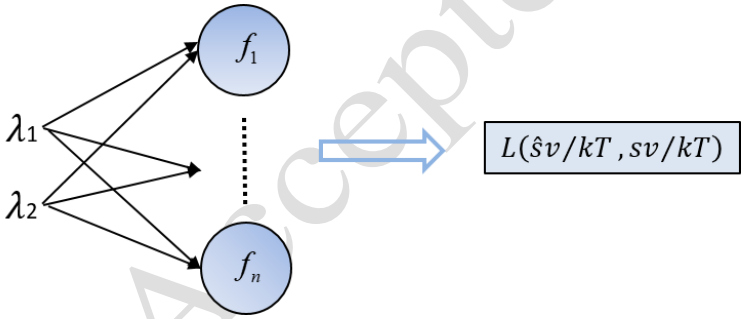


Fig. 10. The schematics of the neural networks liked algorithm for hydrogel under uniaxial load.

In comparison, λ_1, λ_2 and $s\nu/kT$ in the neural networks liked algorithm is like x_1, x_2 and y in the neural networks. Then, we replace the logistic function with $f(\lambda)$ due to the fact that both functions have strong nonlinearity. It should be noted that we can determine $N\nu$, χ, and μ/kT in the neural networks liked algorithm at the same time.

Above is the forward propagation of the neural networks liked algorithm. We then develop the backpropagation to finish the loop of one iteration. First, the differentiation $\hat{s}\nu/kT$ of with respect to L is

$$d\left(\hat{s}\nu/kT\right)=\hat{s}\nu/kT-s\nu/kT. \tag{28}$$

Using the chain rule of differentiation, we can get

$$dN\nu=d\left(\hat{s}\nu/kT\right)\frac{\partial f}{\partial N\nu}=d\left(\hat{s}\nu/kT\right)\left(\lambda_1-\frac{1}{\lambda_1}\right), \tag{29}$$

$$d\chi=d\left(\hat{s}\nu/kT\right)\frac{\partial f}{\partial \chi}=d\left(\hat{\mu}/kT\right)\left(\frac{1}{\lambda_1^2\lambda_2^2}\right), \tag{30}$$

$$d\,\mu/kT=d\left(\hat{s}\nu/kT\right)\frac{\partial f}{\partial\,\mu/kT}=d\left(\hat{\mu}/kT\right)\left(-\lambda_2^2\right). \tag{31}$$

Finally, we update $N\nu$, χ, and μ/kT to iterate:

$$N\nu:=N\nu-\alpha dN\nu, \tag{32}$$

$$\chi:=\chi-\alpha d\chi, \tag{33}$$

$$\mu/kT:=\mu/kT-\alpha d\,\mu/kT. \tag{34}$$

We have implemented the neural networks liked algorithm into Python and the results could be seen in Fig. 11. We input 900 sets of (λ_1, λ_2, $s\nu/kT$). The actual values of $N\nu$, χ, and μ/kT are 0.001, 0.01, and 0, reasonable values taken in many studies (Liu et al., 2015). The learning rate is set to be 5e-5 because it is very easy for the algorithm to converge. We initially set the $N\nu$, χ, and μ/kT to be 100. After 20000 iterations, the algorithm output the value of $N\nu$, χ, and μ/kT as 0.00089437, 0.01002539, and -0.00011973 respectively, which is in a reasonably good agreement with the true value.

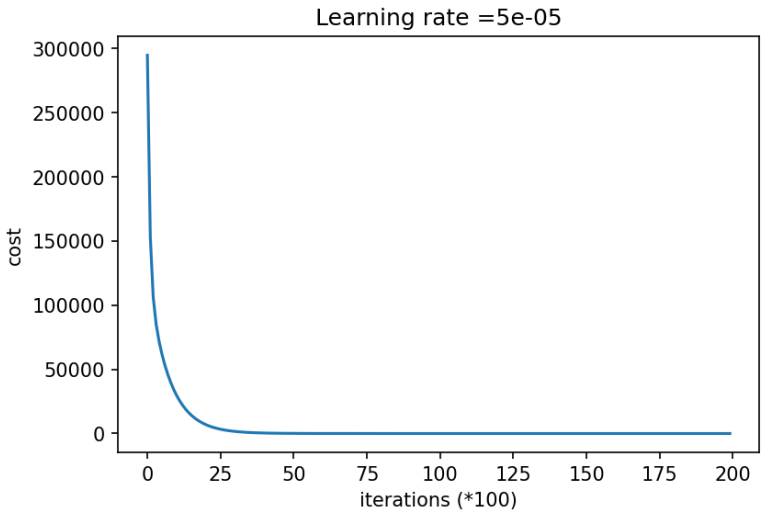


Fig. 11. The cost of the neural networks liked algorithm is plotted as a function of iterations.

Here we demonstrated the effectiveness of neural networks liked algorithm for hydrogel under uniaxial load. With known λ_1, λ_2, and $s\nu/kT$, we used the neural networks liked algorithm to determine the fitting parameter $N\nu$, χ, and μ/kT through iteration at the same time. It should be noted that this neural networks liked algorithm can also be applied to the experimental study of hydrogel. λ_1, λ_2, and $s\nu/kT$ can all be obtained through experiment. So we can determine the value of $N\nu$, χ, and μ/kT through just one loading experiment.

Machine learning is one of the most popular technologies that have the potential to reshape the entire world. It can already make computers synthesis novel art or music. It can also render a medical diagnosis or build an automatic driving system. In Section 5, we will propose several machine learning methods that have potential applications in hydrogel research.

5. Potential applications of machine learning in hydrogel research

In this Section, we hope to use the idea of machine learning to accelerate the current research of the mechanics of hydrogel study. Machine learning can be systematically divided into supervised learning, unsupervised learning and reinforcement learning. The core idea of the

neural networks we exploited in Section 2-4 can be categorized into supervised learning. After systematically studying machine learning, we found that many fully-fledged machine learning technology can be combined with current hydrogel research, as shown in Fig. 12.

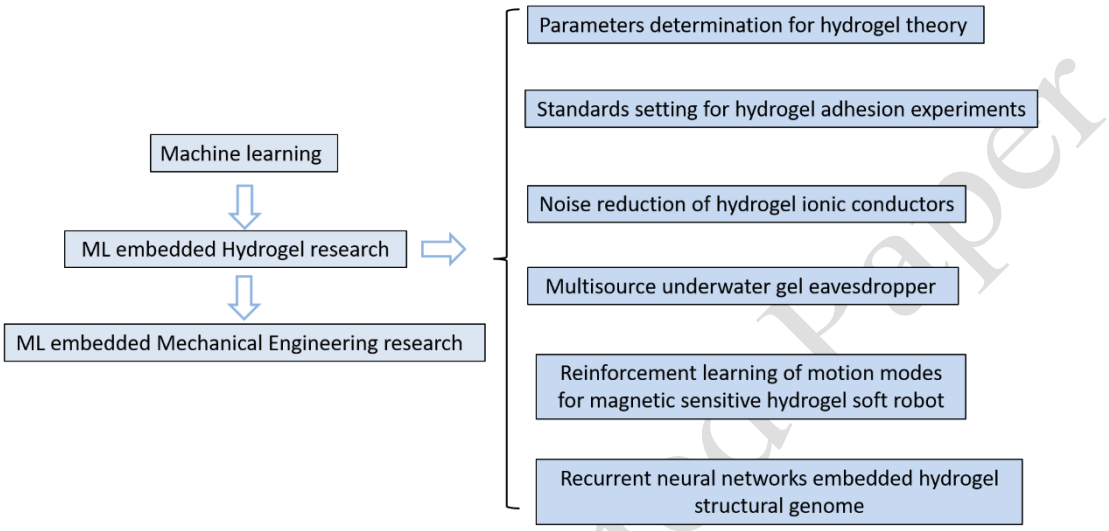


Fig. 12. The schematics of potential applications of machine learning in hydrogel research.

5.1. Parameters determination for hydrogel theory

As presented in Section 2.4, the machine learning embedded method of parameters determination in the constitutional models of hydrogel is a full of research potential. In this paper, we only use the ideology of neural networks to study the constitutional models of neutral hydrogel. Nonetheless, there are several other constitutional models of hydrogels, which can all be studied using the similar machine learning approach to determine their fitting parameters. Classified by their different environmental stimuli, the models can be divided into neutral gel, salt concentration-sensitive gel, pH-sensitive gel, temperature-sensitive gel, photo-thermal sensitive gel and magnetic sensitive gel. Although their theoretical formulations share the same basic formulas, their models are different by considering each respective distinctive free energy density part. For example, for the salt concentration-sensitive hydrogel, except for $N\nu$ and χ, C_0

is another fitting parameter, representing the fixed charges in the gel, those fitting parameters can be determined at the same time using the similar method proposed in this paper.

We talked about the dilemma between converge speed and physical meaning of the parameters in the multi-layer fully-connected neural networks liked algorithm. For future studies, we can focus on design a multi-layer fully-connected neural networks liked algorithm which has both deep layers and parameters with actual physical meanings. This is achievable with at least two nonlinear mechanical models. For example, combing both the large deformation theory of hydrogel and the adhesion theory, specifically the Maugis model, the output of the first layer, stress, is the input of the second layer, which is constructed based on the second nonlinear mechanical models, outputting the contact radius. This kind of design enables the multi-layer fully-connected neural networks liked algorithm to enjoy both deep layers and parameters with actual physical meanings.

5.2. Standards setting for hydrogel adhesion experiments

Analytical and empirical solutions to engineering problems are usually preferred because of their convenience in applications. However, they are not always accessible in complex problems. A new class of solutions, based on machine learning models such as regression trees and neural networks, are proposed and their feasibility and value are demonstrated through the analysis of hydrogel adhesion measurements.

It has been found that both solutions based on regression trees and neural networks can provide accurate results for the fracture toughness measurements, but neural networks-based solutions outperform regression-tree-based solutions in terms of their simplicity (Liu et al., 2020). This example demonstrates that machine learning solutions are a major improvement over analytical and empirical solutions in terms of both reliable functionality and rapid deployment.

When analytical solutions are not available, the use of machine learning solutions can overcome the limitations of empirical solutions and substantially change the way that engineering problems are solved.

Here, specifically for the hydrogel adhesion experiments, there is a distinct inverse problem of identifying adhesion strength based on measured force in peeling experiments. Conventional methods in this field are often computationally or experimentally costly and cannot meet the increasing demand for real-time and high-throughput solutions for advanced manufacturing and clinical practices. Nonetheless, a deep learning approach to address this challenge is achievable by constructing representative sampling spaces of adhesion strength distribution and adopting a conditional generative adversarial net. It is known that the deep learning model can learn high-dimensional mapping via training over a limited portion of the sampling space. So the proposed deep learning approach can bypass the costly iterative solver in conventional methods and can be rapidly deployed with high accuracy, making it particularly suitable for applications such as real-time hydrogel adhesion experimental problems.

5.3. Noise reduction of hydrogel ionic conductors

On one hand, let us briefly talk about the locally weighted linear regression (LWR) algorithm which, assuming there is sufficient training data, makes the choice of features less critical. In LWR algorithm, we set the weight w as:

$$w^{(i)} = \exp\left(-\frac{\left(x^{(i)} - x\right)^2}{2\tau^2}\right), \tag{35}$$

where τ is called the bandwidth parameter.

Note that the weights depend on the particular point x at which we're trying to evaluate x. Moreover, if $|x^{(i)} - x|$ is small, then $w^{(i)}$ is close to 1; and if $|x^{(i)} - x|$ is large, then $w^{(i)}$ is small. Note also that while the formula for the weights takes a form that is cosmetically similar to the density of a Gaussian distribution, the $w^{(i)}$ do not directly have anything to do with Gaussians, and in particular the $w^{(i)}$ are not random variables, normally distributed or otherwise. The parameter τ controls how quickly the weight of a training example falls off with distance of its x;

Locally weighted linear regression is the first example we're seeing of a non-parametric algorithm. The unweighted regression algorithm that we saw earlier is known as a parametric learning algorithm, because it has a fixed, finite number of parameters, which are fit to the data. Once we've fit the parameters and stored them away, we no longer need to keep the training data around to make future predictions. In contrast, to make predictions using locally weighted linear regression, we need to keep the entire training set around. The term "non-parametric" roughly refers to the fact that the amount of stuff we need to keep in order to represent the output grows linearly with the size of the training set.

On the other hand, hydrogels are stretchable, transparent, ionic conductors that can transmit electrical signals of high frequency over long distance, enabling ionic conductor's devices such as artificial muscles, skins and axons. Moreover, ionotronic luminescent devices, ionotronic liquid crystal devices, touchpads, triboelectric generators, artificial eels and gel–elastomer-oil devices can be designed based on hydrogels (Yang and Suo, 2018).

Nonetheless, the noise accompanied by the electrical signal in the hydrogel ionic conductors is one of the puzzles that disables their true application. Here, we propose a LWR embedded noise reduction method for hydrogel ionic conductors. To do so, we can perform a weighted regression of the locally weighted regressions. Based on LWR, we may define the nonparametric

functional regression estimator, which is a locally weighted sum of noise from the training data (this is like locally weighted linear regression, except that instead of predicting *y* we predict a function of noise). Specifically, we can smooth the signal using locally weighted linear regression. We wish to estimate the associated noise by defining the certain function. It has been reported that similar algorithm has successfully achieve noise reduction for quasar spectra (Liu and Bordoloi, 2020). Therefore, the similar approach can be used to reduce noise for hydrogel ionic conductors.

5.4. Multisource underwater gel eavesdropper

In this sub-Section 5.4, we propose a potential application of multisource underwater gel eavesdropper by applying Independent Components Analysis (ICA), a new basis in which to represent the data. ICA is a computational method for separating a multivariate signal into additive subcomponents. This is done by assuming that the subcomponents are non-Gaussian signals and that they are statistically independent from each other. ICA is a special case of blind source separation. A common example application is the "cocktail party problem" of listening to one person's speech in a noisy room (Comon, 1994).

In addition, hydrogel can be used to integrate an easily deformable network of metal nanoparticles in a hydrogel matrix for use as a cavity-free microphone. Since metal nanoparticles can be densely implanted as inclusions, and can even be arranged in coherent arrays, this microphone can detect static loads and air breezes from different angles (Gao et al., 2016).

By combining ICA and the underwater gel eavesdropper device, we can potentially design a multisource underwater gel eavesdropper which can be potentially used to track the sound of whales.

5.5. Reinforcement learning of motion modes for magnetic sensitive hydrogel soft robot

Furthermore, in the reinforcement learning framework, a reward function is provided in the algorithm, which indicates to the learning agent when it is doing well, and when it is doing poorly. In the four-legged walking example, the reward function might give the robot positive rewards for moving forwards, and negative rewards for either moving backwards or falling over. It will then be the learning algorithm's job to figure out how to choose actions over time so as to obtain large rewards. Reinforcement learning has been successful in applications as diverse as autonomous helicopter flight, robot legged locomotion, cell-phone network routing, marketing strategy selection, factory control, and efficient web-page indexing.

It has been reported that printed programmed hydrogels yield fast transformations between complex 3D shapes via magnetic actuation. The approach is based on direct ink writing of an elastomer composite containing ferromagnetic microparticles. By applying a magnetic field to the dispensing nozzle while printing, particles is reoriented along the applied field to impart patterned magnetic polarity to printed filaments (Huang et al., 2020a; Kim et al., 2018).

Reinforcement learning has a huge potential in robot controls. So it is reasonable to use reinforcement learning to train magnetic sensitive hydrogel soft robot to develop complex motion modes. The future study of reinforcement learning embedded hydrogel study can begin with a definition of the Markov decision processes (MDP), which provides the formalism in which reinforcement learning problems are usually posed.

5.6. Recurrent neural networks embedded hydrogel structural genome

Finally, we propose the potential recurrent neural networks embedded hydrogel structural genome study. Recurrent neural networks (RNNs) can be a class of artificial neural networks where connections between nodes form a directed graph along a temporal sequence, which allows it to exhibit temporal dynamic behaviour. RNNs have been successful in applications such as speech recognition, music generation, sentiment classification, DNA Sequence analysis and so on.

Moreover, a new concept, Structure Genome (SG), is proposed to fill the gap between materials genome and structural analysis. SG acts as the basic building block of the structure connecting materials to structures and the mechanics of SG governs the necessary information to link materials genome and structural analysis. Combing RNNs and SG, there is a potential to solve mechanical problems such as failure criterion problems (Liu et al., 2019).

To summarize, machine learning is like the superpower that has great potential to help the hydrogel research. The potential applications can be way much more than what has been listed above.

6. Conclusion Remarks

While the application of machine learning is trending, most of the hydrogel research has not exploited the great property of machine learning. This paper has proposed a machine learning embedded method of parameters determination in the constitutional models of hydrogels. First, inspired by the basic structure of logistic regression, we developed a logistic regression liked algorithm for hydrogel swelling by replacing the sigmoid function with the nonlinear large

deformation theory of neutral gels,, which allows us to determine the fitting parameters $N\nu$ and χ with known swelling ratio λ and chemical potential μ/kT.

Similarly, inspired by the neural networks, the neural networks liked algorithm is developed, which, by its own nature, can effectively solve hydrogel-related problem. The fitting parameters $N\nu$ and χ of the neural networks liked algorithm with one hidden layer still have physical meaning. Nonetheless, due to the influence of the deeper neural networks layers, the fitting parameters of multi-layer fully-connected neural networks liked algorithm don't have physical meaning anymore. In addition, for experimental application purpose, we developed neural networks liked algorithm for hydrogel under uniaxial load, which can determine all the fitting parameters $N\nu$, χ, and μ/kT with one loading experiment. All the codes can be downloaded from http://www.zsliu.net.

Furthermore, we proposed several machine learning embedded potential applications for hydrogel research, which will provide new insights for hydrogel researchers. Local weighted linear regression, independent component analysis, reinforcement learning and other useful tools can all be used to accelerate the study of hydrogel.

Acknowledgement

The authors are grateful for the support from the National Natural Science Foundation of China through grant numbers 11820101001 and 11572236.

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