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Modeling a PEMFC by a support vector machine

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Abstract

This paper reports a modeling study of proton exchange membrane fuel cell (PEMFC) performance by using a support vector machine (SVM). A PEMFC is a nonlinear, multi-variable system that is hard to model by conventional methods. As regards the SVM, it has a superior capability for generalization, and this capability is independent on the dimensionality of the input data. These two merits combine to make it a powerful tool to predict how a PEMFC will behave under different operating conditions. Herein a SVM model of a PEMFC system is built, optimized and tested. First, the model is determined with selected experimental data, and then it is used to predict PEMFC performance. It is shown that the model can make the prediction in 10 ms with the squared correlation coefficient as high as 99.7%. Therefore, the proposed black-box SVM PEMFC model applies to the simulation, real-time control and monitoring of a fuel cell's performance.

Keywords: Fuel cell modeling; Proton exchange membrane fuel cell (PEMFC); Support vector machine (SVM); Support vector regression (SVR)

1. Introduction

A fuel cell, which can provide energy for electric vehicles, power plants and so on, is probably the most promising type of renewable electric power source. The fuel cell vehicle, for example, is acclaimed as the vehicle of the future that almost all manufacturers have made a developmental priority. Among various kinds of fuel cells, the proton exchange membrane fuel cell (PEMFC), with its low operating temperature, high power density, high efficiency, fast startup, quick response and zero emission, is the most suitable for vehicles. A sound model can help size, simulate, evaluate and optimize PEMFC research programs [1], and is thus of great importance to researchers.

The PEMFC system is a nonlinear, multi-variable system that is hard to model. To date, many models have been developed, but most focus on the design of the PEMFC instead of its application. What matters most to PEMFC users, however, is not its relevant internal details but its performance under different operating conditions. What they really need is a behavioral model, with which they can predict PEMFC behavior under various operating conditions.

Motivated by this need and realizing the growing popularity of the support vector machine (SVM) regression application, we decided to make a modeling study of the PEMFC system by using a SVM. The support vector machine was developed by Vapnik [2] on solid VC-theory foundations. It has been used for classification in various domains of pattern recognition and lately, has handled regression problems successfully [3]. Superior generalization performance is obtained from SVM regression and more importantly, the performance does not depend on the dimensionality of the input data. In our study, the proposed SVM model is built, optimized and tested with data obtained from a Ballard MK5-E PEMFC [4]. The experimental results show that cell voltage is predicted with a mean squared error of 0.02% and a squared correlation coefficient of 99.7%.

This paper consists of five sections. The first section serves as an introduction to our study. The second one discusses various existing PEMFC models briefly. The third one is concerned with SVM theories. In the fourth section, the experimental process of building, testing and optimizing our SVM PEMFC model are presented in detail. Conclusions and suggestions for future work are summarized in the last section.

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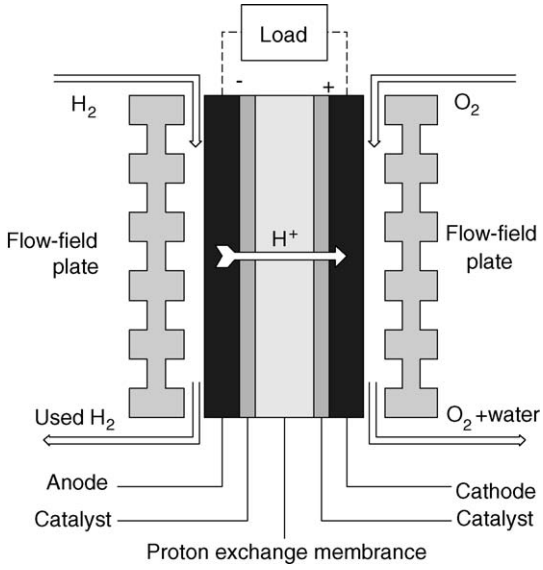

Fig. 1. PEMFC components.

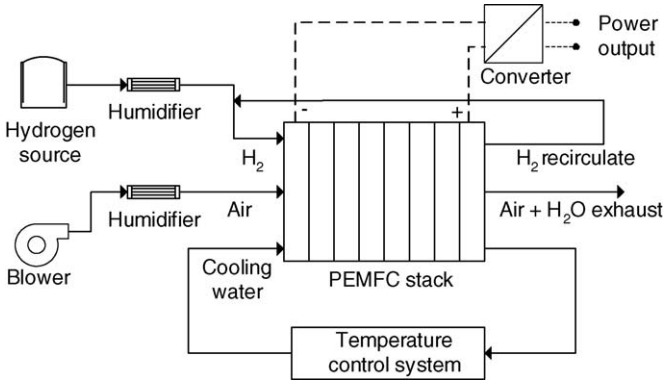

Fig. 2. PEMFC system.

2. Existing PEMFC models

A brief review of various existing PEMFC models is given in this section. Both advantages and disadvantages of the following analytical and experimental models are discussed.

A fuel cell is a chemical reactor that, when fed with fuel and air, can produce electricity continuously. The fuel used is determined by the type of the fuel cell. In the case of a PEMFC, pure hydrogen is commonly used. Pure hydrogen is fed into the anode as fuel and air is fed into the cathode as oxidant. Then, promoted by the electrocatalyst, electrochemical reactions take place, and heat, carbon dioxide and water are produced (Fig. 1).

Some analytical PEMFC models have been put forward, including simplified one-dimensional models [5,6], two-dimensional models [7–9], and a more complex three-dimensional model [10]. Although these models can help analyze and optimize fuel cells in the laboratory context, they have limits. The simplified one-dimensional models are short on accuracy and the two-dimensional and three-dimensional models, with a few immeasurable parameters, are too complicated for most PEMFC users. Consequently, they are not suitable for engineering applications. An empirical modeling approach will be more practical for PEMFC users, from which they can deduce PEMFC stack responses without a knowledge of the internal details.

There are several experimental PEMFC models, among which the most influential one was put forward by Kim et al. [11]

$$U_{\text{cell}} = E_0 - b\log\left(\frac{I}{A_{\text{cell}}}\right) - r\frac{I}{A_{\text{cell}}} - m\exp\left(n\frac{I}{A_{\text{cell}}}\right) \quad (1)$$

The equation expresses the relationship between cell voltage U_{cell} and current I. In it, A_{cell} stands for cell area and other symbols are coefficients: open cell voltage E_0, growth rate of byproducts n, activation coefficient b, ohmic resistance coefficient r and mass transport coefficient m. Eq. (1) provides a good indication of PEMFC performance, but its coefficients relate too closely to operating parameters, such as cell temperature, gas pressure and gas flow rate (Fig. 2). As a result, a given set of operating parameters requires a corresponding set of coefficients. Unless the coefficients change with the operating parameters, the equation produces the wrong results. But it is difficult to keep the operating parameters unchanged for the whole period a PEMFC is working. This drawback greatly restricts the model's application.

Jemei et al. [12] utilized artificial neural network (ANN) methodology and came up with an interesting and powerful solution, i.e. an efficient static PEMFC model. In their study, as experimental and simulated results are very close, the model can be implemented without any difficulty in a complete vehicle powertrain simulation. Highly efficient as it is, however, their model has two main weaknesses. Firstly, although only four experimental learning patterns are needed for the training stage of the network, the training strategy and the topology of ANN are normally determined by experience, which weakens the model's objectivity. Secondly, ANN converges slowly and gets easily trapped in local extremum. Therefore, it is not appropriate for real-time applications.

In short, a new modeling approach is needed to provide a better solution. In the following sections, the SVM-based modeling method will be presented in detail.

3. SVM theories

The support vector machine, based on statistical learning theories or VC-theories, is a novel and powerful tool. It was originally developed at AT&T Bell Laboratories by Vapnik for classification in various domains of pattern recognition, but has recently expanded successfully to deal with regression problems. SVM has a superior ability of generalization to ANN. SVM regression employs the structural risk minimization (SRM) principle to minimize risks rather than the empirical risk minimization (ERM) principle that is used in most traditional ANN models. SVM is also more robust than ANN. In terms of fault-tolerance, ANN behaves unsatisfactorily; all training data, even small noises and errors, can influence its performance. In the case of SVM, however, with the introduction of the ε-insensitive loss function, it uses only part of the training data, i.e. support

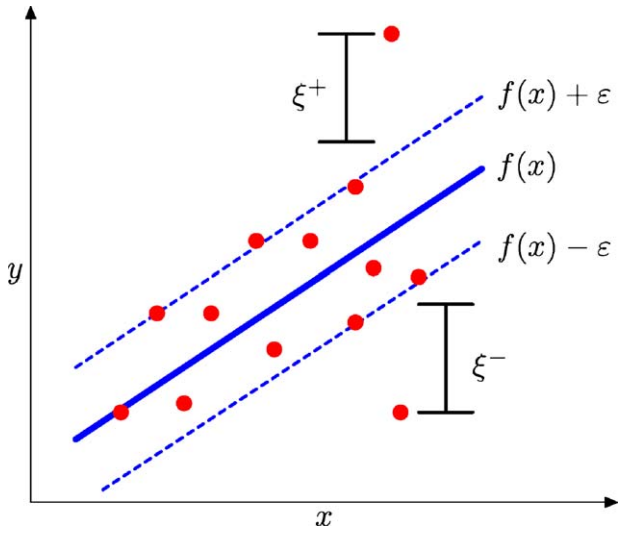

Fig. 3. A linear SVM regression. Points lying outside the ε-tube are named support vectors.

vectors (SVs), to generate output. As a result, the errors smaller than ε are neglected and the notable errors are compensated by slack variables. Next, the theoretical background of SVM will be explained briefly.

For a given data set $D = \{(\mathbf{x}_i, y_i)|i = 1, \ldots, n\} \subset \mathbb{R}^d \times \mathbb{R}$, $\mathbf{x}_i \in \mathbb{R}^d$ is the input data and $y_i \in \mathbb{R}$ is the output data. In a linear case, the mission of SVM regression is to approximate the data set D by a function

$$f(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b \quad \text{with} \quad \mathbf{w} \in \mathbb{R}^d, \quad b \in \mathbb{R} \tag{2}$$

where $\langle \cdot, \cdot \rangle$ denotes the dot product between $\mathbf{w}$ and $\mathbf{x}$ in $\mathbb{R}^d$. Fig. 3 illustrates a linear SVM regression. In a nonlinear case

$$\langle \mathbf{w}, \mathbf{x} \rangle = \sum_{i=1}^{n_{SV}} (\alpha_i^+ - \alpha_i^-) K(\mathbf{x}_i, \mathbf{x}) \tag{3}$$

where $K(\mathbf{x}_i, \mathbf{x})$ is a predefined kernel function, and n_{SV} the number of support vectors. The values of weights α_i^+, α_i^- are decided during the training process. The kernel function is employed to map the nonlinear data into a high dimensional feature space where linear regression is to be performed. Eq. (3) is thus rewritten as

$$f(\mathbf{x}) = \sum_{i=1}^{n_{SV}} (\alpha_i^+ - \alpha_i^-) K(\mathbf{x}_i, \mathbf{x}) + b \tag{4}$$

Support vector regression uses the SRM principle to solve Eq. (4). The SRM principle requires that Eq. (4) be flat, which is subject to the minimum of the functional

$$\Phi(\mathbf{w}, \xi) = \tfrac{1}{2}||\mathbf{w}||^2 + C \sum_{i=1}^{n} (\xi_i^- + \xi_i^+) \tag{5}$$

Constrained by the ε-insensitive loss function

$$L_\varepsilon(y, f(\mathbf{x}, \alpha)) = |y - f(\mathbf{x}, \alpha)|_\varepsilon = \begin{cases} 0, & \text{if} \quad |y - f(\mathbf{x}, \alpha)| \le \varepsilon \\ |y - f(\mathbf{x}, \alpha)| - \varepsilon, & \text{otherwise} \end{cases} \tag{6}$$

where $\varepsilon > 0$ is a predefined constant. The regression algorithm uses the ε-insensitive loss function to describe how the estimated function $f(\mathbf{x})$ deviates from the true one. It accepts errors smaller than ε, but rejects larger ones. The regression can be converted to a convex optimization problem

$$\text{minimum } \Phi(\mathbf{w}, \xi) = \tfrac{1}{2}||\mathbf{w}||^2 + C \sum_{i=1}^{n} (\xi_i^- + \xi_i^+)$$

$$\text{subject to} \begin{cases} L_\varepsilon(y, f(\mathbf{w}, \alpha)) \\ \xi_i^-, \xi_i^+ > 0 \end{cases}$$

where $C > 0$ is a pre-specified constant, and ξ_i^- and ξ_i^+ are slack variables. $||\mathbf{w}||^2$ is the norm of $\mathbf{w}$, and minimum of $\frac{1}{2}||\mathbf{w}||^2$ means that $f(\mathbf{x})$ should be flat. With only the constraint $\frac{1}{2}||\mathbf{w}||^2$, the optimization problem is sometimes infeasible; hence the variables ξ_i^- and ξ_i^+ are added to promise the existence of a solution. Besides, the addition of these two variables allows of some notable errors and makes the algorithm more robust. The constant C adjusts the balance between the flatness and the permitted errors beyond ε. The area between $f(\mathbf{x}) + \varepsilon$ and $f(\mathbf{x}) - \varepsilon$ is called the ε-tube.

Implementing SVM algorithm by mathematical programming is a highly skillful job, but fortunately, some software packages have already been developed. This paper employs LIBSVM [13], an efficient and easy-to-use software for SVM classification and regression.

4. Modeling PEMFC by SVM

For a given PEMFC system, the relation between terminal voltage U and current density I is influenced by many operating parameters: cell temperature T, air flow rate qO_2, hydrogen flow rate qH_2, air pressure P_{O_2}, hydrogen pressure P_{H_2}, relative humidity α, membrane humidity λ, etc. Accordingly, terminal voltage U of PEMFC system is given by

$$U = f(I, T, qO_2, qH_2, P_{O_2}, P_{H_2}, \lambda, \alpha, \ldots) \tag{8}$$

Up to now, no model has ever been able to accommodate all these operating parameters. Our SVM model is no exception. In our experiment, current density I, which is decided by the uncontrollable load, and cell temperature T are taken as variables, and other operating parameters are held constant. Among all the operating parameters, we single out cell temperature T as one of our variables. The reasons for doing so are as follows.

Firstly, it figures significantly in determining terminal voltage U. Secondly, it is easy to measure. Thirdly, although the stack can be operated under a constant pressure and at a constant flow rate, temperature is hard to be held constant in real-world applications. For example, since the stack nominal temperature cannot be attained at startup or when the stack runs at a low power level, cell temperature may vary within a large range. Finally, this simplification does not impair the validity of our

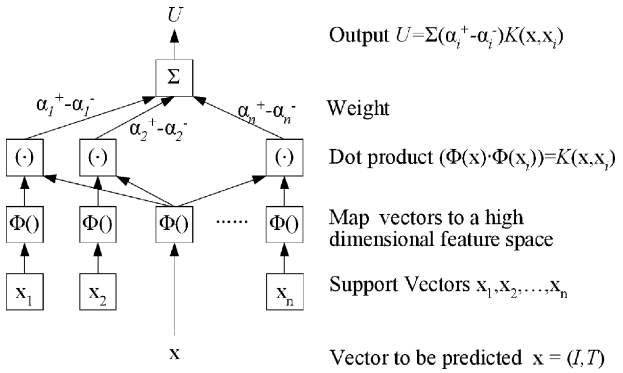

Fig. 4. Illustration of the SVM PEMFC model, which is a feed-forward network. The input is current density and temperature, and the output is voltage. Support vectors and weights are decided during training.

study, which is aimed at modeling PEMFC by SVM. As pointed out before, SVM generalization performance is independent of the dimensionality of the input data. This means that if our SVM model, obtained with the two variables, can make the prediction quite precisely, then a model taking into account more variables can do it with the same degree of precision. Besides, the new multi-dimensional model can be obtained easily; all needed is to add more variables to our model and train it again. Hence in our study Eq. (8) is simplified as

$$U = f(I, T) \tag{9}$$

It follows that the simplified given experimental data set is $D = \{((I, T)_i, U_i)|i = 1, \ldots, n\}$, where $(I, T)_i \in \mathbb{R}^2$ is the two-dimensional input data and $U_i \in \mathbb{R}$ is the output data. The aim of our study is thus to find an SVM model that approximates Eq. (9). The scheme of our proposed model is illustrated in Fig. 4 [14].

Basically, it requires three steps to build an efficient SVM model: preparing training data, training the data to obtain an SVM model, and predicting the new input data with the obtained model [15].

4.1. Preparing training data

Training data ought to cover the entire expected range of operations of the final SVM model. For example, temperatures from 20 to 80 °C and current densities from 0 to 800 mA/cm^2 all should be covered. In most cases, training data should be scaled, normally linearly, to [0, 1] or [−1, +1]. An example of scaled temperature is shown in Table 1. Scaling can increase the training speed and assist in selecting optimal SVM parameters. Another matter worthy of note is that training data and testing data must be scaled to the same interval. In this paper, $U - I$ data obtained at 24, 31, 39 and 72 °C are used as training data, and all those obtained at 56 °C as testing data (Fig. 5). All the data, including averaged cell voltage, current density and temperature, are scaled to [0, 1].

Table 1
An example of cell temperature scaled to [0, 1]

Unscaled (°C)	Scaled
20	0
24	0.067
31	0.183
39	0.317
56	0.6
72	0.867
80	1

4.2. Selecting optimal SVM parameters

The key to obtaining a highly accurate SVM estimation is to choose a proper set of meta-parameters C, ε and kernel parameters. Regression application is essentially more difficult than classification. A lot of work has bee done on support vector classification but little on regression. Fortunately, however, a few recommendations on how to decide on appropriate SVM parameters, though quite contradictory and confusing, have been given in the literature; and several basic rules can be extracted from them [16].

The constant ε is used to find the target function that not only lies as close as possible to the border of the ε-tube but also is as flat as possible. The larger ε is, the flatter the function will be, and the fewer SVs will be. On the other hand, however, a larger ε leads to larger estimation errors. Therefore, the value of ε ought to be determined in a way that it is proportional to the input noise level σ.

The constant C determines the balance between the complexity or flatness of the function and the amount up to which deviations larger than ε are tolerated. Because both C and ε can affect the complexity of the function, they should be adjusted at the same time. This increases the difficulty of selecting the most appropriate parameters. The principle for deciding the value of C is that it is equal to the output range.

It is also important to choose an appropriate kernel function and then assign proper values to its parameters. There are many types of kernels: polynomial kernel, hyperbolic tangent kernel,

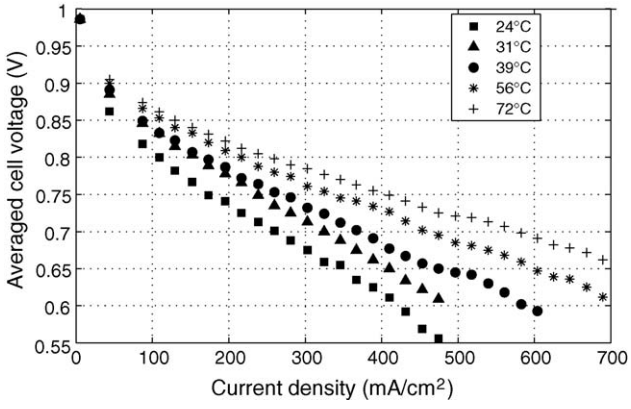

Fig. 5. Characteristics of a Ballard 5 kW MK5-E PEMFC. It is composed of 36 cells; each cell has a 232 cm^2 active area, graphite electrodes, and a Dow membrane. Air pressure P_{O_2} and hydrogen pressure P_{H_2} are both regulated to 3 atm [4].

Radial Base Gaussian Function (RBGF) kernel, B-splines kernel, two-layer neural networks kernel, etc. Polynomial kernels are given by

$$K(x, x_i) = (\langle x, x_i \rangle + c)^p, \quad p \in \mathbb{N}, \quad c > 0 \tag{10}$$

Hyperbolic tangent kernels are given by

$$K(x, x_i) = \tanh(\theta + \phi\langle x, x_i \rangle) \tag{11}$$

RBGF kernels are given by

$$K(x, x_i) = \exp\left(-\frac{||x - x_i||^2}{2\sigma^2}\right) \tag{12}$$

Among all the kernels, RBGF kernel function is the most popular one that ought to be tried first [17], and is thus used in our study.

To determine the optimal parameters, we employ the cross validation method, which is often used in practical applications. The method consists of three steps.

(1) Using four groups of data obtained respectively at 24, 31, 39 and 72 °C as the training data set.
(2) Training SVM with some parameters and predicting other data, and then obtaining the degree of prediction accuracy.
(3) Changing the parameters and repeating the above two steps until a high degree of accuracy is obtained.

With RBGF kernel, ε is set to 0.005. After the above three steps are carried out, the final optimal C is found to be 15 and σ in the kernel is 0.5.

4.3. Predicting with the SVM model

After training, an SVM model is obtained, which can be used to predict new input data. First, the cell voltage at 56 °C with the current density in the range from 0 to 700 mA/cm^2 is predicted. A comparison between the predicted data and the experimental data is then made to evaluate the model's prediction precision (Fig. 6). Next, all the data in the temperature range from 20 to 80 °C and the current density range from 0 to 700 mA/cm^2 are estimated (Fig. 7).

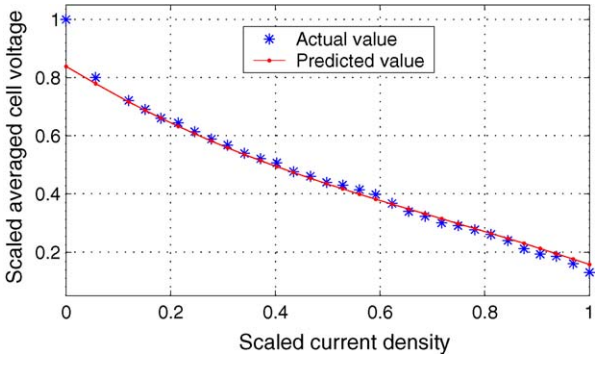

Fig. 6. Averaged cell voltage predicted by the SVM model at 56 °C. Current density varies from 0 to 700 mA/cm^2. All the data have been scaled to [0, 1]. The mean squared error is 0.097% and the squared correlation coefficient is 98.6%.

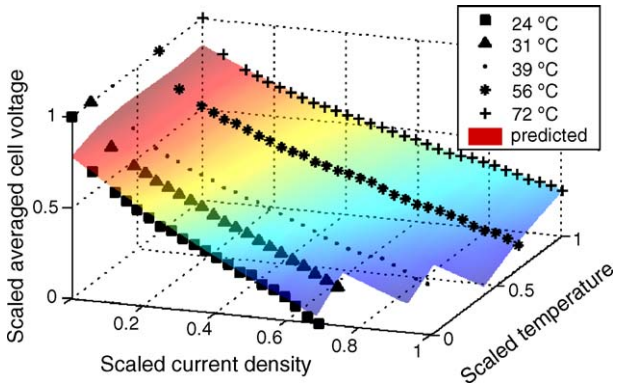

Fig. 7. Averaged cell voltage predicted by the SVM model from 20 to 80 °C. Current density varies from 0 to 700 mA/cm^2. All the data have been scaled to [0, 1].

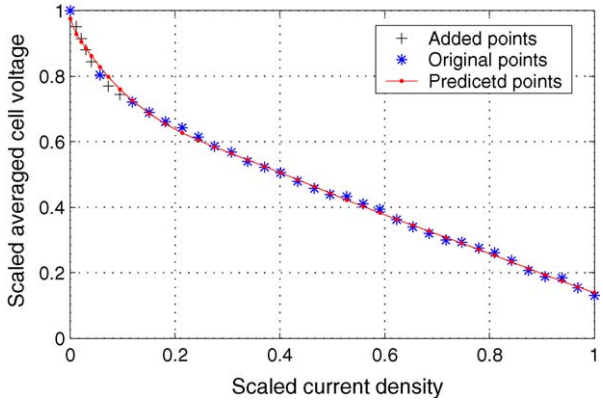

Fig. 8. Averaged cell voltage predicted by the new SVM model at 56 °C. Current density varies form 0 to 700 mA/cm^2. All the data have been scaled to [0, 1]. The mean squared error is 0.02% and the squared correlation coefficient is 99.7%.

Although the results are quite satisfactory, the SVM model can still be improved. As shown in Figs. 6 and 7, there are notable errors between the actual voltage and the predicted voltage at the beginning of the curve. The reason is that while the curve changes greatly at the beginning, the training data are too few to represent the trend of this sharp turn. These few data, however, are regarded as exceptional data points by SVM algorithm. For example, the first point in Fig. 6 is treated as an error and is compensated by slack variables. To describe the curve in accurate detail, we need more data points for the beginning of the curve. Therefore, several data points are supplemented to the beginning of the curve and the new SVM model is trained again. Then the cell voltage at 56 °C is predicted with the new model (Fig. 8). Comparing Fig. 6 with Fig. 8, we can see clearly that the precision at the beginning of the curve is greatly improved.

5. Conclusions and suggestions for future work

An off-line modeling study of a fuel cell using a SVM, which takes PEMFC as the example, is reported in this paper. It is shown that the optimized SVM model is more attractive and more competitive than other modeling solutions in that it possesses a high degree of precision and does not require a pre-knowledge of the

fuel cell. In our study, training a SVM with optimized parameters needs 1583 iterations and only 30 ms on a PIII 800 MHz computer. The time for prediction is no more than 10 ms. Hence, this black-box SVM model is most applicable for simulation, real-time control and monitoring of fuel cell performance.

Among all the operating parameters that can affect the PEMFC performance, only current density and temperature are included in our model. This is because, in accordance with SVM theories, we can incorporate any other operating parameter into a more complete model without degrading the model's generalization performance or complicating the modeling process. Therefore, an online training and prediction algorithm with more variables can be considered in future work.

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