Artificial Neural Network Models of the Ruminal pH in Holstein Steers

Alireza Vakili, Mohsen Danesh Mesgaran and Majid Abdollazade

Abstract— In this study four Holstein steers with rumen fistula fed 7 kg of dry matter (DM) of diets differing in concentrate to alfalfa hay ratios as 60:40, 70:30, 80:20, and 90:10 in a 4 × 4 latin square design. The pH of the ruminal fluid was measured before the morning feeding (0.0 h) to 8 h post feeding. In this study, a two-layered feed-forward neural network trained by the Levenberg-Marquardt algorithm was used for modelling of ruminal pH. The input variables of the network were time, concentrate to alfalfa hay ratios (C/F), non fiber carbohydrate (NFC) and neutral detergent fiber (NDF). The output variable was the ruminal pH. The modeling results showed that there was excellent agreement between the experimental data and predicted values, with a high determination coefficient ($R^2 > 0.96$). Therefore, we suggest using these model-derived biological values to summarize continuously recorded pH data.

Key words—Ruminal pH, Artificial Neural Network (ANN), Non Fiber Carbohydrate, Neutral Detergent Fiber

I. INTRODUCTION

Ruminal acidosis is the consequence of feeding high grain diets to ruminant animals, who are adapted to digest and metabolise predominantly forage diets. Feeding diets that are progressively higher in grain tends to increase milk production, even in diets containing up to 0.75 concentrates [1]. However, short-term gains in milk production from feeding high grain diets are often substantially or completely negated by long-term compromises in cow health. Compromises in dairy cow health due to ruminal acidosis are a concern not only for economic reasons, but also for animal welfare reasons. Sub acute ruminal acidosis is defined as periods of moderately depressed ruminal pH, from about 5.5 to 5.0. Although ruminal pH varies considerably within a day, cows possess a highly developed system to maintain ruminal pH within a physiological range. However, if the acid production from fermentation is more than the system can buffer, ruminal pH compensation fails and ruminal pH may drop drastically.

Alireza Vakili is with the Animal Science Department, Ferdowsi University of Mashhad, Mashhad, Iran. P. O. Box: 91775-1163 (corresponding author to provide phone: 0098-511-7685423; fax: 0098-511-8796845; e-mail: savakili@ um.ac.ir).

Mohsen Danesh Mesgaran is with Animal Science Department, Ferdowsi University of Mashhad, Mashhad, Iran. P. O. Box: 91775-1163 (e-mail: danesh@um.ac.ir).

Majid Abdollazade is with the Mechanical Engineering Department, University of Tehran, (e-mail: m.abdollahzade@gmail.com).

pH fluctuations, specially low pH, affects rumen fermentation and microbial growth [2], but, most current feeding systems for dairy cattle [3]-[4] do not include the effect of pH in their models [5]. In fact, the effects of pH fluctuations on microbial fermentation and nutrient flow have been identified as one of the research needs to improve the prediction of nutrient digestion in the rumen [6]-[7]. The relationship between ruminal pH and dietary variables, and subsequent dairy cow production has not been well documented for cows fed high concentrate diets. Most of the previously ruminal pH prediction models reported were based on the regression analysis methods. Alternatively, a soft-computing method, which is a combination of artificial neural networks seemed to be more appropriate for the ruminal pH prediction. An ANN is a set of nonlinear equations that predicts output variable(s) from input variable(s) in a flexible way using layers of linear regressions and S-shaped functions [8]. Artificial neural networks are new information processing techniques offering solutions to problems that have not been clearly formulated. This paper proposes an artificial neural network approach for modelling of ruminal pH based on time, concentrate to forage ratios, nonfiber carbohydrate and neutral detergent fiber.

II. MATERIALS AND METHOD

Dataset

Four Holstein steers (300 ± 15 kg, body weight) with rumen fistulae were adapted to experimental diets for one week. Steers fed 7 kg of DM of diets differing in concentrate (155 g CP kg-1 of DM; 30% maize, 34% barley, 8% soybean meal, 5% sugar beet pulp, 10% wheat bran, 12% cottonseed meal, 0.3% CaCo3, 0.5% mineral and vitamin premix, 0.2% salt) to forage (155 g CP kg-1 of DM) ratios as 60:40, 70:30, 80:20, and 90:10 in a 4×4 Latin square design (28 days of each period). Ruminal fluid was taken, by suction, via rumen fistula on days 24 to 28 of each period. The pH of the ruminal fluid samples was measured immediately with a portable pH meter (Metrohm 744) before the morning feeding (0.0 h) to 8 h post feeding (interval 15 min) on all ruminal collection days of each experimental period. Data of the consequence days of the each period were then pooled.

ANN Modeling

Neural networks are interconnected processing units which model how human brain performs a particular task. Each of those units, termed neurons, forms a weighted sum of inputs. A constant term, called bias, is then added to each

sum and total sum is passed through a linear, sigmoid or hyperbolic transfer function. Structure of a neuron is depicted in figure 1. Multilayer perceptron (MLP) networks are the most widely used kind of neural networks. Feed-forward neural networks are those which do not form any loop. On the other hand, recurrent neural networks consist of one or more loops. Feed forward networks often include an input layer, one or more hidden layers and an output layer. Typically units in the input layer serve only for transferring the input pattern to the rest of the network, without any processing. Figure 2 shows the structure of a generic three-layered neural network. Finding the optimal network architecture requires trying different combinations. Different number of hidden layers, different number of neurons in each layer and different transfer functions must be examined to achieve the optimal network. It must be noted that too few neurons leads to a network not flexible enough to appropriately model data and on the other hand when there are too many neurons, the network may overfit the data. Numbers of hidden layer neuron are normally chosen by trial an error. Training and learning are two main steps which have to be taken in modeling application. Training of the neural network is normally performed in a supervised manner. It's assumed that a training set, including inputs and desired outputs, is available. In the learning process a neural network constructs an input–output mapping, adjusting the weights and biases at each iteration based on the minimization of some error measure between the output produced and the desired output. Thus, learning entails an optimization process. The error minimization process is repeated until an acceptable criterion for convergence is reached [9].
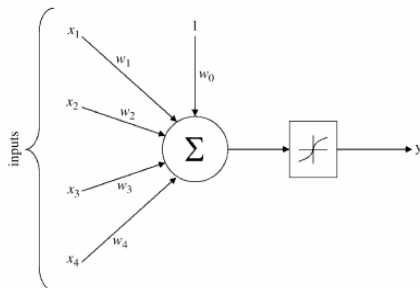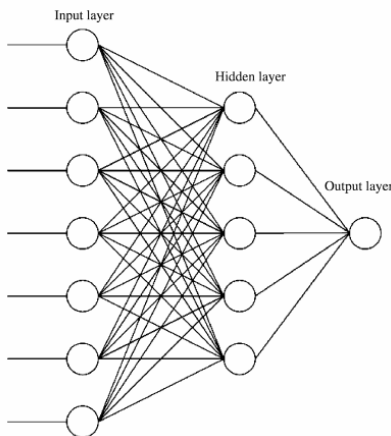

Fig 1. Internal structure of a neuron

Fig 2. Example of a three-layered feed-forward neural network model with a single output unit

The Levenberg-Marquardt algorithm, is a fast learning algorithm which was designed to approach second-order training speed without having to compute the Hessian matrix. When the performance function has the form of a sum of squares (as is typical in training feed forward networks), then the Hessian matrix can be approximated as:

$$H = J^T J$$

$$J(x) = \begin{bmatrix} \dfrac{\partial e_1(x)}{\partial x_1} & \dfrac{\partial e_1(x)}{\partial x_2} & \cdots & \dfrac{\partial e_1(x)}{\partial x_n} \\ \dfrac{\partial e_2(x)}{\partial x_1} & \dfrac{\partial e_2(x)}{\partial x_2} & \cdots & \dfrac{\partial e_2(x)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial e_N(x)}{\partial x_1} & \dfrac{\partial e_N(x)}{\partial x_2} & \cdots & \dfrac{\partial e_N(x)}{\partial x_n} \end{bmatrix}$$

and the gradient can be computed as:

$$g = H^T e$$

Where J is the Jacobean matrix that contains first derivatives of the network errors with respect to the weights and biases, and e is a vector of network errors. The Levenberg-Marquardt algorithm uses this approximation to the Hessian matrix in the following update:

$$x_{k+1} = x_k - \left[J^T J + \mu I \right]^{-1} J^T e$$

Where parameter μ is conveniently modified during the algorithm iterations.

Statistical Parameters

The goodness of fit or accuracy of the model was determined by R-square (R2), mean absolute percentage error (MAPE), root mean squared error (RMSE) and standard deviation error (SDE). Equations formulate these criteria:

$$MAPE = 100 \times \frac{1}{N} \sum_{s=1}^{N} \frac{\left| pH_s^{act} - pH_s^{model} \right|}{pH_s^{act}}$$

$$R^2 = 1 - \frac{\sum_{s=1}^{N} \left(pH_s^{act} - pH_s^{model} \right)^2}{\sum_{s=1}^{N} \left(pH_s^{act} - \bar{p}H_s^{act} \right)^2}$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{s=1}^{N} \left(pH_s^{act} - pH_s^{model} \right)^2}$$

$$SDE = \sqrt{\frac{1}{N} \sum_{s=1}^{N} \left(\frac{\left| pH_s^{act} - pH_s^{model} \right|}{\bar{P}H_s^{act}} - \frac{MAPE}{100} \right)^2}$$

In the above equations, pH_s^{act} and pH_s^{model} are actual and predicted pH respectively. besides $\overline{PH}_s^{act}$ is the average of pH_s^{act} and N is the number of test data. The error criteria are evaluated only using the test data in the comparisons.

Model Development

In this study, several three-layered feed-forward neural networks trained by the Levenberg-Marquardt algorithm were used for modelling of ruminal pH. Efficiency and accuracy of the presented models were demonstrated using real experimental data. The software package MATLAB (Version 2007b) was used to fit a truly connected MLP model to the training dataset. A neural network model consists of an input layer, an output layer, and one or more hidden layers. In this study, the ANN was designed with only one hidden layer with four neurons and one output [Figure 3]. One hidden layer is usually sufficient to approximate any continuous nonlinear function, although more complex networks must be used in special applications [10].

In the present study, the neural network models to predict ruminal pH were developed using two and four input variables: time, C/F, and NFC and NDF concentrations. The training dataset was randomly split into a training dataset (n = 69, i.e., 75% of the data) and a test dataset (n = 23, i.e., 25% of the data).

ANN models for the training and validation data sets are presented in figures 4 and 5. These figures show a comparison of model predictions with the experimental values of ruminal pH. Each model was developed separately for time + C/F, and time + C/F + NFC + NDF. The simplified algebraic equations derived from the ANN models for the prediction of ruminal pH with time + C/F (1) and time + C/F + NFC + NDF (2) are presented as follows:
Model 1:

$$pH = 5.3753 + 0.8812 \times f_1 + 0.2014 \times f_2 + 0.8147 \times f_3 + 0.2014 \times f_4$$
$$f_1 = f(17.5202 + 0.0096 \times Time - 0.2398 \times C/F)$$
$$f_2 = f(-9.0205 + 0.3416 \times Time - 1.5472 \times C/F)$$
$$f_3 = f(-6.4328 - 0.0252 \times Time + 0.1038 \times C/F)$$
$$f_4 = f(30.2528 - 0.0681 \times Time - 0.2503 \times C/F)$$
$$f(x) = \frac{1}{1 + \exp(-x)}$$

Model 2:

$$pH = 6.072 + 1.2012 \times f_1 + 0.4611 \times f_2 - 0.8159 \times f_3 + 0.3313 \times f_4$$
$$f_1 = f(-41.9838 - 0.0177 \times Time + 0.3147 \times NDF + 0.9410 \times NFC - 0.1849 \times C/F)$$
$$f_2 = f(29.8559 + 0.0030 \times Time + 1.0808 \times NDF - 0.5071 \times NFC - 0.3747 \times C/F)$$
$$f_3 = f(0.1214 - 0.0120 \times Time - 0.1532 \times NDF + 0.1857 \times NFC - 0.0377 \times C/F)$$
$$f_4 = f(-11.8424 - 0.0649 \times Time + 0.3928 \times NDF + 0.4916 \times NFC - 0.1551 \times C/F)$$
$$f(x) = \frac{1}{1 + \exp(-x)}$$

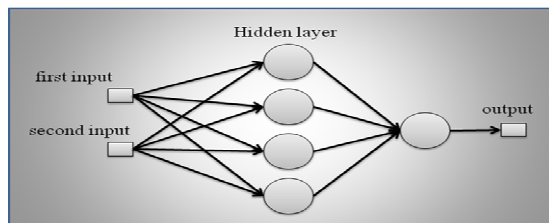Where f (x) is activation function.

Fig 3. Selected neural network structure: two inputs were used for the artificial neural network (ANN): first input is time and the second input is concentrate to alfalfa hay ratios (60: 40, 70: 30, 80: 20 and 90: 10). For the ANN used to predict the ruminal pH, one output was used and the output value was the "ruminal pH".

Table 1. Statistical analysis of the prediction of ruminal pH using the neural network approach

Model	Inputs[1]	R^2	MAPE	SDE	RMSE	Rank
1	Time-C/F	0.9720	0.8314	0.0045	0.0589	1
2	Time-C/F-NFC-NDF	0.9612	0.8787	0.0068	0.0694	2

Statistical parameters[2]

[1]Inputs: C/F = concentrate to alfalfa hay ratios; NFC = Nonfiber carbohydrate (g/kg DM); NDF = Neutral detergent fiber (g/kg DM).
[2]Statistical parameters: R^2 = R-Squared; MAPE = Mean Absolute Percentage Error; SDE = Standard Deviation Error; RMSE = Root Mean Squared Error.

III. RESULTS AND DISCUSSION

In the present study, the input variables of time, C/F, and NFC and NDF concentrations were included in the neural network models because of their potential role in explaining the output variable (ruminal pH). It was previously demonstrated that the amount of fiber in the ration affects rumen pH [11]. The NDF level is inversely related to the more fermentable NFC component of the diet [12]. The balance of carbohydrates in the diet impacts milk production because it affects amount and ratios of ruminal VFA produced, which in turn alters metabolism and partitioning of nutrients [13].
Table 1 summarizes the key statistical measures used to compare performance of the models. The performance of the
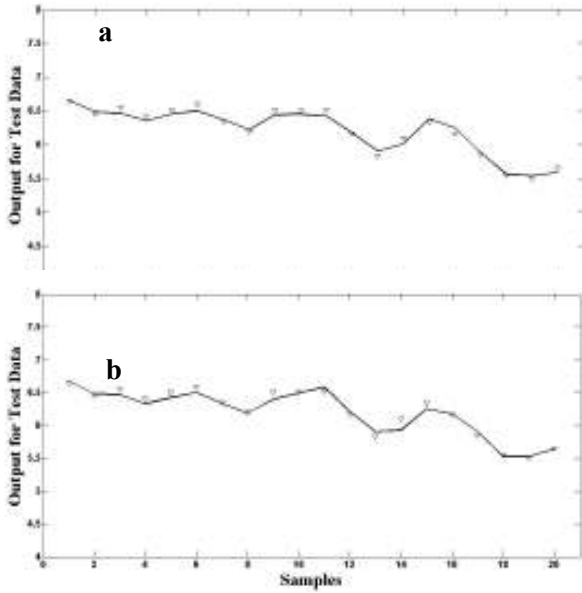
Fig 4. In the developed models ~75% of the data were used for training and ~25% for validation (—: predicted ruminal pH, ∇: actual ruminal pH). The y-axis represents the output for test data. The scale from 4 to 8 on the y-axis represents ruminal pH (a = time + C/F and b = time + C/F + NFC + NDF). C/F = Concentrate to alfalfa hay ratios; NFC = Nonfiber carbohydrate; NDF = Neutral detergent fiber.
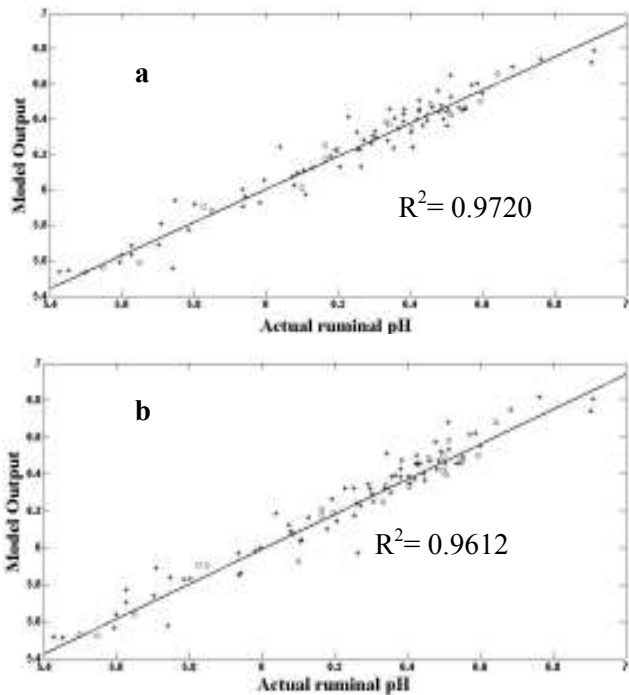

Fig 5. Correlation of neural network models output vs. actual ruminal pH values with training data set (69, *: training data) using the optimal network, with 1 hidden layer with 4 neurons and a test data set (23, ○: test data). The y-axis represents the output of model vs. Actual pH on the x-axis. The scale from 5.4 to 7 on the y-axis and x-axis represent ruminal pH (a = time + C/F, and b = time +

C/F + NFC + NDF). C/F = Concentrate to alfalfa hay ratios; NFC = Nonfiber carbohydrate; NDF = Neutral detergent fiber.

The models were developed by time + C/F gave better results than another model. The error parameter values were the lower for the model was developed by time and C/F; furthermore, the highest R^2 belonged to this model [Table 1]. RMSE, MAPE and SDE parameters became increased for another model, however, correlation coefficient values were> 0.96 for all models [Table 1], which indicated high precision and accuracy. Therefore, time and C/F were considered the optimal factors to use in describing ruminal pH. Researchers have shown that ruminal pH was highly influenced by the C/F and the dietary level of fermentable carbohydrates [14]-[15]-[16]. Results of the present experimental showed that the training procedure for ruminal pH prediction was very successful and that a perfect match was obtained between the measured and the calculated values.

IV. CONCLUSION

Combining neural networks with objective readings might result in powerful predictions. The modelling results showed that there was excellent agreement between the experimental data and predicted values, with a high determination coefficient (R^2 >0.96), showing that the developed models were able to analyze nonlinear multivariant data with very good performance, fewer parameters, and shorter calculation time. Although ANN has been used in many applications in animal science, this is the first study modelling the prediction of ruminal pH using ANN. The use of ANN provides an inexpensive and easy technique for evaluation of ruminal pH. The conceptual ANN model provides a database and an alternative generic framework for the modeling of ruminal pH. These models have potential to be used as an alternative method to control the ruminal acidosis, estimate the ruminal pH, and ensure the dairy cow health. The results indicated that the ANN model can reliably and satisfactorily simulate the system and is a potential alternative tool to be use for practical assessment and biological system development.

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