Wine Quality Estimation System using Deep Neural Network with Reduced Measurable Features

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***Abstract*—This paper presents a wine quality estimation system using deep neural networks. The proposed system is intended for environments with reduced measurable features from inadequate chemical measurement instruments such as homebrewing. A simple feedforward neural network is employed as the core component of the quality estimation system. Input of the system includes chemical profiles of the wine. Output of the system is the wine quality score in the range from 0 to 10. Four feedforward neural network (FNN) models are developed and trained using the same dataset from the online source with different conditions. The first model is developed using the base dataset with 11 input features. The second model is developed using the dataset with the number of input features reduced from 11 to 3 by filling zeroes in most input feature columns. The third model is trained using the dataset with the number of input features reduced from 11 to 3 by removing most input feature columns from the dataset. The last model is trained with the transfer learning approach on the same dataset as the third model. Developed FNN models are tested in wine quality estimation experiments with applicable test sets. Among models developed for environments with input features significantly reduced, the model with transfer learning achieved the most satisfying results across the evaluated metrics.**

***Keywords*—wine quality estimation, reduced input features, FNN, transfer learning, deep neural networks**

I. Introduction

Wine is one of liquors which has been produced and consumed since ancient times. Archaeological evidence suggests that the earliest consumption of wine can be traced back more than 7,000 years [1]. In present days, wine is still widely produced and consumed around the globe, despite the declines in wine consumption during recent years [2]. Production of wines is accessible for both industrial and local sections. Craft wine is one of the wines that usually made by local sections. Due to the growing popularity of craft wines, the global craft wine market size is expected to reach 61.89 billion USD by 2032 [3]. Successful winemaking process results in high quality wines. Several methods exist for measuring wine quality, including the sensory responses and the analysis of wine chemical profiles [4]. Sensory assessment requires professional tasters who typically rely on established frameworks such as the assessment of wine balance, length, intensity, and complexity (BLIC) [5]. On the contrary, the chemical analysis of the wine focuses on measurements of complex markers such as volatile acidity, pH, and alcohol.

Chemical analysis of wine is regarded in recent works as an objective method which can provide reproducible and accurate results. Recent studies have extensively utilized these chemical characteristics to evaluate wine quality, trace authenticity, and map consumer acceptability [6-8]. However, assessing comprehensive chemical properties of the wine requires sophisticated laboratory equipment. These analysis tools cannot be easily accessed by artisanal winemakers and homebrewers who are mostly restricted to basic measurement devices such as a hydrometer [9].

In recent years, machine learning (ML) and artificial intelligence (AI) have emerged as highly effective tools for predicting wine quality. Numerous ML algorithms have been developed and applied to estimate wine quality in the chemical profile analysis. Machine learning algorithms such as XGBoost, Support Vector Machine, and neural networks were successfully applied to classify wine quality based on comprehensive chemical profiles in recent research [10-12]. Despite effectiveness of ML and deep neural networks in developing wine quality prediction systems, these systems rely on comprehensive chemical datasets such as the widely used 11-feature wine quality datasets [10]. Users of these systems require all elements of chemical profile inputs, which cannot be measured practically with basic measurement tools.

Improvement techniques for ML such as transfer learning can be introduced to systems with neural networks, to create a wine quality estimation system for environments with low number of measurable features such as in homebrewing. Transfer learning can improve deep neural network models by leveraging trained patterns from models of similar tasks to create a new model [13]. Therefore, this paper proposes a wine quality estimation system using a deep neural network model for environments with low number of input features. The proposed system reduces the standard 11-feature requirements to three fundamental parameters which can be measured with less effort, including residual sugar, pH, and alcohol. Chemical features of the wine are used as the input. The output of the system is the wine quality score, ranging from 0 to 10. Four feedforward neural network (FNN) models are developed and trained using the same dataset from an online source [14], with differences in the input features. Three of the models are simple FNNs trained with different variants of the dataset, while the remaining model is employed with transfer learning. The FNN models are evaluated in experiments which require the model to estimate the wine quality score based on input features, using applicable wine quality test sets.

Fig. 1. Diagram of the proposed wine quality estimation system.

	A	B	C	D
1	fixed acidity	volatile acidity	citric acid	residual sugar
2	7.4	0.7	0	1.9
3	7.8	0.88	0	2.6

(a)

	A	B	C	D
1	fixed acidity	volatile acidity	citric acid	residual sugar
2	0	0	0	1.9
3	0	0	0	2.6

(b)

	A	B	C	D
1	residual sugar	pH	alcohol	quality
2	1.9	3.51	9.4	5
3	2.6	3.2	9.8	5

(c)

Fig. 2. Examples of data in implemented datasets: (a) base dataset, (b) dataset with zero-filled, (c) dataset with column removal.

The remainder of this paper is organized as follows: Section 2 details the proposed wine quality estimation system, Section 3 explains the experiments and results, and Section 4 concludes this paper with a discussion on future work.

II. Wine Quality Estimation System

The proposed quality estimation system implements a simple feedforward neural network (FNN) as its core module, as illustrated in Fig. 1. The neural network determines quality of the wine based on the input chemical profiles. The output of this neural network is the wine quality score, ranging from 0 to 10, in which 0 refers to the lowest quality and 10 resembles the highest wine quality. Four FNN models were designed and developed through different approaches. These models were developed to investigate the suitable models for homebrewers, who have limited access to complex chemical measurement instruments. Detailed information of the developed FNN models and the applied dataset are described in following subsections.

A. Wine Quality Dataset

Typically, neural network is considered as one of the supervised machine learning algorithms. In machine learning, supervised algorithms utilize labeled data to learn a function that predicts target output from input features [15]. The development of the proposed system also requires data to train the neural network models. From vastly available datasets, the wine quality dataset from Kaggle platform was selected for the development due to the ease of access [14]. The implemented dataset is in the form of a CSV file with 12 columns and 1143 rows. Among 12 columns, 11 columns are the input chemical profiles of the wine, while the remaining column is the output quality score. The 11 input columns are composed of 1. fixed acidity, 2. volatile acidity, 3. citric acid, 4. residual sugar, 5. chlorides, 6. free sulfur dioxide, 7. total sulfur dioxide, 8. density, 9. pH, 10. sulphates, and 11. alcohol. Rows in the dataset were separated manually into the train set and the test set. The first 993 rows are used as the train set, and the remaining 150 rows are included in the test set. The train and the test sets reside in different files.

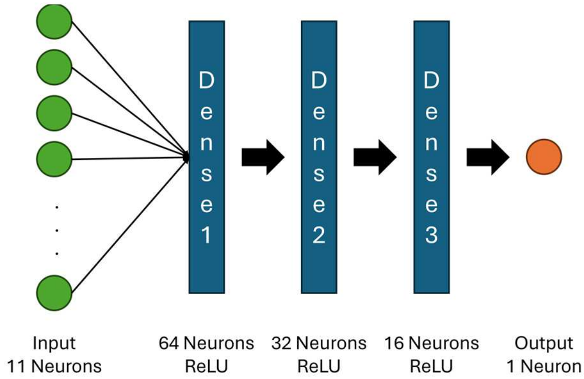

Fig. 3. FNN structure for wine quality estimation with 11 input features.

The base dataset was augmented to create two additional variants for training and testing more neural network models. The dataset was augmented by reducing the number of input features from 11 to 3, as examples displayed in Fig. 2. The remaining features include residual sugar, pH, and alcohol, which are easier to be measured by homebrewers with basic measurement devices. The first variant in Fig. 2 (b) has values in the reduced input feature columns filled with zeroes, while the number of columns remains the same. Zeroes are filled in both train and test sets of data. The second variant in Fig. 2 (c) has the entire column of the reduced features removed from the files. Both the train and the test sets have columns of the input features removed, with only residual sugar, pH, and alcohol remain as input features. The columns of the output quality score remain the same. In total, six separated dataset files are applied in the development of the proposed system.

B. Base NN Models for Wine Quality Estimation

Feedforward neural network can be implied as the simplest model to be implemented in deep learning applications. FNN is normally composed of an input layer, hidden layers for calculations, and the output layer. Typically, FNN learns a function that predicts the target output from input features through the training process, using labeled data. Input features are sent from the input layer to the hidden layers which handle the calculations. The information calculated from the hidden layers is processed further at the output layer to obtain the target output. Many deep FNN models such as [16] contain a significant number of layers and neurons, which can increase complexity during implementations on low-end devices. Thus, simple FNNs are employed as core structures of designed neural network models, increasing accessibility.

Two FNN structures were designed to create three base models for wine quality estimation. Fig. 3 shows the design of the first FNN structure. The first structure consists of an input layer with 11 neurons, an output layer with a single neuron, and 3 dense layers working as hidden layers. The first dense layer contains 64 neurons. The second and third dense layers contain 32 and 16 neurons, respectively. Activation functions of all hidden layers are ReLU. The output layer has no activation function applied. The first structure was used to develop two FNN models with 11 input feature columns. The

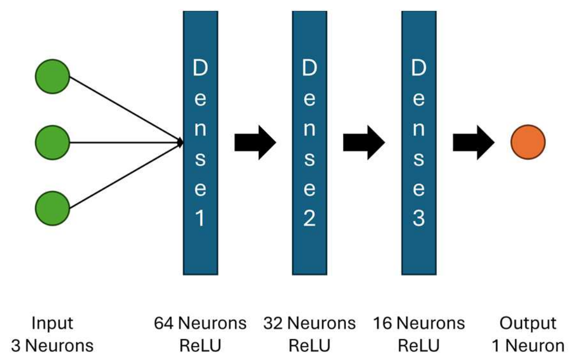

Fig. 4. FNN structure for wine quality estimation with 3 input features.

TABLE I. TRAINING SETTINGS FOR FNN MODELS

Settings	Values
Training : Validation Split	80:20
Loss Function	Mean Squared Error
Optimizer	Adam (Default)
Batch Size	64
Training Epochs	128
Early Stop	On (24 Patience)

second structure has the design as shown in Fig. 4. The second structure possesses the same settings and the same design as the first structure. The only difference is the input layer which comprises only 3 neurons. The second structure was used to develop a simple FNN model with 3 input features.

The development of three base models mainly consisted of the selection of the structure for the model, and the training of the models with designated datasets. The training of three base models employed the same settings and hyperparameters, which are described in Table 1. The 993 rows of the training set were divided further into the actual training set and the validation set. The scale in the division was 80:20, in which 80% of the training set was applied in the actual training, and the remaining 20% was applied for the validation during the training. Adam optimizer was employed in the training with default settings as stated in [17]. Mean squared error (MSE) was applied as the loss function. The actual training dataset was used to train designed models in batches, with the batch size of 64. The maximum epoch was set to 128. An early stop was set for the training, which monitored the changes in the validation loss values with patience setting of 24. This patience setting implies that the training process will be stopped once the validation loss value did not improve, i.e. lower, for 24 epochs. The first and second models implemented the designed structure with 11 inputs. The third model utilized the designed structure with 3 inputs. The first model was trained with the base dataset without data augmentation. The second model was trained through the dataset with zeroes filled in columns of reduced input features. The third model was trained with the dataset which has the reduced features completely removed from the dataset file. Training results of all three base models expressed the same trend in training loss and validation loss values. Fig. 5 (a), Fig. 5 (b), and Fig. 5 (c) illustrate the training losses and validation losses of the first, the second, and the third models,

TABLE II. MEAN SQUARE ERRORS FROM INITIAL EVALUATIONS OF DEVELOPED FNN MODELS

Models	Mean Square Error (MSE)
Model 1 (Base)	0.4165
Model 2 (Zero-Filled Data)	0.4876
Model 3 (Data Removal)	0.4837
Model 4 (Transfer Learning)	0.4725

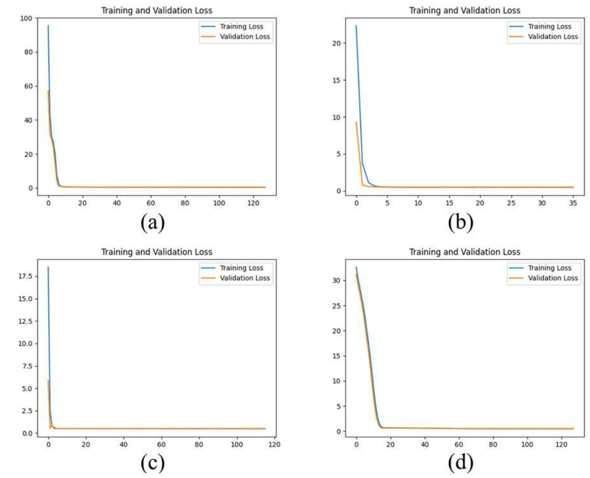

Fig. 5. Training and valudation loss of developed FNN models: (a) the first base model, (b) model with zero-filled data, (c) model with data removal, and (d) the transfer learning model.

respectively. Losses or errors in the training were sharply reduced during early epochs of the training, before saturating in later training epochs. Validation losses from validation datasets of each model also expressed the same characteristics as training losses, with the same sharp reduction in earlier epochs and saturated in later epochs. Trained models were initially evaluated with losses from the validation set of each model, which were calculated through MSE. Results from early evaluations are described in Table 2. The first model achieved the lowest loss with a value of 0.4165, while the second model possesses the highest loss of 0.4876. The third model achieved the loss of 0.4837.

C. FNN Model with Transfer Learning

Initial investigation on developed basic models indicated that models with reduced features achieved higher losses. In order to reduce losses on the model with removed input features, transfer learning approach is applied to the models. Transfer learning is a technique for neural networks which allow the knowledge from one model to be transferred to another that performs similar tasks [14]. In this case, knowledge from the first base model was transferred to create a new model, as the loss was lowest during the evaluation. From performances of the third base model during the initial evaluation, the model created through the transfer learning employs the same dataset as the third model, with similar structure of 3 input features.

Structure of the fourth model with transfer learning is different from the third base model, despite the same training data, as shown in Fig. 6. Input layer of the transfer learning model contains 3 neurons, according to the 3 input features in

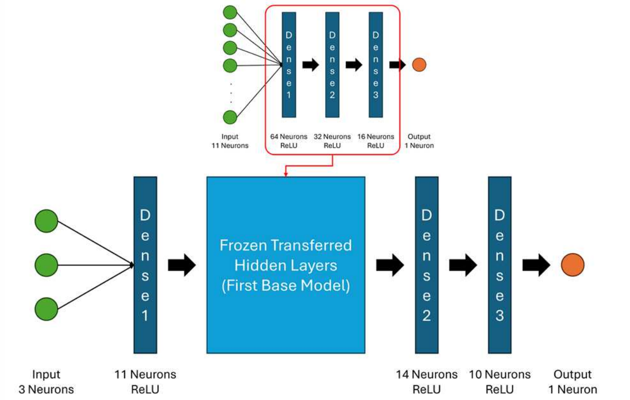

Fig. 6. Structure of the FNN model with transfer learning approach, using knowledge from the first base model.

the dataset. Output layer comprises of a single neuron, with no activation function, to output the wine quality, same as all developed models. The transfer learning model employs all hidden layers from the first base model. These hidden layers from the base model remain frozen throughout the training process, in which all neuron in these layers are not trained. As the first hidden layer of the base model requires 11 inputs, a dense layer, with 11 neuron and ReLU activation, is placed before the layers from the base model to perform as an adapter. Two additional dense layers are also added after the transferred hidden layers to assist in mapping information from the frozen transferred layers to the output. These additional layers contain 14 and 10 neurons, respectively. Activation functions of two additional layers are set to ReLU.

FNN model with transfer learning was trained with the same dataset and the same settings as in the training of the third base model from Table 1. Training results from Fig. 5 (d) showed the similar characteristics in training and validation losses as other trained models. Trained FNN with transfer learning was initially evaluated though the loss calculation using the validation dataset. Initial evaluation result from the model is included in Table 2. The model with transfer leaning achieved the loss of 0.4725 during the evaluation.

III. Experimental Results

The trained FNN models were tested in wine quality estimation experiments. All models were tested with applicable test sets which located in separated files. Models with 11 input neurons, including the first two base models, were tested with the base test set with no augmentation and the test set with zeroes filled in reduced feature columns, since both test sets contain 11 input feature columns. Models with 3 inputs, including the third base model and the transfer learning model, were tested with the test set which contains only 3 input feature columns. In total, there were six tests conducted in wine quality estimation experiments. Each test has the model predicts the wine quality score based on input features for 150 times, according to 150 rows in each test set.

Estimation performances from each FNN model were evaluated using mean squared errors (MSE), mean absolute errors (MAE), and R squared scores (R^2). The applied metrics were calculated from estimated quality scores, which resulted from the developed models. From two types of errors applied, the implemented formula for the MSE calculations can be mathematically described as

$$MSE = \frac{1}{n}\left(\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2\right) \quad (1)$$

where *MSE* is the calculated mean squared error, Y is the actual wine quality score in the test set, $\hat{Y}$ is the predicted quality score, and n is the total number of test data rows, which remains 150 in all tests. MAE values of experimental results were calculated from the equation described as

$$MAE = \frac{1}{n}\left(\sum_{i=1}^{n}\left|Y_i - \hat{Y}_i\right|\right) \quad (2)$$

where *MAE* is the calculated mean absolute error, Y is the actual wine quality score, $\hat{Y}$ is the predicted score, and n is the total number of test data rows. Apart from the errors, the results from each model were also measured through the coefficient of determination or the R^2 score. The R^2 score determines the effectiveness of the model in the fitting of the data, which refers to each test set during experiments. The implemented equation for the calculations of R2 scores is described as

$$R^2 = 1 - \frac{\sum_i (Y_i - f_i)^2}{\sum_i (Y_i - \bar{Y})^2} \quad (3)$$

where R^2 is the calculated R^2 score, Y is the actual wine quality score, f is the predicted score, and $\bar{Y}$ is the average wine quality score in the test set. Values of R^2 scores are normally in the range from 0 to 1. R^2 score of 1 indicates that the model perfectly fits the data. R^2 score of 0 means the model cannot explain variability in the data. The prediction performance of the model with 0 R^2 score is just the same as the horizontal line representing the average prediction target, which is the average wine quality score in each test. R^2 score can have its value below 0 or negative R^2 score, which indicates that the model performs worse than the horizontal average line.

Experimental results which evaluated through the applied metrics are presented in Table 3. Experimental results from the test set with all available 11 input features suggest the significant performances of the first model which trained through the data with all input features. The first model achieved 0.5733 MSE, 0.5669 MAE, and 0.2307 R^2 score. The second model trained with zero-filled dataset performed much worse on the 11 inputs test set, with 96.2648 MSE, 7.642 MAE, and the R^2 score of -128.1644. The model trained with zero-filled dataset performed with more favorable results with the test set with zeroes filled in every input columns, except for residual sugar, pH, and alcohol. For experiments with the zero-filled test set, the second base model achieved 0.6559 MSE, 0.5891 MAE, and 0.1198 R^2 score, while the first base model achieved 13.3911 MSE, 3.5673 MAE, and the R^2 score of -16.9677. The last two experiments conducted on the test set with 3 input features, including residual sugar, pH, and alcohol. The models included in last two experiments were the third based model and the model with transfer learning implemented. Results from experiments on the test set with reduced feature columns provide promising results from both tested models. The third base model trained with removed features dataset achieved 0.6488 MSE, 0.5852 MAE, and 0.1293 R^2 score. The transfer learning model performed with slightly better results by achieving 0.6391 MSE, 0.5876 MAE, and the R^2 score of 0.1423.

TABLE III. RESULTS FROM DEEP NN MODELS IN WINE QUALITY ESTIMATION EXPERIMENTS

Models	MSE	MAE	R^2 Score
Base Test Set Experiments			
Model 1 (Base)	0.5733	0.5669	0.2307
Model 2 (Zero-Filled Data)	96.2648	7.642	-128.1644
Model 3 (Data Removal)	-	-	-
Model 4 (Transfer Learning)	-	-	-
Zero-Filled Test Set Experiments			
Model 1 (Base)	13.3911	3.5673	-16.9677
Model 2 (Zero-Filled Data)	0.6559	0.5891	0.1198
Model 3 (Data Removal)	-	-	-
Model 4 (Transfer Learning)	-	-	-
Data Removed Test Set Experiments			
Model 1 (Base)	-	-	-
Model 2 (Zero-Filled Data)	-	-	-
Model 3 (Data Removal)	0.6488	0.5852	0.1293
Model 4 (Transfer Learning)	0.6391	0.5876	0.1423

Results from six experiments revealed that the model which trained with the base data set of 11 input features performed the best among the developed models, in which lowest errors and the most R^2 score were achieved from the model. The outcomes of the experiments were expected, as more input features and more data can result in models with better accuracies. However, once the input features are not available from the measurements, the models trained with the dataset that have these unavailable features entirely removed from the file performed slightly better than the use of zero-filled data. Comparing the best results from the third base model trained and the second base model, MSE of the third model was lower by 1%, MAE was lower by 0.6%, and the R^2 score was higher by 7.9%. Results from the transfer learning model was similar to the third base model in terms of errors, in which MSE was lower by 1.5%, but the MAE was slightly higher by 0.4%. In term of the R^2 score, the transfer learning model performed with a noticeably better result, with R^2 score higher than the third base model by 10%. Comparing the transfer learning model with the second base model, MSE was lower by 2.5%, MAE was lower by 0.2%, and R^2 score was higher by 18.7%. However, performance of the model with transfer learning is noticeably inferior to the first model trained with all input features, with 11.4% higher in MSE, 3.6% higher in MAE, and 38.3% lower R^2 score. Despite inferior performances to the model with abundant input features, the model with transfer learning has proved to be viable for initial wine quality estimation in situations where most measurable features are unavailable.

Although developed models provided promising results in wine quality estimation, there are rooms for improvements which should be investigated further. One of the points is that the best R^2 score acquired was 0.2307, which was moderately higher than the use of the mean horizontal line for estimation. This can be caused by various factors, such as the absence of feature engineering, the range of target quality scores, and the source of the quality scores. Dataset in the training of all models were employed without feature engineering prior. The data remain the same as the source throughout the training. The target quality scores is also suspected to be another factor that affect performances of the models. Most values in the quality column in the datasets are ranging from 5 to 6, which can cause the trained models to predict mostly 5 and 6. The source of wine quality scores in datasets can also lower the performances of trained models, as the scores were given by human wine tasters. The quality scores provided by human wine tasters can be subjective. There is a high possibility that some quality scores in the datasets are noises. Despite the fact that the model with transfer learning has proved to be viable for initial wine quality estimation, the addressed problems need to be studied in future investigations.

IV. CONCLUSION

This paper presented a wine quality estimation system using deep neural networks, for the situations where most measurable wine features are unavailable. The quality estimation system consists of a deep neural network which accepts the chemical profiles of the wine as input, and output the quality score on the scale of 0 to 10. Four similar deep NN models were developed and trained with different datasets based on the same source. The first model was trained with the base dataset from Kaggle with all 11 input features, including fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol. The second model was trained with the dataset which has all columns of input features filled with zeroes, except the residual sugar, pH, and alcohol. The third model trained with the dataset which has all columns of input features entirely removed from the file, except for residual sugar, pH, and alcohol. The fourth model applied the same dataset as the third model, with addition of the transfer learning approach applied during the training. All developed models were tests with applicable wine quality test sets. Results from the models were evaluated by MSE, MAE, and R^2 score. Among developed models for reduced input features conditions, the model applied with transfer learning approach yielded the most satisfying results across evaluated metrics.

Future work can include the investigations on designs of deep neural network models for wine chemical profiles predictions, feature selection and feature engineering for the wine quality datasets, customized and improved datasets for wine quality scores with different types of wines, and wine brewing controls for homebrewing environments.

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