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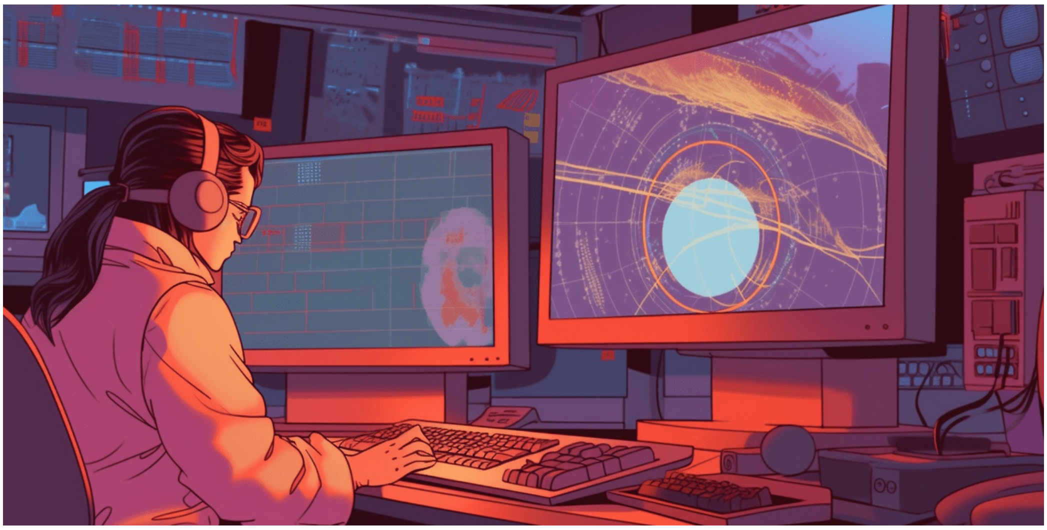

Interpreting the loss functions of Artificial neural networks in cancer research

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Abstract

Artificial Neural Networks (ANNs) have become a popular tool in cancer research for their ability to learn complex relationships between input variables and clinical outcomes. One of the crucial components of ANNs is the loss function, It measures the difference between the output that was anticipated and the output that was produced. In cancer research, different loss functions are used depending on the nature of the research question and the type of data being analyzed. The optimal loss function is critical to ensure optimal performance of the ANN model. The Mean Squared Error (MSE) and Root Mean Squared Error (RMSE) are used in regression tasks, while Cross-Entropy (CE) is often used in classification tasks. The optimal selection of loss function depends on the specific research question and data being analyzed.

Keywords: artificial intelligence, artificial neural networks, error, cancer, research.

Introduction

The dimensions of artificial neural networks (ANNs) to understand intricate correlations between input factors and clinical outcomes has made them a desirable tool in the field of cancer research. The loss function, which is used to measure the divergence between the output that is anticipated and what is actually produced, is one of the most important elements of ANNs[1]. Depending on the nature of the research topic and the type of data being examined, many loss functions are employed in cancer research. The Mean Squared Error (MSE) loss function is commonly used in regression tasks, such as predicting tumor size or survival time. It calculates the average squared difference between the predicted and actual output[2]. The Root Mean Squared Error (RMSE) is a variant of MSE that calculates the square root of the average squared difference, which provides a more interpretable metric of the error. The Cross-Entropy (CE) loss function is often used in classification tasks[3], such as predicting whether a tumor is malignant or benign. It measures the difference between the predicted probability distribution and the actual class distribution. The selection of the appropriate loss function depends on the specific research question and the data being analyzed. In cancer research, the optimal choice of loss function can help to improve the accuracy of the ANN model, ultimately leading to more accurate cancer diagnosis, prognosis, and treatment. Here in our short report, we look into the popular loss functions used in ANN.

Mean squared error

The mean squared error (MSE) is a popular loss function employed in regression problems and artificial neural networks (ANN) to predict a continuous value based on input features. For instance, in medical domains, predicting the survival rate of cancer patients based on their medical history and diagnostic details is a regression problem that can be solved using MSE. The MSE calculates the average squared difference between the predicted output and the true output for all the training examples in a dataset. The formula for MSE involves dividing the sum of squared errors by the number of training examples. When designing a multilayer perceptron (MLP) neural network to utilize the MSE as the loss function, the output layer should utilize an activation function that produces a continuous output, such as the linear activation function. The linear activation function merely sums the weighted inputs to the neuron without applying any nonlinearity[4]. Therefore, it can generate any value and is appropriate for regression problems where the predicted output is continuous. In addition to the linear activation function, other activation functions, such as the sigmoid function, tanh function, and ReLU function, can be employed in the hidden layers of the MLP network. The MSE is commonly used in cancer research as a loss function in regression problems, with the linear activation function being a suitable choice for the output layer of an MLP neural network when predicting a continuous output. The selection of an activation function for the hidden layers is influenced by the problem being solved and the nature of the data.

Root mean squared error

The RMSE metric can be used to evaluate the performance of artificial neural networks, such as multilayer perceptron models, in predicting important clinical outcomes. These outcomes may include the progression or regression of a tumor, response to chemotherapy, or survival rates of cancer patients. In this context, the RMSE metric provides a valuable tool for assessing the predictive performance of these models[5]. By quantifying the difference between predicted and true outcomes, researchers can gain insights into the accuracy and reliability of their models. Furthermore, the RMSE can be used to compare the performance of different models or parameter configurations, allowing researchers to select the best approach for their specific application. Similar to the mean squared error (MSE), the RMSE quantifies the difference between the predicted output and the true output for each training example. However, the RMSE is obtained by taking the square root of the MSE, which simplifies its interpretation since it is expressed in the same units as the target variable. Overall, the root mean squared error is a valuable metric for cancer researchers utilizing artificial neural networks in their predictive modeling efforts. Its ability to provide information on both the magnitude and direction of errors makes it a powerful tool for evaluating model performance and optimizing predictive accuracy.

Cross entropy error

The cross-entropy error, also known as log loss, is a widely used loss function for classification problems in MLP neural networks[6]. It measures the dissimilarity between the predicted probabilities and the true probabilities of the classes. This loss function is particularly useful in cancer research, where the accurate classification of cancer types can have significant clinical implications. The cross-entropy error is calculated by summing the logarithmic difference between the predicted and true probabilities for each class, weighted by a binary indicator for the true class label. This loss function penalizes the network more if it is highly confident about the wrong class and less if it is less confident. This is in contrast to other loss functions like mean squared error, which penalizes the network proportionally to the squared difference between the predicted and true values, regardless of the confidence of the network. To use the cross-entropy error as the loss function in an MLP neural network for cancer classification, the output layer should use an activation function that produces a probability distribution over the classes, such as the softmax function[7]. The softmax function normalizes the output of the network so that it represents a probability distribution over the classes. It measures the dissimilarity between the predicted and true probabilities of the classes and penalizes the network more if it is highly confident about the wrong class. The use of an appropriate activation function in the output layer, such as the softmax function, is crucial for accurate and efficient training of the network.

RMSE vs Cross entropy error

The selection of an appropriate loss function is an important consideration in the design of a machine learning model. RMSE and cross-entropy error are two commonly used loss functions, each with its own unique characteristics that make it suitable for specific types of tasks. RMSE is commonly used in regression problems, where the target variable is a continuous value[8]. This loss function calculates the average difference between the predicted output and the true output for each training example. The RMSE is effective in penalizing the network proportionally to the difference between the predicted and true values and is particularly useful when the magnitude of the error is critical. On the other hand, cross-entropy error is typically used in classification problems, where the target variable is a categorical variable. This loss function measures the dissimilarity between the predicted probabilities and the true probabilities of the classes. Cross-entropy error penalizes the network more heavily when it is highly confident about the wrong class and less when it is less confident[9]. This approach is different from RMSE, which penalizes the network based on the difference between the predicted and true values. The key difference between RMSE and cross-entropy error is their suitability for different types of problems and how they penalize the network for incorrect predictions. RMSE is ideal for regression problems and penalizes the network based on the difference between the predicted and true values. In contrast, cross-entropy error is well-suited for classification problems and penalizes the network based on the predicted probabilities of the classes. In conclusion, researchers must carefully consider the selection of loss function based on the specific requirements of the task. The decision to use either RMSE or cross-entropy error should be based on the nature of the problem and the desired outcome. Ultimately, the selection of an appropriate loss function can significantly impact the accuracy and performance of the model.

Interpreting the RMSE

Interpretation of RMSE values in cancer research requires careful consideration of several factors. Firstly, the accuracy and completeness of the input data must be assessed, as the model's predictive ability is only as good as the quality of the data used to train it. Additionally, the complexity of the model must be considered, as overly complex models may overfit to the training data and perform poorly on new data. A smaller RMSE value would indicate a more accurate prediction of the clinical outcome being modeled. For example, in a study predicting tumor size, a smaller RMSE value would suggest that the predicted tumor sizes are closer to the actual tumor sizes. Similarly, in a study predicting survival rates, a smaller RMSE value would indicate that the predicted survival rates are closer to the actual survival rates. However, interpretation of RMSE values should not be considered in isolation. Other performance metrics, such as sensitivity, specificity, and area under the curve (AUC), should also be evaluated to ensure a comprehensive evaluation of the model's predictive ability[10]. Moreover, clinical relevance should be taken into account, as a model with high predictive accuracy but limited clinical relevance may not provide much value to clinicians. Interpretation of RMSE values must be done in conjunction with other relevant metrics, assessment of data quality, and consideration of the model's clinical relevance to ensure a comprehensive evaluation of the model's performance.

Conclusion

The choice of loss function is critical to ensure optimal performance of the ANN model. The Mean Squared Error (MSE) and Root Mean Squared Error (RMSE) are used in regression tasks, while Cross-Entropy (CE) is often used in classification tasks. The optimal selection of loss function depends on the specific research question and data being analyzed, and can ultimately improve accuracy in cancer diagnosis, prognosis, and treatment.

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