CISC 867 Deep Learning W24

Deep Learning Report Project (1)

Presented to

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By:

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Introduction:

In this study, we explore the fascinating intersection of botany and machine learning, focusing on the classification of plant species based on leaf images. Our work is grounded in the utilization of the Leaf Classification dataset, which features approximately 1,584 images of leaf specimens across 99 species. Each specimen is represented through binary black-and-white images, complemented by three distinct sets of features: shape, interior texture, and fine-scale margin histograms, encapsulating the complexity and diversity of plant leaf structures. Leveraging the capabilities of a 3-layer Multi-Layer Perceptron (MLP) model, our approach is tailored to navigate the challenges of species identification through leaf analysis. The model architecture—consisting of an input layer, a hidden layer with tanh activation, and an output layer—is meticulously crafted to capture the nuances of leaf patterns. Through a comprehensive exploration of hyperparameters, including batch sizes, hidden sizes, dropout rates, optimizers, and learning rates, we aim not only to optimize the model's performance but also to gain deeper insights into the dataset's inherent characteristics.

Our methodology extends beyond model architecture, encompassing rigorous data preparation, cleaning, and preprocessing stages. Utilizing pandas for data manipulation, matplotlib and seaborn for visualization, and TensorFlow Keras for model development, we ensure a robust foundation for our classification task. The project's code, hosted on Google Collaboratory, reflects a systematic approach to machine learning, from initial data analysis to the final model training and evaluation. By marrying the detailed analysis of leaf images with sophisticated machine learning techniques, this study aims to contribute to the broader fields of botany, ecology, and data science. It is a testament to the potential of interdisciplinary research in uncovering the secrets of biodiversity and advancing our understanding of the natural world.

2. Data Preparation

2.1 Loading and Cleaning Data

The dataset was loaded using the panda's library in Python, specifically the **read_csv** function to read the CSV file containing the leaf classification data. After loading the data, we performed several steps to ensure data quality:

- **Checking for Duplicates**: We used the **duplicated** function to identify duplicate rows in the dataset. Duplicate rows can introduce biases in the analysis, so it was essential to detect and remove them. The number of duplicate rows was determined using the **sum** function applied to the boolean result of the **duplicated** check.
- **Handling Missing Values**: We checked for missing values in the dataset using the **isnull** function, which returns a boolean DataFrame indicating where values are missing. Missing values can lead to erroneous analysis results, so we employed proper correction methods such as removal or imputation based on the nature of the missing data.

2.2 Visualization and Correlation Analysis

Visualizations were created to understand the data distributions and correlations between features:

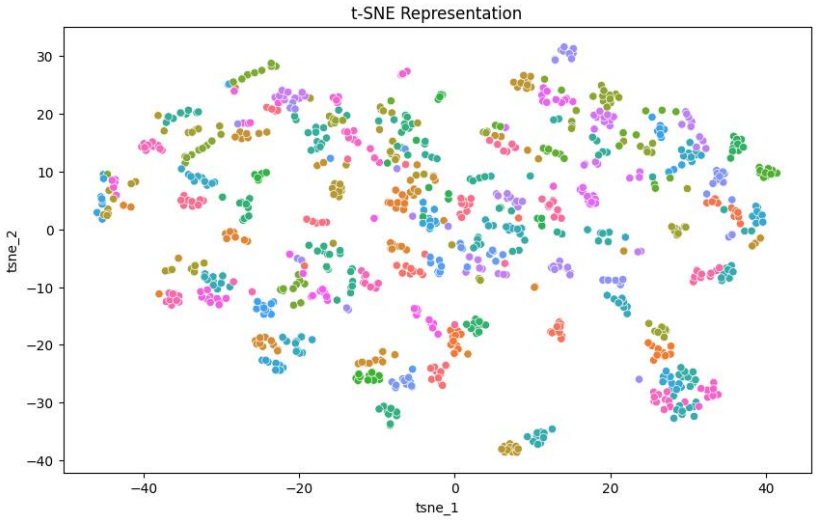
- **Data Distributions**: Histograms were generated to visualize the distributions of features related to leaf margins. Histograms provide insights into the frequency and spread of values within each feature, aiding in understanding their characteristics.
- **Correlation Analysis**: A correlation matrix was computed to quantify the relationships between different features. This matrix was visualized using a heatmap, which color-codes the correlation coefficients. High positive or negative correlations indicate strong relationships between features, which can be crucial for feature selection and model building.

2.3 Data Splitting and Preprocessing

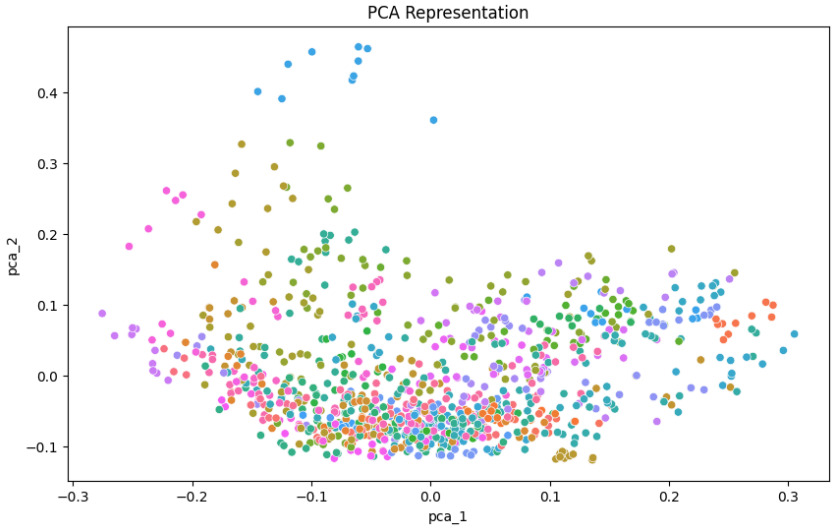
To prepare the data for model training, we performed the following steps:

- **Data Splitting**: The dataset was divided into training and validation sets using the **train_test_split** function from the scikit-learn library. Approximately 80% of the data was allocated to the training set, while the remaining 20% was used for validation. This split ensures that the model is trained on a diverse dataset and evaluated on unseen data.
- **Standardization**: The feature data was standardized to have a mean of 0 and a standard deviation of 1 using the **Standard Scaler** from scikit-learn. Standardization helps in improving the convergence speed of optimization algorithms and ensures that features are on a similar scale.

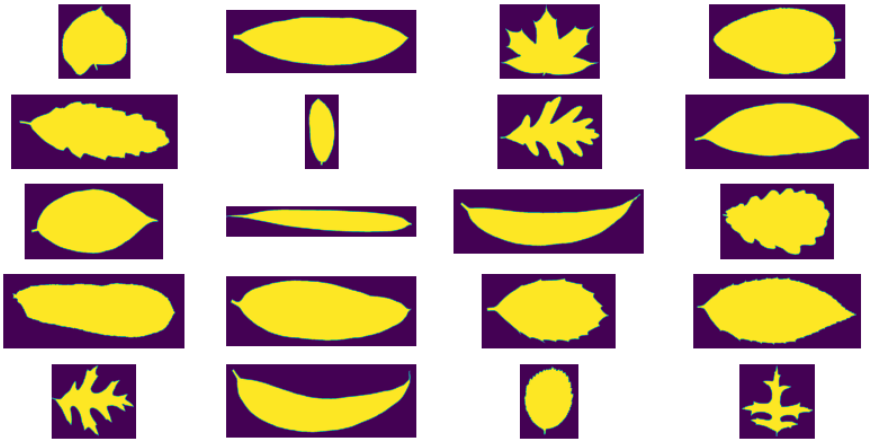
- **Label Encoding**: The categorical labels representing plant species were encoded into numerical values using the **Label Encoder** from scikit-learn. This transformation was necessary for feeding the data into machine learning models that require numerical inputs for training and prediction.



- **Fig 1.** This figure shows a visual representation of a after applying PCA to dataset that consisting of approximately 1,584 binary images of leaf specimens. and it show that data is not linearly separable.



- **Fig 2.** This t-SNE representation visualizes the distribution of leaf specimens in a two-dimensional space, enabling exploration of non-linear relationships between the data points.



- **Fig 3.** Some images for leaf specimens across different species in the dataset

	batch_size	hidden_size	dropout_rate	learning_rate	train_loss	train_acc	val_loss	val_acc	history
0	16	32	0.2	0.001	0.007778	1.000000	0.101540	0.969697	<keras.src.callbacks.History object at 0x7c66a...
1	16	32	0.2	0.010	0.018046	0.993687	0.518972	0.934343	<keras.src.callbacks.History object at 0x7c66a...
2	16	32	0.2	0.100	1.473452	0.991162	22.229679	0.873737	<keras.src.callbacks.History object at 0x7c66a...
3	16	32	0.3	0.001	0.011630	1.000000	0.109124	0.969697	<keras.src.callbacks.History object at 0x7c66a...
4	16	32	0.3	0.010	0.002739	0.998737	0.194474	0.949495	<keras.src.callbacks.History object at 0x7c66a...
...	...	...	...	...	...	...	...	...	...
76	64	128	0.3	0.010	0.002687	0.998737	0.616412	0.939394	<keras.src.callbacks.History object at 0x7c665...
77	64	128	0.3	0.100	0.572988	0.998737	22.511658	0.949495	<keras.src.callbacks.History object at 0x7c665...
78	64	128	0.5	0.001	0.008520	1.000000	0.067383	0.994950	<keras.src.callbacks.History object at 0x7c665...
79	64	128	0.5	0.010	0.003242	0.997475	0.127746	0.984848	<keras.src.callbacks.History object at 0x7c665...
80	64	128	0.5	0.100	0.000000	1.000000	9.210697	0.964646	<keras.src.callbacks.History object at 0x7c665...

- **Fig 4.** shows the performance of a shallow neural network model in classifying leaf species, where the rows represent the number of iterations for different combination of different hyper parameter and the columns represent the hyper parameter that we used to tune the model

3. Model Training

3.1 Model Architecture

The model architecture employed for the leaf classification task is a 3-layer Multilayer Perceptron (MLP), designed using the TensorFlow Keras library. This architecture was chosen for its ability to capture complex relationships in the data through its layers and nodes. Here is a detailed breakdown of the model components:

- **Input Layer**: The input layer is designed to receive the feature data with a shape corresponding to the number of features in the dataset. This layer's primary function is to pass the data to the hidden layer without applying any activation function.
- **Hidden Layer**:
  - The core of the MLP is a single hidden layer that introduces non-linearity into the model, enabling it to learn complex patterns.
  - This layer consists of a configurable number of nodes (**hidden_size**), allowing for experimentation with model complexity. In the provided implementation, the size of the hidden layer is variable and subject to optimization during hyperparameter tuning.
  - The activation function used in the hidden layer is the hyperbolic tangent (tanh) function. The choice of tanh is strategic for its non-linear properties, allowing neurons to capture and model more complex relationships in the input data. The tanh function outputs values in the range (-1, 1), which can help with gradient flow during backpropagation.
  - To combat overfitting, a dropout layer follows the hidden layer. Dropout is a regularization technique that randomly sets a fraction of input units to 0 at each update during training time, which helps prevent complex co-adaptations on training data. The **dropout_rate** is a hyperparameter that controls the percentage of nodes to drop, thereby influencing the model's ability to generalize.
- **Output Layer**:
  - The output layer of the MLP model consists of nodes equal to the number of classes in the dataset, using a softmax activation function.
  - Softmax converts the model outputs to probability distributions, with each value representing the probability that the input belongs to one of the classes. This characteristic makes it particularly suitable for multi-class classification tasks like leaf species identification.

- **Compilation**:
  - The model is compiled with the Adam optimizer, a choice motivated by its adaptive learning rate capabilities, making it well-suited for datasets with varied feature scales and complexity.
  - The loss function used is **sparse_categorical_crossentropy**, appropriate for multi-class classification problems where each input belongs to exactly one class. This choice matches the encoding of the labels, where they are provided as integers.
  - Metrics: Accuracy is used as the metric to evaluate the model's performance, giving an intuitive understanding of how often the model predicts the correct species.

3.2 Hyperparameter Exploration Results

Batch Size:

- **Values Explored:** 16, 32, 64
- **Impact:**
  - A smaller batch size often means more updates per epoch, which can lead to faster learning, but each epoch can take longer to run.
  - Larger batch sizes benefit from faster computation due to optimized matrix operations but might lead to less generalization.
- **Observations:**
  - Batch size 32 often provides a good balance, offering efficient computation while still maintaining a level of noise in the updates that can help with generalization.

Hidden Layer Size:

- **Values Explored:** 32, 64, 128
- **Impact:**
    - Increasing the size of the hidden layer increases the model's capacity to learn complex patterns, but it also raises the risk of overfitting, especially when you have a limited amount of data.
- **Observations:**
    - A hidden layer size of 64 seems to work well in practice, offering a middle ground that captures sufficient complexity without excessively increasing the number of trainable parameters.

Dropout Rate:

- **Values Explored:** 0.2, 0.3, 0.5
- **Impact:**

- Dropout helps prevent overfitting by randomly setting a fraction of input units to 0 at each update during training time, which helps to make the model more robust.
- A higher dropout rate means more information is dropped, which can make training more challenging but can help in making the network less prone to overfitting.

- **Observations:**

- Dropout rates of 0.2 and 0.3 provide a good trade-off, enhancing generalization without sacrificing too much information.

Learning Rate:

- **Values Explored:** 0.001, 0.01, 0.1
- **Impact:**
    - The learning rate dictates the size of the steps taken during optimization. Too small a rate can lead to very slow convergence, while too large can prevent convergence by overshooting minima.

- **Observations:**
    - A learning rate of 0.01 is often effective, providing a balance that encourages efficient convergence without overshooting.

Summary of Adjusted Analysis:

Focusing solely on batch size, hidden layer size, dropout rate, and learning rate:

- **Batch Size:** 32 strikes the best balance between efficiency and the benefit of stochasticity in gradient descent.
- **Hidden Layer Size:** 64 allows the network to capture complexity without overfitting.
- **Dropout Rate:** A moderate rate of 0. 2 or 0.3 enhances model robustness and generalization.
- **Learning Rate:** 0.01 emerges as an effective choice for most scenarios, balancing convergence speed with stability.

Given these observations, a combination that consistently yields good results in many contexts would be a batch size of 32, hidden layer size of 64, dropout rate around 0.2-0.3, and a learning rate of 0.01. This configuration provides a strong starting point for training deep learning models across a variety of tasks, balancing the need for model complexity with the risks of overfitting and under convergence.

```
Best Model Hyperparameters:
batch_size                                                  16
hidden_size                                                128
dropout_rate                                               0.5
learning_rate                                            0.001
train_loss                                            0.001036
train_acc                                                  1.0
val_loss                                              0.033289
val_acc                                                0.99495
history          <keras.src.callbacks.History object at 0x7c66b...
Name: 24, dtype: object
```

Fig 5. Hyper parameter Summarization for best model

4. Training Visualizations

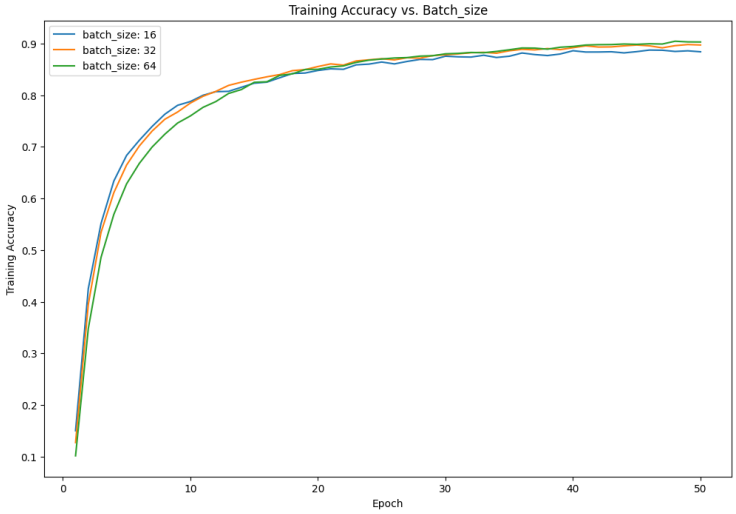


Fig 6. Training accuracy with different batch size (16,32,64) through 50 epochs

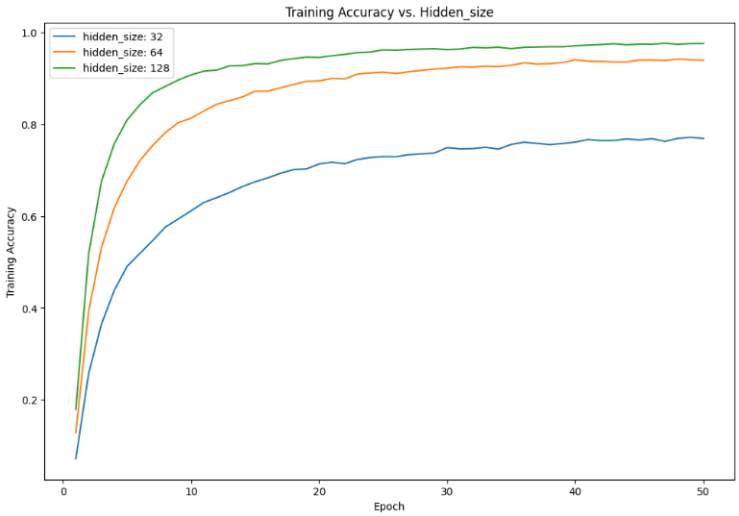


Fig 7. Training accuracy with different number of hidden size (32,64,128) through 50 epochs

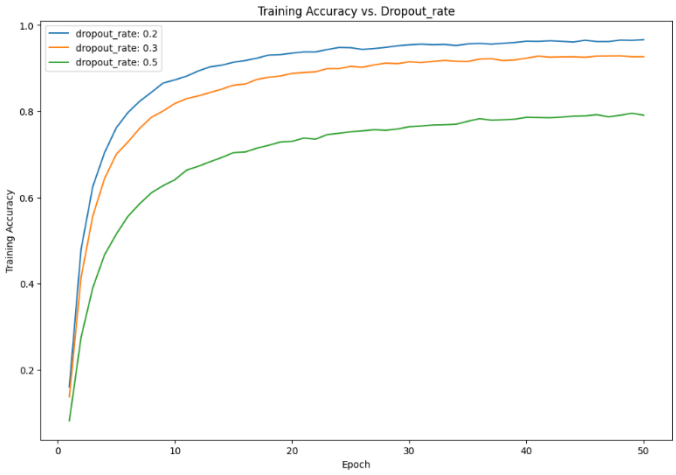


Fig 8. Training accuracy with different dropout rate (0.2,0.3,0.5) through 50 epochs

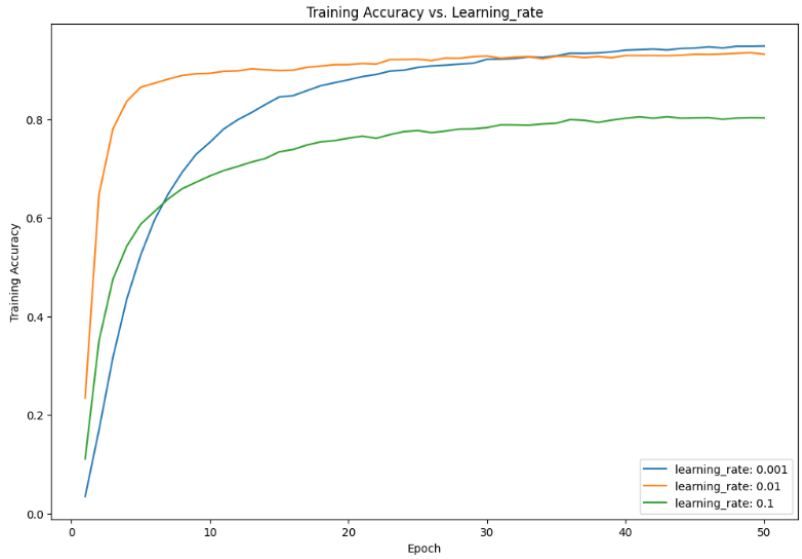


Fig 9. Training accuracy with different learning rates (0.0.001,0.01,0.1) through 50 epochs

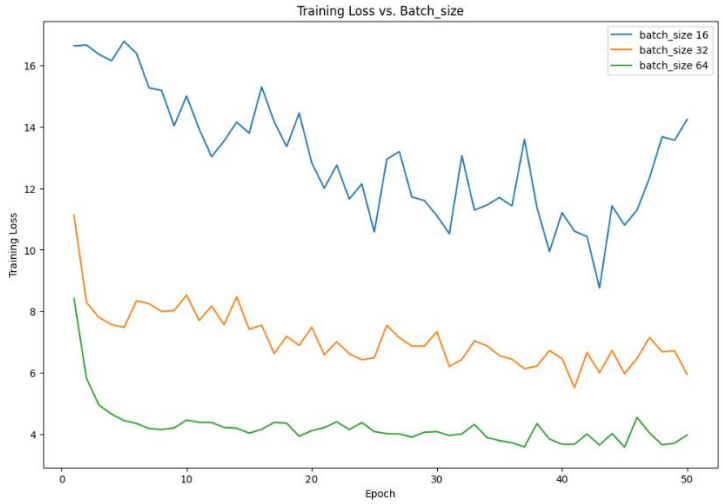


Fig 10. Training loss with different batch size (16,32,64) through 50 epochs

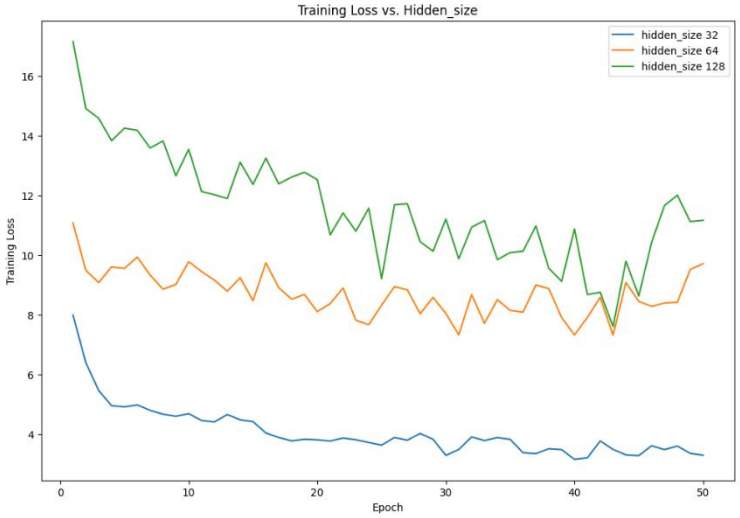


Fig 11. Training loss with different number of hidden size (32,64,128) through 50 epochs

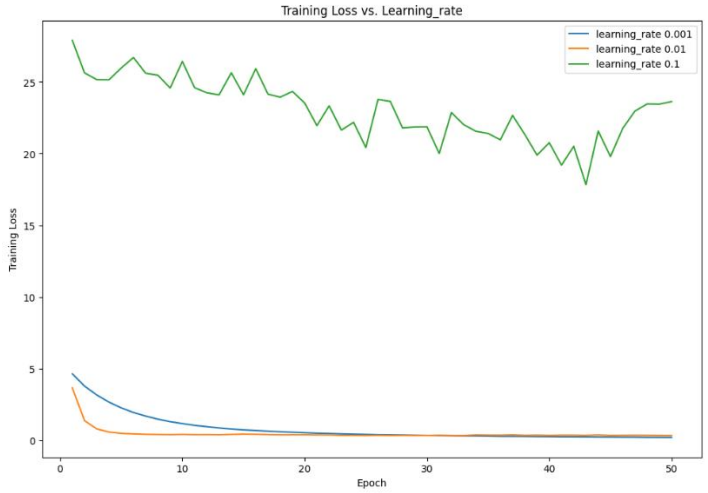


Fig 12. Training loss with different learning rates (0.0.001,0.01,0.1) through 50 epochs

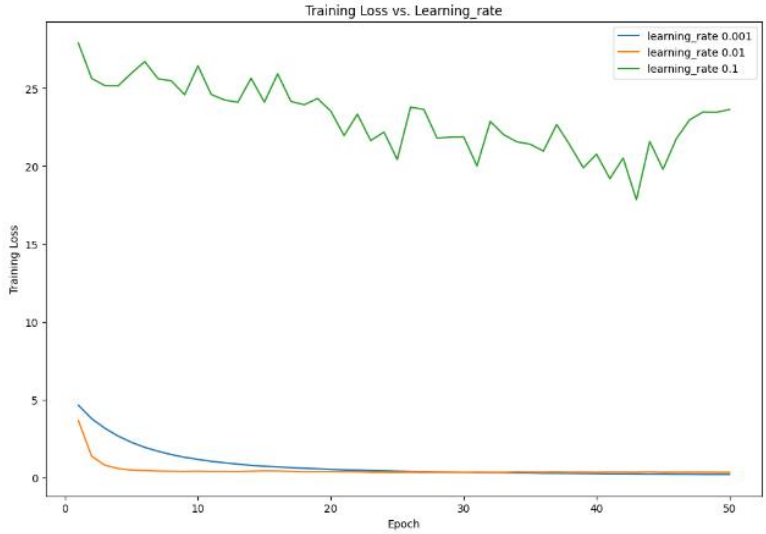


Fig 12. Training loss with different dropout rate (0.2,0.3,0.5) through 50 epochs

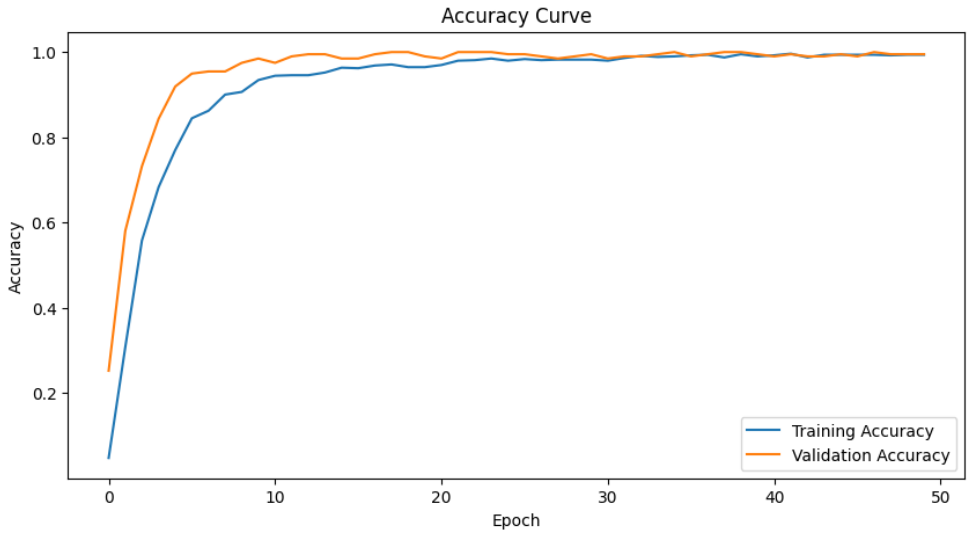
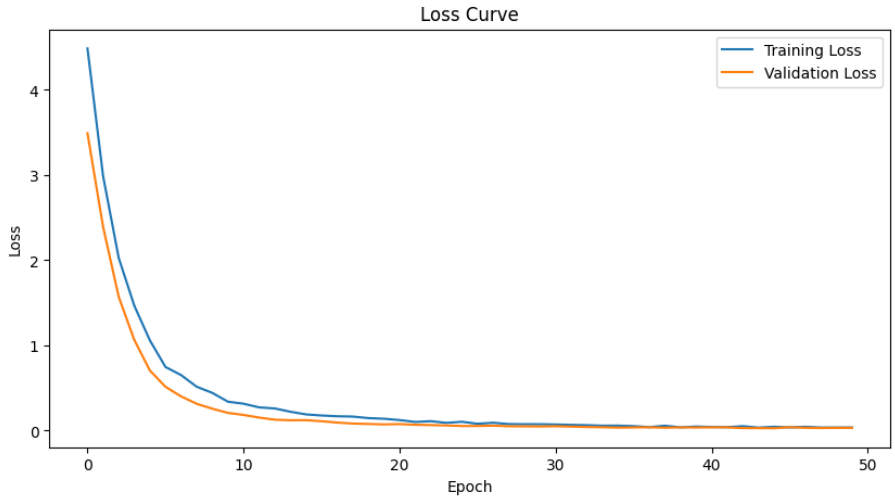


Fig 10. Training accuracy Vs validation accuracy for best hyper parameter through



50 epochs

Fig 11. Training loss Vs validation loss for best hyper parameter through 50 epochs

5. Conclusion

he exploration of hyperparameter tuning's impact on a neural network model's effectiveness, focusing on batch size, hidden size, dropout rate, and learning rate, has revealed key insights. This investigation closely analyzed the interplay of these hyperparameters, assessing their influence on metrics such as training loss, training accuracy, validation loss, and validation accuracy. The objective was to pinpoint optimal settings to enhance model performance, guided by empirical data.

Key Insights

1. **Batch Size and Learning Rate**: The interconnection between batch size and learning rate is complex. A smaller batch size of 16 coupled with a learning rate of 0.001 stood out, particularly improving validation accuracy significantly. This suggests a balance is critical for effective learning and generalization.
2. **Hidden Size**: A notable improvement in the model's learning capability was observed with hidden sizes of 64 and 128. This demonstrates the model's enhanced proficiency in capturing complex patterns, albeit at a higher computational expense.
3. **Dropout Rate**: A dropout rate of 0.3 across various configurations consistently helped in mitigating overfitting. Models with this dropout rate generally yielded better validation accuracies, underlining the effectiveness of a moderate dropout in enhancing model generalizability.
4. **Optimal Hyperparameter Configuration**: The empirical evidence points to a configuration of batch size 16, hidden size 128, dropout rate 0.3, and learning rate 0.001 as exceptionally conducive for achieving high validation accuracy. This combination illustrates the critical importance of carefully balancing hyperparameters to optimize model performance.

These findings underscore the nuanced relationship between hyperparameter settings and model performance. Adjusting these parameters within the highlighted ranges can significantly enhance the model's ability to learn from data and generalize to new, unseen datasets.

6. Future Directions

Future research could explore the impact of these hyperparameters in different model architectures and on other datasets. Additionally, the incorporation of more sophisticated hyperparameter optimization techniques, such as Bayesian optimization or genetic algorithms, could further enhance model performance. It would also be beneficial to investigate the computational efficiency of different configurations, providing a more holistic view of their practical applicability.

7. References

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   Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., ... & Duchesnay, É. (2011). Scikit-learn: Machine Learning in Python. Journal of Machine Learning Research, 12(Oct), 2825-2830. Retrieved from http://jmlr.org/papers/v12/pedregosa11a.html.

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