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Deep Learning

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By

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Building ANN from Scratch

Multilayer and Multiclass ANN on Iris dataset

Exercise 4: Multilayer ANN for Classification on Iris Dataset

Objective:

We will extend the neural network by adding multiple hidden layers to solve a multi-class classification problem using the Iris dataset. The goal is to classify different species of iris flowers based on input features like sepal length, sepal width, petal length, and petal width.

1. **Multilayer Perceptron (MLP) for Classification:**
    1. We will build a deeper neural network by adding multiple hidden layers. This will allow the model to capture more complex patterns in the data for multi-class classification.
2. **Softmax Activation for Multi-Class Classification:**
    1. In the output layer, we will apply the **softmax activation function**. This will help the network output probabilities for each class (setosa, versicolor, virginica), making it suitable for multi-class classification.
3. **Loss Function - Categorical Cross-Entropy:**
    1. We will use **categorical cross-entropy** as the loss function, which is optimal for multi-class problems like this one.

Steps in the Code for Building a Multilayer ANN from Scratch for the Iris Dataset

Step 1: Import Libraries

Description: This step imports the necessary libraries and modules for data manipulation, dataset loading, splitting, standardization, and accuracy measurement.

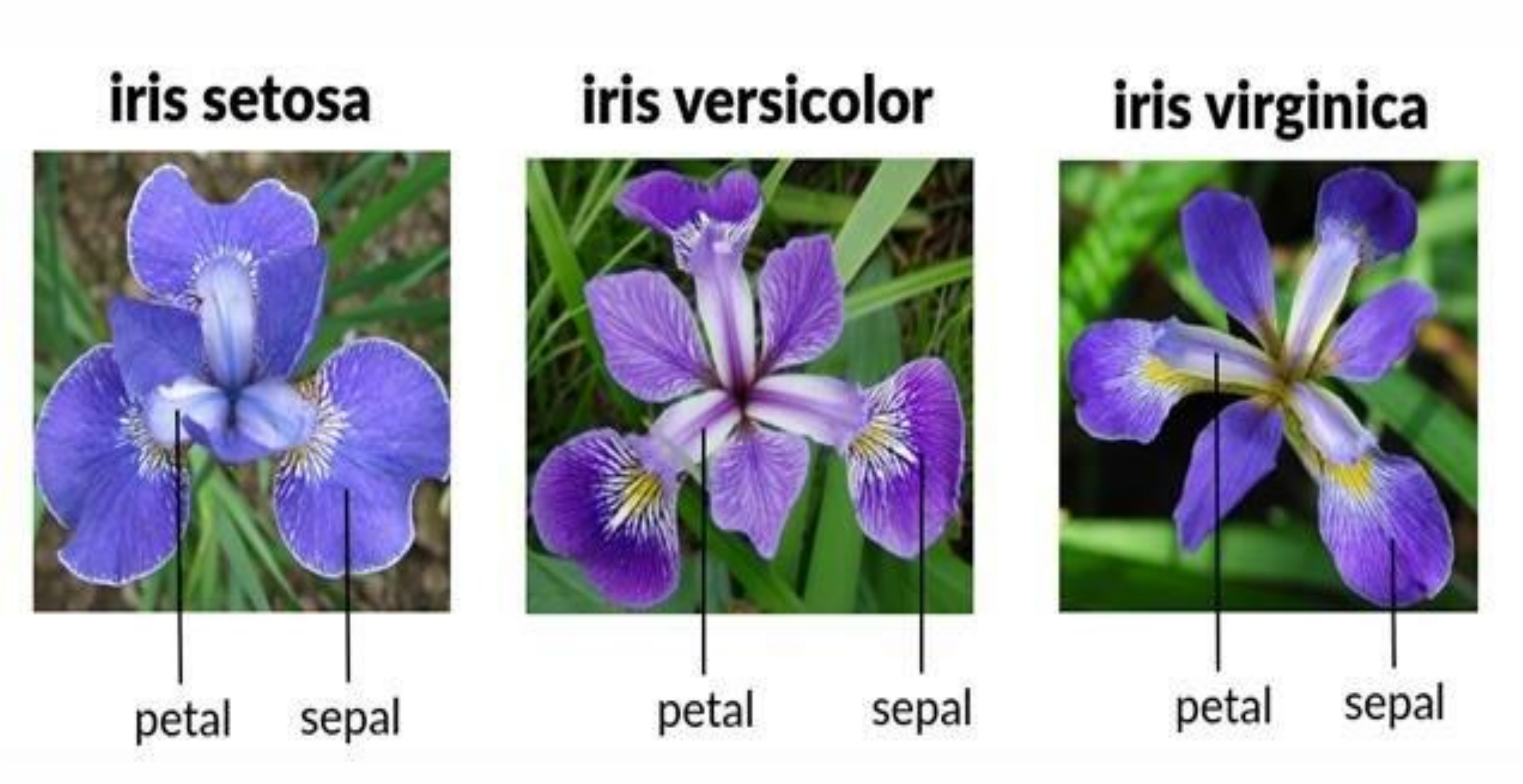
```
import numpy as np
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import accuracy_score
```

Step 2: Load the Iris Dataset

Description: load the Iris dataset and extracts the features and target labels:

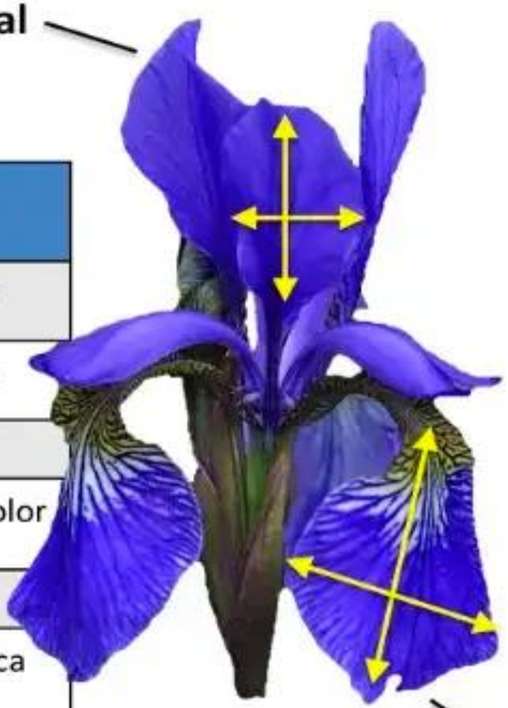
- X: Contains the feature data (sepal length, sepal width, petal length, petal width).
- y: Contains the target labels (species of the iris).

```
data = load_iris()
X = data.data
y = data.target
```


iris setosa
iris versicolor
iris virginica
petal
sepal
petal
sepal
petal
sepal

Samples
(instances, observations)

	Sepal length	Sepal width	Petal length	Petal width	Class label
1	5.1	3.5	1.4	0.2	Setosa
2	4.9	3.0	1.4	0.2	Setosa
...					
50	6.4	3.5	4.5	1.2	Versicolor
...					
150	5.9	3.0	5.0	1.8	Virginica



Features
(attributes, measurements, dimensions)

Class labels
(targets)

Step3 : Convert Labels to One-Hot Encoding

Description: This step converts the target variable into a one-hot encoded format:

- **Function Definition**: The one_hot_encoding function creates a one-hot encoded representation of the target labels using NumPy's eye function, which generates a 2D identity matrix. For example, if a sample belongs to class 1, it will be represented as [0, 1, 0].
- num_classes: Specifies the number of unique classes (3 for the Iris dataset).
- y_one_hot: The resulting one-hot encoded labels, which are used for multi-class classification.

One-Hot Encoding: An Overview

One-hot encoding is a technique used in machine learning and data processing to convert categorical variables into a numerical format.

Example: One-Hot Encoding on a Sample Dataset

Sample Dataset

Consider a simple dataset with a feature "Color":

ID	Color
1	Red
2	Green
3	Blue
4	Green
5	Red

The transformed dataset after one-hot encoding would look like this:

ID	Color	Color_Red	Color_Green	Color_Blue
1	Red	1	0	0
2	Green	0	1	0
3	Blue	0	0	1
4	Green	0	1	0
5	Red	1	0	0

```python
# Convert labels to one-hot encoding
def one_hot_encoding(y, num_classes):
    return np.eye(num_classes)[y]

y_one_hot = one_hot_encoding(y, num_classes=3)
```

- **y**: The array of target labels (class indices).
- **num_classes**: The total number of unique classes present in the target variable.
- **np.eye(num_classes)**: This function from the NumPy library creates an identity matrix of size num_classes x num_classes. An identity matrix has ones on the diagonal and zeros elsewhere.

For instance, if num_classes is 3, the output will look like this:

```
[[1. 0. 0.]
 [0. 1. 0.]
 [0. 0. 1.]]
```

- **[y]**: This indexing operation selects rows from the identity matrix. Each entry in the target array y acts as an index to the identity matrix, effectively selecting the corresponding one-hot encoded vector for each class label.
- For example, if y is [0, 1, 2, 1], the function will map:
    - 0 → [1, 0, 0] (Setosa)
    - 1 → [0, 1, 0] (Versicolor)
    - 2 → [0, 0, 1] (Virginica)
    - 1 → [0, 1, 0] (Versicolor)
- **Return Value**: The function returns a 2D array where each row corresponds to the one-hot encoded vector for the respective class label in y.

- Here, we call the one_hot_encoding function with y and num_classes set to 3 (since there are three classes in the Iris dataset).
- The result is stored in y_one_hot, which will be a 2D array with shape (n_samples, n_classes) where n_samples is the number of samples in the dataset and n_classes is the number of unique classes (3 in this case).

Step 4 : Split the Dataset and Standardize Features

Description:

- **Split Dataset**: This part divides the dataset into training and testing sets:
  - train_test_split: A utility function that randomly splits the data.
  - X_train, y_train: The training data and corresponding one-hot encoded labels.
  - X_test, y_test: The testing data and corresponding labels.
  - test_size=0.2: Indicates that 20% of the data will be reserved for testing.
  - random_state=42: Ensures that the random splitting is reproducible.
- **Standardize Features**: This part standardizes the feature values:
  - StandardScaler: Used to standardize the features to have a mean of 0 and a standard deviation of 1.
  - fit_transform(): Computes the mean and standard deviation from the training data and applies the transformation.
  - transform(): Standardizes the testing data using the same statistics from the training data.

```python
# Split the dataset into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y_onehot, test_size=0.2, random_state=42)

# Standardize the features
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

Step 5: Initialize Weights and Biases

Description: This step initializes weights and biases for each layer:

- Weights are initialized using a normal distribution to introduce randomness.
- Biases are initialized to zeros, which is a common practice.

```python
def initialize_parameters(input_size, hidden_size1, hidden_size2, output_size):
    np.random.seed(42)  # For reproducibility

    # Weights and biases for input to first hidden layer
    weights_input_hidden1 = np.random.randn(input_size, hidden_size1) * 0.01
    bias_hidden1 = np.zeros((1, hidden_size1))

    # Weights and biases for first hidden layer to second hidden layer
    weights_hidden1_hidden2 = np.random.randn(hidden_size1, hidden_size2) * 0.01
    bias_hidden2 = np.zeros((1, hidden_size2))

    # Weights and biases for second hidden layer to output layer
    weights_hidden2_output = np.random.randn(hidden_size2, output_size) * 0.01
    bias_output = np.zeros((1, output_size))

    return {
        "weights_input_hidden1": weights_input_hidden1,
        "bias_hidden1": bias_hidden1,
        "weights_hidden1_hidden2": weights_hidden1_hidden2,
        "bias_hidden2": bias_hidden2,
        "weights_hidden2_output": weights_hidden2_output,
        "bias_output": bias_output
    }
```

Step 6: Define Activation Functions and compute loss function (CCE)

Description: This step defines the activation functions used in the network:

- **Sigmoid**: Used for the hidden layers, it introduces non-linearity.
- **Softmax**: Used for the output layer, it converts logits into probabilities for multi-class classification.

```python
def sigmoid(z):
    return 1 / (1 + np.exp(-z))

def sigmoid_derivative(z):
    s = sigmoid(z)
    return s * (1 - s)

def softmax(z):
    exp_z = np.exp(z - np.max(z, axis=1, keepdims=True))
    return exp_z / np.sum(exp_z, axis=1, keepdims=True)
```

$$\mathrm{CCE} = -\frac{1}{N}\sum_{j=1}^{N}\sum_{i=1}^{K} y_{ij}\cdot\log(\hat{y}_{ij}+\epsilon)$$

where:

- N is the number of samples in the batch.
- K is the number of classes.
- y_{ij} is the true label for class i of sample j (either 0 or 1 in a one-hot encoded format).
- $\hat{y}_{ij}$ is the predicted probability for class i of sample j.
- ϵ is a small constant (e.g., 1×10^{-8}) added to avoid taking the logarithm of zero.

```python
def compute_loss(y_true, y_pred):
    """Calculate the cross-entropy loss."""
    loss = -np.mean(np.sum(y_true * np.log(y_pred + 1e-8), axis=1))
    return loss
```

•y_true is multiplied element-wise with the logarithm of y_pred. The expression np.log(y_pred + 1e-8) takes the log of each predicted probability in y_pred.

•The small constant 1e-8 is added to y_pred to avoid taking the logarithm of zero, which is undefined and would cause computational errors.

np.sum(..., axis=1):
•This sums the values across each row (i.e., across the classes) for every sample in the batch.

np.mean(...):
•np.mean calculates the average of the cross-entropy values across all samples in the batch.

The negative sign at the beginning ensures the result is positive, as cross-entropy is defined to be a positive measure.

step7: Forward Propagation

Define a function to perform forward propagation:

Compute the hidden layer activation by applying the sigmoid function. Compute the output layer activation using the softmax function.

Implement the function forward():

(X, weights_input_hidden1, bias_hidden1, weights_hidden1_hidden2, bias_hidden2, weights_hidden2_output, bias_output)

```
lef forward(X, weights_input_hidden1, bias_hidden1, weights_hidden1_hidden2, bias_hidden2, weights_hidden2_output, bias_output):
    # First hidden layer
    z_hidden1 = np.dot(X, weights_input_hidden1) + bias_hidden1
    a_hidden1 = sigmoid(z_hidden1)

    # Second hidden layer
    z_hidden2 = np.dot(a_hidden1, weights_hidden1_hidden2) + bias_hidden2
    a_hidden2 = sigmoid(z_hidden2)

    # Output layer
    z_output = np.dot(a_hidden2, weights_hidden2_output) + bias_output
    a_output = softmax(z_output)

    return a_hidden1, a_hidden2, a_output, z_hidden1, z_hidden2, z_output
```

step8: Backward Propagation

Define a function to perform backward propagation:

Compute gradients of the loss function with respect to weights and biases using the chain rule. Update gradients for the weights and biases of both layers. Implement the function backward():

(X, y, a_hidden1, a_hidden2, a_output, z_hidden1, z_hidden2, weights_hidden1_hidden2, weights_hidden2_output)

```python
def backward(X, y, a_hidden1, a_hidden2, a_output, z_hidden1, z_hidden2, weights_hidden1_hidden2, weights_hidden2_output):
    m = y.shape[0]

    # Output layer gradients
    dz_output = a_output - y
    dw_hidden2_output = np.dot(a_hidden2.T, dz_output) / m
    db_output = np.sum(dz_output, axis=0, keepdims=True) / m

    # Second hidden layer gradients
    dz_hidden2 = np.dot(dz_output, weights_hidden2_output.T) * sigmoid_derivative(z_hidden2)
    dw_hidden1_hidden2 = np.dot(a_hidden1.T, dz_hidden2) / m
    db_hidden2 = np.sum(dz_hidden2, axis=0, keepdims=True) / m

    # First hidden layer gradients
    dz_hidden1 = np.dot(dz_hidden2, weights_hidden1_hidden2.T) * sigmoid_derivative(z_hidden1)
    dw_input_hidden1 = np.dot(X.T, dz_hidden1) / m
    db_hidden1 = np.sum(dz_hidden1, axis=0, keepdims=True) / m

    return dw_input_hidden1, db_hidden1, dw_hidden1_hidden2, db_hidden2, dw_hidden2_output, db_output
```

step9: Train the Neural Network

Define a function to train the network:

Use the forward and backward propagation functions to update weights and biases over multiple epochs. Print the loss value at regular intervals (e.g., every 100 epochs) to monitor training progress. Implement the function train():

Description: This step begins the training loop for the network:

- **Forward Pass**: Calculate activations for each layer using the weights and biases.
- **Compute Loss**: Calculate the loss using the categorical cross-entropy function.
- **Backward Pass**: Calculate gradients to update weights and biases (not fully shown here).

```python
def train(X_train, y_train, input_size, hidden_size1, hidden_size2, output_size, learning_rate=0.01, epochs=1000):
    # Initialize parameters with two hidden layers
    parameters = initialize_parameters(input_size, hidden_size1, hidden_size2, output_size)

    for epoch in range(epochs):
        # Forward pass
        a_hidden1, a_hidden2, a_output, z_hidden1, z_hidden2, z_output = forward(
            X_train,
            parameters["weights_input_hidden1"], parameters["bias_hidden1"],
            parameters["weights_hidden1_hidden2"], parameters["bias_hidden2"],
            parameters["weights_hidden2_output"], parameters["bias_output"]
        )

        # Compute loss
        loss = compute_loss(y_train, a_output)

        # Backward pass
        dw_input_hidden1, db_hidden1, dw_hidden1_hidden2, db_hidden2, dw_hidden2_output, db_output = backward(
            X_train, y_train, a_hidden1, a_hidden2, a_output, z_hidden1, z_hidden2,
            parameters["weights_hidden1_hidden2"], parameters["weights_hidden2_output"]
        )

        # Update weights and biases
        parameters["weights_input_hidden1"] -= learning_rate * dw_input_hidden1
        parameters["bias_hidden1"] -= learning_rate * db_hidden1
        parameters["weights_hidden1_hidden2"] -= learning_rate * dw_hidden1_hidden2
        parameters["bias_hidden2"] -= learning_rate * db_hidden2
        parameters["weights_hidden2_output"] -= learning_rate * dw_hidden2_output
        parameters["bias_output"] -= learning_rate * db_output

        # Print loss every 100 epochs
        if epoch % 100 == 0:
            print(f'Epoch {epoch}, Loss: {loss}')

    return parameters
```

step10: make Predictions and Evaluate the Model

Define a function to make predictions:

Use the trained network to compute probabilities for the test set and predict the class with the highest probability. Define a function to evaluate the model:

Calculate the accuracy of the predictions by comparing them with the true labels of the test set.

Implement the functions predict() and evaluation code:

```python
def predict(X, parameters):
    """Make predictions using the trained weights."""
    a_hidden1, a_hidden2, a_output, _, _, _ = forward(
        X,
        parameters["weights_input_hidden1"], parameters["bias_hidden1"],
        parameters["weights_hidden1_hidden2"], parameters["bias_hidden2"],
        parameters["weights_hidden2_output"], parameters["bias_output"]
    )
    return np.argmax(a_output, axis=1)

# Train the neural network with two hidden layers
input_size = X_train.shape[1]
hidden_size1 = 10  # Size of the first hidden layer
hidden_size2 = 10  # Size of the second hidden layer
output_size = y_train.shape[1]
learning_rate = 0.01
epochs = 1000

# Train the model
parameters = train(X_train, y_train, input_size, hidden_size1, hidden_size2, output_size, learning_rate, epochs)

# Make predictions and evaluate
y_pred = predict(X_test, parameters)
y_true = np.argmax(y_test, axis=1)
accuracy = accuracy_score(y_true, y_pred)
print(f'Accuracy: {accuracy * 100:.2f}%')
```