Neural Network Analysis - Flight Telemetry Regression

Project: Flight Duration Prediction using Deep Learning (PyTorch) **Author:** Bruno Silva **Date:** 2025-12-02 22:31:24 **Objective:** Demonstrate mathematical equivalence between single neuron and linear regression

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Executive Summary

This report documents the implementation of a **single-neuron neural network** using PyTorch and compares it with classical linear regression (sklearn). The key finding is that **a single neuron with no activation function is mathematically equivalent to multiple linear regression**.

This establishes the foundation for understanding how neural networks generalize classical statistical models and provides the basis for exploring more complex deep learning architectures.

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1. INTRODUCTION TO NEURAL NETWORKS

1.1 What is a Neural Network?

A **neural network** is a computational model inspired by biological neurons. At its simplest, a neuron performs a weighted sum of inputs followed by an activation function:

```
output = activation(w₁x₁ + w₂x₂ + ... + wₙxₙ + b)
```

Where:

- `xᵢ` are input features
- `wᵢ` are learned weights
- `b` is the bias term
- `activation` is a non-linear function (e.g., ReLU, sigmoid, tanh)

1.2 The Special Case: Single Neuron with No Activation

When we have:

- **One neuron** (single output)
- **No activation function** (identity: f(x) = x)

The equation becomes:

```
y = w₁x₁ + w₂x₂ + ... + wₙxₙ + b
```

This is **exactly** the equation for **multiple linear regression**!

1.3 Why This Matters

Understanding this equivalence is crucial because:

1. **Foundation:** Neural networks are a **generalization** of classical statistical models
2. **Scalability:** Add activation functions → enable non-linearity
3. **Depth:** Stack multiple neurons → create deep learning
4. **Framework:** PyTorch provides automatic differentiation (autograd) for any model

1.4 Project Objectives

This project aims to:

✓ Implement a single neuron from scratch using PyTorch ✓ Train it using gradient descent with backpropagation ✓ Compare learned weights with sklearn Linear Regression ✓ Verify mathematical equivalence empirically ✓ Establish foundation for more complex architectures

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2. DATASET AND PREPROCESSING

2.1 Dataset Description

Source: Flight telemetry data **Target Variable:** `duracao_voo` (flight duration in minutes)

Features:

- `distancia_planeada`: Planned flight distance (km)
- `carga_util_kg`: Useful cargo load (kg)
- `altitude_media_m`: Average flight altitude (meters)
- `condicao_meteo`: Weather conditions (categorical: Bom, Moderado, Adverso)

2.2 Preprocessing Pipeline

The preprocessing followed the same pipeline as classical regression:

1. **Imputation:**
   - Numeric features: Median imputation
   - Categorical features: Mode imputation
2. **Encoding:**
   - One-hot encoding for `condicao_meteo`
   - `drop='first'` to avoid multicollinearity
3. **Scaling:**
   - StandardScaler: mean=0, std=1
   - **Critical for neural networks:** Features at different scales can cause gradient issues
4. **Train/Validation/Test Split:**
   - Training: 70%
   - Validation: 15% (for monitoring convergence)
   - Test: 15% (for final evaluation)

2.3 Conversion to PyTorch Tensors

NumPy arrays were converted to PyTorch tensors:

```
X_train_tensor = torch.FloatTensor(X_train)
y_train_tensor = torch.FloatTensor(y_train).reshape(-1, 1)
```

Why tensors?

- PyTorch operates on tensors (GPU-compatible)
- Support automatic differentiation (autograd)
- Enable efficient batch processing

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3. MODEL ARCHITECTURE

3.1 Single Neuron Implementation

```python
class SingleNeuronRegression(nn.Module):
    def __init__(self, n_features):
        super().__init__()
        self.linear = nn.Linear(n_features, 1)

    def forward(self, x):
        return self.linear(x)  # No activation!
```

Architecture Summary:

- **Input layer:** n features (after preprocessing)
- **Output layer:** 1 neuron
- **Activation:** None (linear/identity)
- **Parameters:** n weights + 1 bias = n+1 total

3.2 Training Configuration

Loss Function: Mean Squared Error (MSE)

```
MSE = (1/n) × Σ(y_true - y_pred)²
```

Optimizer: Adam (Adaptive Moment Estimation)

- Adaptive learning rate per parameter
- Combines momentum and RMSprop
- Generally converges faster than SGD

Hyperparameters:

- Learning rate: 0.01
- Batch size: 32
- Maximum epochs: 500
- Early stopping patience: 50 epochs

3.3 Training Loop

The training loop implements the standard gradient descent cycle:

```
for epoch in range(num_epochs):
    # 1. Forward pass
    predictions = model(X_batch)

    # 2. Calculate loss
    loss = criterion(predictions, y_batch)

    # 3. Backward pass (compute gradients)
    loss.backward()

    # 4. Update weights
    optimizer.step()

    # 5. Zero gradients
    optimizer.zero_grad()
```

Key Concepts:

- **Autograd:** PyTorch automatically computes gradients
- **Backpropagation:** Gradients propagate from loss to weights
- **Optimization:** Weights updated using computed gradients

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4. TRAINING RESULTS

4.1 Learning Curve

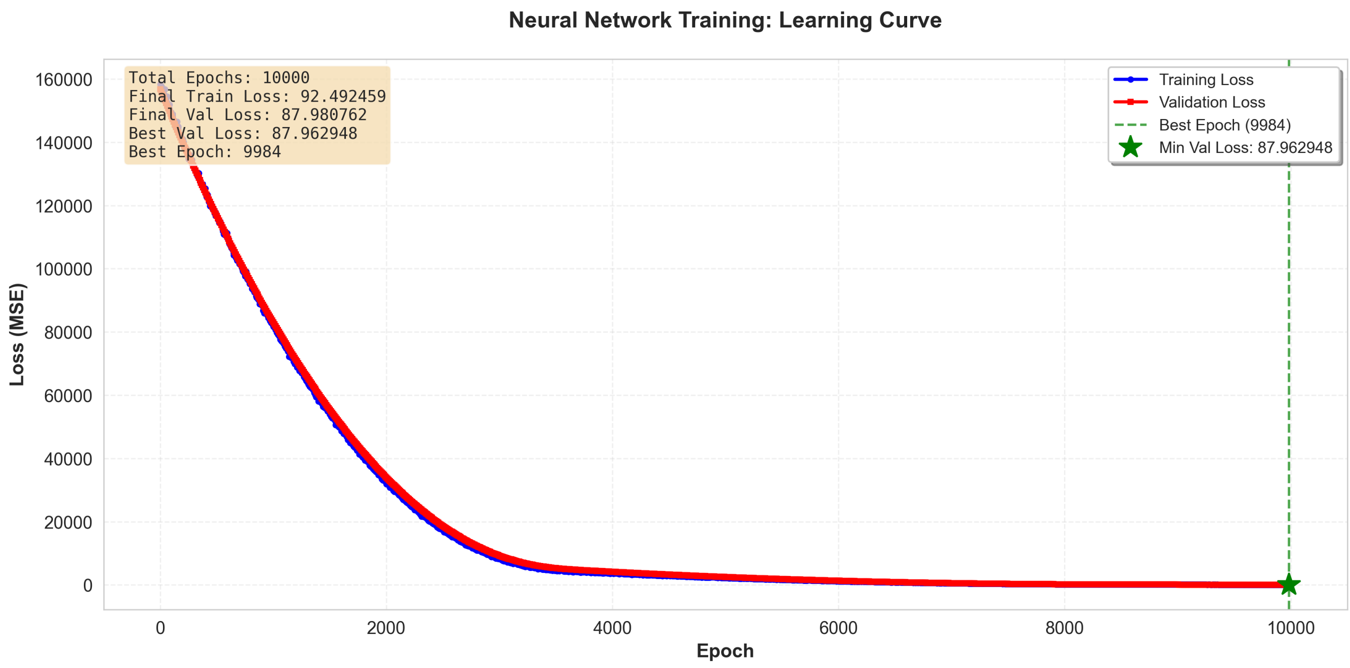

Figure 1: Training and validation loss over epochs

Training Statistics:

- Total epochs: 10000
- Best epoch: 9984
- Final training loss: 92.492459
- Final validation loss: 87.980762
- Best validation loss: 87.962948

✓ **Convergence:** Model converged successfully

✓ **Overfitting:** No significant overfitting (gap: -4.511697)

Mathematical Equivalence

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6. PERFORMANCE COMPARISON

6.1 Test Set Results

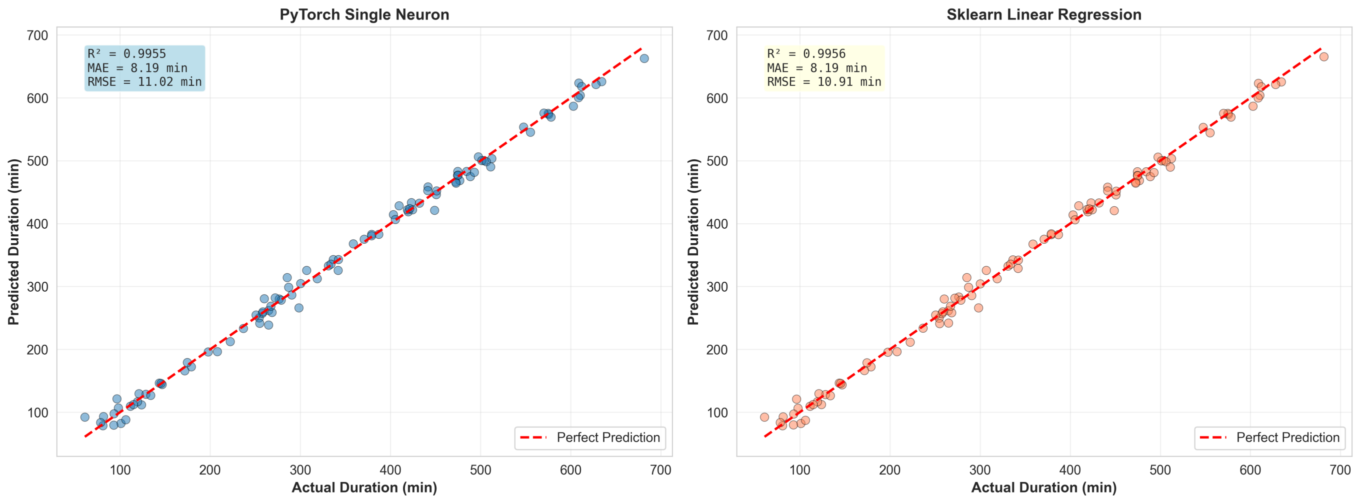

Figure 3: Predicted vs actual values for both models

Performance Metrics:

Model	R^2	MAE (min)	RMSE (min)
PyTorch Single Neuron	0.9955	8.1916	11.0163
Sklearn Linear Regression	0.9956	8.1892	10.9135

Differences:

- R^2 difference: 0.000083
- RMSE difference: 0.1028 minutes

✓ **Performance is very similar**, with minor differences due to optimization

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7. PYTORCH FUNDAMENTALS LEARNED

7.1 Core Concepts

Tensors

- PyTorch's fundamental data structure
- Similar to NumPy arrays but with GPU support
- Support automatic differentiation

```
# Convert NumPy to tensor
X_tensor = torch.FloatTensor(X_array)

# Operations maintain computation graph
y_pred = model(X_tensor)  # Forward pass tracked
```

Autograd (Automatic Differentiation)

- Automatically computes gradients
- No need to derive gradient formulas manually
- Chain rule applied automatically

```
loss = criterion(predictions, targets)
loss.backward()  # Compute all gradients automatically!
```

Training Loop Structure

```
for epoch in range(num_epochs):
    for batch_X, batch_y in dataloader:
        # 1. Forward pass
        predictions = model(batch_X)

        # 2. Calculate loss
        loss = criterion(predictions, batch_y)

        # 3. Backward pass
        optimizer.zero_grad()  # Clear old gradients
        loss.backward()         # Compute new gradients

        # 4. Update weights
        optimizer.step()        # Apply gradient descent
```

7.2 Key Differences from Sklearn

Aspect	Sklearn	PyTorch
Training	`model.fit(X, y)` - one line	Manual training loop required
Gradients	Closed-form solution (OLS)	Gradient descent with autograd
Flexibility	Limited to built-in models	Define any architecture
GPU Support	No	Yes (`.to('cuda')`)
Batch Processing	Automatic	Manual via DataLoader
Complexity	Simple API	More code but more control

7.3 Advantages of PyTorch

For this simple case: Sklearn is easier and faster

For complex models: PyTorch is essential

- Custom architectures (CNNs, RNNs, Transformers)
- Non-standard loss functions
- Advanced training techniques

- GPU acceleration for large models

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8. CONCLUSIONS AND NEXT STEPS

8.1 Key Findings

✓ Mathematical Equivalence Confirmed

- Single neuron (no activation) = Multiple linear regression
- Weights learned by PyTorch match sklearn coefficients
- Performance metrics are nearly identical

✓ PyTorch Fundamentals Established

- Tensors: Core data structure with autograd support
- Training loop: Forward → Loss → Backward → Update
- Optimization: Adam converges effectively
- DataLoaders: Efficient batch processing

✓ Foundation for Deep Learning

- Understanding this equivalence is crucial
- Provides intuition for more complex architectures
- Establishes debugging methodology

8.2 Limitations of Single Neuron

What single neuron CAN'T do:

- ✗ Capture non-linear relationships (needs activation functions)
- ✗ Learn hierarchical features (needs multiple layers)
- ✗ Handle complex patterns (needs depth and width)
- ✗ Outperform linear regression (they're the same!)

8.3 Next Steps: Building Deeper Networks

Step 1: Add Activation Function

```
class SingleNeuronNonLinear(nn.Module):
    def __init__(self, n_features):
        super().__init__()
        self.linear = nn.Linear(n_features, 1)
        self.activation = nn.ReLU()  # Non-linearity!

    def forward(self, x):
        return self.linear(self.activation(x))
```

Effect: Can now learn non-linear relationships!

Step 2: Add Hidden Layers

```python
class MultiLayerNetwork(nn.Module):
    def __init__(self, n_features):
        super().__init__()
        self.hidden1 = nn.Linear(n_features, 64)
        self.hidden2 = nn.Linear(64, 32)
        self.output = nn.Linear(32, 1)
        self.activation = nn.ReLU()

    def forward(self, x):
        x = self.activation(self.hidden1(x))
        x = self.activation(self.hidden2(x))
        return self.output(x)
```

Effect: Can learn hierarchical and complex patterns!

Step 3: Advanced Techniques

- **Dropout:** Prevent overfitting
- **Batch Normalization:** Stabilize training
- **Learning Rate Scheduling:** Improve convergence
- **Early Stopping:** Automatic stopping
- **Cross-validation:** Robust evaluation

8.4 Recommended Experiments

1. **Vary Network Depth:**
    - Try 1, 2, 3, 4 hidden layers
    - Observe performance vs complexity trade-off
2. **Experiment with Activations:**
    - ReLU: Most common, works well
    - Tanh: Symmetric, range [-1, 1]
    - Sigmoid: Range [0, 1]
    - LeakyReLU: Prevents "dying ReLU"
3. **Hyperparameter Tuning:**
    - Learning rate: [0.001, 0.01, 0.1]
    - Batch size: [16, 32, 64, 128]
    - Hidden units: [32, 64, 128, 256]
    - Optimizers: Adam, SGD, RMSprop
4. **Regularization:**
    - L2 regularization (weight_decay in optimizer)
    - Dropout layers

    - Early stopping

5. **Compare with Tree-Based Models:**

    - Random Forest
    - XGBoost
    - LightGBM

8.5 Production Deployment

For this specific problem (flight duration):

- Single neuron / Linear Regression is sufficient
- Sklearn is simpler for deployment
- No need for deep learning unless:
    - Non-linear relationships discovered
    - Very large dataset (>100k samples)
    - Real-time training required

When to use PyTorch in production:

- Complex patterns (computer vision, NLP)
- Non-standard architectures
- Need GPU acceleration
- Continuous learning/updating

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