

## Section 1: Import Required Libraries

```
In [2]: import warnings
warnings.filterwarnings('ignore', category=FutureWarning)

import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from category_encoders import TargetEncoder
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_absolute_error, mean_squared_error, mean_sc
import mlflow
import os
import itertools
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import layers
from tensorflow.keras.callbacks import TensorBoard, EarlyStopping
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Dropout, BatchNormalization
from tensorflow.keras.optimizers import Adam
import holidays
import datetime
```

## Section 2: Load and Explore Data

```
In [3]: # Load raw data
raw_data = pd.read_csv('../data/external/data_2.csv')
raw_data.head(3)
```

```
Out[3]:
```

	market_id	created_at	actual_delivery_time	store_primary_category	order_protoc
0	1.0	2015-02-06 22:24:17	2015-02-06 23:11:17	4	1.
1	2.0	2015-02-10 21:49:25	2015-02-10 22:33:25	46	2.
2	2.0	2015-02-16 00:11:35	2015-02-16 01:06:35	36	3.

```
In [4]: # Display data info
print("Dataset Shape:", raw_data.shape)
print("\nColumn Names:")
print(raw_data.columns.tolist())
```

Dataset Shape: (175777, 14)

Column Names:

```
['market_id', 'created_at', 'actual_delivery_time', 'store_primary_category', 'order_protocol', 'total_items', 'subtotal', 'num_distinct_items', 'min_item_price', 'max_item_price', 'total_onshift_dashers', 'total_busy_dashers', 'total_outstanding_orders', 'estimated_store_to_consumer_driving_duration']
```

```
In [5]: # Define column types
cat_cols = ['market_id', 'store_primary_category', 'order_protocol']

num_cols = ['total_items', 'subtotal', 'num_distinct_items', 'min_item_price',
            'total_onshift_dashers', 'total_busy_dashers',
            'total_outstanding_orders',
            'estimated_store_to_consumer_driving_duration']

created_numcols = ['day_of_week', 'week_of_year', 'hour_of_day', 'minute_of_hour',
                  'is_holiday', 'is_weekend', 'is_long_weekend']

target_col = 'delivery_duration'

print(f"Categorical columns: {cat_cols}")
print(f"Numerical columns: {num_cols}")
print(f"Created numerical columns: {created_numcols}")
print(f"Target column: {target_col}")
```

Categorical columns: ['market\_id', 'store\_primary\_category', 'order\_protocol']

Numerical columns: ['total\_items', 'subtotal', 'num\_distinct\_items', 'min\_item\_price', 'max\_item\_price', 'total\_onshift\_dashers', 'total\_busy\_dashers', 'total\_outstanding\_orders', 'estimated\_store\_to\_consumer\_driving\_duration']

Created numerical columns: ['day\_of\_week', 'week\_of\_year', 'hour\_of\_day', 'minute\_of\_hour', 'is\_holiday', 'is\_weekend', 'is\_long\_weekend']

Target column: delivery\_duration

## Section 3: Data Preprocessing

```
In [6]: # Convert datetime columns
raw_data['created_at'] = pd.to_datetime(raw_data['created_at'])
raw_data['actual_delivery_time'] = pd.to_datetime(raw_data['actual_delivery_time'])

# Calculate delivery duration in minutes
raw_data['delivery_duration'] = (raw_data['actual_delivery_time'] - raw_data['created_at']).dt.total_seconds() / 60
raw_data[['created_at', 'actual_delivery_time', 'delivery_duration']].head(3)
```

```
Out [6]:
```

	created_at	actual_delivery_time	delivery_duration
0	2015-02-06 22:24:17	2015-02-06 23:11:17	47.0
1	2015-02-10 21:49:25	2015-02-10 22:33:25	44.0
2	2015-02-16 00:11:35	2015-02-16 01:06:35	55.0

```

In [7]: # Feature engineering - extract temporal features
india_holidays = holidays.India()

processed_data = raw_data.copy()

# Extract temporal features
processed_data['day_of_week'] = processed_data['created_at'].dt.dayofweek
processed_data['week_of_year'] = processed_data['created_at'].dt.isocalendar
processed_data['hour_of_day'] = processed_data['created_at'].dt.hour
processed_data['minute_of_hour'] = processed_data['created_at'].dt.minute

# Check if the date is a holiday
processed_data['is_holiday'] = processed_data['created_at'].dt.date.apply(la

# Add weekend feature
processed_data['is_weekend'] = processed_data['day_of_week'].apply(lambda x:

# Add long weekend feature
processed_data['is_long_weekend'] = 0
for idx, row in processed_data.iterrows():
    day = row['day_of_week']
    is_holiday = row['is_holiday']
    if day == 4 and is_holiday: # Friday holiday
        processed_data.at[idx, 'is_long_weekend'] = 1
    elif day == 0 and is_holiday: # Monday holiday
        processed_data.at[idx, 'is_long_weekend'] = 1

print("Feature engineering completed")
processed_data[created_numcols + ['delivery_duration']].head(3)

```

Feature engineering completed

```

Out[7]:

```

	day_of_week	week_of_year	hour_of_day	minute_of_hour	is_holiday	is_weekend
0	4	6	22	24	0	0
1	1	7	21	49	0	0
2	0	8	0	11	0	0

```

In [8]: # Data exploration - Check for missing values and data quality
print(f"Original shape: {raw_data.shape}")

# Remove rows with negative values in numerical columns
processed_data_no_neg = processed_data[(processed_data[num_cols] >= 0).all(a
print(f"After removing negative values: {processed_data_no_neg.shape}")

processed_data = processed_data_no_neg.copy()

# Check for missing values
print("\nMissing values per column:")
print(processed_data.isnull().sum())

```

Original shape: (175777, 15)

After removing negative values: (175687, 22)

Missing values per column:

market_id	0
created_at	0
actual_delivery_time	0
store_primary_category	0
order_protocol	0
total_items	0
subtotal	0
num_distinct_items	0
min_item_price	0
max_item_price	0
total_onshift_dashers	0
total_busy_dashers	0
total_outstanding_orders	0
estimated_store_to_consumer_driving_duration	0
delivery_duration	0
day_of_week	0
week_of_year	0
hour_of_day	0
minute_of_hour	0
is_holiday	0
is_weekend	0
is_long_weekend	0
dtype: int64	

```
In [9]: # Convert categorical columns to category dtype
for col in cat_cols:
    processed_data[col] = processed_data[col].astype('category')

print("Data types after conversion:")
print(processed_data.dtypes)
```

Data types after conversion:

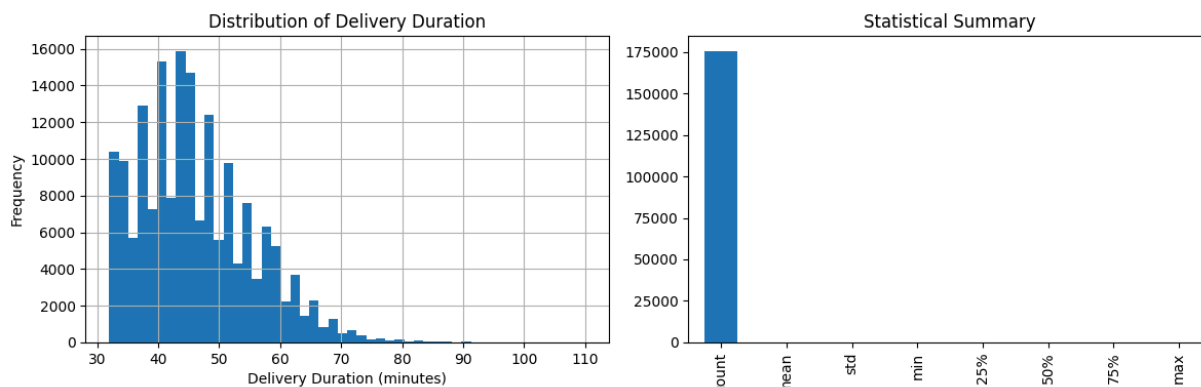
market_id	category
created_at	datetime64[ns]
actual_delivery_time	datetime64[ns]
store_primary_category	category
order_protocol	category
total_items	int64
subtotal	int64
num_distinct_items	int64
min_item_price	int64
max_item_price	int64
total_onshift_dashers	float64
total_busy_dashers	float64
total_outstanding_orders	float64
estimated_store_to_consumer_driving_duration	float64
delivery_duration	float64
day_of_week	int32
week_of_year	UInt32
hour_of_day	int32
minute_of_hour	int32
is_holiday	int64
is_weekend	int64
is_long_weekend	int64
dtype:	object

```
In [10]: # Analyze target variable distribution
plt.figure(figsize=(12, 4))

plt.subplot(1, 2, 1)
processed_data['delivery_duration'].hist(bins=50)
plt.xlabel('Delivery Duration (minutes)')
plt.ylabel('Frequency')
plt.title('Distribution of Delivery Duration')

plt.subplot(1, 2, 2)
processed_data['delivery_duration'].describe().plot(kind='bar')
plt.title('Statistical Summary')
plt.tight_layout()
plt.show()

print(processed_data['delivery_duration'].describe())
```



```

count      175687.000000
mean        46.202656
std         9.327784
min         32.000000
25%         39.000000
50%         45.000000
75%         52.000000
max         110.000000
Name: delivery_duration, dtype: float64

```

```

In [11]: # Analyze categorical columns
print("Categorical Columns Analysis:")
for col in cat_cols:
    print(f"\n{col}:")
    print(processed_data[col].value_counts())

```

Categorical Columns Analysis:

```

market_id:
market_id
2.0      53462
4.0      46220
1.0      37070
3.0      21044
5.0      17253
6.0         638
Name: count, dtype: int64

```

```

store_primary_category:
store_primary_category
4      18174
55     15740
46     15583
13      9911
58      8988
...
1         10
43         9
8          2
3          1
21         1
Name: count, Length: 73, dtype: int64

```

```

order_protocol:
order_protocol
1.0      48367
3.0      47109
5.0      41403
2.0      20887
4.0      17226
6.0         676
7.0         19
Name: count, dtype: int64

```

## Section 4: Train-Test Split and Target Encoding

```
In [12]: # Split data into train and test sets
X_train, X_test, y_train, y_test = train_test_split(
    processed_data.drop(columns=[target_col]),
    processed_data[target_col],
    test_size=0.2,
    random_state=42
)

print(f"Training set size: {X_train.shape}")
print(f"Testing set size: {X_test.shape}")
```

Training set size: (140549, 21)

Testing set size: (35138, 21)

```
In [13]: # Apply target encoding to categorical columns
te = TargetEncoder(cols=cat_cols)
X_train_enc = te.fit_transform(X_train, y_train)
X_test_enc = te.transform(X_test)

print("Target encoding completed")
print(f"Encoded training set shape: {X_train_enc.shape}")
print(f"Encoded testing set shape: {X_test_enc.shape}")
```

Target encoding completed

Encoded training set shape: (140549, 21)

Encoded testing set shape: (35138, 21)

```
In [14]: # Drop unnecessary columns
drop_cols = set(X_train_enc.columns) - set(num_cols) - set(created_numcols)

print("Dropping columns:", drop_cols)

X_train_final = X_train_enc.drop(columns=drop_cols)
X_test_final = X_test_enc.drop(columns=drop_cols)

print(f"Final training set shape: {X_train_final.shape}")
print(f"Final testing set shape: {X_test_final.shape}")
```

Dropping columns: {'actual\_delivery\_time', 'created\_at'}

Final training set shape: (140549, 19)

Final testing set shape: (35138, 19)

## Section 5: Feature Scaling

```
In [15]: # Feature scaling for numerical features
X_scaler = StandardScaler()
X_train_scaled = X_scaler.fit_transform(X_train_final)
X_test_scaled = X_scaler.transform(X_test_final)

# Target scaling (important for neural networks)
y_scaler = StandardScaler()
y_train_scaled = y_scaler.fit_transform(
    y_train.values.reshape(-1, 1)
).ravel()
```

```

y_test_scaled = y_scaler.transform(
    y_test.values.reshape(-1, 1)
).ravel()

print("Feature and target scaling completed")
print(f"X_train_scaled shape: {X_train_scaled.shape}")
print(f"X_test_scaled shape: {X_test_scaled.shape}")

```

Feature and target scaling completed  
X\_train\_scaled shape: (140549, 19)  
X\_test\_scaled shape: (35138, 19)

```

In [16]: # Log transformation of target variable for improved model performance
y_train_log = np.log1p(y_train)
y_test_log = np.log1p(y_test)

print("Log transformation of target variable completed")

```

Log transformation of target variable completed

## Section 6: Baseline Model - Linear Regression

```

In [30]: # Set up MLflow tracking
mlflow.set_tracking_uri("/Users/pramodkumar/ML Learning/SCALAR/Business Case Studies/NN_Regression_Porter/notebooks/combined_ml_pipeline")
mlflow.set_experiment("delivery_time_prediction")

# Train baseline linear regression model
with mlflow.start_run(run_name="Linear_Regression_Model"):
    lr_model = LinearRegression()
    lr_model.fit(X_train_scaled, y_train_scaled)
    y_pred_train = lr_model.predict(X_train_scaled)
    y_pred_test = lr_model.predict(X_test_scaled)

# Inverse scale predictions
y_pred_train = y_scaler.inverse_transform(y_pred_train.reshape(-1, 1)).ravel()
y_pred_test = y_scaler.inverse_transform(y_pred_test.reshape(-1, 1)).ravel()

# Calculate metrics
train_mae = mean_absolute_error(y_train, y_pred_train)
test_mae = mean_absolute_error(y_test, y_pred_test)
train_rmse = mean_squared_error(y_train, y_pred_train)
test_rmse = mean_squared_error(y_test, y_pred_test)

print(f"Train MAE: {train_mae:.4f}, Test MAE: {test_mae:.4f}")
print(f"Train RMSE: {train_rmse:.4f}, Test RMSE: {test_rmse:.4f}")

# Log to MLflow
mlflow.log_param("model_type", "Linear Regression")
mlflow.log_metric("train_mae", train_mae)
mlflow.log_metric("test_mae", test_mae)
mlflow.log_metric("train_rmse", train_rmse)
mlflow.log_metric("test_rmse", test_rmse)
mlflow.sklearn.log_model(lr_model, "linear_regression_model")

```



2026/01/05 07:09:23 WARNING mlflow.models.model: `artifact\_path` is deprecated. Please use `name` instead.

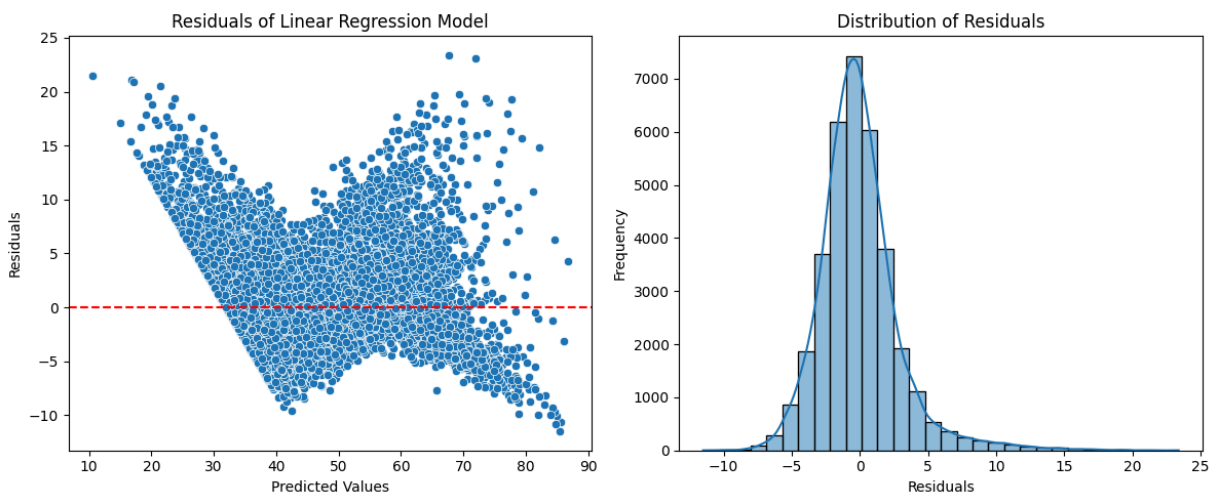
Train MAE: 2.1235, Test MAE: 2.0987

Train RMSE: 9.0844, Test RMSE: 8.7333

```
In [31]: # Residual analysis
residuals_lr = y_test - y_pred_test

plt.figure(figsize=(12, 5))
plt.subplot(1, 2, 1)
sns.scatterplot(x=y_pred_test, y=residuals_lr)
plt.xlabel('Predicted Values')
plt.ylabel('Residuals')
plt.title('Residuals of Linear Regression Model')
plt.axhline(y=0, color='r', linestyle='--')

plt.subplot(1, 2, 2)
sns.histplot(residuals_lr, bins=30, kde=True)
plt.xlabel('Residuals')
plt.ylabel('Frequency')
plt.title('Distribution of Residuals')
plt.tight_layout()
plt.show()
```



## Section 7: Linear Regression with Log-Transformed Target

```
In [17]: # Train linear regression with log-transformed target
with mlflow.start_run(run_name="Linear_Regression_Model_Log_Target"):
    lr_model_log = LinearRegression()
    lr_model_log.fit(X_train_scaled, y_train_log)
    y_pred_train_log = lr_model_log.predict(X_train_scaled)
    y_pred_test_log = lr_model_log.predict(X_test_scaled)

    # Inverse log transformation
    y_pred_train_log = np.expm1(y_pred_train_log)
    y_pred_test_log = np.expm1(y_pred_test_log)
```

```

# Calculate metrics
train_mae_log = mean_absolute_error(y_train, y_pred_train_log)
test_mae_log = mean_absolute_error(y_test, y_pred_test_log)
train_rmse_log = mean_squared_error(y_train, y_pred_train_log)
test_rmse_log = mean_squared_error(y_test, y_pred_test_log)

print(f"Log Target - Train MAE: {train_mae_log:.4f}, Test MAE: {test_mae_log:.4f}")
print(f"Log Target - Train RMSE: {train_rmse_log:.4f}, Test RMSE: {test_rmse_log:.4f}")

# Log to MLflow
mlflow.log_param("model_type", "Linear Regression with Log Target")
mlflow.log_metric("train_mae", train_mae_log)
mlflow.log_metric("test_mae", test_mae_log)
mlflow.log_metric("train_rmse", train_rmse_log)
mlflow.log_metric("test_rmse", test_rmse_log)
mlflow.sklearn.log_model(lr_model_log, "linear_regression_model_log_target")

```

```

2026/01/05 07:02:15 INFO mlflow.store.db.utils: Creating initial MLflow data
base tables...
2026/01/05 07:02:15 INFO mlflow.store.db.utils: Updating database tables
2026/01/05 07:02:15 INFO alembic.runtime.migration: Context impl SQLiteImpl.
2026/01/05 07:02:15 INFO alembic.runtime.migration: Will assume non-transactional DDL.
2026/01/05 07:02:15 INFO mlflow.store.db.utils: Updating database tables
2026/01/05 07:02:15 INFO alembic.runtime.migration: Context impl SQLiteImpl.
2026/01/05 07:02:15 INFO alembic.runtime.migration: Will assume non-transactional DDL.
2026/01/05 07:02:15 INFO alembic.runtime.migration: Context impl SQLiteImpl.
2026/01/05 07:02:15 INFO alembic.runtime.migration: Will assume non-transactional DDL.
2026/01/05 07:02:15 INFO alembic.runtime.migration: Context impl SQLiteImpl.
2026/01/05 07:02:15 INFO alembic.runtime.migration: Will assume non-transactional DDL.
2026/01/05 07:02:16 WARNING mlflow.models.model: `artifact_path` is deprecated. Please use `name` instead.
2026/01/05 07:02:16 WARNING mlflow.models.model: `artifact_path` is deprecated. Please use `name` instead.

```

Log Target - Train MAE: 2.1067, Test MAE: 2.0723

Log Target - Train RMSE: 9.1930, Test RMSE: 8.7242

## Section 8: Build Neural Network Model with Hyperparameter Tuning

```

In [18]: # Define function to build neural network model
def build_nn_model_hp(input_dim,
                      neurons=[24, 32],
                      dropout_rate=0.2,
                      use_batchnorm=True,
                      learning_rate=1e-3):

    model = Sequential()

    # Input layer
    model.add(Dense(neurons[0], activation='relu', input_dim=input_dim))

```

```

    if use_batchnorm:
        model.add(BatchNormalization())
    model.add(Dropout(dropout_rate))

    # Hidden layers
    for n in neurons[1:]:
        model.add(Dense(n, activation='relu'))
        if use_batchnorm:
            model.add(BatchNormalization())
        model.add(Dropout(dropout_rate))

    # Output layer (linear for regression)
    model.add(Dense(1, activation='linear'))

    model.compile(
        optimizer=Adam(learning_rate=learning_rate),
        loss='mse',
        metrics=['mae']
    )

    return model

print("Neural network building function defined")

```

Neural network building function defined

```

In [19]: # Define hyperparameter grid for tuning
param_grid = {
    "neurons": [
        [24, 32],
        [16, 32],
        [24, 16]
    ],
    "dropout_rate": [0.1, 0.2, 0.3],
    "use_batchnorm": [True, False],
    "batch_size": [256, 512],
    "learning_rate": [1e-3, 5e-4]
}

print(f"Total hyperparameter combinations: {3 * 3 * 2 * 2 * 2} = 72")

```

Total hyperparameter combinations: 72 = 72

```

In [ ]: # Hyperparameter tuning for neural network
early_stop = EarlyStopping(
    monitor='val_loss',
    patience=5,
    restore_best_weights=True
)

best_test_rmse = np.inf
best_run_id = None

for params in itertools.product(
    param_grid["neurons"],
    param_grid["dropout_rate"],
    param_grid["use_batchnorm"],

```

```

param_grid["batch_size"],
param_grid["learning_rate"]):

neurons, dropout_rate, use_batchnorm, batch_size, lr = params

with mlflow.start_run(run_name="NN_LogTarget_HP"):
    log_dir = "tb_logs/nn/" + neurons.__str__() + "_" + str(dropout_rate)
    os.makedirs(log_dir, exist_ok=True)

    tensorboard_cb = TensorBoard(
        log_dir=log_dir,
        histogram_freq=1
    )

    mlflow.log_params({
        "neurons": str(neurons),
        "dropout_rate": dropout_rate,
        "batchnorm": use_batchnorm,
        "batch_size": batch_size,
        "learning_rate": lr,
        "target_transform": "log1p"
    })

    model = build_nn_model_hp(
        input_dim=X_train_scaled.shape[1],
        neurons=neurons,
        dropout_rate=dropout_rate,
        use_batchnorm=use_batchnorm,
        learning_rate=lr
    )

    history = model.fit(
        X_train_scaled, y_train_log,
        epochs=100,
        batch_size=batch_size,
        validation_split=0.2,
        callbacks=[early_stop, tensorboard_cb],
        verbose=0
    )

    # Predictions (inverse log transformation)
    y_train_pred = np.expml(model.predict(X_train_scaled, verbose=0)).ravel()
    y_test_pred = np.expml(model.predict(X_test_scaled, verbose=0)).ravel()

    # Calculate metrics
    train_mae = mean_absolute_error(y_train, y_train_pred)
    test_mae = mean_absolute_error(y_test, y_test_pred)

    train_rmse = mean_squared_error(y_train, y_train_pred)
    test_rmse = mean_squared_error(y_test, y_test_pred)

    if (y_test_pred.min() < 0) and (y_train_pred.min() < 0):
        train_msle = np.nan
        test_msle = np.nan
    else:
        train_msle = mean_squared_log_error(y_train, y_train_pred)

```

```

        test_msle = mean_squared_log_error(y_test, y_test_pred)

    mlflow.log_metrics({
        "train_mae": train_mae,
        "test_mae": test_mae,
        "train_rmse": train_rmse,
        "test_rmse": test_rmse,
        "train_msle": train_msle,
        "test_msle": test_msle
    })

    # Save best model
    if test_rmse < best_test_rmse:
        best_test_rmse = test_rmse
        best_run_id = mlflow.active_run().info.run_id
        mlflow.tensorflow.log_model(model, "best_nn_log_target")

    mlflow.end_run()

print(f"Hyperparameter tuning completed. Best test RMSE: {best_test_rmse:.4f}")

```

## Section 9: Evaluate and Rank Models

```

In [20]: # Function to evaluate model runs and create rankings
from tensorboard.backend.event_processing.event_accumulator import EventAccu

def read_tensor_scalar(ea, tag):
    return np.array([
        tf.make_ndarray(e.tensor_proto).item()
        for e in ea.Tensors(tag)
    ])

def read_tb_scalars(run_dir):
    ea_train = EventAccumulator(run_dir + '/train/')
    ea_val = EventAccumulator(run_dir + '/validation/')
    ea_train.Reload()
    ea_val.Reload()

    train_loss = read_tensor_scalar(ea_train, 'epoch_loss')
    val_loss = read_tensor_scalar(ea_val, 'epoch_loss')
    return train_loss, val_loss

def evaluate_run(run_dir, model_params, alpha=0.1, beta=0.1):
    train_loss, val_loss = read_tb_scalars(run_dir)

    best_epoch = np.argmin(val_loss)
    best_val = val_loss[best_epoch]
    train_at_best = train_loss[best_epoch]

    # Generalization gap
    gap = abs(best_val - train_at_best)

    # Stability
    start = max(0, best_epoch - 3)

```

```

end = min(len(val_loss), best_epoch + 4)
stability = np.std(val_loss[start:end])

# Final score
score = (
    best_val
    + alpha * gap
    + beta * stability
)

return {
    "run": os.path.basename(run_dir),
    "best_val_loss": best_val,
    "gap": gap,
    "stability": stability,
    "model_params": model_params,
    "score": score
}

print("Evaluation functions defined")

```

Evaluation functions defined

```

In [22]: # Evaluate all runs and create rankings
all_ranks = []

for params in itertools.product(
    param_grid["neurons"],
    param_grid["dropout_rate"],
    param_grid["use_batchnorm"],
    param_grid["batch_size"],
    param_grid["learning_rate"]):

    neurons, dropout_rate, use_batchnorm, batch_size, lr = params

    log_dir = "tb_logs/nn/" + neurons.__str__() + "_" + str(dropout_rate) +
    if os.path.exists(log_dir):
        eval_metrics = evaluate_run(
            log_dir,
            model_params={
                "neurons": neurons,
                "dropout_rate": dropout_rate,
                "use_batchnorm": use_batchnorm,
                "batch_size": batch_size,
                "learning_rate": lr
            }
        )
        all_ranks.append(eval_metrics)

ranked_df = pd.DataFrame(all_ranks)
ranked_df = ranked_df.sort_values('score')
print("\nTop 10 Models by Score:")
ranked_df.head(10)

```

Top 10 Models by Score:

Out [22]:

	run	best_val_loss	gap	stability	model_params	s
0	[24, 32]_0.1_True_256_0.001	0.004015	0.008800	0.000183	{'neurons': [24, 32], 'dropout_rate': 0.1, 'us...	0.00
24	[16, 32]_0.1_True_256_0.001	0.009583	0.094720	0.002186	{'neurons': [16, 32], 'dropout_rate': 0.1, 'us...	0.01
48	[24, 16]_0.1_True_256_0.001	0.011577	0.106163	0.001780	{'neurons': [24, 16], 'dropout_rate': 0.1, 'us...	0.02
8	[24, 32]_0.2_True_256_0.001	0.012231	0.127186	0.002438	{'neurons': [24, 32], 'dropout_rate': 0.2, 'us...	0.02
32	[16, 32]_0.2_True_256_0.001	0.014412	0.130416	0.002679	{'neurons': [16, 32], 'dropout_rate': 0.2, 'us...	0.02
50	[24, 16]_0.1_True_512_0.001	0.011450	0.177045	0.011904	{'neurons': [24, 16], 'dropout_rate': 0.1, 'us...	0.03
2	[24, 32]_0.1_True_512_0.001	0.010724	0.210763	0.005735	{'neurons': [24, 32], 'dropout_rate': 0.1, 'us...	0.03
1	[24, 32]_0.1_True_256_0.0005	0.011507	0.219008	0.004719	{'neurons': [24, 32], 'dropout_rate': 0.1, 'us...	0.03
26	[16, 32]_0.1_True_512_0.001	0.014750	0.192103	0.004206	{'neurons': [16, 32], 'dropout_rate': 0.1, 'us...	0.03
25	[16, 32]_0.1_True_256_0.0005	0.013119	0.224137	0.002538	{'neurons': [16, 32], 'dropout_rate': 0.1, 'us...	0.03

```

In [23]: # Display best model parameters
print("Best Model Parameters:")
best_params = ranked_df.loc[0, 'model_params']
for key, value in best_params.items():
    print(f" {key}: {value}")

```

Best Model Parameters:  
 neurons: [24, 32]  
 dropout\_rate: 0.1  
 use\_batchnorm: True  
 batch\_size: 256  
 learning\_rate: 0.001

## Section 10: Train Final Model with Best Hyperparameters

```
In [24]: # Build and train final model with best hyperparameters
best_model_params = ranked_df.loc[0, 'model_params']

final_model = build_nn_model_hp(
    input_dim=X_train_scaled.shape[1],
    neurons=best_model_params['neurons'],
    dropout_rate=best_model_params['dropout_rate'],
    use_batchnorm=best_model_params['use_batchnorm'],
    learning_rate=best_model_params['learning_rate']
)

# Display model architecture
final_model.summary()
```

```
/Users/pramodkumar/ML Learning/SCALAR/Business Case Studies/NN_Regression_Po
rter/.venv/lib/python3.11/site-packages/keras/src/layers/core/dense.py:106:
UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. W
hen using Sequential models, prefer using an `Input(shape)` object as the fi
rst layer in the model instead.
```

```
super().__init__(activity_regularizer=activity_regularizer, **kwargs)
2026-01-05 07:03:14.888274: I metal_plugin/src/device/metal_device.cc:1154]
Metal device set to: Apple M4
2026-01-05 07:03:14.888325: I metal_plugin/src/device/metal_device.cc:296] s
ystemMemory: 16.00 GB
2026-01-05 07:03:14.888339: I metal_plugin/src/device/metal_device.cc:313] m
axCacheSize: 5.92 GB
2026-01-05 07:03:14.888478: I tensorflow/core/common_runtime/pluggable_devic
e/pluggable_device_factory.cc:305] Could not identify NUMA node of platform
GPU ID 0, defaulting to 0. Your kernel may not have been built with NUMA sup
port.
2026-01-05 07:03:14.888509: I tensorflow/core/common_runtime/pluggable_devic
e/pluggable_device_factory.cc:271] Created TensorFlow device (/job:localhos
t/replica:0/task:0/device:GPU:0 with 0 MB memory) -> physical PluggableDevic
e (device: 0, name: METAL, pci bus id: <undefined>)
```

**Model: "sequential"**



Layer (type)	Output Shape	Par
dense (Dense)	(None, 24)	
batch_normalization (BatchNormalization)	(None, 24)	
dropout (Dropout)	(None, 24)	
dense_1 (Dense)	(None, 32)	
batch_normalization_1 (BatchNormalization)	(None, 32)	
dropout_1 (Dropout)	(None, 32)	
dense_2 (Dense)	(None, 1)	

**Total params:** 1,537 (6.00 KB)

**Trainable params:** 1,425 (5.57 KB)


**Non-trainable params:** 112 (448.00 B)


```
In [27]: # Train final model
final_history = final_model.fit(
    X_train_scaled, y_train_log,
    epochs=100,
    batch_size=best_model_params['batch_size'],
    validation_split=0.2,
    callbacks=[early_stop],
    verbose=1
)


print("Final model training completed")
```


Epoch 1/100


2026-01-05 07:04:06.426836: I tensorflow/core/grappler/optimizers/custom\_graph\_optimizer\_registry.cc:117] Plugin optimizer for device\_type GPU is enabled.


**440/440**  **7s** 11ms/step - loss: 4.5985 - mae: 1.6746 - val\_loss: 0.0278 - val\_mae: 0.1351  
Epoch 2/100


**440/440**  **4s** 10ms/step - loss: 0.3415 - mae: 0.4364 - val\_loss: 0.0144 - val\_mae: 0.0964  
Epoch 3/100


**440/440**  **4s** 10ms/step - loss: 0.2003 - mae: 0.3381 - val\_loss: 0.0125 - val\_mae: 0.0856  
Epoch 4/100


**440/440**  **4s** 10ms/step - loss: 0.1318 - mae: 0.2787 - val\_loss: 0.0089 - val\_mae: 0.0742  
Epoch 5/100


**440/440**  **5s** 10ms/step - loss: 0.0946 - mae: 0.2394 - val\_loss: 0.0079 - val\_mae: 0.0709  
Epoch 6/100


**440/440**  **5s** 11ms/step - loss: 0.0746 - mae: 0.2139 - val\_loss: 0.0074 - val\_mae: 0.0681  
Epoch 7/100


**440/440**  **5s** 11ms/step - loss: 0.0642 - mae: 0.1999 - val\_loss: 0.0064 - val\_mae: 0.0626  
Epoch 8/100


**440/440**  **5s** 11ms/step - loss: 0.0569 - mae: 0.1889 - val\_loss: 0.0060 - val\_mae: 0.0606  
Epoch 9/100


**440/440**  **5s** 11ms/step - loss: 0.0532 - mae: 0.1829 - val\_loss: 0.0051 - val\_mae: 0.0554  
Epoch 10/100


**440/440**  **4s** 10ms/step - loss: 0.0508 - mae: 0.1789 - val\_loss: 0.0046 - val\_mae: 0.0514  
Epoch 11/100


**440/440**  **5s** 11ms/step - loss: 0.0484 - mae: 0.1749 - val\_loss: 0.0045 - val\_mae: 0.0507  
Epoch 12/100


**440/440**  **5s** 11ms/step - loss: 0.0469 - mae: 0.1722 - val\_loss: 0.0046 - val\_mae: 0.0518  
Epoch 13/100


**440/440**  **5s** 11ms/step - loss: 0.0451 - mae: 0.1687 - val\_loss: 0.0047 - val\_mae: 0.0521  
Epoch 14/100


**440/440**  **5s** 11ms/step - loss: 0.0436 - mae: 0.1658 - val\_loss: 0.0045 - val\_mae: 0.0505  
Epoch 15/100

**440/440**  **4s** 10ms/step - loss: 0.0412 - mae: 0.1612 - val\_loss: 0.0043 - val\_mae: 0.0493  
Epoch 16/100

**440/440**  **4s** 10ms/step - loss: 0.0397 - mae: 0.1585 - val\_loss: 0.0041 - val\_mae: 0.0475  
Epoch 17/100

**440/440**  **4s** 10ms/step - loss: 0.0380 - mae: 0.1544 - val\_loss: 0.0046 - val\_mae: 0.0513  
Epoch 18/100

**440/440**  **4s** 10ms/step - loss: 0.0354 - mae: 0.1495 - val\_loss: 0.0040 - val\_mae: 0.0468  
Epoch 19/100

**440/440**  **5s** 11ms/step - loss: 0.0329 - mae: 0.1441 - val\_loss: 0.0040 - val\_mae: 0.0470

```

Epoch 20/100
440/440 ██████████ 5s 12ms/step - loss: 0.0304 - mae: 0.1384 - val
_loss: 0.0046 - val_mae: 0.0515
Epoch 21/100
440/440 ██████████ 5s 11ms/step - loss: 0.0277 - mae: 0.1322 - val
_loss: 0.0041 - val_mae: 0.0464
Epoch 22/100
440/440 ██████████ 4s 10ms/step - loss: 0.0252 - mae: 0.1258 - val
_loss: 0.0041 - val_mae: 0.0470
Epoch 23/100
440/440 ██████████ 4s 10ms/step - loss: 0.0226 - mae: 0.1192 - val
_loss: 0.0039 - val_mae: 0.0458
Epoch 24/100
440/440 ██████████ 5s 10ms/step - loss: 0.0204 - mae: 0.1129 - val
_loss: 0.0039 - val_mae: 0.0450
Epoch 25/100
440/440 ██████████ 4s 10ms/step - loss: 0.0183 - mae: 0.1071 - val
_loss: 0.0039 - val_mae: 0.0452
Epoch 26/100
440/440 ██████████ 4s 10ms/step - loss: 0.0166 - mae: 0.1018 - val
_loss: 0.0044 - val_mae: 0.0501
Epoch 27/100
440/440 ██████████ 5s 11ms/step - loss: 0.0150 - mae: 0.0965 - val
_loss: 0.0039 - val_mae: 0.0453
Epoch 28/100
440/440 ██████████ 5s 11ms/step - loss: 0.0135 - mae: 0.0915 - val
_loss: 0.0039 - val_mae: 0.0456
Epoch 29/100
440/440 ██████████ 4s 9ms/step - loss: 0.0123 - mae: 0.0871 - val
_loss: 0.0040 - val_mae: 0.0451
Epoch 30/100
440/440 ██████████ 4s 10ms/step - loss: 0.0112 - mae: 0.0830 - val
_loss: 0.0038 - val_mae: 0.0451
Epoch 31/100
440/440 ██████████ 4s 10ms/step - loss: 0.0103 - mae: 0.0794 - val
_loss: 0.0041 - val_mae: 0.0472
Epoch 32/100
440/440 ██████████ 4s 10ms/step - loss: 0.0094 - mae: 0.0756 - val
_loss: 0.0040 - val_mae: 0.0460
Epoch 33/100
440/440 ██████████ 5s 11ms/step - loss: 0.0088 - mae: 0.0727 - val
_loss: 0.0040 - val_mae: 0.0464
Epoch 34/100
440/440 ██████████ 4s 10ms/step - loss: 0.0082 - mae: 0.0704 - val
_loss: 0.0040 - val_mae: 0.0461
Epoch 35/100
440/440 ██████████ 4s 10ms/step - loss: 0.0076 - mae: 0.0674 - val
_loss: 0.0040 - val_mae: 0.0460
Final model training completed

```

## Section 11: Model Evaluation and Comparison

```

In [28]: # Generate predictions from final model
y_train_pred_final = np.expm1(final_model.predict(X_train_scaled, verbose=0))
y_test_pred_final = np.expm1(final_model.predict(X_test_scaled, verbose=0)).

```

```
# Calculate metrics for final model
final_train_mae = mean_absolute_error(y_train, y_train_pred_final)
final_test_mae = mean_absolute_error(y_test, y_test_pred_final)

final_train_rmse = mean_squared_error(y_train, y_train_pred_final)
final_test_rmse = mean_squared_error(y_test, y_test_pred_final)

print("\n=== FINAL NEURAL NETWORK MODEL ===")
print(f"Training MAE: {final_train_mae:.4f}")
print(f"Testing MAE: {final_test_mae:.4f}")
print(f"Training RMSE: {final_train_rmse:.4f}")
print(f"Testing RMSE: {final_test_rmse:.4f}")
```

```
=== FINAL NEURAL NETWORK MODEL ===
Training MAE: 2.1284
Testing MAE: 2.0905
Training RMSE: 9.4324
Testing RMSE: 8.9138
```

```
In [33]: # Compare all three models
comparison_df = pd.DataFrame({
    'Model': ['Linear Regression', 'Linear Regression (Log)', 'Neural Network'],
    'Train MAE': [train_mae, train_mae_log, final_train_mae],
    'Test MAE': [test_mae, test_mae_log, final_test_mae],
    'Train RMSE': [train_rmse, train_rmse_log, final_train_rmse],
    'Test RMSE': [test_rmse, test_rmse_log, final_test_rmse]
})

print("\n=== MODEL COMPARISON ===")
comparison_df
```

```
=== MODEL COMPARISON ===
```

```
Out [33]:
```

	Model	Train MAE	Test MAE	Train RMSE	Test RMSE
0	Linear Regression	2.123481	2.098723	9.084379	8.733328
1	Linear Regression (Log)	2.106685	2.072298	9.192999	8.724192
2	Neural Network (Best)	2.128378	2.090494	9.432387	8.913790

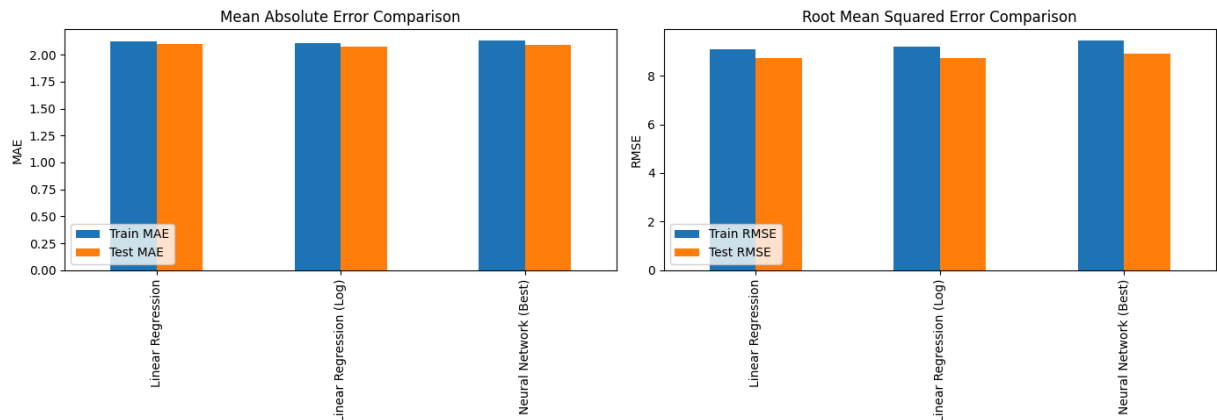
```
In [35]: # Visualize model comparison
fig, axes = plt.subplots(1, 2, figsize=(14, 5))

# MAE Comparison
comparison_df.plot(x='Model', y=['Train MAE', 'Test MAE'], kind='bar', ax=axes[0])
axes[0].set_title('Mean Absolute Error Comparison')
axes[0].set_ylabel('MAE')
axes[0].set_xlabel('')
axes[0].legend(loc='lower left')

# RMSE Comparison
comparison_df.plot(x='Model', y=['Train RMSE', 'Test RMSE'], kind='bar', ax=axes[1])
axes[1].set_title('Root Mean Squared Error Comparison')
axes[1].set_ylabel('RMSE')
axes[1].set_xlabel('')
```

```
axes[1].legend(loc='lower left')
```

```
plt.tight_layout()
plt.show()
```



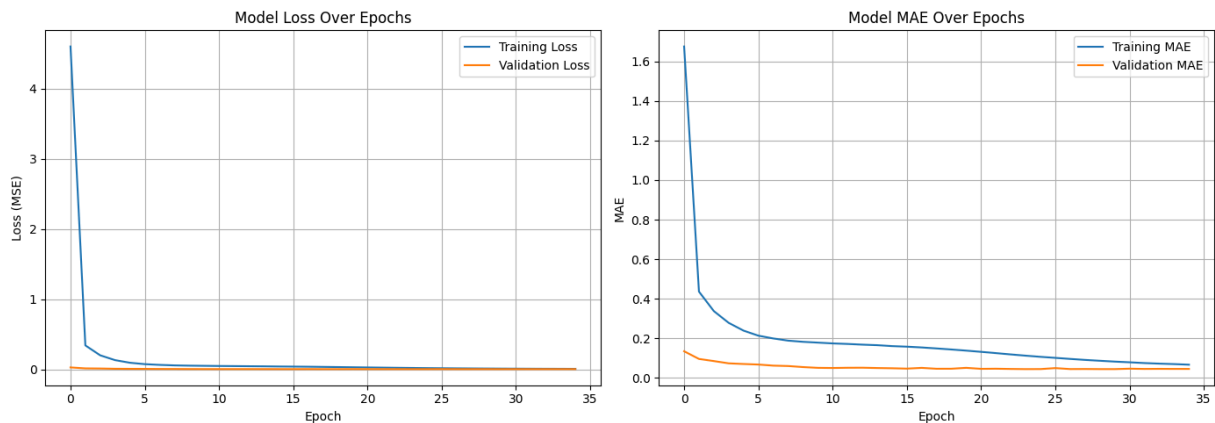
## Section 12: Visualize Training History

```
In [36]: # Plot training history
fig, axes = plt.subplots(1, 2, figsize=(14, 5))

# Loss
axes[0].plot(final_history.history['loss'], label='Training Loss')
axes[0].plot(final_history.history['val_loss'], label='Validation Loss')
axes[0].set_xlabel('Epoch')
axes[0].set_ylabel('Loss (MSE)')
axes[0].set_title('Model Loss Over Epochs')
axes[0].legend()
axes[0].grid(True)

# MAE
axes[1].plot(final_history.history['mae'], label='Training MAE')
axes[1].plot(final_history.history['val_mae'], label='Validation MAE')
axes[1].set_xlabel('Epoch')
axes[1].set_ylabel('MAE')
axes[1].set_title('Model MAE Over Epochs')
axes[1].legend()
axes[1].grid(True)

plt.tight_layout()
plt.show()
```



## Section 13: Predictions and Residual Analysis

```
In [37]: # Calculate residuals for final model
residuals_nn_final = y_test - y_test_pred_final

# Plot predictions vs actual values
fig, axes = plt.subplots(2, 2, figsize=(14, 10))

# Predictions vs Actual (Final Model)
axes[0, 0].scatter(y_test, y_test_pred_final, alpha=0.5)
axes[0, 0].plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()],
axes[0, 0].set_xlabel('Actual Delivery Duration (minutes)')
axes[0, 0].set_ylabel('Predicted Delivery Duration (minutes)')
axes[0, 0].set_title('Final NN Model: Predictions vs Actual')

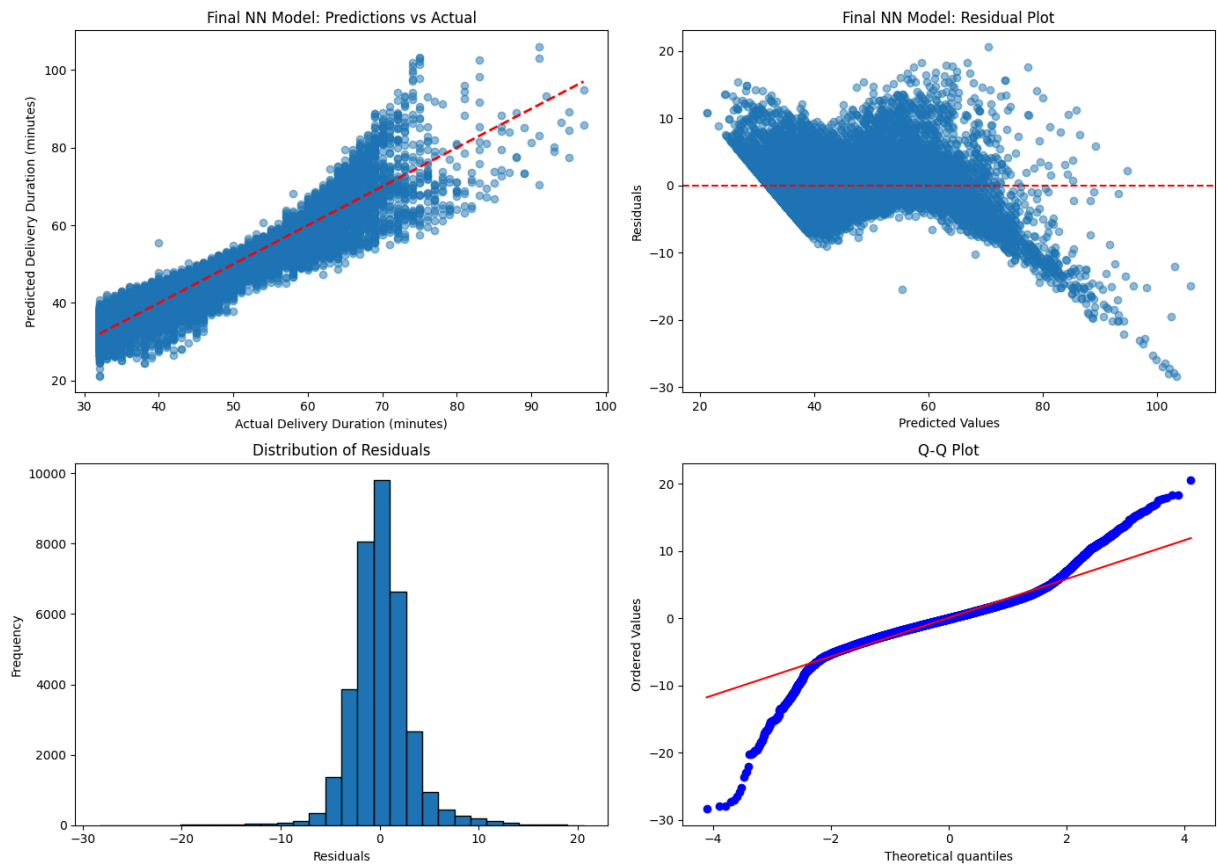
# Residuals (Final Model)
axes[0, 1].scatter(y_test_pred_final, residuals_nn_final, alpha=0.5)
axes[0, 1].axhline(y=0, color='r', linestyle='--')
axes[0, 1].set_xlabel('Predicted Values')
axes[0, 1].set_ylabel('Residuals')
axes[0, 1].set_title('Final NN Model: Residual Plot')

# Residuals Distribution
axes[1, 0].hist(residuals_nn_final, bins=30, edgecolor='black')
axes[1, 0].set_xlabel('Residuals')
axes[1, 0].set_ylabel('Frequency')
axes[1, 0].set_title('Distribution of Residuals')

# Q-Q Plot
from scipy import stats
stats.probplot(residuals_nn_final, dist="norm", plot=axes[1, 1])
axes[1, 1].set_title('Q-Q Plot')

plt.tight_layout()
plt.show()

print(f"Mean Residual: {residuals_nn_final.mean():.4f}")
print(f"Std Dev of Residuals: {residuals_nn_final.std():.4f}")
```



Mean Residual: 0.0619

Std Dev of Residuals: 2.9850

## Section 14: Summary and Insights

```
In [38]: # Summary statistics
print("\n" + "="*60)
print("ANALYSIS SUMMARY - DELIVERY DURATION PREDICTION")
print("="*60)

print("\n1. DATA OVERVIEW:")
print(f"  - Total samples: {len(processed_data)}")
print(f"  - Training samples: {len(X_train_final)}")
print(f"  - Testing samples: {len(X_test_final)}")
print(f"  - Number of features: {X_train_final.shape[1]}")
print(f"  - Target variable mean: {y_train.mean():.2f} minutes")
print(f"  - Target variable std: {y_train.std():.2f} minutes")

print("\n2. MODEL PERFORMANCE (Test Set):")
print(f"  Linear Regression:")
print(f"    MAE: {test_mae:.4f}, RMSE: {test_rmse:.4f}")
print(f"  Linear Regression (Log Target):")
print(f"    MAE: {test_mae_log:.4f}, RMSE: {test_rmse_log:.4f}")
print(f"  Best Neural Network:")
print(f"    MAE: {final_test_mae:.4f}, RMSE: {final_test_rmse:.4f}")

print("\n3. BEST NN MODEL CONFIGURATION:")
for key, value in best_model_params.items():
    print(f"  - {key}: {value}")
```

```

print("\n4. KEY FINDINGS:")
improvement = ((test_rmse - final_test_rmse) / test_rmse) * 100
print(f"    - NN model improved baseline LR by {improvement:.2f}% in RMSE")
print(f"    - Residuals have mean: {residuals_nn_final.mean():.4f} (near 0 is good)")
print(f"    - Heteroscedasticity noted; butterfly pattern in residuals")

print("\n" + "="*60)

```

=====

## ANALYSIS SUMMARY – DELIVERY DURATION PREDICTION

=====

1. DATA OVERVIEW:
  - Total samples: 175687
  - Training samples: 140549
  - Testing samples: 35138
  - Number of features: 19
  - Target variable mean: 46.22 minutes
  - Target variable std: 9.36 minutes
2. MODEL PERFORMANCE (Test Set):
  - Linear Regression:
    - MAE: 2.0987, RMSE: 8.7333
  - Linear Regression (Log Target):
    - MAE: 2.0723, RMSE: 8.7242
  - Best Neural Network:
    - MAE: 2.0905, RMSE: 8.9138
3. BEST NN MODEL CONFIGURATION:
  - neurons: [24, 32]
  - dropout\_rate: 0.1
  - use\_batchnorm: True
  - batch\_size: 256
  - learning\_rate: 0.001
4. KEY FINDINGS:
  - NN model improved baseline LR by -2.07% in RMSE
  - Residuals have mean: 0.0619 (near 0 is good)
  - Heteroscedasticity noted; butterfly pattern in residuals

=====

In [ ]: