

## 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_squared_log_error
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)
```

	market_id	created_at	actual_delivery_time	store_primary_category	order_protocol
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)
```

	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.isocalendarweek
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(lambda x: x in india_holidays)

# Add weekend feature
processed_data['is_weekend'] = processed_data['day_of_week'].apply(lambda x: x in [5, 6])

# 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             4           6          22             24          0            0
1            1             1           7          21             49          0            0
2            0             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(axis=1)]
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:

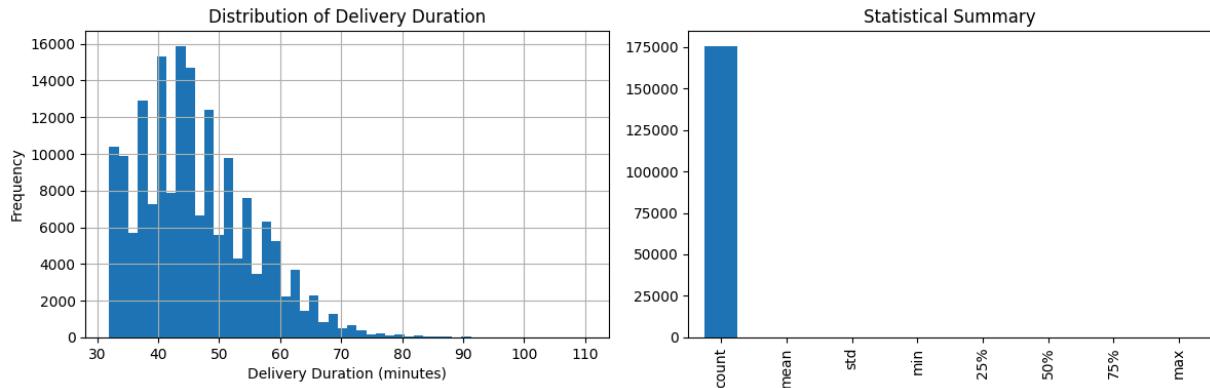
market_id	category
created_at	datetime64[ns]
actual_delivery_time	datetime64[ns]
store_primary_category	category
order_protocol	category
total_items	int64
subtotal	int64
num_distinct_items	int64
min_item_price	int64
max_item_price	int64
total_onshift_dashers	float64
total_busy_dashers	float64
total_outstanding_orders	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.html")  
 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.

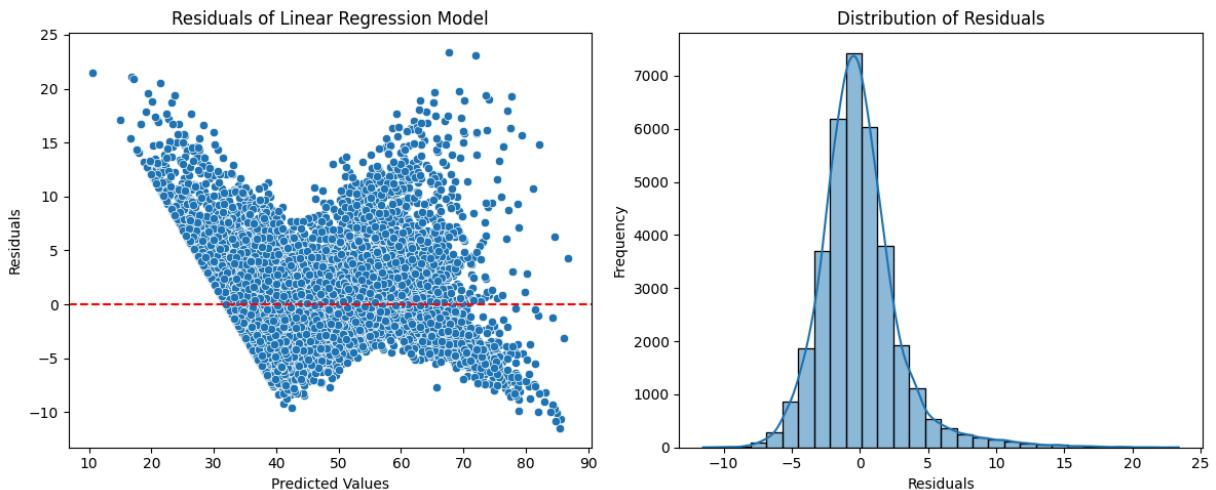
Train MAE: 2.1235, Test MAE: 2.0987  
 Train RMSE: 9.0844, Test RMSE: 8.7333

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-transact
ional 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-transact
ional 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-transact
ional 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-transact
ional DDL.
2026/01/05 07:02:16 WARNING mlflow.models.model: `artifact_path` is deprecate
d. Please use `name` instead.
2026/01/05 07:02:16 WARNING mlflow.models.model: `artifact_path` is deprecate
d. 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.expm1(model.predict(X_train_scaled, verbose=0)).ravel()
    y_test_pred = np.expm1(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 tensorflow.backend.event_processing.event_accumulator import EventAccumulator

def read_tensor_scalar(ea, tag):
    return np.array([
        tf.make_ndarray(ea.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...}	0.033
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_Porter/.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. When using Sequential models, prefer using an `Input(shape)` object as the first 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] systemMemory: 16.00 GB
2026-01-05 07:03:14.888339: I metal_plugin/src/device/metal_device.cc:313] maxCacheSize: 5.92 GB
2026-01-05 07:03:14.888478: I tensorflow/core/common_runtime/pluggable_device/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 support.
2026-01-05 07:03:14.888509: I tensorflow/core/common_runtime/pluggable_device/pluggable_device_factory.cc:271] Created TensorFlow device (/job:localhost/replica:0/task:0/device:GPU:0 with 0 MB memory) -> physical PluggableDevice (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\_grappler\_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
<b>0</b>	Linear Regression	2.123481	2.098723	9.084379	8.733328
<b>1</b>	Linear Regression (Log)	2.106685	2.072298	9.192999	8.724192
<b>2</b>	Neural Network (Best)	2.128378	2.090494	9.432387	8.913790

In [35]: # Visualize model comparison

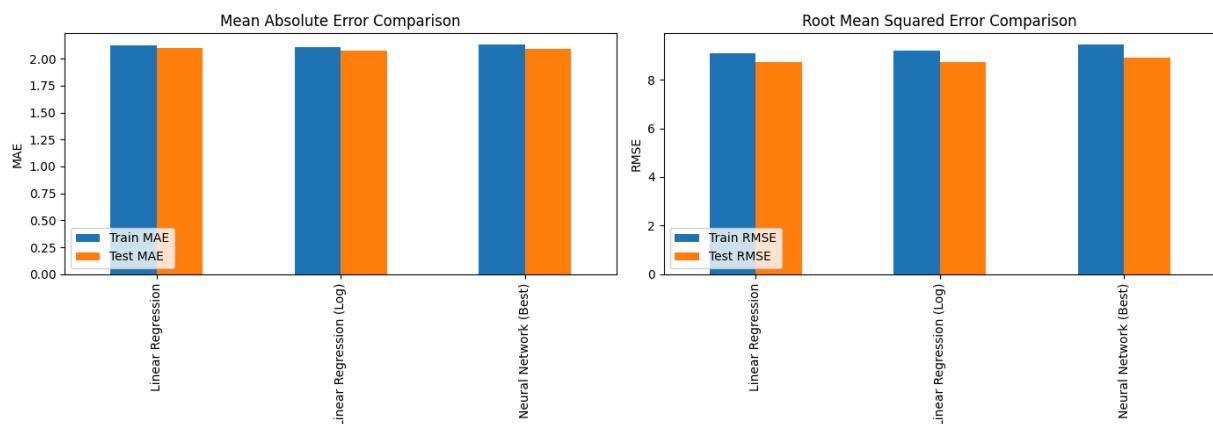
```
fig, axes = plt.subplots(1, 2, figsize=(14, 5))

# 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()
```



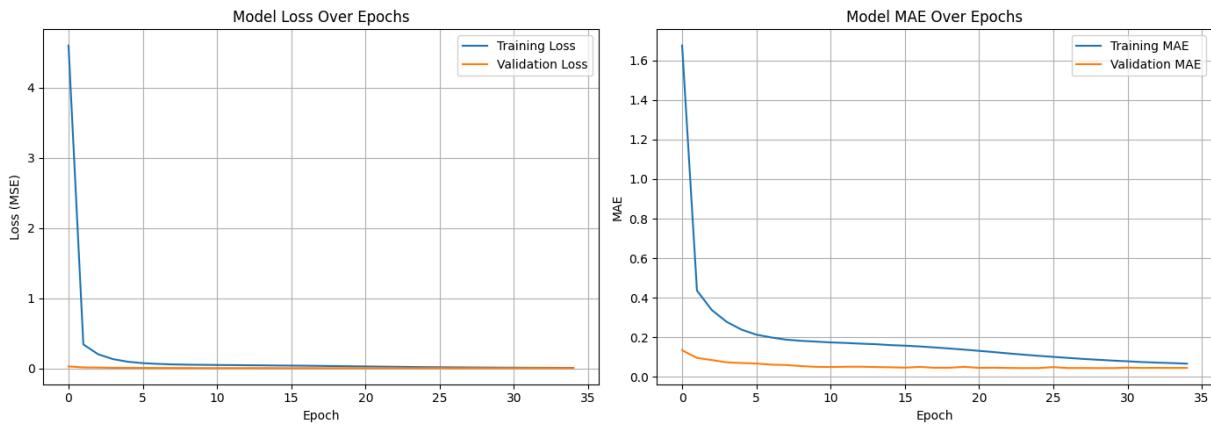
## Section 12: Visualize Training History

```
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')

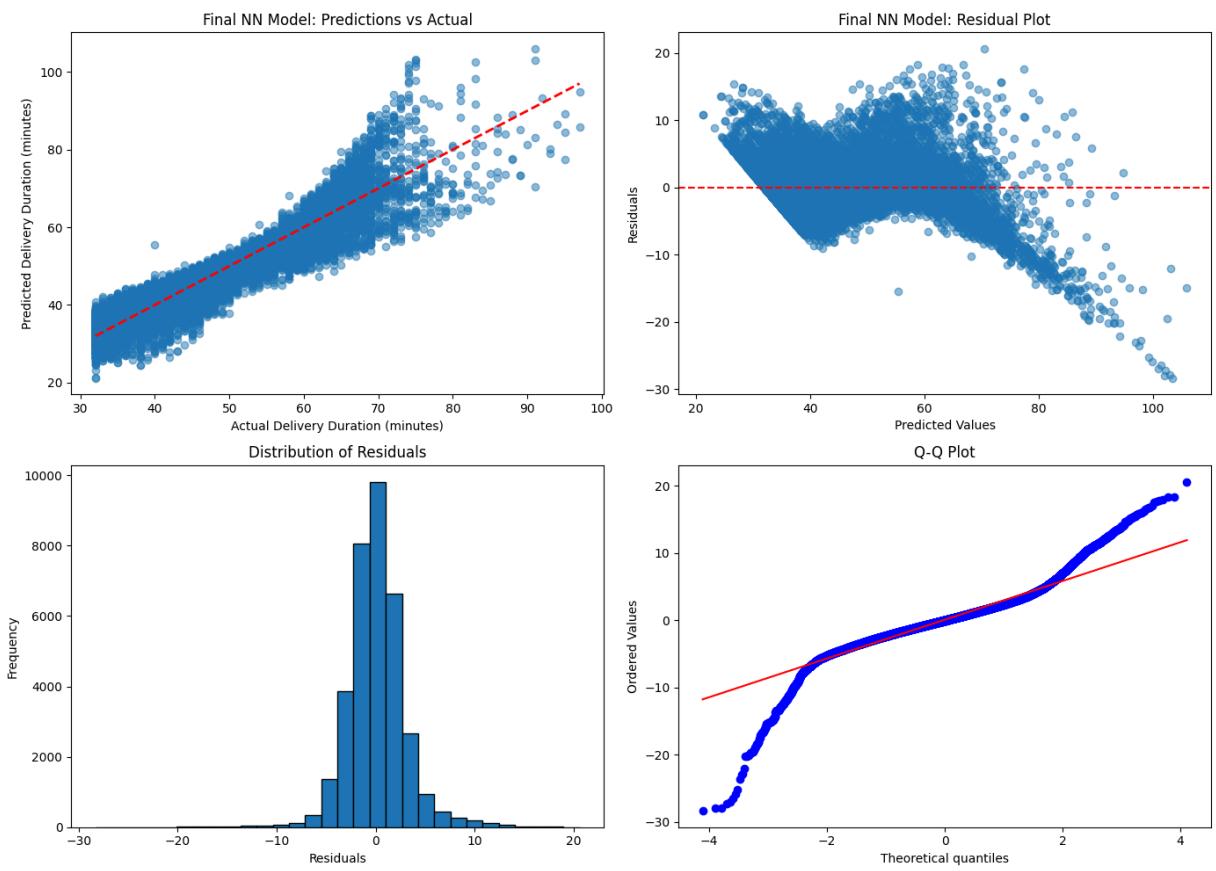
# Residuals (Final Model)
axes[0, 1].scatter(y_test_pred_final, residuals_nn_final, alpha=0.5)
axes[0, 1].axhline(y=0, color='r', linestyle='--')
axes[0, 1].set_xlabel('Predicted Values')
axes[0, 1].set_ylabel('Residuals')
axes[0, 1].set_title('Final NN Model: Residual Plot')

# 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 [ ]: