MERC_DEMO

July 6, 2024

# 1 HEAL Data2Action (D2A) Program - Emulator for RESPOND Model via LSTM

## 1.1 Introduction

The RESPOND model is a cohort-based simulation model designed to assist researchers in exploring and investigating overdose rates associated with the opioid misuse crisis in the United States. Using the results from RESPOND, researchers were able to explore combinations of community-level interventions to determine important factors associated with overdose rates. However, the simulation structure of RESPOND is complicated, and the model is computationally intensive. An alternative approach would be to construct emulators capable of returning approximations of the underlying simulation model.

In this notebook, we will build a Long Short-Term Memory (LSTM) neural network model to emulate the RESPOND model. The LSTM model will be trained on the RESPOND model data and used to predict the number of overdose deaths in a given week for a specific group. The LSTM model will be evaluated based on the root mean squared error (RMSE) of the predictions.

[7]:
```
import os
data_dir = 'Model Data'

import numpy as np
import pandas as pd
import time
from sklearn.preprocessing import MinMaxScaler
import tensorflow as tf
from tensorflow.keras.models import Sequential, load_model
from tensorflow.keras.layers import LSTM, Dense
import matplotlib.pyplot as plt
import math
from sklearn.metrics import mean_squared_error
from kerastuner.tuners import Hyperband

np.random.seed(42)
tf.random.set_seed(42)
```

## 1.2 Data Preprocessing

We first load the RESPOND model data and preprocess it for training the LSTM model. To be noted, due to privacy concerns, the specific data used in this notebook is not provided. However, the data is structured in a way that is compatible with the LSTM model. The data consists of the following columns:

- `time_step`: The time step of the simulation.
- `group_id`: The group identifier.
- `count`: The number of overdose deaths in a given week for a specific group.
- `treatment`: The treatment status of the group.
- `agegrp`: The age group of the group.
- `sex`: The sex of the group.
- `oud`: The opioid use disorder status of the group.

[ ]:
```
long_data1 = pd.read_csv(os.path.join(data_dir, 'long_data1.csv'), index_col=0)
```

The function `create_grouped_dataset` is used to create a grouped dataset from the RESPOND model data. It groups the data by `group_id` and creates sequences of length `n_time_steps` for each group. The function takes the following parameters:

- `data`: The RESPOND model data.
- `n_time_steps`: The number of time steps to consider in the LSTM model.
- `feature`: The feature to predict.

[11]:
```
def create_grouped_dataset(data, n_time_steps=7, feature='count'):
    grouped_data = []
    grouped_labels = []
    group_ids = data['group_id'].unique()

    for group in group_ids:
        group_data = data[data['group_id'] == group][feature].values
        for i in range(len(group_data) - n_time_steps + 1):
            grouped_data.append(group_data[i:i + n_time_steps])
            grouped_labels.append(group_data[i:i + n_time_steps])

    return np.array(grouped_data), np.array(grouped_labels)
```

[12]:
```
# feature selection
feature = 'count'
data = long_data1[['time_step', 'group_id', feature, "treatment", "agegrp",␣
↪"sex", "oud"]]

# sort by group_id and time_step
data = data.sort_values(by=['group_id', 'time_step'])

# we have 7 time point in this data set
n_time_steps = 7
X, y = create_grouped_dataset(data, n_time_steps, feature)
```

```
# reshape data
X = X.reshape(X.shape[0], X.shape[1], 1)
y = y.reshape(y.shape[0], y.shape[1])

# scale the data
scaler_X = MinMaxScaler(feature_range=(0, 1))
scaler_y = MinMaxScaler(feature_range=(0, 1))
X_train = scaler_X.fit_transform(X.reshape(-1, 1)).reshape(X.shape)
y_train = scaler_y.fit_transform(y)
```

### 1.3 Model Training

We use Hyperband tuning to search for the best hyperparameters for the LSTM model. The hyperparameters include the number of LSTM units, the activation function, and the number of LSTM layers.

[13]:
```
def build_model(hp):
    model = Sequential()
    model.add(LSTM(units=hp.Int('units_base', min_value=32, max_value=256,␣
 ↪step=32),
                   activation=hp.Choice('activation_base', values=['relu',␣
 ↪'tanh', 'sigmoid']),
                   return_sequences=True,
                   input_shape=(n_time_steps, 1)))

    for i in range(hp.Int('num_layers', 1, 10)):
        model.add(LSTM(
            units=hp.Int(f'units_{i}', min_value=32, max_value=256, step=32),
            activation=hp.Choice(f'activation_{i}', values=['relu', 'tanh',␣
 ↪'sigmoid']),
            return_sequences=True))

    model.add(LSTM(units=hp.Int('units_final', min_value=32, max_value=256,␣
 ↪step=32),
                   activation=hp.Choice('activation_final', values=['relu',␣
 ↪'tanh', 'sigmoid'])))
    model.add(Dense(n_time_steps))

    model.compile(optimizer='adam', loss='mean_squared_error')

    return model
```

[ ]:
```
tuner = Hyperband(
    build_model,
    objective='val_loss',
    max_epochs=200,
```

```
    factor=3,
    directory='hyperband_search',
    project_name='lstm_tuning')
```

[15]:
```
tuner.search(X_train, y_train, epochs=200, validation_data=(X_train, y_train))

best_model = tuner.get_best_models(num_models=1)[0]

best_hyperparameters = tuner.get_best_hyperparameters(num_trials=1)[0]
print(f"Best hyperparameters: {best_hyperparameters.values}")
```

```
Trial 254 Complete [03h 28m 37s]
val_loss: 0.007067888509482145

Best val_loss So Far: 3.5989630760013824e-06
Total elapsed time: 2d 03h 20m 33s
Best hyperparameters: {'units_base': 256, 'activation_base': 'relu',
'num_layers': 1, 'units_0': 256, 'activation_0': 'tanh', 'units_final': 224,
'activation_final': 'tanh', 'units_1': 192, 'activation_1': 'relu', 'units_2':
128, 'activation_2': 'tanh', 'units_3': 192, 'activation_3': 'sigmoid',
'units_4': 128, 'activation_4': 'tanh', 'units_5': 32, 'activation_5': 'tanh',
'units_6': 96, 'activation_6': 'relu', 'units_7': 192, 'activation_7':
'sigmoid', 'units_8': 96, 'activation_8': 'relu', 'units_9': 256,
'activation_9': 'sigmoid', 'tuner/epochs': 200, 'tuner/initial_epoch': 67,
'tuner/bracket': 4, 'tuner/round': 4, 'tuner/trial_id': '0142'}
```

We save the best model.

[ ]:
```
best_model.save('best_model.h5')
```

Then we load the best model and fit it to the training data.

[ ]:
```
def fit_model(model, X_train, y_train, scaler_y, epochs=200, initial_epoch=10,
 ↪batch_size=32, validation_data=None, fit=True):
    history = None
    fit_time = None

    if fit:
        start_time = time.time()
        history = model.fit(X_train, y_train, epochs=epochs,
 ↪initial_epoch=initial_epoch, batch_size=batch_size,
 ↪validation_data=validation_data, verbose=1)
        end_time = time.time()
        fit_time = end_time - start_time

    train_predict = model.predict(X_train)

    train_predict = scaler_y.inverse_transform(train_predict)
```

```
    return history, train_predict, fit_time

model = load_model('best_model.h5')
model.summary()
history, train_predict, fit_time = fit_model(model, X_train, y_train, scaler_y,␣
↪epochs=200, initial_epoch=0, batch_size=32, validation_data=(X_train,␣
↪y_train), fit=False)
```

[37]:
```
print(fit_time)
```

```
733.4378037452698
```

### 1.4 Evaluate Model

We tried to evaluate the model by calculating the root mean squared error (RMSE) for the full data, small count data, and large count data. The small count data is defined as the data where the maximum count change is less than or equal to 200, and the large count data is defined as the data where the maximum count change is greater than 200.

[57]:
```
def model_rmse(y_train, train_predict):
    y_small_index = np.where(y_train < 200)[0]
    y_large_index = np.where(y_train >= 200)[0]
    y_train_samll= y_train[y_small_index]
    y_train_large = y_train[y_large_index]

    train_predict_samll = train_predict[y_small_index]
    train_predict_large = train_predict[y_large_index]

    train_score_full = math.sqrt(mean_squared_error(y_train, train_predict))
    train_score_small = math.sqrt(mean_squared_error(y_train_samll,␣
↪train_predict_samll))
    train_score_large = math.sqrt(mean_squared_error(y_train_large,␣
↪train_predict_large))

    print(f'RMSE for full data: {train_score_full:.2f}')
    print(f'RMSE for small count: {train_score_small:.2f}')
    print(f'RMSE for large count: {train_score_large:.2f}')

    return train_score_full, train_score_small, train_score_large

model_rmse(y, train_predict)
```

```
RMSE for full data: 15.62
RMSE for small count: 6.40
RMSE for large count: 40.88
```

[57]:
```
(15.620350329658793, 6.401010495058592, 40.87666222949874)
```

[52]:
```
def individual_predict(ids, x_scaler, y_scaler, model, data, n_time_steps=7,␣
↪feature='count'):
    actual_vs_predicted = {}

    for group_id in ids:
        group_data = data[data['group_id'] == group_id][feature].values
        X_group = group_data[:n_time_steps].reshape(1, n_time_steps, 1)
        X_group = x_scaler.transform(X_group.reshape(-1, 1)).reshape(X_group.
↪shape)

        start_time = time.time()
        predicted = model.predict(X_group)
        predicted = y_scaler.inverse_transform(predicted).flatten()
        end_time = time.time()
        predict_time = end_time - start_time

        actual_vs_predicted[group_id] = {
            "actual": group_data[:n_time_steps],
            "predicted": predicted,
            "predict_time": predict_time
        }

    return actual_vs_predicted

def plot_results(actual_vs_predicted, selected_group_ids, col_count=3):

    plot_count = len(selected_group_ids)
    n_rows = math.ceil(plot_count / col_count)
    n_cols = min(plot_count, col_count)

    fig, axs = plt.subplots(n_rows, n_cols, figsize=(5 * n_cols, 4 * n_rows))
    if n_rows == 1:
        axs = np.expand_dims(axs, axis=0)
    if n_cols == 1:
        axs = np.expand_dims(axs, axis=1)

    for i, group_id in enumerate(selected_group_ids):
        actual_data = actual_vs_predicted[group_id]['actual']
        predicted_data = actual_vs_predicted[group_id]['predicted']
        time_steps = np.arange(len(actual_data))

        ax = axs[i // n_cols, i % n_cols]

        # Plot actual values
        ax.plot(time_steps, actual_data, label=f'RESPOND')
        ax.scatter(time_steps, actual_data, s=50)
```

```
        # Plot predicted values
        ax.plot(time_steps, predicted_data, linestyle='--', label=f'LSTM')
        ax.scatter(time_steps, predicted_data, s=50)

        ax.set_title(f'Group {group_id}')
        ax.set_xlabel('Time (by week)')
        ax.set_ylabel('Count')
        ax.legend()

    for j in range(i + 1, n_rows * n_cols):
        fig.delaxes(axs[j // n_cols, j % n_cols])

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

[ ]:
```
def calculate_changes(df):
    reference_count = df[df['time_step'] == 157]['count'].values[0]
    df['count_change'] = reference_count - df['count']
    df['data_split'] = 'small_change' if df['count_change'].abs().max() <= 200␣
 ↪else 'large_change'
    return df

change_data = long_data1.groupby('group_id').apply(calculate_changes)

large_change_id = change_data[change_data['data_split'] ==␣
 ↪'large_change']['group_id'].unique()
small_change_id = change_data[change_data['data_split'] ==␣
 ↪'small_change']['group_id'].unique()
```

### 1.4.1 Full data prediction plot

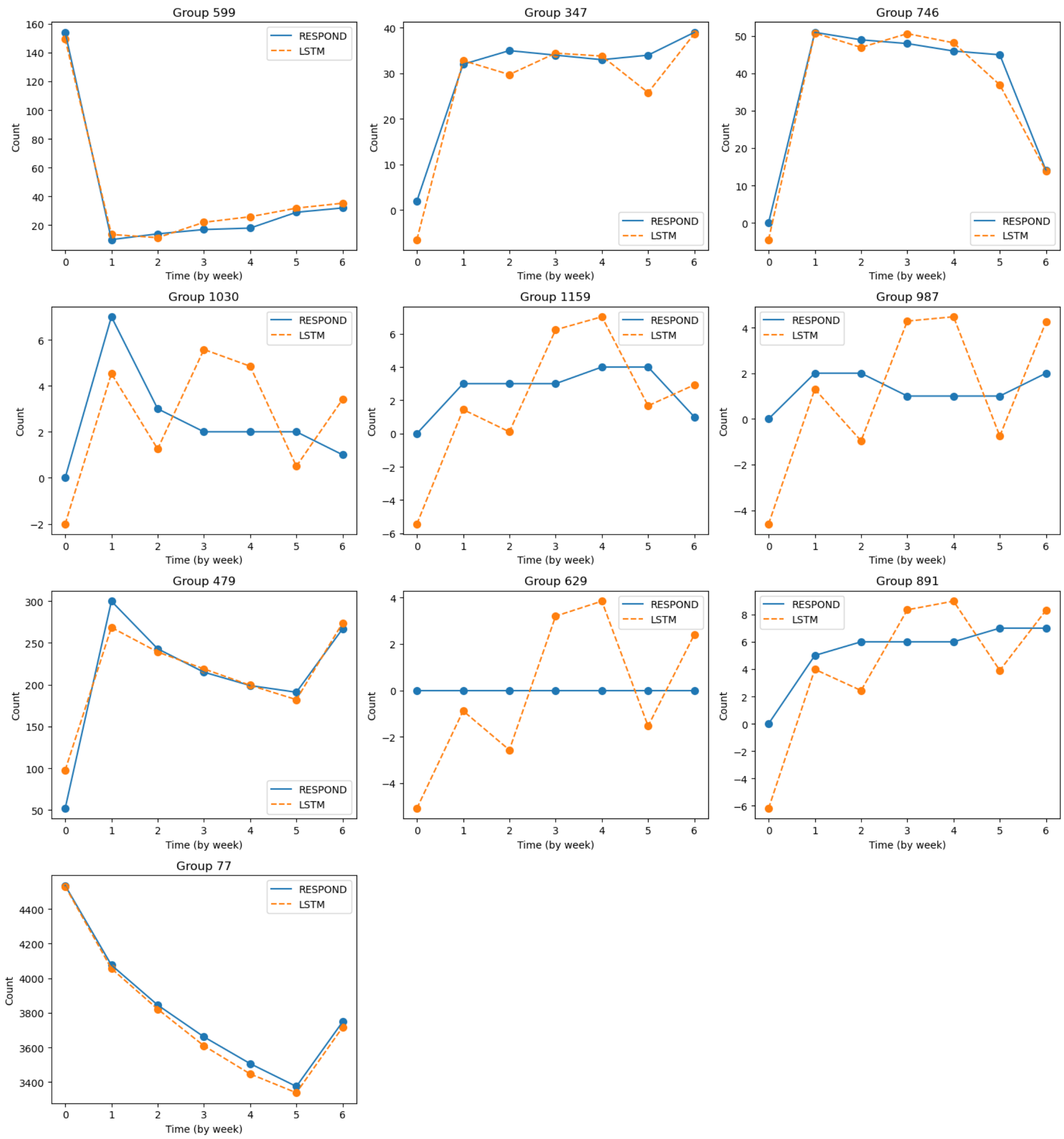
[53]:
```
selected_group_ids = np.random.choice(data['group_id'].unique(), 10,␣
 ↪replace=False)
actual_vs_predicted = individual_predict(selected_group_ids, scaler_X,␣
 ↪scaler_y, model, data, n_time_steps, feature)

plot_results(actual_vs_predicted, selected_group_ids)

print(actual_vs_predicted)
```

```
1/1               0s 76ms/step
1/1               0s 28ms/step
1/1               0s 26ms/step
1/1               0s 23ms/step
1/1               0s 25ms/step
1/1               0s 27ms/step
1/1               0s 28ms/step
```

```
1/1              0s 25ms/step
1/1              0s 27ms/step
1/1              0s 23ms/step
```




```
{599: {'actual': array([154,  10,  14,  17,  18,  29,  32]), 'predicted':
array([149.43364 ,  13.576566,  11.347096,  22.014423,  25.905779,
        31.876785,  35.296215], dtype=float32), 'predict_time':
0.09722709655761719}, 347: {'actual': array([ 2, 32, 35, 34, 33, 34, 39]),
'predicted': array([-6.4614086, 32.818176 , 29.746708 , 34.43696  , 33.801594 ,
       25.778023 , 38.69705  ], dtype=float32), 'predict_time':
0.045269012451171875}, 746: {'actual': array([ 0, 51, 49, 48, 46, 45, 14]),
```

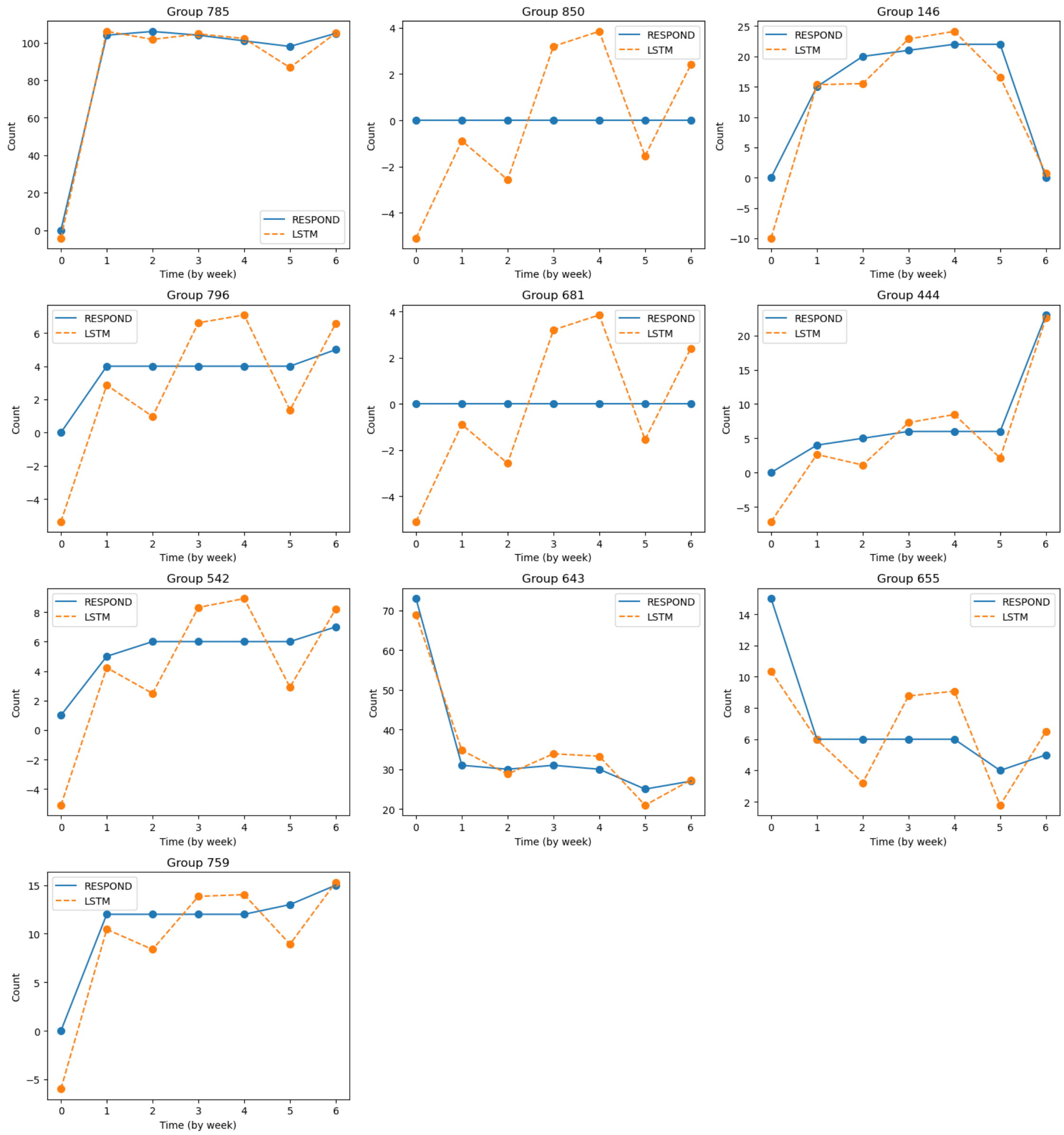
'predicted': array([-4.5236073, 50.840565 , 46.96814  , 50.6631   , 48.197704 ,
       36.938488 , 13.852169 ], dtype=float32), 'predict_time':
0.043237924575805664}, 1030: {'actual': array([0, 7, 3, 2, 2, 2, 1]),
'predicted': array([-2.008466  ,  4.530183  ,  1.2513322 ,  5.5791216 ,
4.8494253 ,
        0.50191426,  3.4144742 ], dtype=float32), 'predict_time':
0.043473005294799805}, 1159: {'actual': array([0, 3, 3, 3, 4, 4, 1]),
'predicted': array([-5.4364157 ,  1.44239   ,  0.10608691,  6.238548  ,
7.022839  ,
        1.6720356 ,  2.9288843 ], dtype=float32), 'predict_time':
0.04244494438171387}, 987: {'actual': array([0, 2, 2, 1, 1, 1, 2]), 'predicted':
array([-4.60081  ,  1.3036627, -0.9598608,  4.281967 ,  4.470721 ,
       -0.7533574,  4.2477355], dtype=float32), 'predict_time':
0.04518413543701172}, 479: {'actual': array([ 52, 300, 243, 215, 199, 191,
267]), 'predicted': array([ 97.68999, 268.54868, 239.18053, 218.95021,
199.37335, 182.11827,
       274.02496], dtype=float32), 'predict_time': 0.04700613021850586}, 629:
{'actual': array([0, 0, 0, 0, 0, 0, 0]), 'predicted': array([-5.0932107 ,
-0.88518554, -2.5721662 ,  3.2025125 ,  3.8495805 ,
       -1.5435262 ,  2.4097953 ], dtype=float32), 'predict_time':
0.047688961029052734}, 891: {'actual': array([0, 5, 6, 6, 6, 7, 7]),
'predicted': array([-6.196713 ,  3.9865513,  2.4336252,  8.340449 ,  8.976584 ,
        3.9063473,  8.315856 ], dtype=float32), 'predict_time':
0.04333090782165527}, 77: {'actual': array([4536, 4076, 3845, 3661, 3506, 3374,
3748]), 'predicted': array([4531.294 , 4055.8074, 3821.4683, 3609.3413,
3446.4731, 3337.4763,
       3716.639 ], dtype=float32), 'predict_time': 0.040868282318115234}}

### 1.4.2 Small count data prediction plot

[54]:
```
selected_group_ids_small = np.random.choice(small_change_id, 10, replace=False)
actual_vs_predicted = individual_predict(selected_group_ids_small, scaler_X,␣
 ↪scaler_y, model, data, n_time_steps, feature)

plot_results(actual_vs_predicted, selected_group_ids_small)
```

```
1/1            0s 40ms/step
1/1            0s 25ms/step
1/1            0s 26ms/step
1/1            0s 24ms/step
1/1            0s 28ms/step
1/1            0s 26ms/step
1/1            0s 24ms/step
1/1            0s 24ms/step
1/1            0s 23ms/step
1/1            0s 25ms/step
```



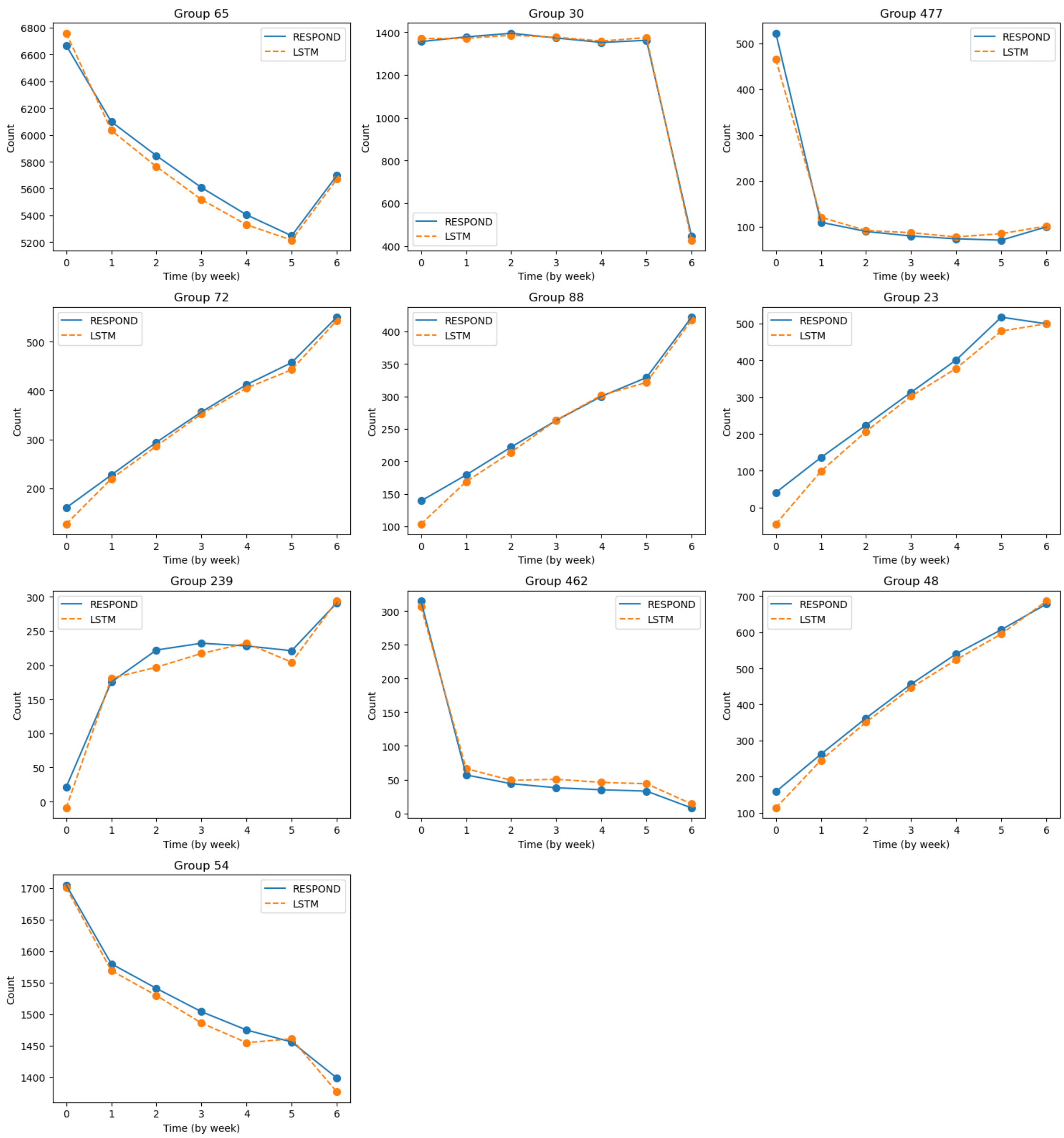

### 1.4.3 Large count data prediction plot

[55]:
```
selected_group_ids_large = np.random.choice(large_change_id, 10, replace=False)
actual_vs_predicted = individual_predict(selected_group_ids_large, scaler_X,␣
↪scaler_y, model, data, n_time_steps, feature)

plot_results(actual_vs_predicted, selected_group_ids_large)
```

```
1/1              0s 27ms/step
1/1              0s 25ms/step
1/1              0s 22ms/step
```

```
1/1              0s 26ms/step
1/1              0s 26ms/step
1/1              0s 24ms/step
1/1              0s 25ms/step
1/1              0s 27ms/step
1/1              0s 26ms/step
1/1              0s 26ms/step
```




[42]: