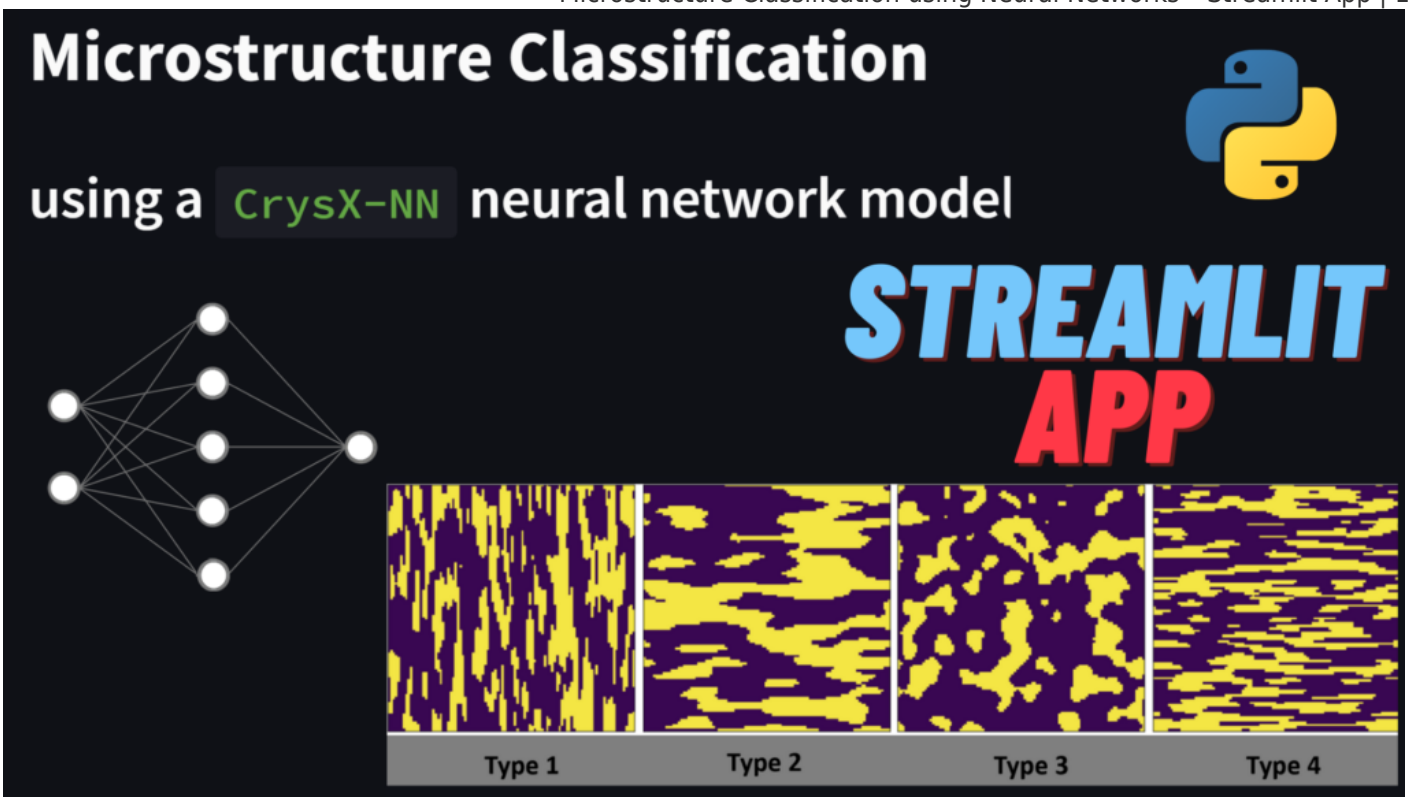

In this post, I demonstrate a Streamlit app that I have created that can be used to classify microstructures of different types.

I trained a neural network using CrysX-NN library, on synthetic microstructures of 4 types as shown in this notebook.

Check out the Streamlit App below (Source code is provided below the app)

https://share.streamlit.io/manassharma07/microstructure_classification_app/main/Microstructure_Classification_CrysX-NN_app.py

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Source Code:

```
import streamlit as st
import matplotlib.pyplot as plt
import numpy as np
rng = np.random.default_rng()
from pymks import (
    generate_multiphase,
)
from crysx_nn import network
import session_state
from streamlit.script_runner import RerunException
from streamlit.script_request_queue import RerunData

state = session_state.get(rndm_indx=5)

@st.cache
```

```
def create_and_load_model():
    nInputs = 100*100 # No. of nodes in the input layer
    neurons_per_layer = [500, 4] # Neurons per layer (excluding the input layer)
    activation_func_names = ['ReLU', 'Softmax']
    nLayers = len(neurons_per_layer)
    nEpochs = 4
    batchSize = 32 # No. of input samples to process at a time for optimization
    # Create the crysx_nn neural network model
    model = network.nn_model(nInputs=nInputs, neurons_per_layer=neurons_per_layer,
activation_func_names=activation_func_names, batch_size=batchSize, device='CPU',
init_method='Xavier')
    # Load the preoptimized weights and biases
    model.load_model_weights('NN_crysx_microstructure_96_weights_streamlit')
    model.load_model_biases('NN_crysx_microstructure_96_biases_streamlit')
    return model

@st.cache
def generate_microstructures(nSamples_per_type, width, height):
    grain_sizes = [(30, 5), (10, 40), (15, 15), (5, 30)]
    seeds = [10, 99, 4, 36]

    data_synth = np.concatenate([
        generate_multiphase(shape=(nSamples_per_type, width, height),
grain_size=grain_size,
            volume_fraction=(0.5, 0.5),
            percent_variance=0.2,
            # seed=seed
        )
        for grain_size, seed in zip(grain_sizes, seeds)
    ])
    return data_synth

microstructure_data = generate_microstructures(20,100,100)
microstructures_labels =
np.concatenate([np.ones(20)*0,np.ones(20)*1,np.ones(20)*2,np.ones(20)*3])

model = create_and_load_model()

# @st.cache
def make_sidebar():
    # st.sidebar.markdown("## [CrysX-NN](https://github.com/manassharma07/crysx_nn)")
    st.sidebar.write('\n\n ## Neural Network Library Used')
    st.sidebar.image('logo_crysx_nn-min.png')
    st.sidebar.caption('https://github.com/manassharma07/crysx_nn')
    st.sidebar.write('## Neural Network Architecture Used')
    st.sidebar.write('1. **Inputs**: Flattened 100x100=10,000')
    st.sidebar.write('2. **Hidden layer** of size **500** with **ReLU** activation
Function')
    st.sidebar.write('3. **Output layer** of size **4** with **Softmax** activation
Function')
    st.sidebar.write('Training was done for 4 epochs with Categorical Cross Entropy
Loss function using [Stochastic Gradient Descent; learning rate=0.02; batch size of
```

```
32].')
    st.sidebar.image('neural_network_visualization_25.png')
    st.sidebar.caption('Nerual Network Schematic')

make_sidebar()

st.write('# Microstructure Classification')
st.write('## using a `CrysX-NN` neural network model')

st.write('### We have microstructures of 4 types:')

col1, col2, col3, col4 = st.columns(4)
col1.header('Type 1')
col1.write('This  has 6 times more grain boundaries along the x-axis than the y-axis.')
col2.header('Type 2')
col2.write('This has 4 times more grain boundaries along the y-axis than the x-axis.')
col3.header('Type 3')
col3.write('This has the same number of grain boundaries along the x-axis as well as
the y-axis.')
col4.header('Type 4')
col4.write('This has 6 times more grain boundaries along the y-axis than the x-axis.')

st.image('microstructures_4_types-min.png')

st.write('### The following is a random `100x100` pixel picture of a microstructure of
one of these 4 types.')

## The pyplot takes up a lot of screen
# fig, ax = plt.subplots()
# ax.imshow(microstructure_data[state.rndm_indx,:,:])
# ax.set_axis_off()
# st.pyplot(fig)

# So we use matplotlib to save an image instead
plt.imsave('processed_tensor.png',microstructure_data[state.rndm_indx,:,:],
cmap='viridis')
st.image('processed_tensor.png', width=200)

st.write('### Can you guess which type is it?')

option = st.selectbox('Your Answer',
     ('Choose an option', 'Type 1', 'Type 2', 'Type 3', 'Type 4'), key=state.rndm_indx)


if option != 'Choose an option':
    st.write('You selected:', option)
    st.write('### True Type: '+str(int(microstructures_labels[state.rndm_indx])+1))
    input = (microstructure_data[state.rndm_indx,:,:] - 0.5) / 0.5
    input = input.reshape(1, 10000)
    predictions = model.predict(input.astype(np.float32), loss_func_name='BCE')
    # Get the maximum probability
    certainty = np.max(predictions)
```

```
    # Get the index of the maximum probability
    output = np.argmax(predictions)
    # st.write(predictions)
    st.write('### Neural Network Prediction : '+str(int(output+1)))
    st.write('### Certainty: '+ str(certainty*100)+' %')

if st.button('Next sample'):
    state.rndm_indx = rng.integers(0, microstructure_data.shape[0])
    # option = st.selectbox('Your Answer',
    #  ('Choose an option', 'Type 1', 'Type 2', 'Type 3', 'Type 4'))
    option = None
    raise RerunException(RerunData())
st.write('### Code used for training the neural network: [Jupyter
Notebook](https://github.com/manassharma07/crysx_nn/blob/main/examples/Microstructures_
Classification_CPU.ipynb)')
```

Manas Sharma

I’m a physicist specializing in computational material science with a PhD in Physics from Friedrich-Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, and Machine Learning related apps and software from time to time. Can code in most of the popular languages. I like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

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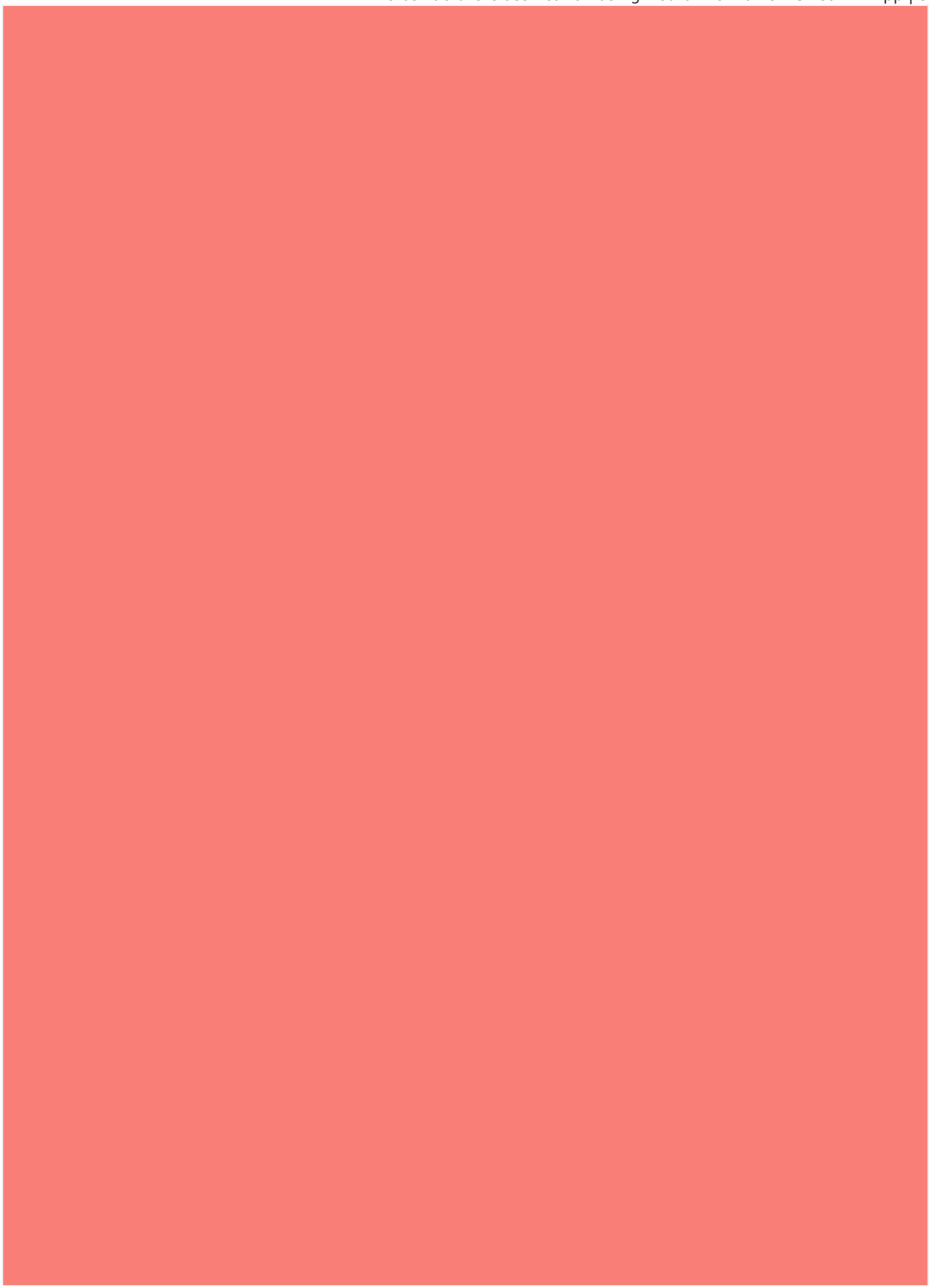

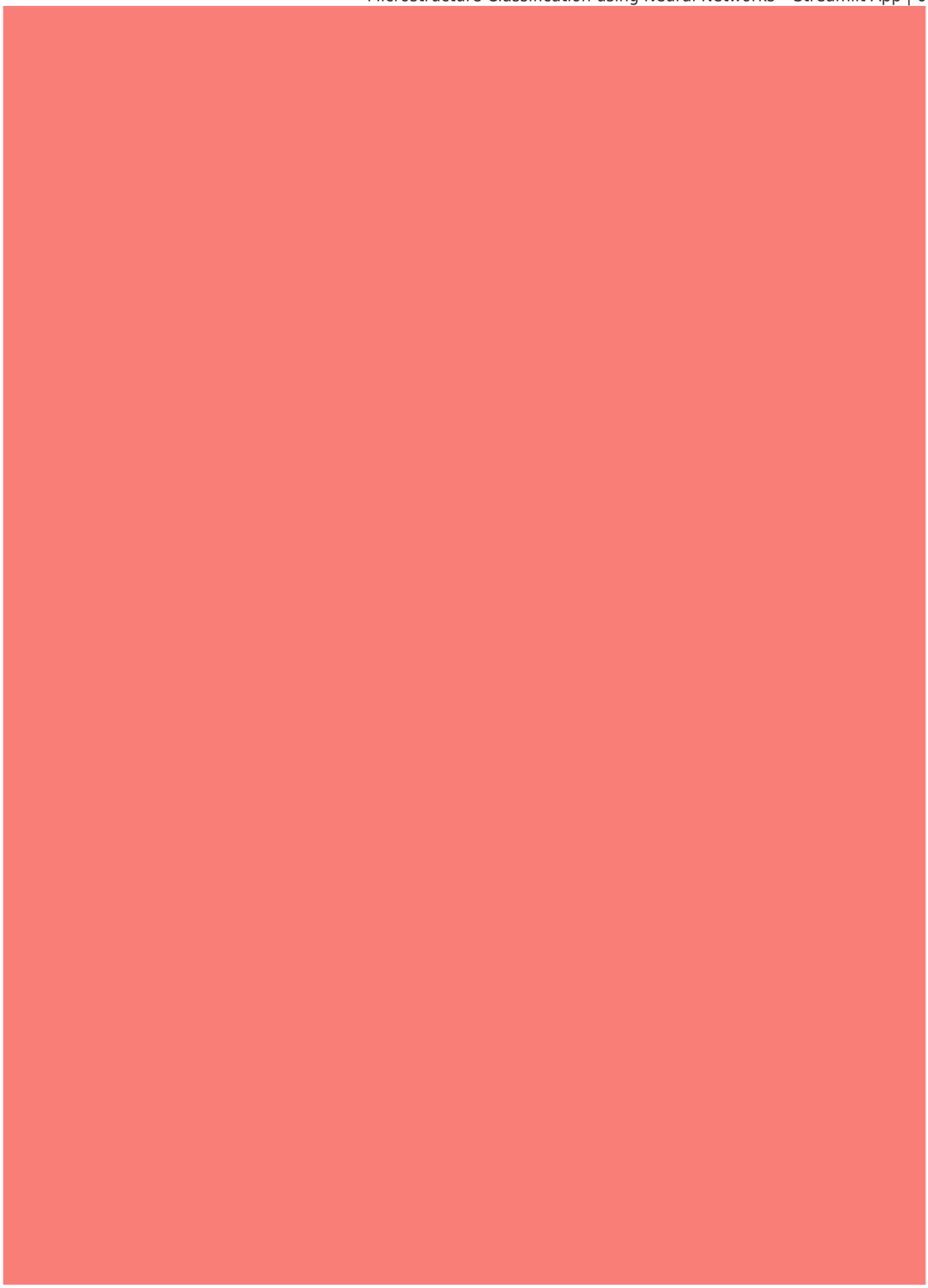

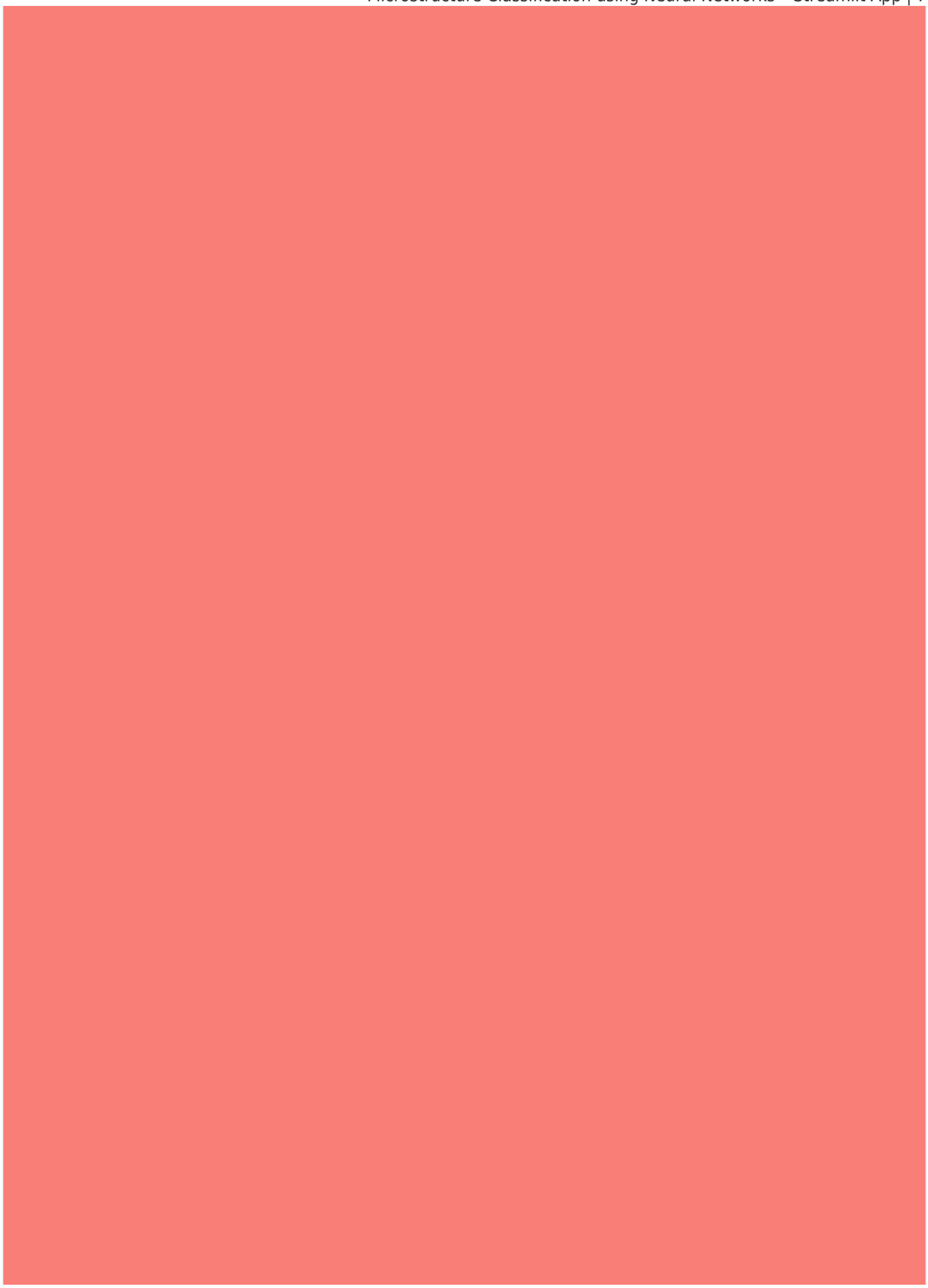

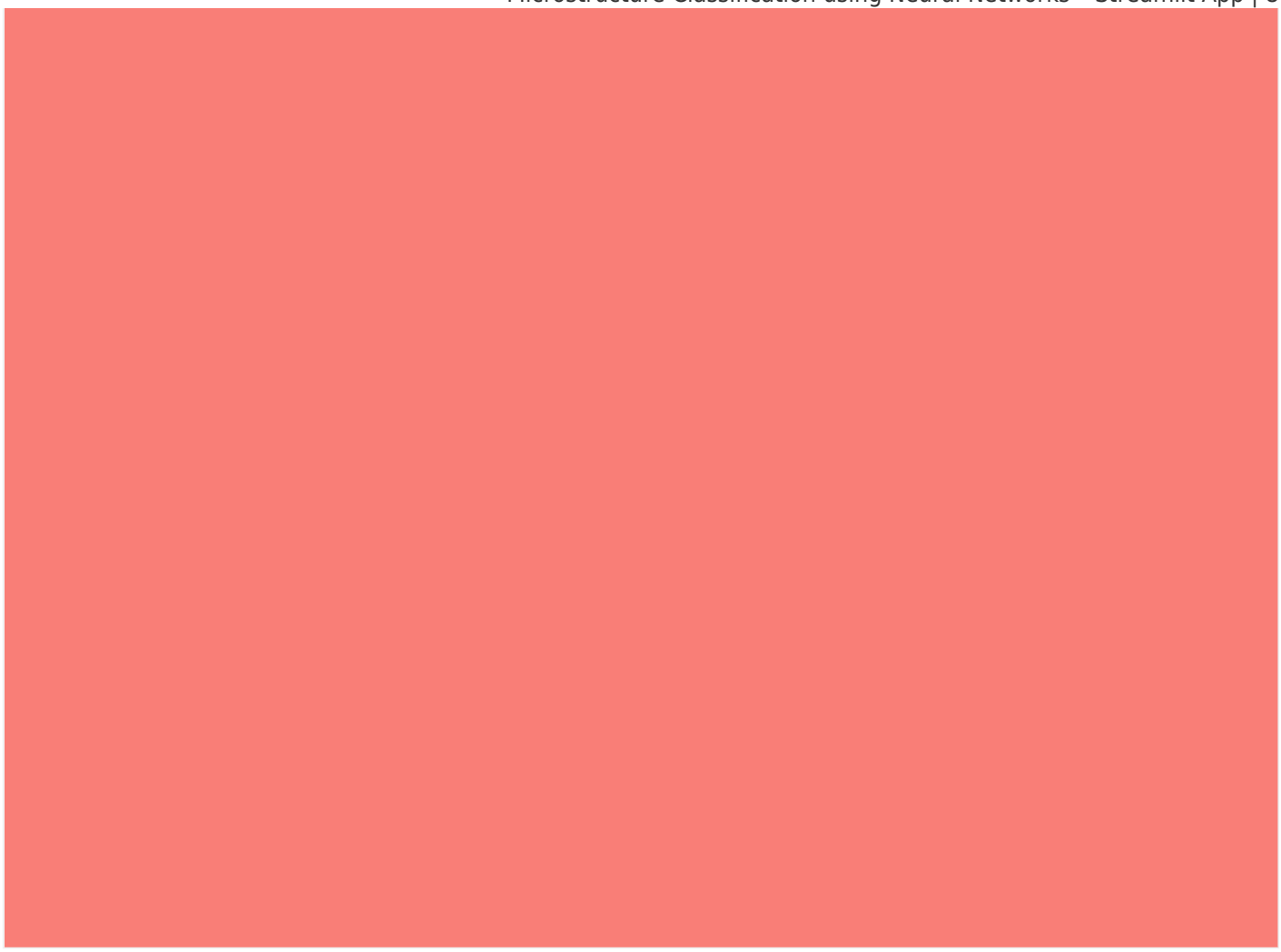

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