## PILSTM

## April 13, 2025

[1]: import numpy as np import os

```
import sys
import gym
import zipfile
import autograd
import matplotlib.gridspec as gridspec
# Use tf.random.set seed for TensorFlow 2.0 and above
#from scipy.signal.waveforms import square
import matplotlib.pyplot as plt
from scipy.integrate import solve_ivp
from sklearn.model_selection import train_test_split
import random
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras.models import Sequential, model_from_json
from keras.layers import Dense
from keras.layers import Input
from tensorflow.keras import layers
2025-04-13 00:03:15.314761: I external/local_xla/xla/tsl/cuda/cudart_stub.cc:32]
Could not find cuda drivers on your machine, GPU will not be used.
2025-04-13 00:03:15.513475: I external/local xla/xla/tsl/cuda/cudart_stub.cc:32]
Could not find cuda drivers on your machine, GPU will not be used.
2025-04-13 00:03:15.590707: E
external/local_xla/xla/stream_executor/cuda/cuda_fft.cc:485] Unable to register
cuFFT factory: Attempting to register factory for plugin cuFFT when one has
already been registered
2025-04-13 00:03:15.774702: E
external/local_xla/xla/stream_executor/cuda/cuda_dnn.cc:8454] Unable to register
cuDNN factory: Attempting to register factory for plugin cuDNN when one has
already been registered
2025-04-13 00:03:15.813402: E
external/local_xla/xla/stream_executor/cuda/cuda_blas.cc:1452] Unable to
register cuBLAS factory: Attempting to register factory for plugin cuBLAS when
one has already been registered
2025-04-13 00:03:16.077384: I tensorflow/core/platform/cpu_feature_guard.cc:210]
This TensorFlow binary is optimized to use available CPU instructions in
```

```
performance-critical operations.
To enable the following instructions: AVX2 FMA, in other operations, rebuild
TensorFlow with the appropriate compiler flags.
2025-04-13 00:03:17.664630: W
tensorflow/compiler/tf2tensorrt/utils/py_utils.cc:38] TF-TRT Warning: Could not
find TensorRT
```

```
[15]: # @title Hp meristor's state variable:
from IPython.display import display, Math

latex_equation = r"""
  \text{State variable:}\quad \frac{dw}{dt} = \mu_\text{v} \cdot \left(\loguad \frac{R_{\text{on}}}{D^2} \right) \cdot i(t) \cdot f(w) \\
  \text{Window function:}\quad f(w) = {w(1 - w)}\\
  \text{state variable in this code is w:}\quad w = \frac{X}{D}
  """
  display(Math(latex_equation))
```

 $\begin{array}{ll} \text{State variable:} & \frac{dw}{dt} = \mu_{\text{v}} \cdot \left(\frac{R_{\text{on}}}{D^2}\right) \cdot i(t) \cdot f(w) \\ \text{Window function:} & f(w) = w(1-w) \\ \text{state variable in this code is w:} & w = \frac{X}{D} \end{array}$ 

```
[2]: import numpy as np
    import matplotlib.pyplot as plt
    from scipy.integrate import solve_ivp
    from sklearn.preprocessing import StandardScaler, MinMaxScaler
    # ----- Physical Parameters -----
    frequency = 1
    A train = 1.5
    W_train = 2 * np.pi * frequency
    mu_v = 10**4
    D = 60
    r_on = 0.1
    r_off = 16
    r0 = 4
    w0 = (r0 - r_off) / (r_on - r_off)
    points_per_period = 600
    total_points = 10 * points_per_period
    # ----- Solving ODE -----
    def f(t, w, A, W, mu_v, D, r_on, r_off):
        k = mu_v * (r_on / D**2)
```

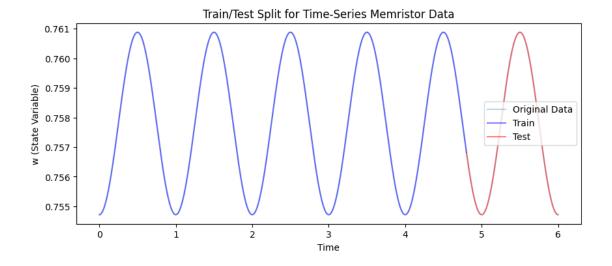
```
f_w = w * (1 - w)
   r = r_on * w + r_off * (1 - w)
   I = A * np.sin(W * t) / r
   return I * f_w * k
t_all = np.linspace(0, 6, total_points)
sol_all=solve_ivp(f, (0, 6), [w0], t_eval=t_all, args=(A_train, W_train, mu_v,_u
\rightarrowD, r_on, r_off),
          method='RK45', max_step=0.001)
w_all = sol_all.y[0]
v_all = A_train * np.sin(W_train * t_all)
r_all = r_on * w_all + r_off * (1 - w_all)
I_all = v_all / r_all
X_{all} = np.column_stack([t_all[:-1], w_all[:-1], I_all[:-1]])
y_all = w_all[1:]
# ------ Split Data -----
test ratio = 0.2
test_size = int(test_ratio * len(X_all))
test_index = np.arange(len(X_all) - test_size, len(X_all))
train_index = np.arange(0, len(X_all) - test_size)
X_train, X_test = X_all[train_index], X_all[test_index]
y_train, y_test = y_all[train_index], y_all[test_index]
print(X_train.shape)
print(X_test.shape)
print(y_train.shape)
print(y_test.shape)
plt.figure(figsize=(10, 4))
plt.plot(t_all[:-1], w_all[:-1], label="Original Data", alpha=0.3)
plt.plot(X_train[:, 0], y_train, color='blue', alpha=0.5, label='Train')
plt.plot(X_test[:, 0], y_test, color='red', alpha=0.5, label='Test')
plt.xlabel("Time")
plt.ylabel("w (State Variable)")
plt.title("Train/Test Split for Time-Series Memristor Data")
#plt.grid()
plt.legend()
plt.savefig("rungkutta_train_test.pdf")
plt.show()
```

```
from sklearn.preprocessing import StandardScaler, MinMaxScaler
import numpy as np
scaler_time = StandardScaler()
X_train[:, 0] = scaler_time.fit_transform(X_train[:, 0].reshape(-1, 1)).
→flatten()
X_test[:, 0] = scaler_time.transform(X_test[:, 0].reshape(-1, 1)).flatten()
scaler_features = MinMaxScaler(feature_range=(-1, 1))
X_train[:, 1:] = scaler_features.fit_transform(X_train[:, 1:])
X_test[:, 1:] = scaler_features.transform(X_test[:, 1:])
scaler_y = MinMaxScaler(feature_range=(-1, 1))
y_train_scaled = scaler_y.fit_transform(y_train.reshape(-1, 1))
y_test_scaled = scaler_y.transform(y_test.reshape(-1, 1))
X_train_scaled = X_train.copy()
X_test_scaled = X_test.copy()
# ----- Create Sequences -----
sequence_length = 10 #
def create_sequences(X, y, sequence_length):
   X_seq, y_seq = [], []
   for i in range(len(X) - sequence_length):
       X_seq.append(X[i:i+sequence_length])
       y_seq.append(y[i+sequence_length])
   return np.array(X_seq), np.array(y_seq).reshape(-1, 1)
X_train_seq, y_train_seq = create_sequences(X_train_scaled, y_train_scaled,_u
⇒sequence_length)
X_test_seq, y_test_seq = create_sequences(X_test_scaled, y_test_scaled, u
 ⇔sequence_length)
print("Mean of X_train_scaled:", np.mean(X_train, axis=0))
print("Std of X_train_scaled:", np.std(X_train, axis=0))
print("Mean of X_test_scaled:", np.mean(X_test, axis=0))
print("Std of X_test_scaled:", np.std(X_test, axis=0))
print("Mean of y_train_scaled:", np.mean(y_train_scaled))
print("Std of y_train_scaled:", np.std(y_train_scaled))
```

```
print("Mean of y_test_scaled:", np.mean(y_test_scaled))
print("Std of y_test_scaled:", np.std(y_test_scaled))

print(f'X_train_seq shape: {X_train_seq.shape}, y_train_seq shape: {y_train_seq.shape}')
print(f'X_test_seq shape: {X_test_seq.shape}, y_test_seq shape: {y_test_seq.shape}')
```

(4800, 3) (1199, 3) (4800,) (1199,)



```
Mean of X_train_scaled: [-6.65671222e-17 3.04609012e-02 2.26622042e-02] Std of X_train_scaled: [1. 0.70298873 0.71031816] Mean of X_test_scaled: [2.16470271 -0.12662702 -0.09072466] Std of X_test_scaled: [0.24979159 0.70958015 0.68660316] Mean of y_train_scaled: 0.03060324437440435 Std of y_train_scaled: 0.7028492870931501 Mean of y_test_scaled: -0.12719823824974452 Std of y_test_scaled: 0.7100073018388313 X_train_seq shape: (4790, 10, 3), y_train_seq shape: (4790, 1) X_test_seq shape: (1189, 10, 3), y_test_seq shape: (1189, 1)
```

```
[3]: import numpy as np
import random
import matplotlib.pyplot as plt
import tensorflow as tf
```

```
from tensorflow.keras.layers import Dense, Input, LSTM # Import LSTM here
from tensorflow.keras import Sequential, regularizers
from tensorflow.keras.layers import Dropout
class PhysicsInformedRNN(tf.keras.Model):
   def __init__(self, **kwargs):
       super().__init__(**kwargs)
       self.RNN = Sequential([
           LSTM(35, return sequences=True, activation='tanh', L
 →kernel_regularizer=tf.keras.regularizers.12(1e-4)),
           Dropout (0.06),
           LSTM(39, return_sequences=True, activation='tanh', __

→kernel_regularizer=tf.keras.regularizers.12(1e-4)), #
           Dropout (0.06),
           Dense(29, activation='tanh', kernel_regularizer=tf.keras.
 ⇔regularizers.12(1e-4)),
           Dense(1,)
       ])
   def call(self, inputs):
       return self.RNN(inputs)
   def build(self, input_shape):
       self.RNN.build(input shape)
       super().build(input_shape)
pinn_rnn = PhysicsInformedRNN()
pinn_rnn.build((None, sequence_length, 3))
pinn_rnn.summary()
from tensorflow.keras.optimizers import Adam
from tensorflow.keras.callbacks import ModelCheckpoint
import tensorflow as tf
import matplotlib.pyplot as plt
```

WARNING: All log messages before absl::InitializeLog() is called are written to STDERR
I0000 00:00:1744490008.960806 6129 cuda\_executor.cc:1015] successful NUMA node read from SysFS had negative value (-1), but there must be at least one NUMA node, so returning NUMA node zero. See more at https://github.com/torvalds/linux/blob/v6.0/Documentation/ABI/testing/sysfs-bus-pci#L344-L355
2025-04-13 00:03:28.961320: W

tensorflow/core/common\_runtime/gpu/gpu\_device.cc:2343] Cannot dlopen some GPU libraries. Please make sure the missing libraries mentioned above are installed properly if you would like to use GPU. Follow the guide at https://www.tensorflow.org/install/gpu for how to download and setup the required libraries for your platform.

Skipping registering GPU devices...

Model: "physics\_informed\_rnn"

```
Layer (type)

Output Shape

Param #

sequential (Sequential)

?

18,350
```

Total params: 18,350 (71.68 KB)

Trainable params: 18,350 (71.68 KB)

Non-trainable params: 0 (0.00 B)

```
[4]: NO = 1
Nf = X_train_seq.shape[0]
Nd = y_train_seq.shape[0]

#col_weights = tf.Variable(1.0)  # for ode loss
#u_weights = tf.Variable(1.0)  # for ic loss
#data_weights = tf.Variable(1.5)  # for data loss
#________

col_weights = tf.Variable(tf.ones(Nf), dtype=tf.float32)  #weight of ODE
data_weights = tf.Variable(tf.ones(Nd), dtype=tf.float32)  #weight of data
u_weights = tf.Variable(tf.ones(NO), dtype=tf.float32)

optimizer_col_weights = tf.keras.optimizers.Adam(learning_rate=1e-2)
optimizer_data_weights = tf.keras.optimizers.Adam(learning_rate=1e-4)

print("Shape of col_weights:", col_weights.shape)
print("Shape of ode_res:", data_weights .shape)

print("done")
```

Shape of col\_weights: (4790,) Shape of ode\_res: (4790,) done

```
[5]: def compute_loss(X, y_true, model, col_weights, u_weights, data_weights):
        X = tf.convert_to_tensor(X, dtype=tf.float32)
        y_true = tf.convert_to_tensor(y_true, dtype=tf.float32)
        with tf.GradientTape(persistent=True) as tape:
            w_pred_sequence = model(X)
            w_pred = w_pred_sequence[:, -1, :]
            I t = X[:, -1, 0:1]
            w_{prev} = X[:, -1, 1:2]
            T = X[:, -1, 2:3]
            f_w = w_pred * (1 - w_pred)
            with tf.GradientTape() as g:
                g.watch(T)
                inputs = tf.concat([I_t,w_prev, T], axis=1)
                w_pred_g = model(tf.expand_dims(inputs, axis=1)) # (batch_size, 1,_
      →3)
            dw_dt = g.gradient(w_pred_g, T)
            ode_res = dw_dt - mu_v * (r_on / D**2) * I_t * f_w
            ode_loss = tf.reduce_mean(tf.square(col_weights[:, tf.newaxis] *__
      →ode_res))
            data_loss = tf.reduce_mean(tf.square(data_weights * (w_pred - y_true)))
            \#ic\_input = tf.convert\_to\_tensor([[0.0, y\_train[0], X\_train[0, 2]]], U
      \hookrightarrow dtype=tf.float32)
            ic_input = X[:, 0:1, :]
            ic_pred = model(ic_input)[:, -1, :]
            ic_true = tf.convert_to_tensor(y_train[0], dtype=tf.float32)
            ic_loss = tf.reduce_mean(tf.square(u_weights * (ic_pred - ic_true)))
            total_loss = data_loss + ode_loss + ic_loss
            return total_loss, ode_loss, data_loss, ic_loss
```

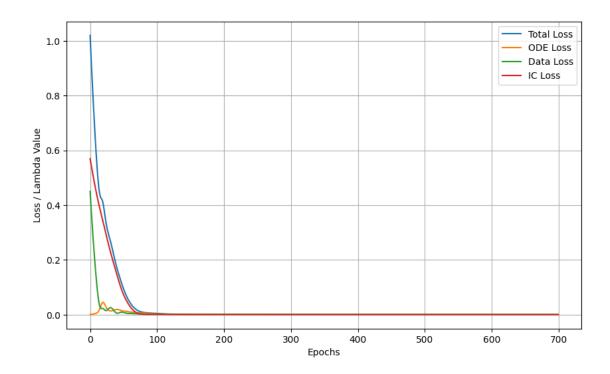
```
from tensorflow.keras.optimizers.schedules import ExponentialDecay
#earning_rate = tf.keras.optimizers.schedules.ExponentialDecay(
   #initial_learning_rate=1e-3
    #ecay_steps=10000 ,
   #ecay rate=0.75
learning_rate=1e-3
optimizer=tf.keras.optimizers.Adam(learning rate, clipnorm=1.0)
epochs=700
train_loss_record,ode_loss_record,data_loss_record,ic_loss_record=[],[],[],[]
for epoch in range(epochs):
   with tf.GradientTape(persistent=True) as tape:
        total_loss, ode_loss, data_loss, ic_loss = compute_loss(X_train_seq,_
 →y_train_seq
                                                , pinn_rnn, col_weights,_

    u_weights, data_weights)

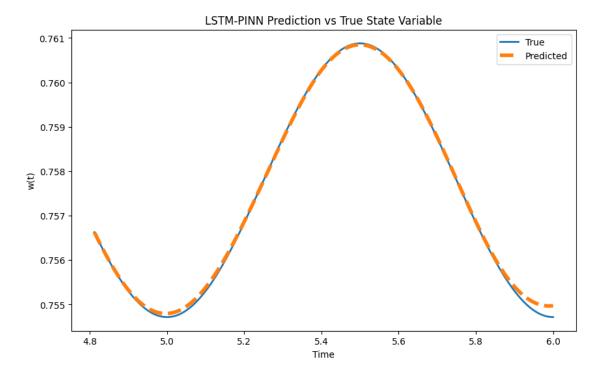
   grads = tape.gradient(total_loss, pinn_rnn.trainable_variables)
   grads_data = tape.gradient(data loss, pinn rnn.trainable_variables)
   grads_ode = tape.gradient(ode_loss, pinn_rnn.trainable_variables)
   grads_col = tape.gradient(ode_loss, col_weights)
   grads_data_weights = tape.gradient(data_loss, data_weights)
   optimizer.apply_gradients(zip(grads, pinn_rnn.trainable_variables))
   if grads col is not None:
        optimizer_col_weights.apply_gradients(zip([grads_col], [col_weights]))
   if grads_data_weights is not None:
        optimizer_data_weights.apply_gradients(zip([grads_data_weights],__
 train_loss_record.append(total_loss.numpy())
   ode loss record.append(ode loss.numpy())
   data_loss_record.append(data_loss.numpy())
    ic_loss_record.append(ic_loss.numpy())
```

```
if (epoch + 1) \% 100 == 0:
        print(f"Epoch {epoch+1}/{epochs} | "
              f"Total Loss: {train_loss_record[-1]:.6f} | "
              f"ODE Loss: {ode_loss_record[-1]:.6f} | "
              f"Data Loss: {data_loss_record[-1]:.6f} | "
              f"IC Loss: {ic_loss_record[-1]:.6f} | ")
# ----- Plot Adaptive Lambda Values -----
plt.figure(figsize=(10, 6))
plt.plot(train_loss_record, label='Total Loss')
plt.plot(ode_loss_record, label='ODE Loss')
plt.plot(data_loss_record, label='Data Loss')
plt.plot(ic_loss_record, label='IC Loss')
plt.xlabel("Epochs")
plt.ylabel("Loss / Lambda Value")
plt.legend()
plt.grid(True)
plt.show()
Epoch 100/700 | Total Loss: 0.004325 | ODE Loss: 0.002554 | Data Loss: 0.000665
| IC Loss: 0.001106 |
Epoch 200/700 | Total Loss: 0.000526 | ODE Loss: 0.000045 | Data Loss: 0.000055
| IC Loss: 0.000426 |
Epoch 300/700 | Total Loss: 0.000265 | ODE Loss: 0.000013 | Data Loss: 0.000020
| IC Loss: 0.000232 |
Epoch 400/700 | Total Loss: 0.000132 | ODE Loss: 0.000007 | Data Loss: 0.000009
| IC Loss: 0.000116 |
Epoch 500/700 | Total Loss: 0.000061 | ODE Loss: 0.000004 | Data Loss: 0.000005
| IC Loss: 0.000052 |
Epoch 600/700 | Total Loss: 0.000027 | ODE Loss: 0.000003 | Data Loss: 0.000003
| IC Loss: 0.000021 |
Epoch 700/700 | Total Loss: 0.000012 | ODE Loss: 0.000002 | Data Loss: 0.000002
```

| IC Loss: 0.000008 |



```
[6]: w_pred_seq = pinn_rnn.predict(X_test_seq)
    w_pred = w_pred_seq[:, -1, :]
    w_pred_original = scaler_y.inverse_transform(w_pred)
    y_test_original = scaler_y.inverse_transform(y_test_seq)
    t_test_plot = t_all[len(t_all) - len(w_pred_original):]
    # ----- Plotting -----
    plt.figure(figsize=(10, 6))
    plt.plot(t_test_plot, y_test_original, label='True', linewidth=2)
    plt.plot(t_test_plot, w_pred_original, label='Predicted', linestyle='--',
      →linewidth=4)
    plt.xlabel('Time')
    plt.ylabel('w(t)')
    plt.title('LSTM-PINN Prediction vs True State Variable')
    plt.savefig("testlstm.pdf")
    plt.legend()
    plt.show()
```

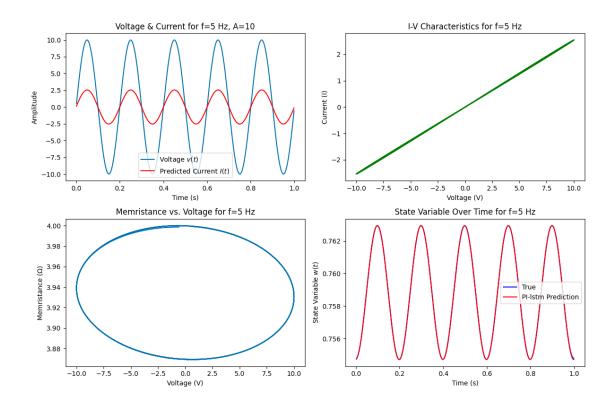


Model saved at: ./models/my\_pinn\_model.keras
 Model loaded successfully!

```
[9]: import numpy as np
    import matplotlib.pyplot as plt
    from scipy.integrate import solve_ivp
    from sklearn.preprocessing import StandardScaler, MinMaxScaler
    import tensorflow as tf
    # ----- Physical Parameters -----
    frequency = 5
    A train = 10
    W_train = 2 * np.pi * frequency
    mu v = 10**4
    D = 60
    r_on = 0.1
    r_off = 16
    r0 = 4
    w0 = (r0 - r_off) / (r_on - r_off)
    points_per_period = 600
    total_points = 10 * points_per_period
    # ----- ODE Solver -----
    def f(t, w, A, W, mu_v, D, r_on, r_off):
       k = mu_v * (r_on / D**2)
        f w = w * (1 - w)
        r = r_{on} * w + r_{off} * (1 - w)
        I = A * np.sin(W * t) / r
        return I * f_w * k
    t_all = np.linspace(0, 1, total_points)
    sol_all = solve_ivp(
        f, (0, 1), [w0], t_eval=t_all,
        args=(A_train, W_train, mu_v, D, r_on, r_off),
        method='RK45',
        max_step=0.001
    )
    # ----- Data Preparation -----
    w_all = sol_all.y[0]
    v_all = A_train * np.sin(W_train * t_all)
    r_all = r_on * w_all + r_off * (1 - w_all)
    I_all = v_all / r_all
    X_{all} = np.column_stack([t_all[:-1], w_all[:-1], I_all[:-1]])
    y_all = w_all[1:]
    # ----- Data Normalization -----
    X_all_scaled = X_all.copy()
```

```
scaler_time = StandardScaler()
X_all_scaled[:, 0] = scaler_time.fit_transform(X_all_scaled[:, 0].reshape(-1,_
 →1)).flatten()
scaler_features = MinMaxScaler(feature_range=(-1, 1))
X_all_scaled[:, 1:] = scaler_features.fit_transform(X_all_scaled[:, 1:])
scaler_y = MinMaxScaler(feature_range=(-1, 1))
y_all_scaled = scaler_y.fit_transform(y_all.reshape(-1, 1))
# ----- Create Sequences -----
sequence_length = 10
def create_sequences(X, y, sequence_length):
   X_seq, y_seq = [], []
   for i in range(len(X) - sequence_length):
       X_seq.append(X[i:i+sequence_length])
       y_seq.append(y[i+sequence_length])
   return np.array(X_seq), np.array(y_seq).reshape(-1, 1)
X_seq, y_seq = create_sequences(X_all_scaled, y_all_scaled, sequence_length)
# ----- PINN Prediction -----
w_pred_seq_new = pinn_rnn.predict(X_seq)
w_pred = w_pred_seq_new[:, -1, :]
w_pred_original_new = scaler_y.inverse_transform(w_pred)
y_all_rescaled = scaler_y.inverse_transform(y_seq)
t_test_plot = t_all[:len(w_pred_original_new)]
# ----- Compute Memristance and Current -----
r_M_pred = r_on * w_pred_original_new + r_off * (1.0 - w_pred_original_new)
print(f"Shape of v_all[:-1]: {v_all[:-1].shape}")
print(f"Shape of r_M_pred.flatten(): {r_M_pred.flatten().shape}")
min_length = min(len(v_all[:-1]), len(r_M_pred.flatten()))
v_all_adjusted = v_all[:min_length]
r_M_pred_adjusted = r_M_pred.flatten()[:min_length]
I_pred_new = v_all_adjusted / r_M_pred_adjusted
# ----- Data Trimming -----
t_trimmed = t_all[:min_length][sequence_length:]
v_trimmed = v_all[:min_length][sequence_length:]
I_trimmed = I_pred_new[sequence_length:]
w_trimmed = w_pred_original_new[:min_length][sequence_length:]
y_trimmed = y_all_rescaled[:min_length][sequence_length:]
```

```
# ----- Visualization -----
fig, axes = plt.subplots(2, 2, figsize=(12, 8))
# Voltage and Current vs. Time
axes[0, 0].plot(t_trimmed, v_trimmed, '#0072B2', label='Voltage $v(t)$')
axes[0, 0].plot(t_trimmed, I_trimmed, 'r', label='Predicted Current $I(t)$')
axes[0, 0].set_xlabel('Time (s)')
axes[0, 0].set ylabel('Amplitude')
axes[0, 0].set_title(f'Voltage & Current for f={frequency} Hz, A={A_train}')
axes[0, 0].legend()
# I-V Characteristics
axes[0, 1].plot(v_trimmed, I_trimmed, 'g-', label='PI-lstm Prediction')
axes[0, 1].set_xlabel('Voltage (V)')
axes[0, 1].set_ylabel('Current (I)')
axes[0, 1].set_title(f'I-V Characteristics for f={frequency} Hz')
# Memristance vs. Voltage
axes[1, 0].plot(v_trimmed, r_M_pred_adjusted[sequence_length:], '#0072B2')
axes[1, 0].set_xlabel('Voltage (V)')
axes[1, 0].set ylabel('Memristance (\Omega)')
axes[1, 0].set_title(f'Memristance vs. Voltage for f={frequency} Hz')
# State Variable w(t) Comparison
axes[1, 1].plot(t_trimmed, y_trimmed, label='True', color='blue')
axes[1, 1].plot(t_trimmed, w_trimmed, 'r', label='PI-lstm Prediction')
axes[1, 1].set_xlabel('Time (s)')
axes[1, 1].set_ylabel('State Variable $w(t)$')
axes[1, 1].set_title(f'State Variable Over Time for f={frequency} Hz')
axes[1, 1].legend()
plt.tight layout()
plt.savefig(f"piMemristor_Plots_square{frequency}Hz.pdf", format="pdf", __
 ⇔bbox inches="tight")
plt.show()
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                   Os 2ms/step
Shape of v_all[:-1]: (5999,)
Shape of r_M_pred.flatten(): (5989,)
```



```
[14]: import numpy as np
      import matplotlib.pyplot as plt
      from scipy.integrate import solve_ivp
      from sklearn.preprocessing import StandardScaler, MinMaxScaler
      import tensorflow as tf
      # ----- Physical Parameters ----
      frequency = 5
      A_{\text{train}} = 10
      W_train = 2 * np.pi * frequency
      mu v = 10**4
      D = 60
      r_on = 0.1
      r_off = 16
      r0 = 4
      w0 = (r0 - r_off) / (r_on - r_off)
      points_per_period = 600
      total_points = 10 * points_per_period
      # Voltage function
      def v(t):
```

```
return A_train* signal.square(W_train * t)
# ----- ODE Solver -----
def f(t, w, A, W, mu_v, D, r_on, r_off):
   k = mu_v * (r_on / D**2)
   f_w = w * (1 - w)
   r = r_on * w + r_off * (1 - w)
   I = v(t) / r
   return I * f_w * k
t_all = np.linspace(0, 1, total_points)
sol_all = solve_ivp(
   f, (0, 1), [w0], t_eval=t_all,
   args=(A_train, W_train, mu_v, D, r_on, r_off),
   method='RK45',
   max_step=0.001
)
# ----- Data Preparation -----
w_all = sol_all.y[0]
v_{all} = v(t_{all})
r_all = r_on * w_all + r_off * (1 - w_all)
I_all = v_all / r_all
X_{all} = np.column_stack([t_all[:-1], w_all[:-1], I_all[:-1]])
y_all = w_all[1:]
# ----- Data Normalization -----
X_all_scaled = X_all.copy()
scaler_time = StandardScaler()
X_all_scaled[:, 0] = scaler_time.fit_transform(X_all_scaled[:, 0].reshape(-1,_
→1)).flatten()
scaler features = MinMaxScaler(feature range=(-1, 1))
X_all_scaled[:, 1:] = scaler_features.fit_transform(X_all_scaled[:, 1:])
scaler_y = MinMaxScaler(feature_range=(-1, 1))
y_all_scaled = scaler_y.fit_transform(y_all.reshape(-1, 1))
# ----- Create Sequences -----
sequence_length = 10
def create_sequences(X, y, sequence_length):
   X_{seq}, y_{seq} = [], []
   for i in range(len(X) - sequence_length):
       X_seq.append(X[i:i+sequence_length])
       y_seq.append(y[i+sequence_length])
   return np.array(X_seq), np.array(y_seq).reshape(-1, 1)
```

```
X seq, y_seq = create sequences(X_all_scaled, y_all_scaled, sequence_length)
# ----- PINN Prediction -----
w_pred_seq_new = pinn_rnn.predict(X_seq)
w_pred = w_pred_seq_new[:, -1, :]
w_pred_original_new = scaler_y.inverse_transform(w_pred)
y_all_rescaled = scaler_y.inverse_transform(y_seq)
t_test_plot = t_all[:len(w_pred_original_new)]
# ----- Compute Memristance and Current -----
r_M_pred = r_on * w_pred_original_new + r_off * (1.0 - w_pred_original_new)
print(f"Shape of v_all[:-1]: {v_all[:-1].shape}")
print(f"Shape of r_M_pred.flatten(): {r_M_pred.flatten().shape}")
min_length = min(len(v_all[:-1]), len(r_M_pred.flatten()))
v_all_adjusted = v_all[:min_length]
r_M_pred_adjusted = r_M_pred.flatten()[:min_length]
I_pred_new = v_all_adjusted / r_M_pred_adjusted
# ----- Data Trimming -----
t_trimmed = t_all[:min_length][sequence_length:]
v trimmed = v all[:min length][sequence length:]
I_trimmed = I_pred_new[sequence_length:]
w_trimmed = w_pred_original_new[:min_length][sequence_length:]
y_trimmed = y_all_rescaled[:min_length][sequence_length:]
# ----- Visualization -----
fig, axes = plt.subplots(2, 2, figsize=(12, 8))
# Voltage and Current vs. Time
axes[0, 0].plot(t_trimmed, v_trimmed, '#0072B2', label='Voltage $v(t)$')
axes[0, 0].plot(t_trimmed, I_trimmed, 'r', label='Predicted Current $I(t)$')
axes[0, 0].set_xlabel('Time (s)')
axes[0, 0].set_ylabel('Amplitude')
axes[0, 0].set title(f'Voltage & Current for f={frequency} Hz, A={A train}')
axes[0, 0].legend()
# I-V Characteristics
axes[0, 1].plot(v_trimmed, I_trimmed, 'g-', label='PI-lstm Prediction')
axes[0, 1].set_xlabel('Voltage (V)')
axes[0, 1].set_ylabel('Current (I)')
axes[0, 1].set_title(f'I-V Characteristics for f={frequency} Hz')
```

```
# Memristance vs. Voltage
axes[1, 0].plot(v_trimmed, r_M_pred_adjusted[sequence_length:], '#0072B2')
axes[1, 0].set_xlabel('Voltage (V)')
axes[1, 0].set_ylabel('Memristance (\Omega)')
axes[1, 0].set_title(f'Memristance vs. Voltage for f={frequency} Hz')
# State Variable w(t) Comparison
axes[1, 1].plot(t_trimmed, y_trimmed, label='True', color='blue')
axes[1, 1].plot(t_trimmed, w_trimmed, 'r', label='PI-lstm Prediction')
axes[1, 1].set xlabel('Time (s)')
axes[1, 1].set_ylabel('State Variable $w(t)$')
axes[1, 1].set_title(f'State Variable Over Time for f={frequency} Hz')
axes[1, 1].legend()
plt.tight_layout()
plt.savefig(f"piMemristor_Plots_square{frequency}Hz.pdf", format="pdf", 
 ⇔bbox_inches="tight")
plt.show()
```

