Accelerated Fitting of Band-Excitation Piezoresponse Force Microscopy

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Background

- Atomic Force Microscope measures the piezoresponse of material during ferroelectric switching.
- Generates hyperspectral dataset [60 (x), 60 (y), 96 (voltage), 4 (cycles), 64 (frequencies)].
- Hard to turn data into actionable information on the microscope.

Motivation

- Simple Harmonic Oscillation (SHO) and Piezoelectric Loop Fitting takes around 6-8 hours (that is too slow) for single experiment, in addition, to being computationally inefficient.
- Goal: accelerate the SHO and loop fitting processes by developing pre-trained deep recurrent neural networks with a fully unsupervised approach in the form of an autoencoder which is able to learn a sparse and thus interpretable latent space of piezoelectric loops.

Model Architecture and Algorithm

1st Order Method (Adam):
- Uses 1st order derivative
- Gradient descent is used to update weights of DNN and reach to global minimum
- Most popular optimizer, but did not work for this problem

2nd Order Methods (Trust-Region CG and AdaHessian)
- Uses 2nd order derivative
- Worked well for both fitting types

Model Architecture:

- PyTorch
- TensorFlow
- Keras

Optimization Methods


Results

After 5 minutes of training:
- Total MSE for SHO fitting = 0.1118
- Total MSE for loops fitting = 0.0265

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References


Summary

- Possibility of real-time analysis of BEPS
- Improved experimental efficiency (5 minutes to train; previous method - 6 hours)
- Extraction of larger amount of information from experiments
- Applications in other spectroscopic imaging techniques