Accelerated Fitting of Band-Excitation Piezoresponse Force Microscopy

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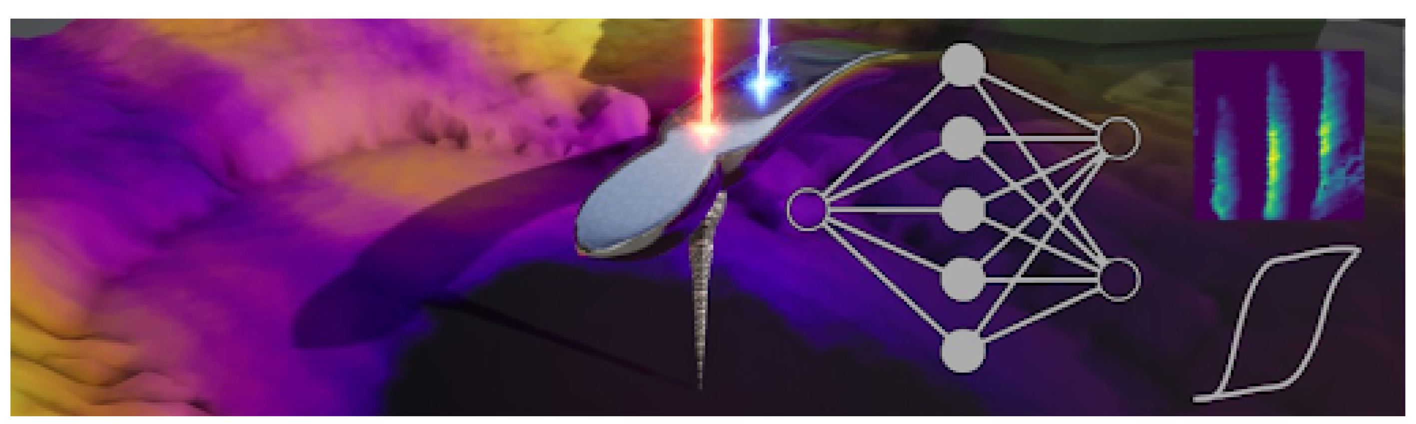
Background

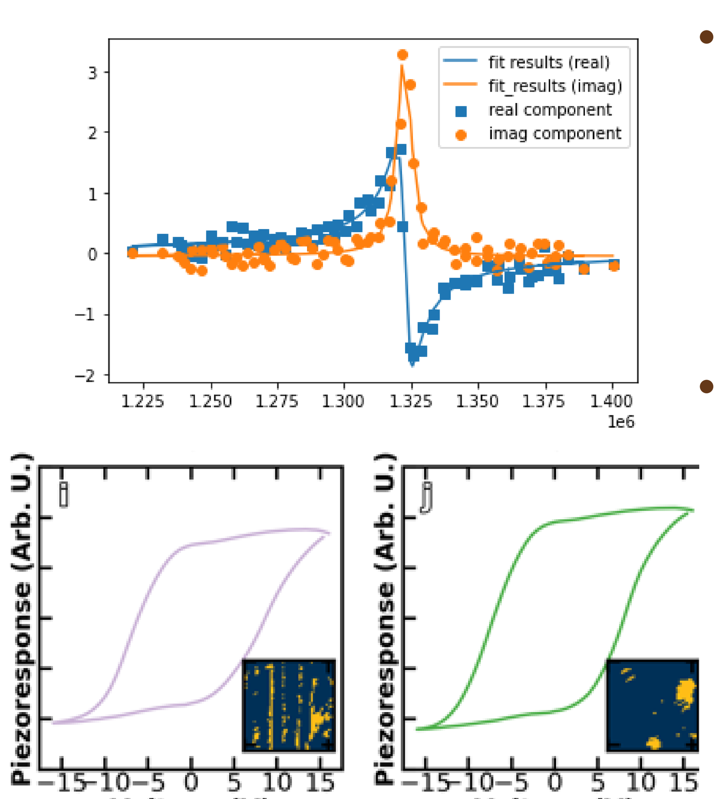
- Atomic Force Microscope measures the piezoresponse of material during ferroelectric switching.
- Generates hyperspectral dataset [60 (x), 60 (y), 96 (voltage), 4 (cycles), 64 (frequencies)].
- Hard to turn data into actionable information on the microscope.



(Agar et al., 2019)

- Following fitting, the raw data from this experiment at every pixel (x,y size = 60, 60) measures the <u>amplitude (A), phase (ϕ), resonance frequency (ω), and quality factor (Q)</u> of the cantilever resonance.

Motivation



(Agar et al., 2019)

- Simple Harmonic Oscillation (SHO) and Piezoelectic Loop Fitting takes around <u>6-8 hours (that is too slow)</u> for single experiment, in addition, to being <u>computationally inneficient</u>.
- *<u>Goal</u>: accelerate the SHO and loop fitting processes by developing pre-trained deep reccurent 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.*

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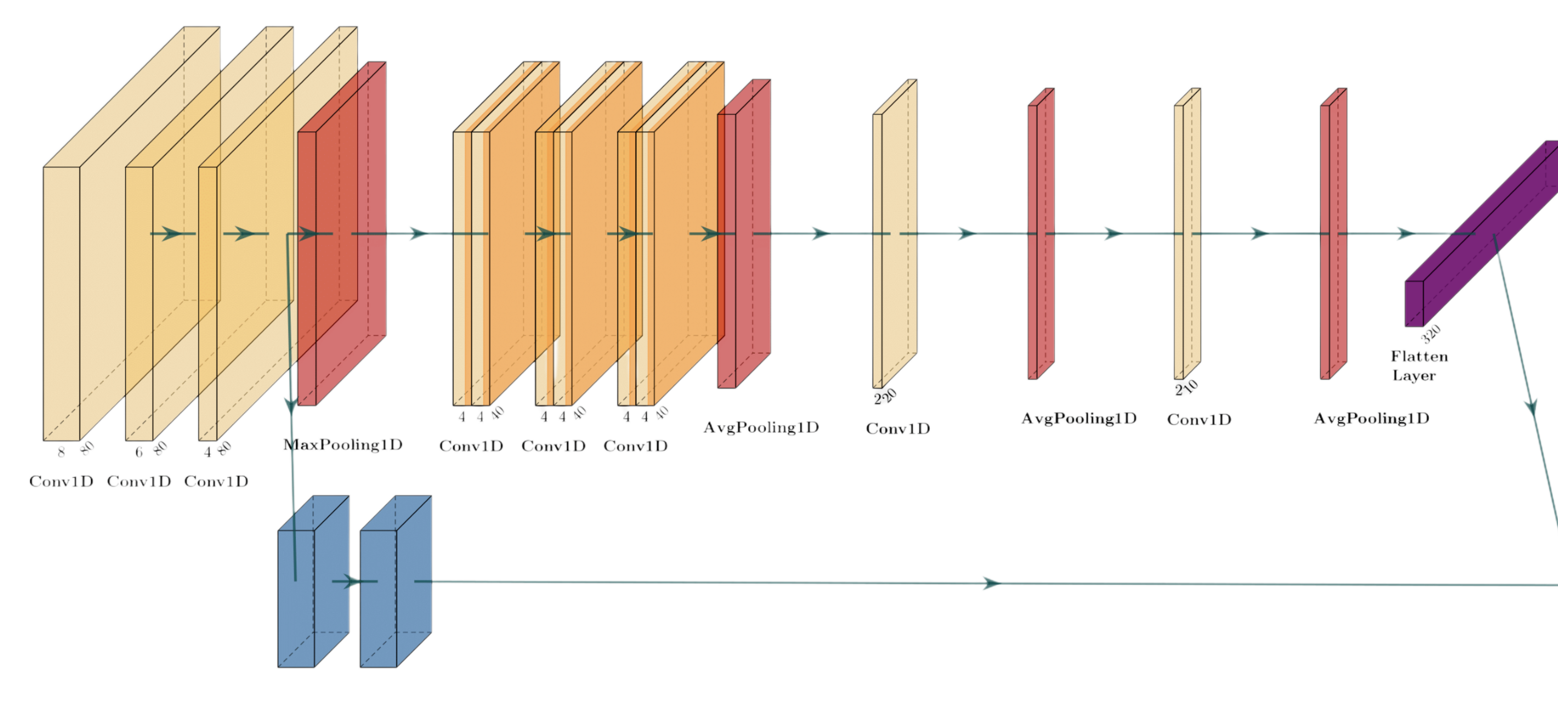
Model Architecture and Algorithm



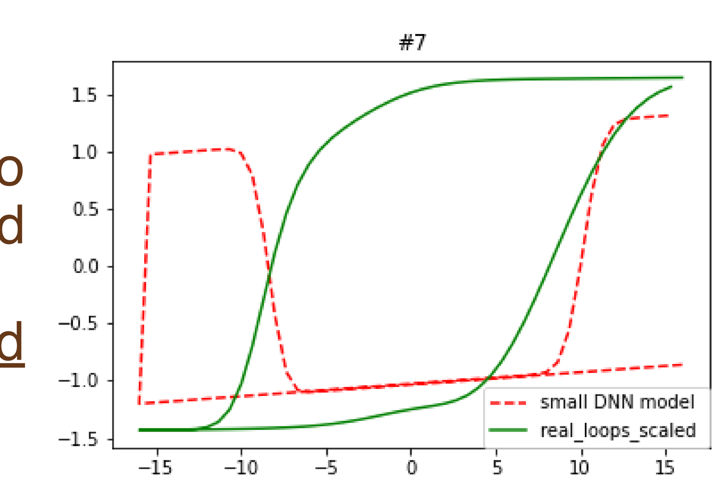
PyTorch
TensorFlow + Keras

1.
$$f(A, w_0, Q, \phi) = \frac{A*i\phi*w_0*Q}{Q*w_{vec}^2 - iw_{vec}*w_0 - Q*w_0^2}$$

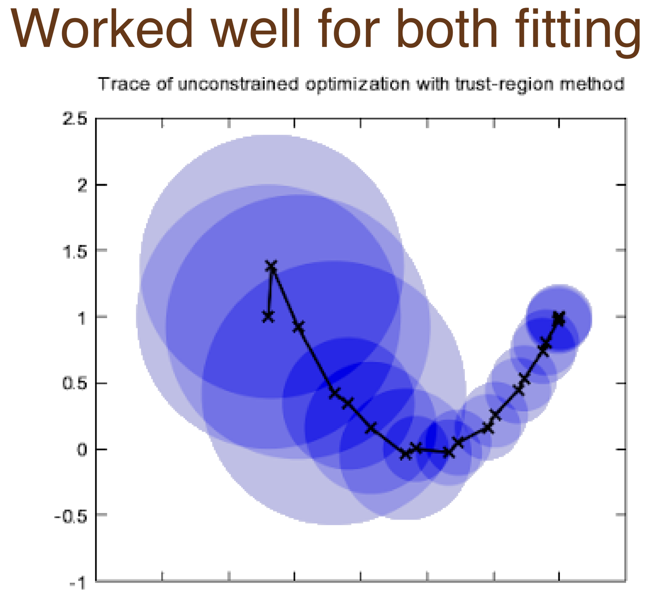
2.
$$\sigma_1 = \frac{b_1+b_2}{2} + \frac{b_2-b_1}{2} + erf\left(\frac{V-b_7}{b_5}\right)$$
$$\sigma_1 = \frac{b_4+b_3}{2} + \frac{b_3-b_4}{2} + erf\left(\frac{V-b_8}{b_6}\right)$$
$$\Gamma_1 = \frac{a_1+a_2}{2} + \frac{a_2-a_1}{2} + erf\left(\frac{V-A_u}{\sigma_1}\right) + a_3V$$
$$\Gamma_2 = \frac{a_4+a_3}{2} + \frac{a_3-a_4}{2} + erf\left(\frac{V-A_l}{\sigma_2}\right) + a_3V$$

Optimization Methods

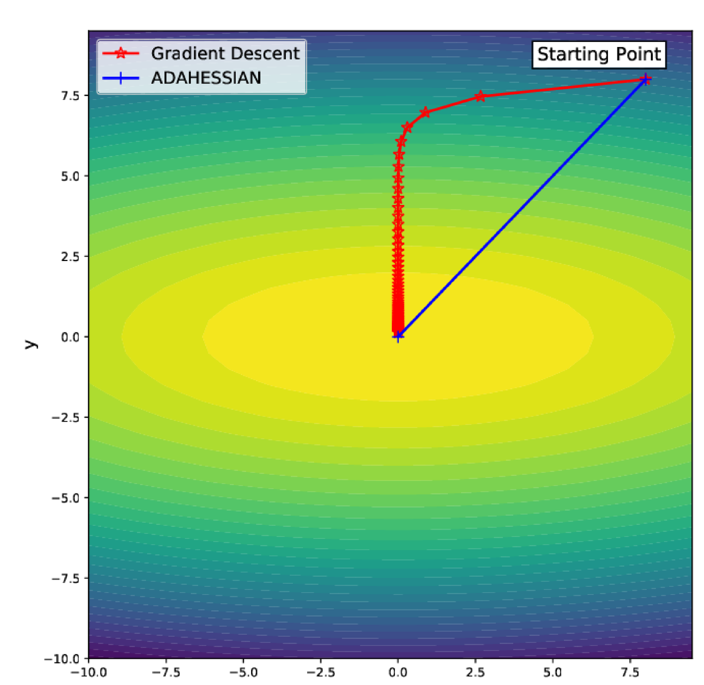
<u>1st Order Method (Adam):</u>
- Uses 1st order derivative
- Gradient descent is used to update weights of DNN and reach to global minimum
- Most popular optimizer, <u>but did not work for this problem</u>



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

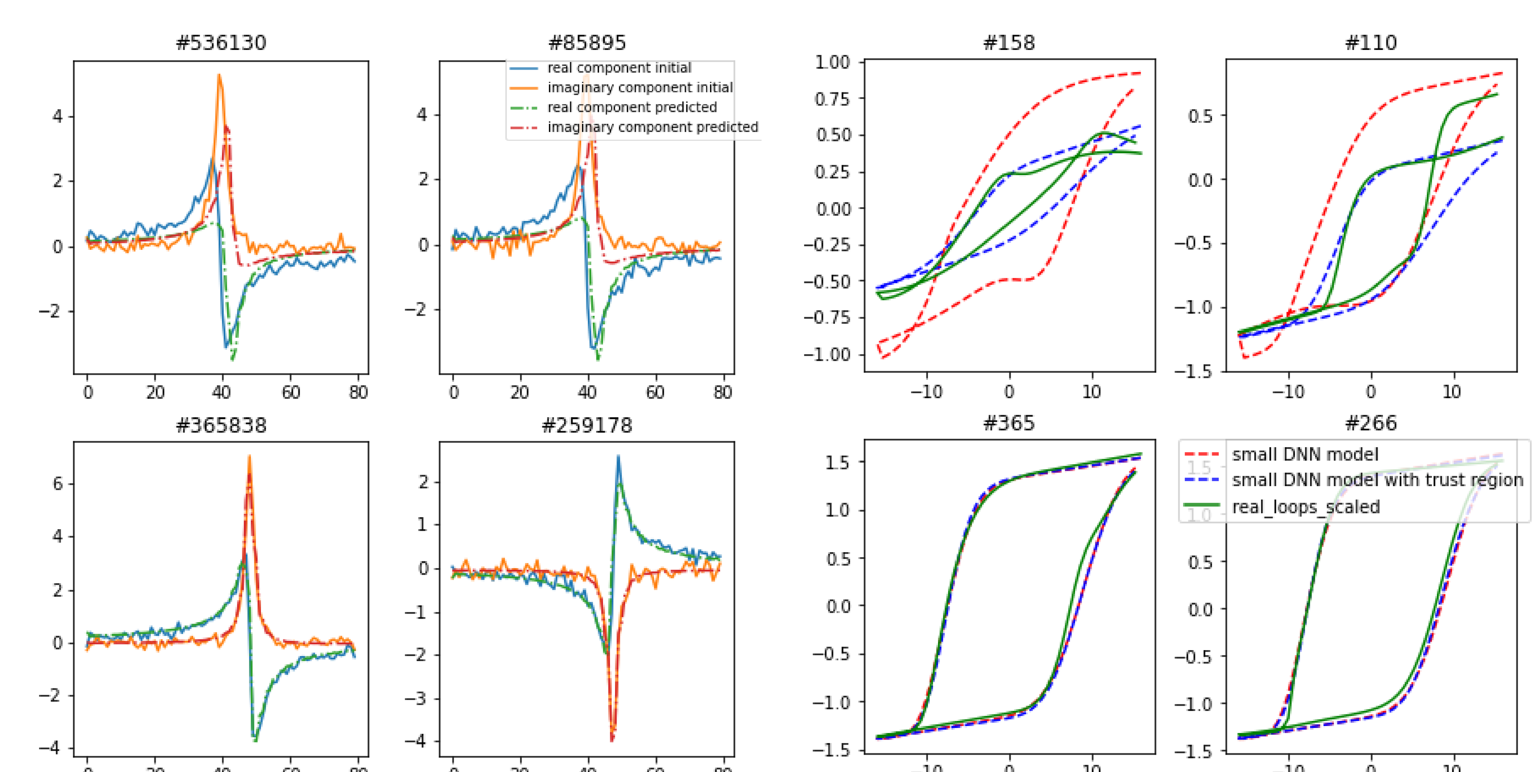


(Ye, 2014)

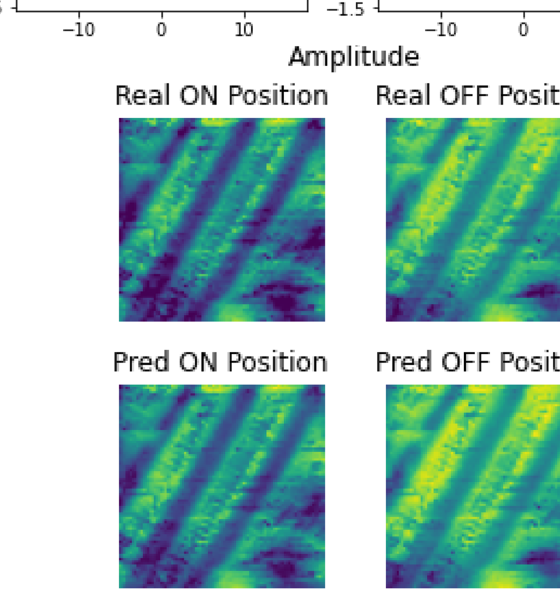


(Yao et al., 2020)

Results



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



References

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2. Ye, W. (2014). Trust-region methods. Retrieved October 23, 2020, from https://optimization.mccormick.northwestern.edu/index.php/Trust-region_methods
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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