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Rapid Fitting of Band-Excitation Piezoresponse Force Microscopy Using Physics Constrained Unsupervised Neural Networks

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Imaging nanoscale dynamics and response in materials requires imaging techniques with high spatial and temporal resolution. To meet this need, various scanning-probe spectroscopic imaging modes have emerged to understand electrochemical and ionic mobility and dynamics, ferroelectric switching dynamics, and dynamics mechanical responses of materials under external perturbations. These techniques collect large, high-dimensional data that is difficult and time-consuming to analyze. Practically, most analysis happens long after the experiments have been completed. This hinders researchers'abilities to use real-time feedback to conduct experiments on sensitive samples with a creative inquiry.

Machine learning techniques like principle component analysis (PCA), linear and non-linear clustering and non-negative matrix factorization have accelerated analysis. However, these techniques are computationally inefficient, highly dependent on prior estimates, and unable to interpret some complex features physically.

We developed a fully unsupervised deep neural network (DNN) that can be constrained to a known empirical governing equation. This is achieved by training an encoder to predict the model parameters, which are decoded by the underlying empirical expression. As long as the empirical expression is differentiable, it can be trained using stochastic gradient descent.

We evaluate this concept on a benchmark band-excitation piezoresponse force microscopy (BE-PFM) to predict amplitude, phase, cantilever resonance frequency, and dissipation from a simple harmonic oscillator (SHO) model. To extract further insights from piezoelectric hysteresis loops, which were calculated from fit results, it is common to fit the loops to a 9-parameter empirical function that extracts parameters related to the shape of the loop.

We demonstrated several important breakthroughs:

1. Speed –we can train our model to conduct 1.38 million SHO fits in less than 5 minutes and can conduct inference in <3 seconds with a batch size of 1024 on free computing resources (PCIe P100 on Google Colab);
2. Robustness –We demonstrate that SHO and hysteresis loop fit results have narrower and more physically reasonable distributions than least-square fitting (LSQF) results;
3. Signal-to-noise ratio –Our model performs well and provides physically interpretable results on artificially noisy data where well-designed conventional LSQF pipelines fail;
4. Real-time –We conduct quantized-aware training to deploy this model on an FPGA. Simulations predict streaming inference at <50 μs, orders of magnitude faster than the data acquisition and sufficiently fast for real-time control of automated experiments.

This work provides an automated methodology to develop physics-conforming, robust, fast approximation of noisy data with real-time (sub-ms) streaming inference. We demonstrate the efficacy of this methodology on a benchmark BE-PFM dataset. However, the approach broadly applies to spectroscopic fitting when the empirical expression is known. This approach provides a pathway for real-time interpretation and controls from high-velocity data sources ubiquitous in experimental science.

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