

Hybrid Machine Learning to Classify STM Tip States

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Scanning tunneling microscopy (STM) is the premier technique for atomic-scale imaging. By raster scanning a surface with an atomically sharp tip, an image topography can be deduced via the amount of tunneling current induced by quantum tunneling electrons. A serious drawback is the maintenance of the tip itself. The state that it is in can be inferred only by the images taken, a process that is not only time consuming, but also unreliable.

A solution to the problem of classifying these STM tip states is to train a neural network on years of already-collected data. Once trained, the programme aims to identify the tip state of the STM based on the image and spectroscopy data.

Given the constraints of what would be an unreliable and time-consuming labeling process, the script uses hybrid learning, incorporating large sets of unlabeled training data and smaller sets of labeled data. This allows the network to learn invariance to physically irrelevant information, while also learning what the expected classes of data are to look like.

Aims and Methods

The aim of this project was to construct the best learning algorithm to classify a broad selection of STM data of Si(111)-7x7 (image crops, adatom images and spectroscopy data) into groupings based on the tip state. This amounts to training the learner to ignore details that do not depend on the tip state.

To address this requires the learner to have access to a large set of varied image data, else features that are not relevant for tip state identification may be used to falsely classify the image. On the other hand, the process of labeling such a large set of images is not only impractical, but there is often disagreement even amongst experts as to the particular tip state used for a given image.

The first means by which the data were clustered was a simple t-stochastic neighbour embedding (t-SNE). This crude technique demonstrated the extent to which the layers to be added must be specifically tailored to this specific form of image. The approach was

then refined by the addition of a ResNet-50 neural network trained on ImageNet that places like STM images close together in feature space, and unlike ones apart. This was heavily influenced by irrelevant image features, prompting the use of a contrastive loss. This loss trains the learner to recognise an image and a transformed one as belonging to the same class, aiding in learning to ignore unimportant image features. A supervised contrastive layer was then added to finetune the learner and give it deliberately curated images from which to build its classes from. The learner was then made multi-modal, incorporating both adatom and spectroscopy data in its feature vectors.

Results

The results demonstrated that the process of classifying STM tip states is a more involved procedure than many other image classification problems in machine learning. While more qualitative good/bad tip classification has been

achieved by convolutional neural networks, the process of identifying the specific configuration of the tip has eluded the standard methods of image classification by machine learning.

The final model of the learner consisted of two layers: an unsupervised blind image quality assessment (BIQA) contrastive learning network, trained on ImageNet, that takes in a large dataset of unlabelled STM image and spectroscopy data to build the backbone; and a supervised contrastive (SupCon) classifier script for fine-tuning of the network's weights and header. The high-dimensional feature space of the data is then visualised using t-SNE and examined to review the performance of the network.

The multi-modal approach of including both two types of image data (square image crops and adatom images) and spectroscopy data provided the learner with as much tip

state-dependent information as possible, while the hybrid aspect allows for a much smaller labeled dataset to be used.

Experience

The opportunity to partake in this research has

been indispensable when considering my future prospects. Not only have I gained strong proficiency in machine learning and the experimental methods of STM, I feel as though no other avenue could give me so much experience as part of a research team. The nature of scientific collaboration, and how my role as an individual integrates into it, has been at the forefront of my time during this project. This has been invaluable to me, as someone looking to undergo a PhD in the future, as I feel much more confident within the research environment. My skill in communicating, presenting and explaining concepts and new ideas has increased significantly. I am now very comfortable discussing papers, presenting my work, and proposing new approaches. The on-the-go learning necessary to undertake serious research has also been extremely engaging, not just because the subject matter concerns the latest research, but also that it was inherently tied to my own immediate research objectives, with new ideas put into practice at a stimulating pace. Prior to research for this project, I was unaware of the current limitations of STM; being a part of improving such vital technology has been a fascinating experience, and I eagerly await engagement in future research.

