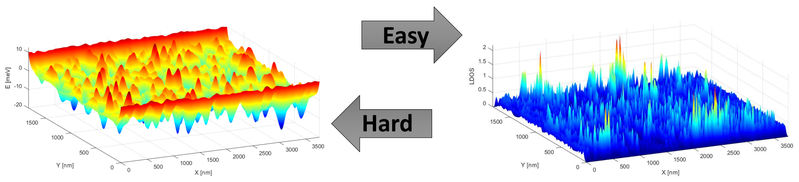
MACHINE LEARNING FOR DISORDERED 2D ELECTRON SYSTEMS

Dominic Bernardi, An Vuong, Diego Lopez, Michael Hilke

Center of the Physics of Materials, Department of Physics, McGill University, Montreal, Quebec, Canada

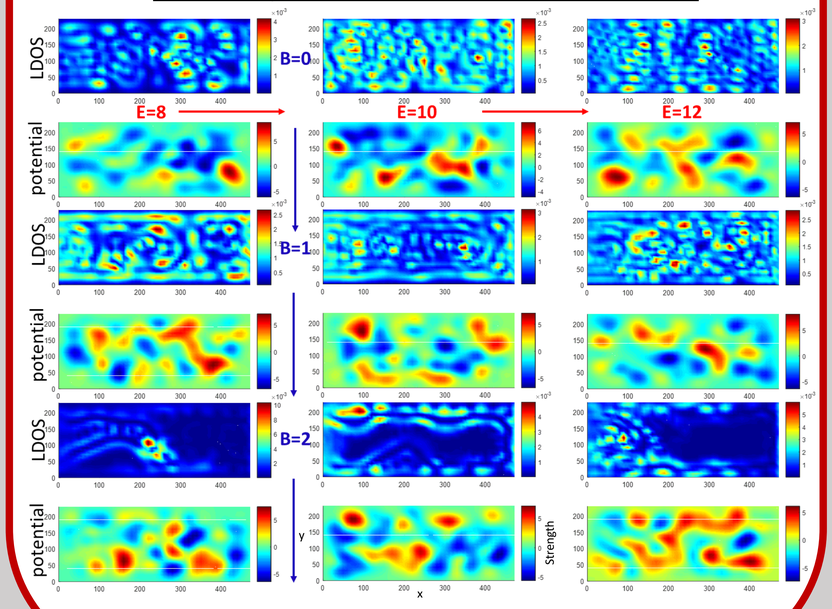
LOCAL DENSITY OF STATES

Disorder Potential *LDOS*



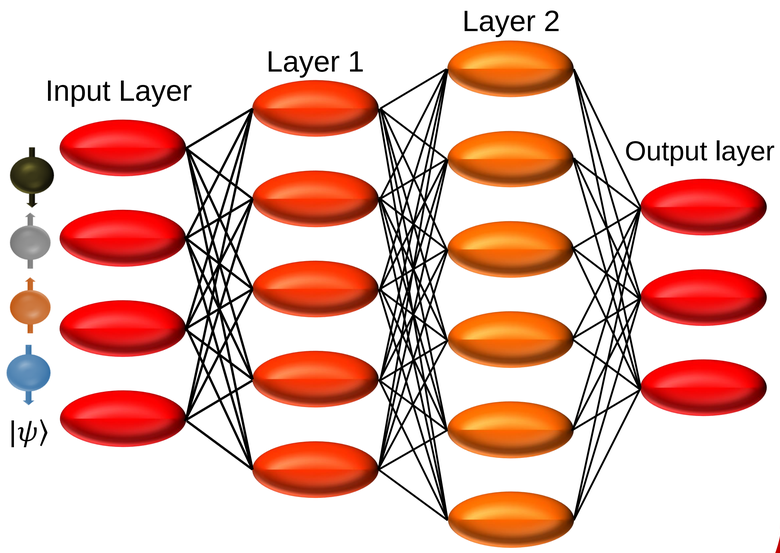
$$LDOS_E(r) = \sum_i |\psi_i|^2 \, \delta(E - E_i) = Im\{G_E(r, r')\}$$

LDOS Dependence on Different Variables



MACHINE LEARNING

QC	Quantum data – classical machine
CQ	Classical data – quantum machine
QQ	Quantum data – quantum machine

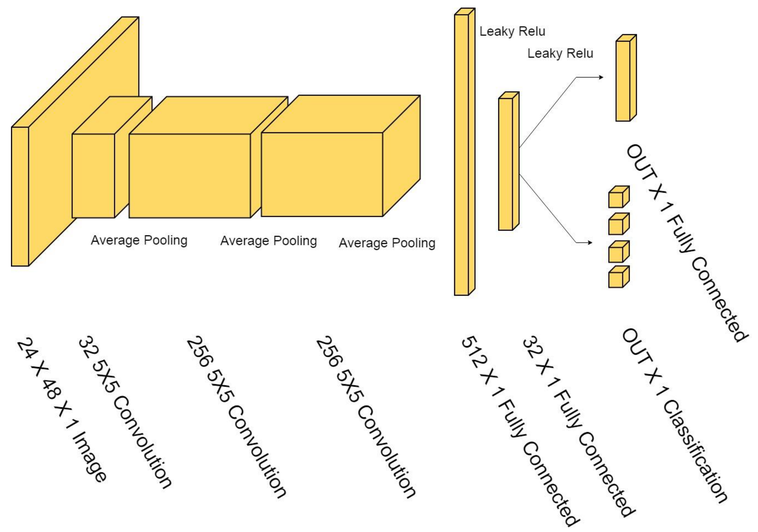


Quantum Data – Classical Machine

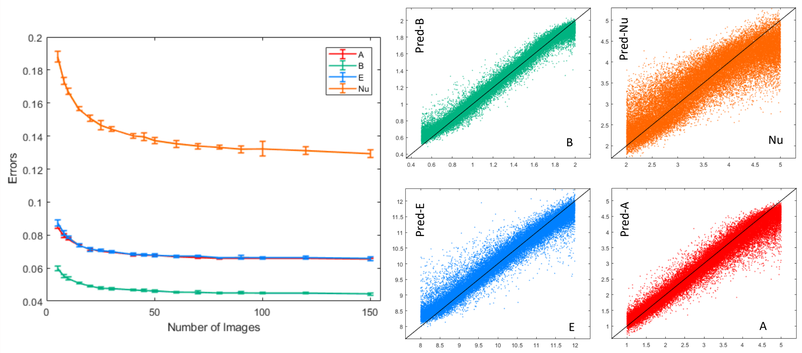
ABSTRACT

We present a novel approach for computing the disorder potential properties in a 2-dimensional disordered electron system from the directly measurable quantity of local density of states (LDOS). In this approach, we apply a convolution neural network to an LDOS input map and train it to predict several continuous variables, such as the disorder strength, the Fermi energy, the magnetic field, the potential correlation length, and the impurity shape. The training set was generated by producing random potential maps with random values of these parameters, from which the LDOS maps were calculated via an iterative Green's function method. We show results obtained with a neural network trained on 50,000 samples which is able to predict the correct potential properties with a relative error as low as 3% on some of the parameters. The results show that convolution neural networks can be a viable method of predicting the potential properties from the LDOS in disordered conductors, but also raises the prospect that such techniques can be applied to a wide variety of complex problems in quantum mechanics.

NETWORKS

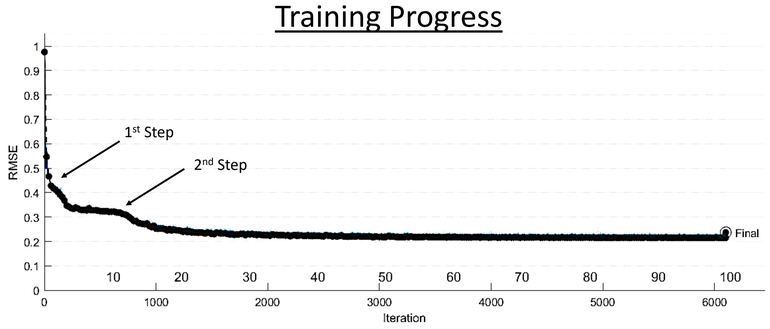


Regression Performance



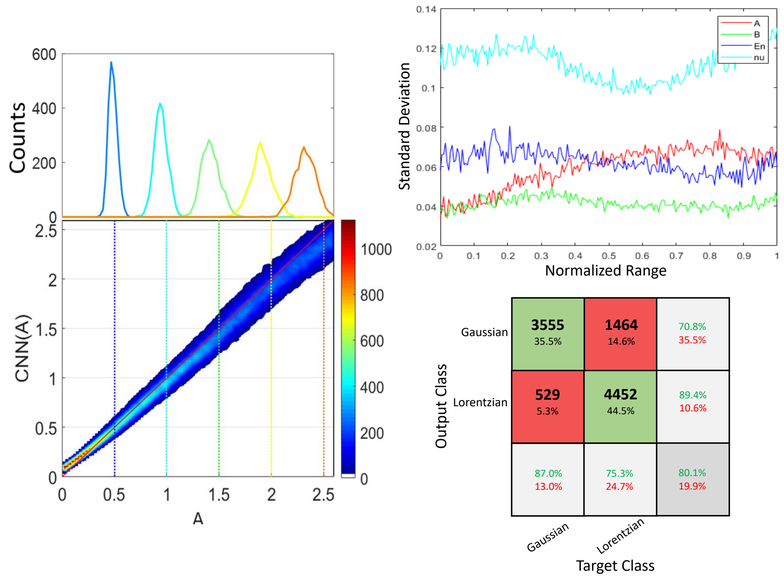
LEFT: Plot of the errors of disorder strength (A), magnetic field (B), the Fermi energy (E), and the potential correlation length (Nu) versus the number of images used in training a regression network. RIGHT: Plots of the true value versus prediction from the trained regression network of the individual variables (A, B, E, and Nu) trained on 50,000 images. The dots correspond to the prediction, whereas the black line corresponds to the real values. The color of the plot on the right corresponds to the variable of the same color on the left plot. The errors are 0.065, 0.045, 0.066, and 0.131 for A, B, E and Nu, respectively.

Training Progress



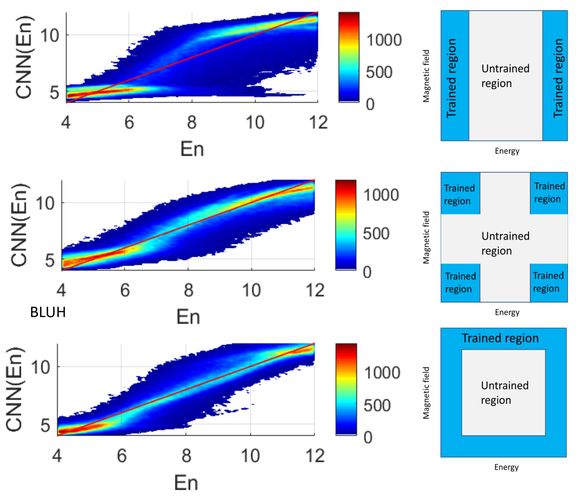
Plot of root mean squared error versus number of iterations when training a regression network with 50,000 different images generated by varying the four variables shown above. The black dots covering the training progress show the validation confirming the accuracy of the network. Because the error is a sum of the individual errors of the four variables, the RMSE has two significant drops where the network begins to learn the less dominant features. If the training progress is stopped before the first step, only B has been learned. Similarly, stopping before the second step shows random predictions for only Nu. This behavior mirrors the different learnabilities shown in the previous figures.

RESULTS



LEFT: Plot of the true value versus prediction from the trained regression network of amplitude (A). Color chart indicates the total number of counts in a region. Cross-sections of some regions are shown above. TOP RIGHT: Plot of the standard deviation between the true value and prediction from the same network on the left on amplitude (A), magnetic field (B), energy (E) and shape factor (nu) in a normalized range. BOTTOM RIGHT: Confusion matrix of a trained classification network on classifying the shape of impurity introduced in the data.

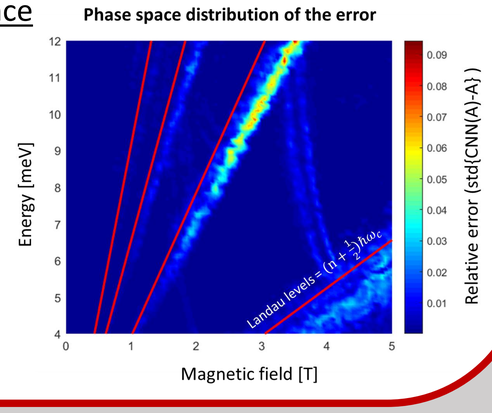
Interpolation



Training a regression network on data limited to certain regions changes the quality of the predictions. Restricting which values of energy and magnetic field the network is trained on has significant effects on the networks predictive capabilities. The three graphs show the correct values of energy plotted against the values predicted by the regression network. All were trained with 36% of the total energy/magnetic field phase space covered in different patterns. The top and middle do not expose the network to every possible value of energy at any point. The bottom trains on every value of energy but only for high and low magnetic field.

Physical Significance

The relative error of the Convolution Neural Network prediction on amplitude is found to depend on energy and magnetic field. The error follows a pattern, which can be ascribed to Landau levels. Here, the prediction error is maximum close to Landau levels because of the corresponding change in filling factor.



Conclusion

Using regression networks proves to be an effective way to predict the disorder potential properties from the local density of states. Although classification networks are used more frequently for problems related to image recognition, the regression networks' ability to simultaneously learn several different variables that define the disorder potential make it significantly more useful. The number of categories that can be learned via classification network is limited by the size of the network. With multiple variables being learned, the total number of categories increases quickly and renders classification useless. Moreover, regression networks are able to predict the relationship between the disorder potential and the local density of states in regions on which it was not trained. This feature is not observed when using classification networks, making it unfavorable for the purpose of our study.

Along with the accurate predictive capability of regression networks, studying the accuracy as a function of different parameters reveals a physical correlation to the learnability within the problem. Even though the connection between a property's physical meaning and the network's learnability of said property is unclear, some behaviors attributed to physically significant phenomena such as Landau levels were observed. This shows that regression networks could potentially guide research along with solving the complicated problems for which they were trained.