Machine Learning in Theoretical Condensed Matter Physics

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Machine Learning Overview

Supervised learning

Train network with large amount of **labelled data** (input-output pairs): Reduce **cost function** (distance measure between network output and labels) via gradient descent.

Verify network performance on distinct test data.

Unsupervised learning

Use unlabelled data, network learns to cluster data/find structure/learn probability distribution of features

Holy grail of the field

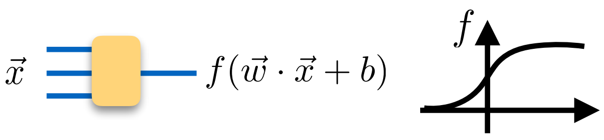
So far, we have focussed on supervised techniques, but are currently also exploring unsupervised methods.

Artificial Neural Networks

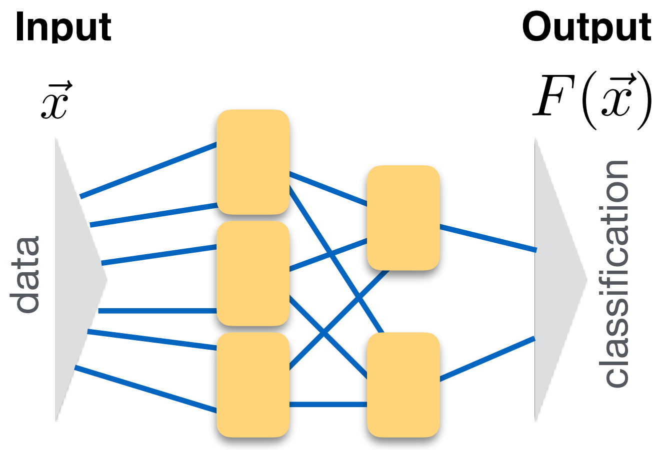
goal: learn complicated function $\hat{F}(\vec{x})$ with $\dim(\vec{x}) \gg 1$ from examples by finding

$$\min_F \mathrm{Error}[F, \hat{F}]$$

Individual neuron: combination of linear map (weights + biases) and nonlinear activation function



Deep network: many layers of neurons



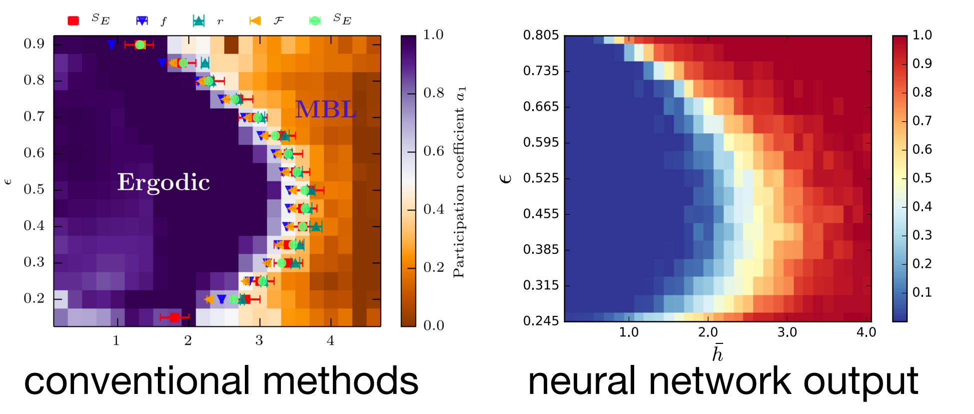
Condensed Matter Applications

Phase Classification

Idea: train with quantities pertaining to known phases of matter and apply network to classify quantities from unknown phases

$$\mathrm{Error}[F,\hat{F}] = -\sum_{\vec{x}\in\mathrm{TD}}\sum_{i=1}^{2}\hat{F}_i(\vec{x})\log F_i(\vec{x}) + \mu\sum_{\vec{w}}|\vec{w}|^2 - \delta\sum_{\vec{x}\in\mathrm{TR}}\sum_{i=1}^{2}F_i(\vec{x})\log F_i(\vec{x})$$

Phase diagram of a discordered spin-chain exhibiting many-body localization (MBL):



see also: **Physical Review B 95, 245134 (2017)**

Quantum State Compression

Goal: Learn a quantum wave function

Ψ_i, with $i = 1 \ldots N$

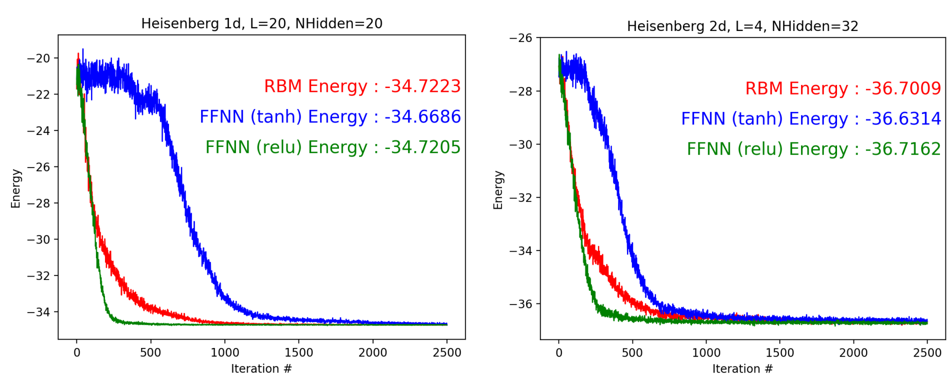
where N is exponentially large in the system size,

using a network with

$n \ll N$ free parameters

Ansatz: $\ln(\Psi)(\vec{\sigma}) = W^{(2)} A\left(W^{(1)}\vec{\sigma} + \vec{b}\right)$

$\text{e.g. } A(x) = \tanh(x) \text{ or } ReLu(x)$



see: **Carleo et. al. Science 355 (6325), 602-606**