Machine Learning Many-Body Models

ML4MS

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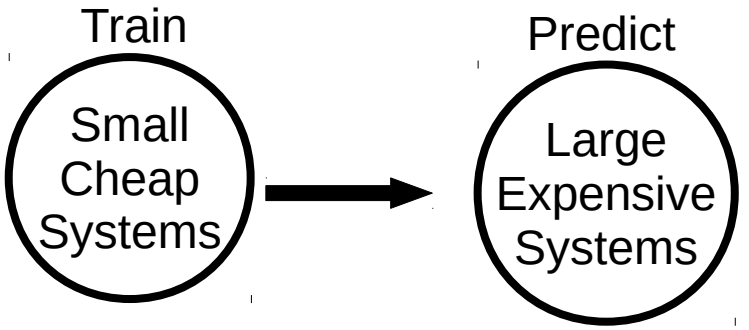
Motivation

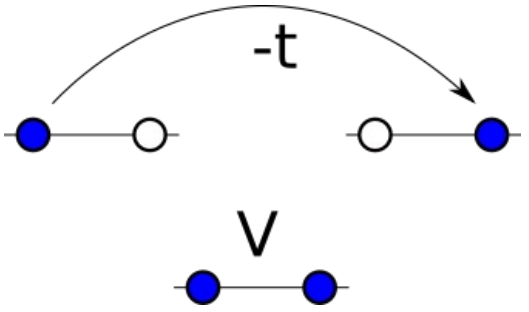
- Lattice Models used to study strongly correlated electrons
  - Systems with F electrons
  - Mott transition
- Number of configurations increases exponentially with the number of particles & sites
  - Exact Diagonalization unfeasible for large systems

Goal

- Predict finite temperature properties
  - By training on small systems
- Method is general for any lattice model
- As an example we use the 1-D Spinless Hubbard Model



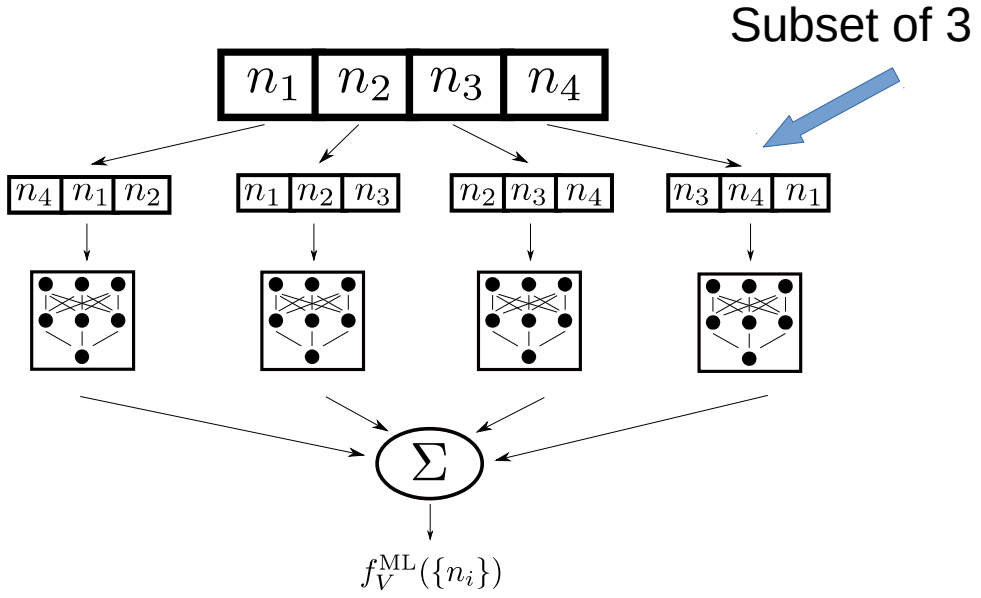
$$\hat{H} = -t \sum_{i=1}^{L} (\hat{c}_i^\dagger \hat{c}_{i+1} + \text{h.c.}) + V \sum_{i=1}^{L} \hat{n}_i \hat{n}_{i+1} + \sum_{i=1}^{L} \epsilon_i \hat{n}_i$$



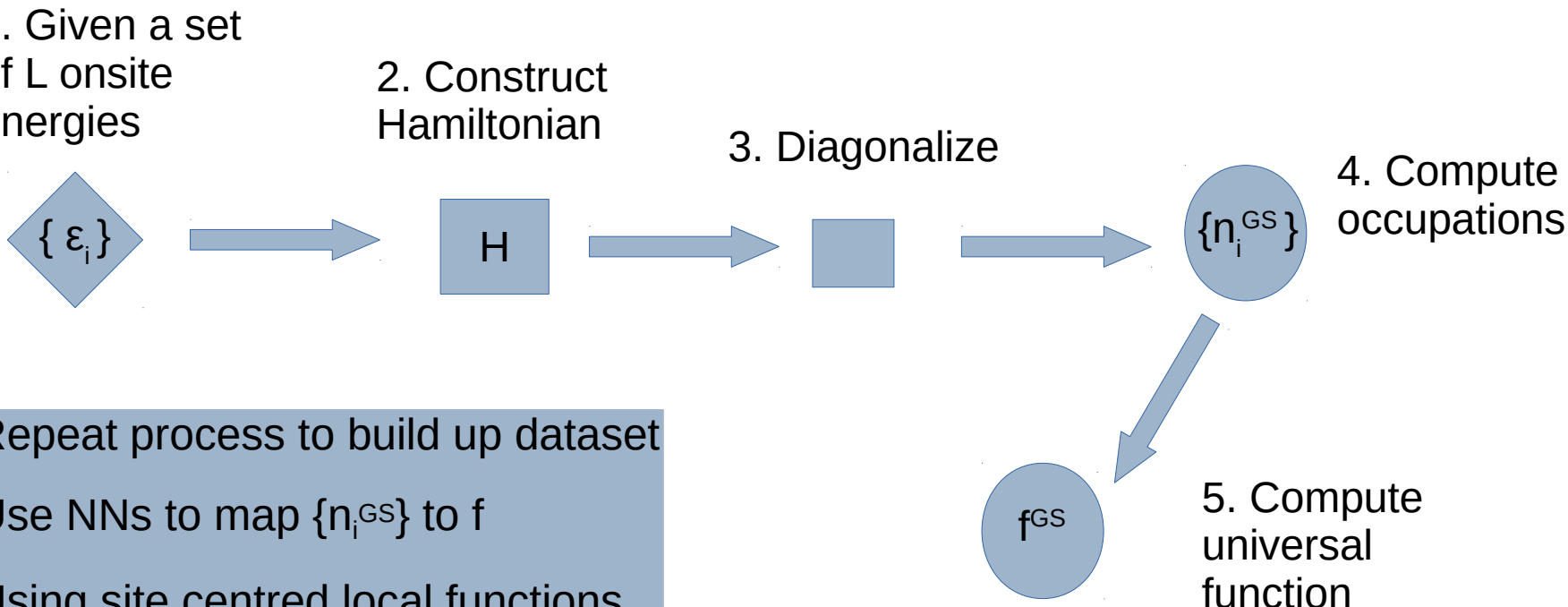
Representation

- HK Theorem – Lattice DFT
- Write F as a sum of site centred local functions
- Size of local subset is a hyperparameter
- We use neural networks – universal approximator

$$E = F(\{n_i\}) + \sum_{i=1}^{L} n_i \epsilon_i$$



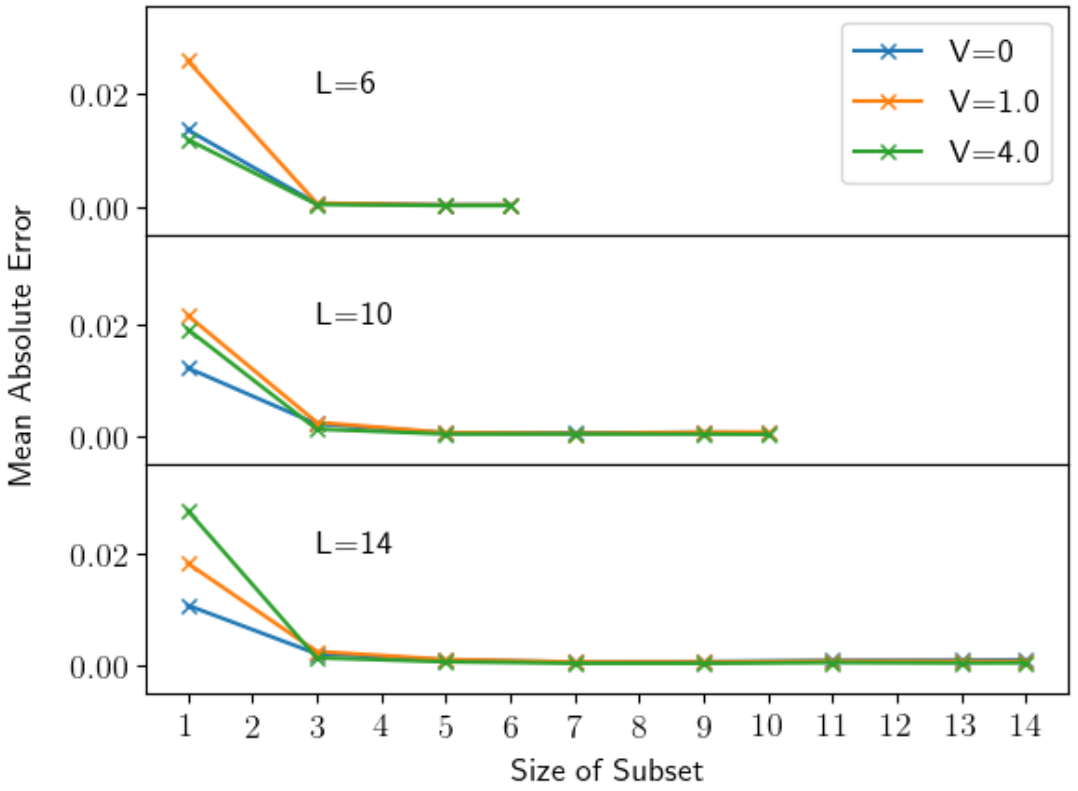
Generating the Dataset

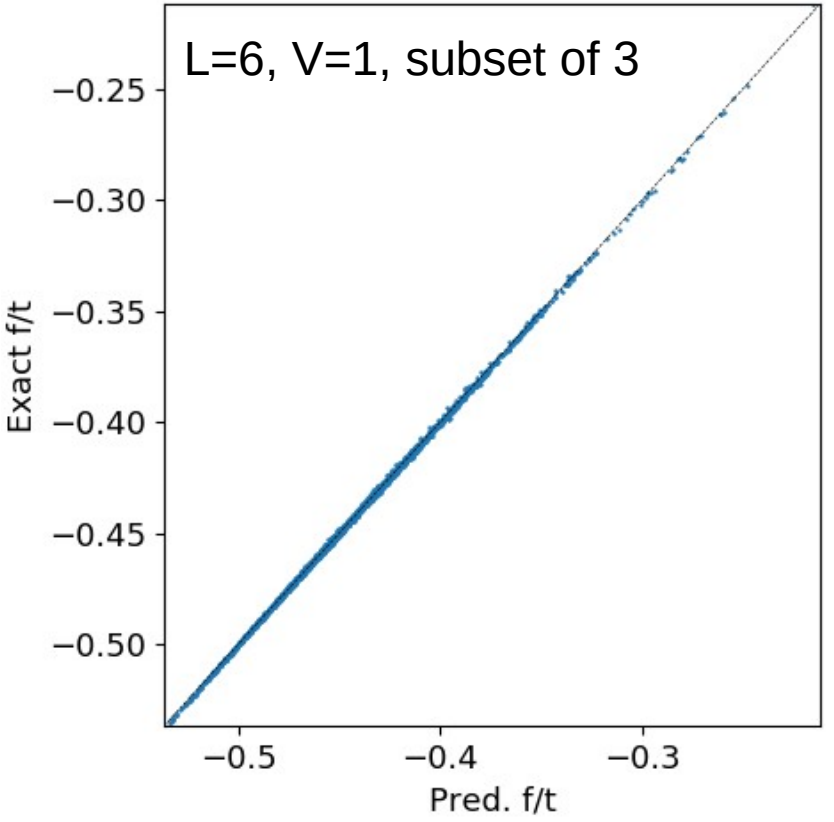


- Repeat process to build up dataset
- Use NNs to map $\{n_i^{GS}\}$ to f
- Using site centred local functions

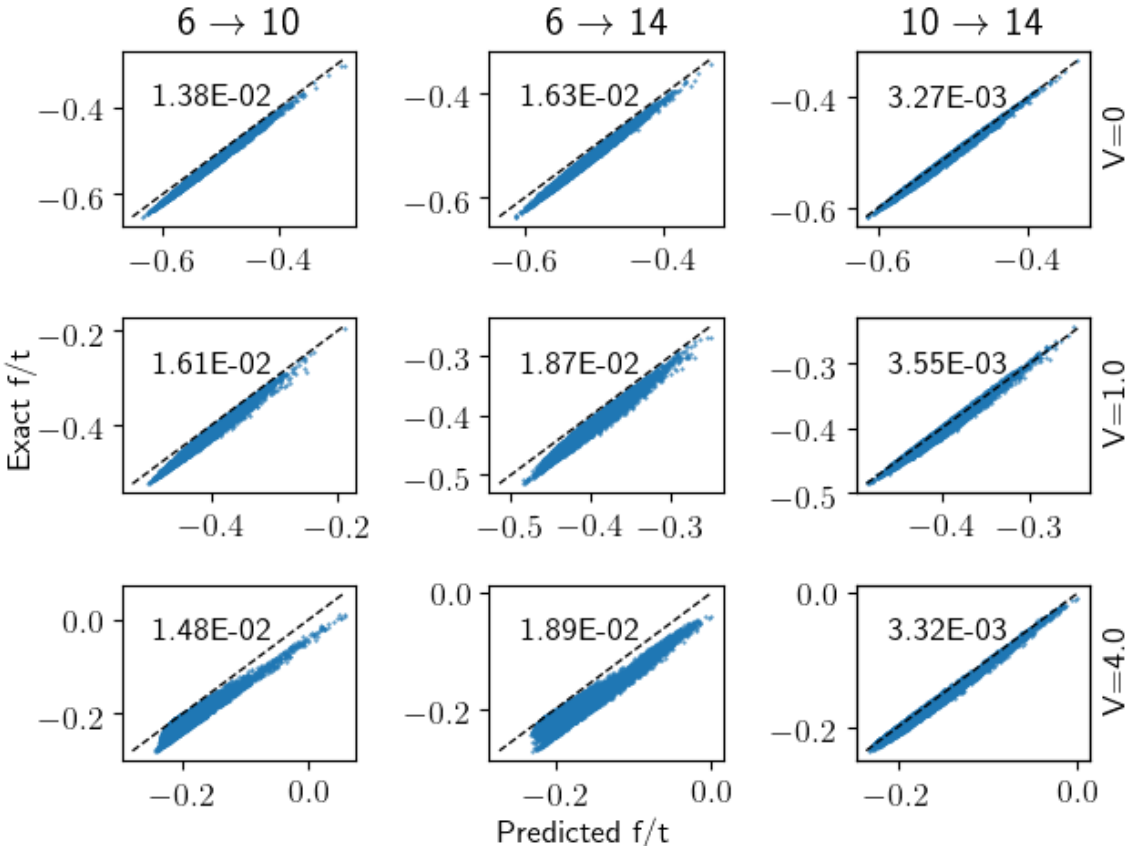
$$E = F(\{n_i\}) + \sum_{i=1}^{L} n_i \epsilon_i$$

How local is the energy?





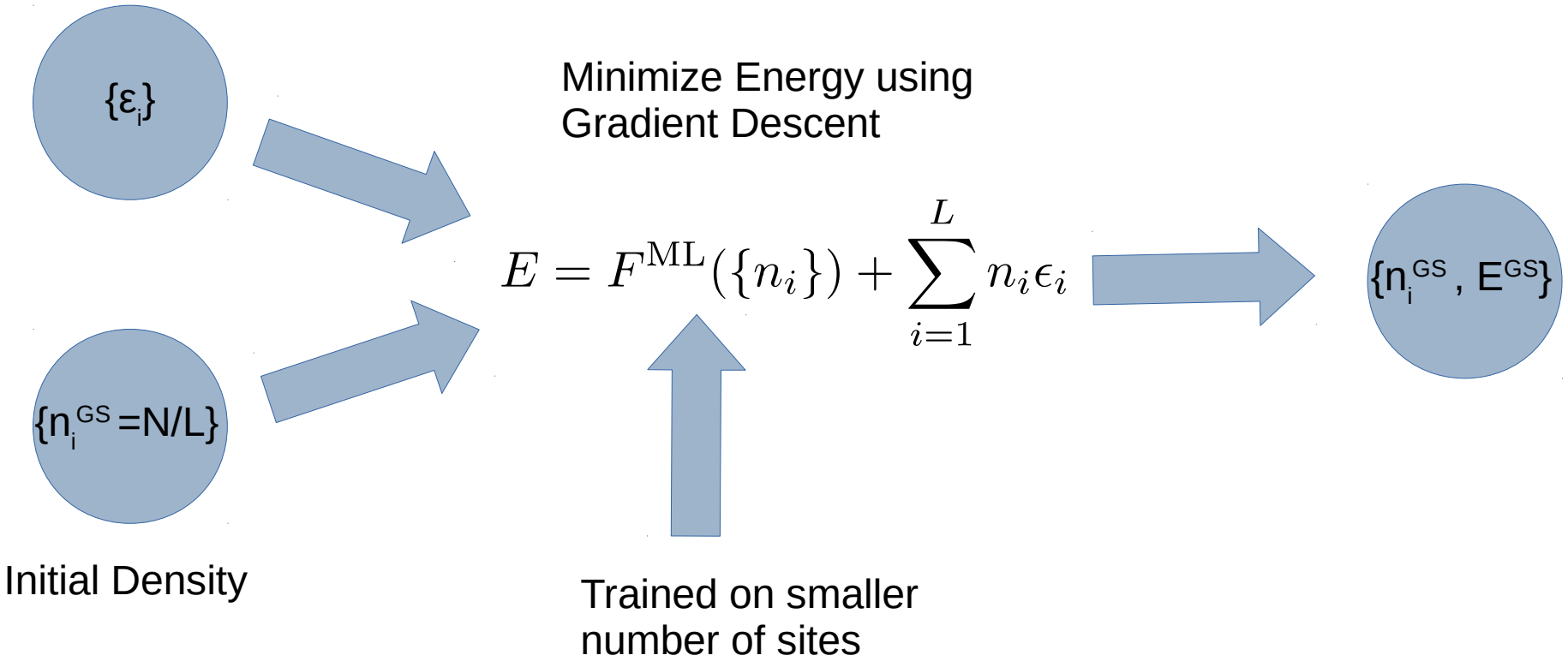
Larger Predictions



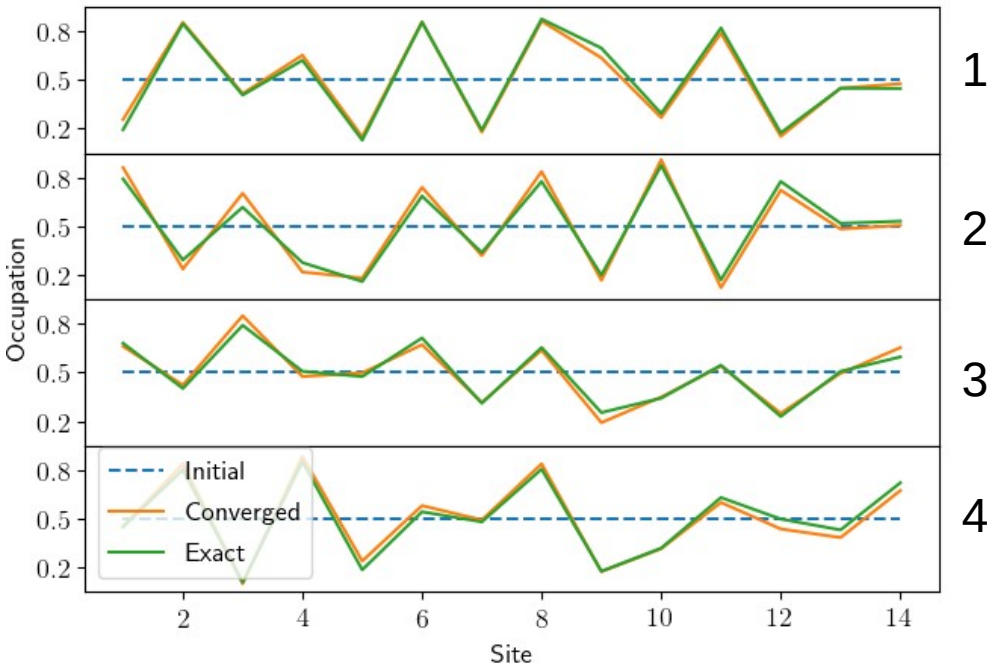
The Error of f:

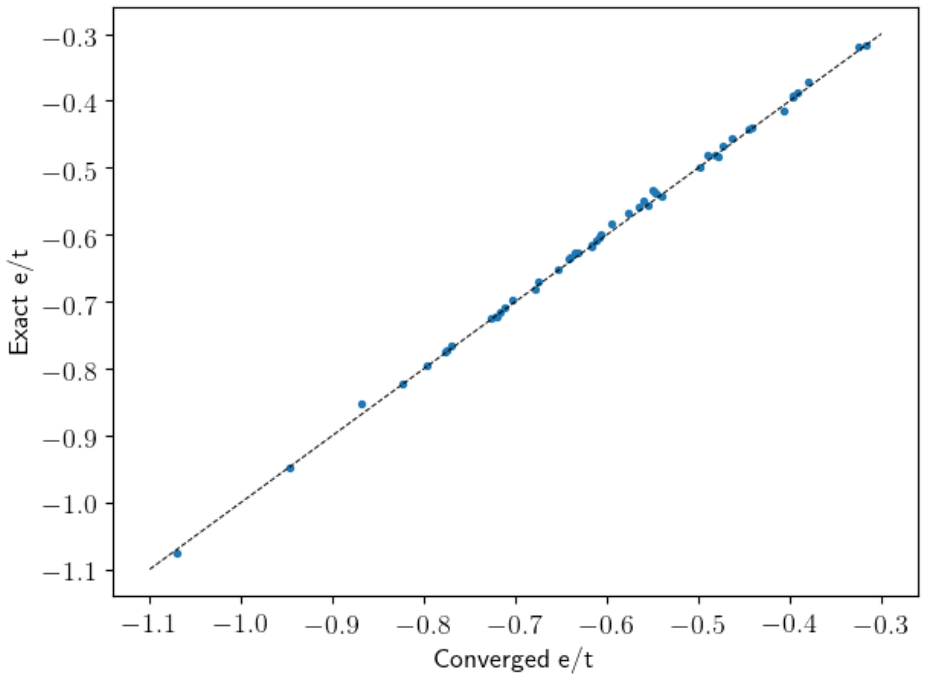
- Decreases by training on larger lattices
- Independent of V

Starting from the Onsite Energies

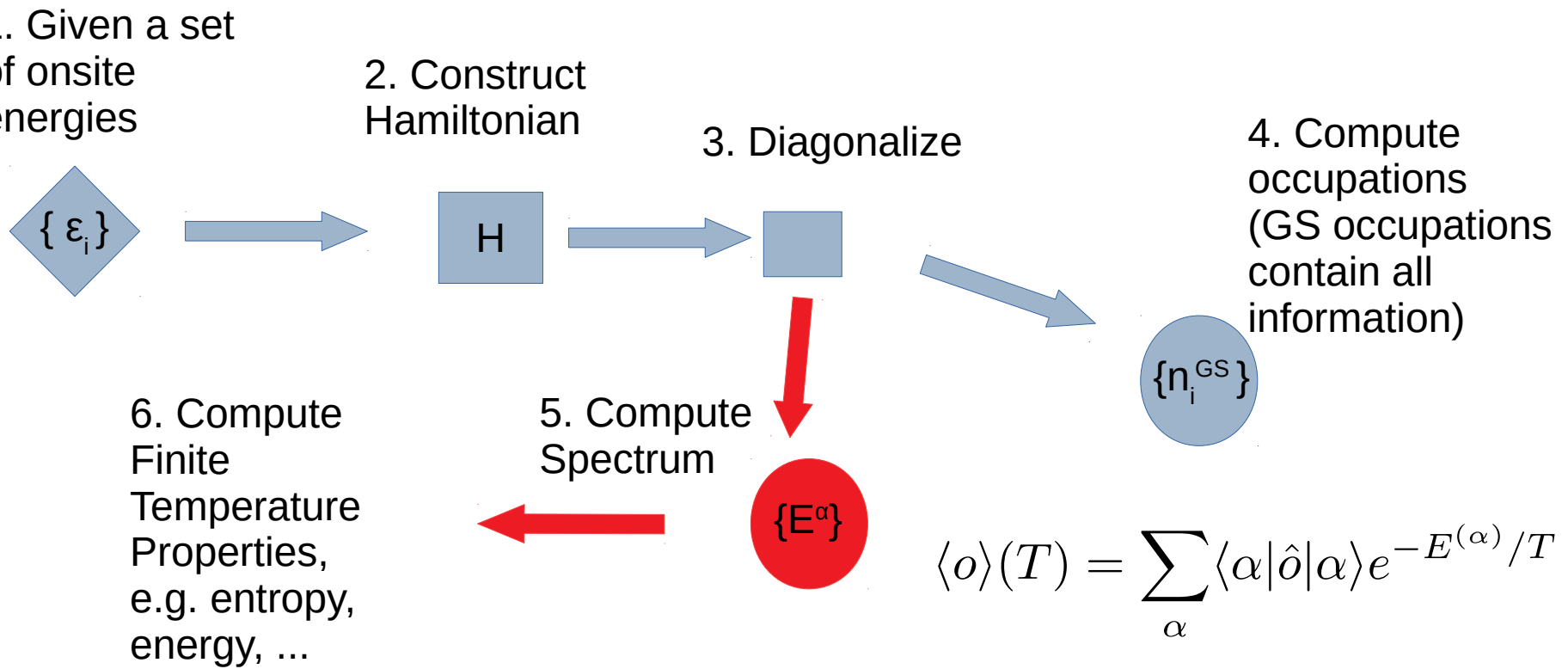


Minimization - L10 to L14





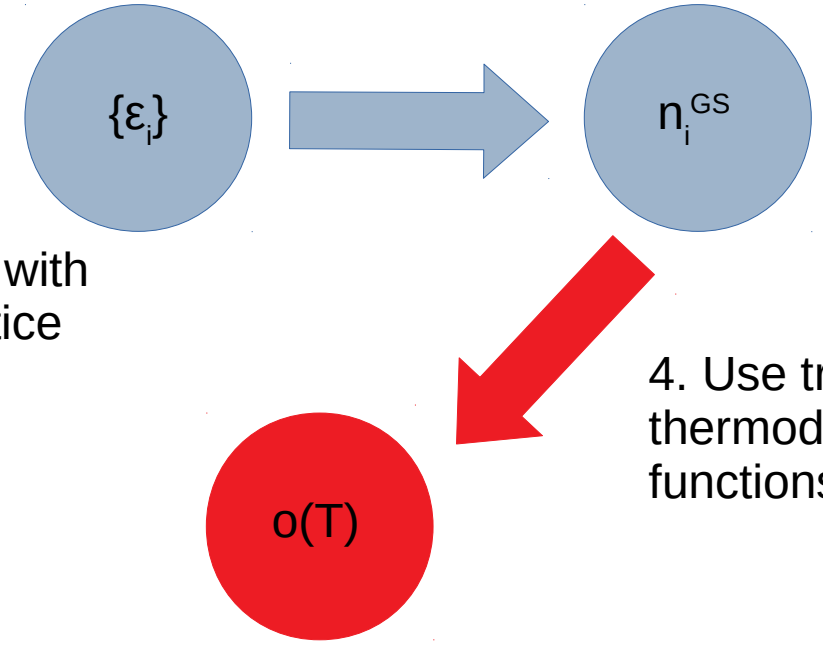
Finte Temperature



Then we use ML to map: $\{n_i^{GS}, T\}$ to o(T)

Workflow

1. Train NNs on data with computable number of sites



2. Onsite Energies with larger lattice size

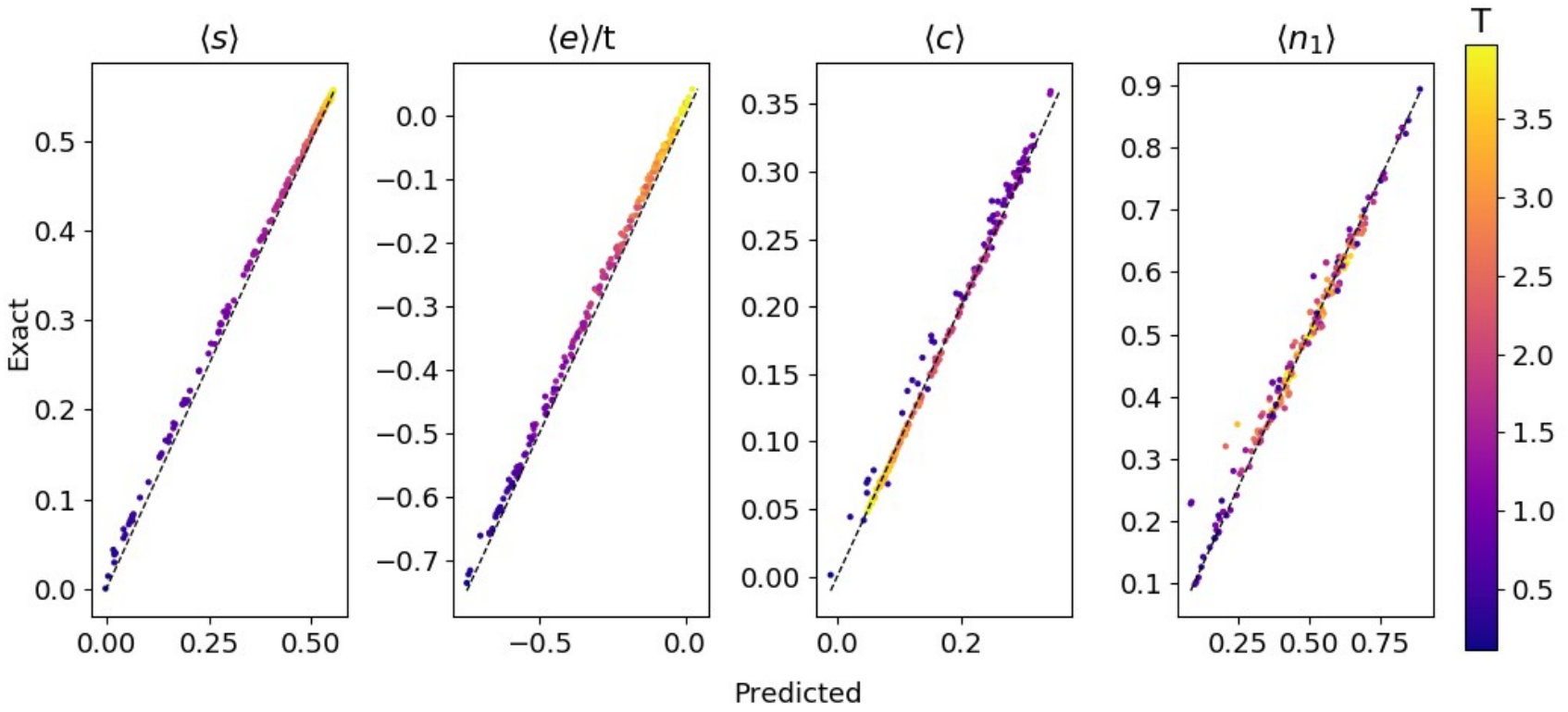
3. Find density that minimizes the energy

4. Use trained thermodynamic functions

Neural Network 1: $\{n_i^{GS}\}$ -> f

Neural Network 2: $\{n_i^{GS}, T\}$ -> o(T)

Thermodynamics - L10 to L14



Conclusions & Future Work

- Introduced local site representation
  - Independent of number of sites
  - Method is generalizable to other lattice models
- Using Spinless Extended Hubbard Model
  - Compute density from onsite energies
  - Framework for predicting finite temperature quantities from onsite energies

- Extend to 2 & 3 dimensions
- Allow hopping to vary – new geometries
- Incorporate Spin

Machine learning density functional theory for the Hubbard model
James Nelson, Rajarshi Tiwari, and Stefano Sanvito
Phys. Rev. B 99, 075132

New work: Arxiv Preprint Forthcoming

Thanks for your attention!

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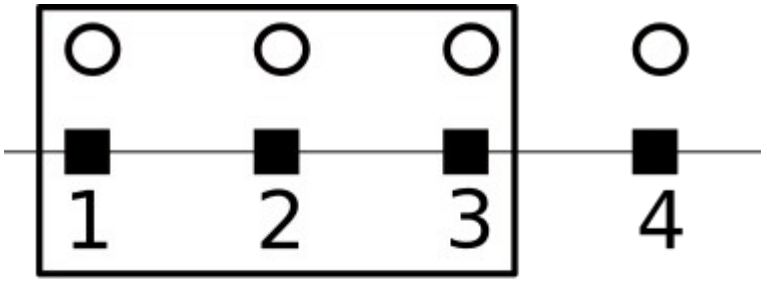
Hamiltonian Matrix

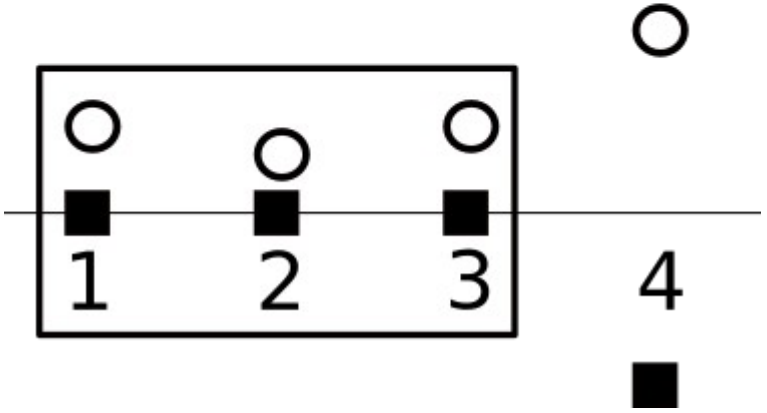
- For a L site lattice with N electrons
- Introduce a basis set $\{|s\rangle\}$ and expand the wavefunction: $|\psi\rangle = \sum_s |s\rangle\langle s|\psi\rangle = \sum_s \psi_s |s\rangle$
- Using the Schrodiinger equation we get an eigenvalue problem: $\sum_s \langle r|\hat{H}|s\rangle\psi_s = E\psi_r$

Density vs Onsites



$f(\epsilon_1, \epsilon_2, \epsilon_3)$

Gives the same value for bth systems



$f(n_1, n_2, n_3)$

Is different – since the densities are different