Solving the travelling salesman problem through variational Monte Carlo

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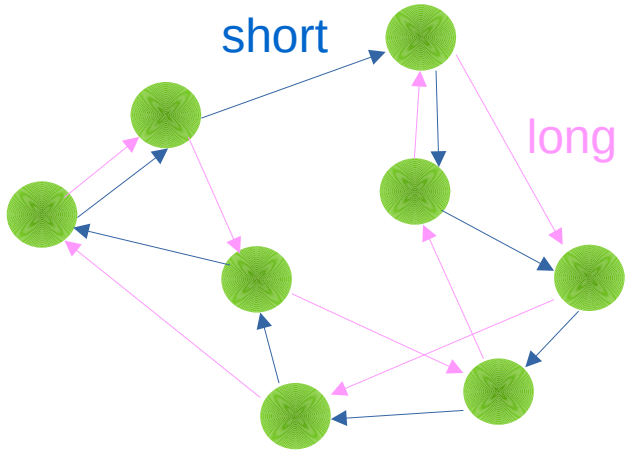
Travelling Salesman Problem (TSP):

Given a set of N locations and a distance matrix d_{ij}, find the shortest path that visits each location exactly once, returning to the origin



Translate

Position of location i in the tour

$$\boldsymbol{n} = (n_1, n_2, \ldots, n_N)$$

Configuration of a physical system

$$\hat{H}|\Psi(\boldsymbol{n})\rangle = E|\Psi(\boldsymbol{n})\rangle$$

Energy and Hamiltonian account for total distance of the tour.

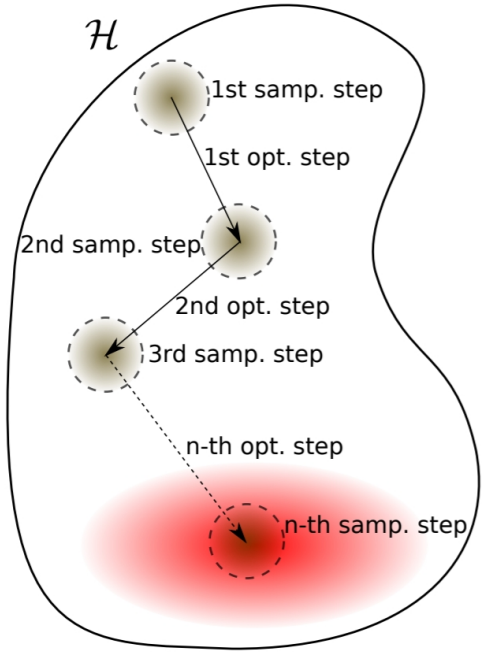
$$\langle \hat{H} \rangle = \sum_{i=1}^{N} d_{n_i, n_{(i+1) \mod N}}$$

Intractable Hilbert space

$$|\mathcal{H}| = N^N$$

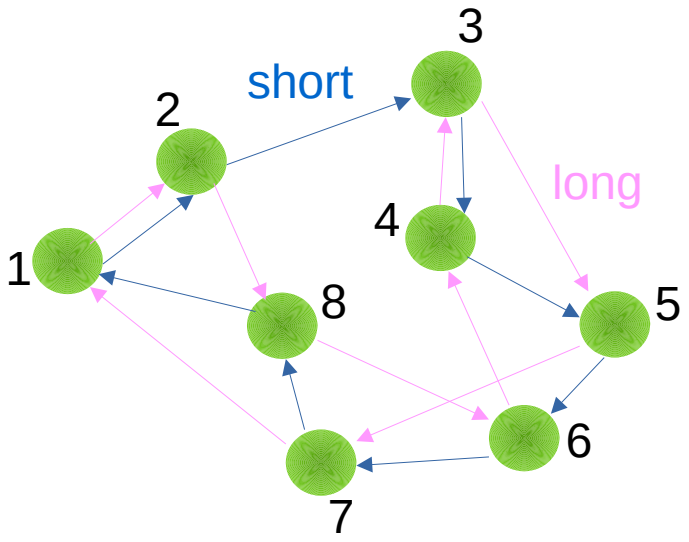
Ground State

[Taken from J. Phys. Soc. Jpn. 89, 094002 (2020)]



Variational Monte Carlo with neural network ansatz efficiently finds ground states (i.e. shortest paths to the TSP) of many-body systems.

Travelling Salesman Problem map to N N-level systems



How do we refer to a specific tour?

Pink path → $(1,2,8,6,4,3,5,7) \mapsto |1,2,8,6,4,3,5,7\rangle$

Blue path → $(1,2,3,4,5,6,7,8) \mapsto |1,2,3,4,5,6,7,8\rangle$

- All occupations must be different
- First position of the tour fixed to be 1
- Energy of each state must be equivalent to the tour distance.
- Mapping N N-level systems to qubits requires N log(N) qubits, which is better than current N^2 qubits proposals.

N N-level system Hamiltonian for the TSP

$$\hat{D}_{ij} : \mathcal{H}_i \otimes \mathcal{H}_j \to \mathcal{H}_i \otimes \mathcal{H}_j$$

Acts on a pair of N-level systems

Single N-level system

$$\hat{D}_{ij} = \mathrm{diag}(d_{1,1} + p, d_{1,2}, \ldots, d_{1,N}, d_{2,1}, \ldots, d_{2,N}, \ldots, d_{N,N} + p) - o$$

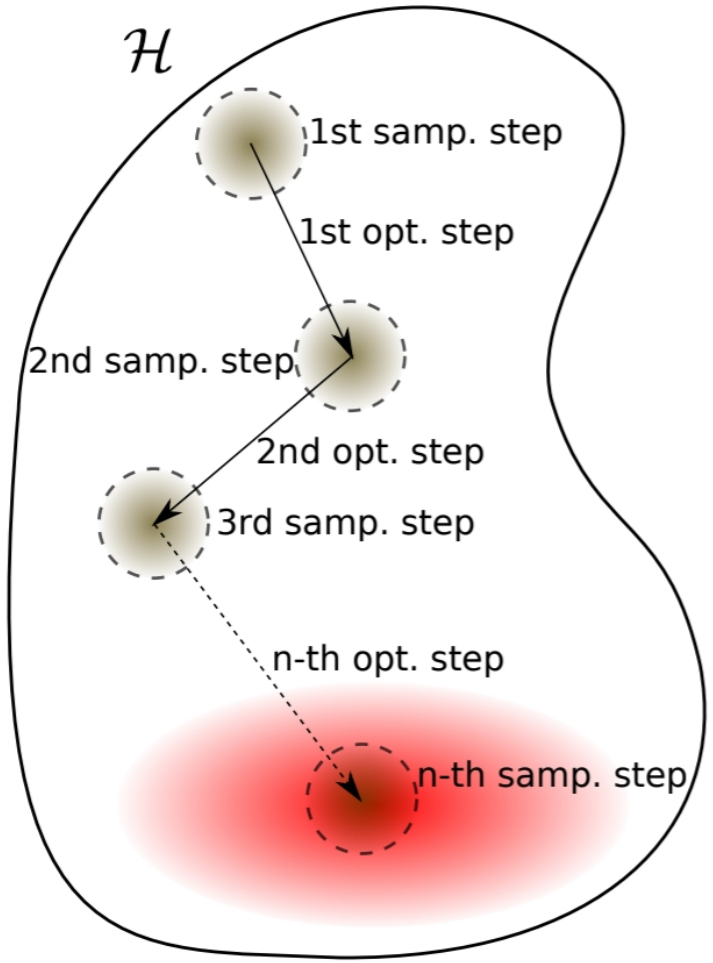
Penalisation term appearing if states of system i and system j are in the same occupation.

Diagonal offset to make terms out of the diagonal large with respect to diagonal terms.

$$\hat{H} = \hat{D}_{1,2} + \hat{D}_{2,3} + \ldots + \hat{D}_{N-1,N} + \hat{D}_{N,1}$$

Tour positions

Ground state of the TSP Hamiltonian



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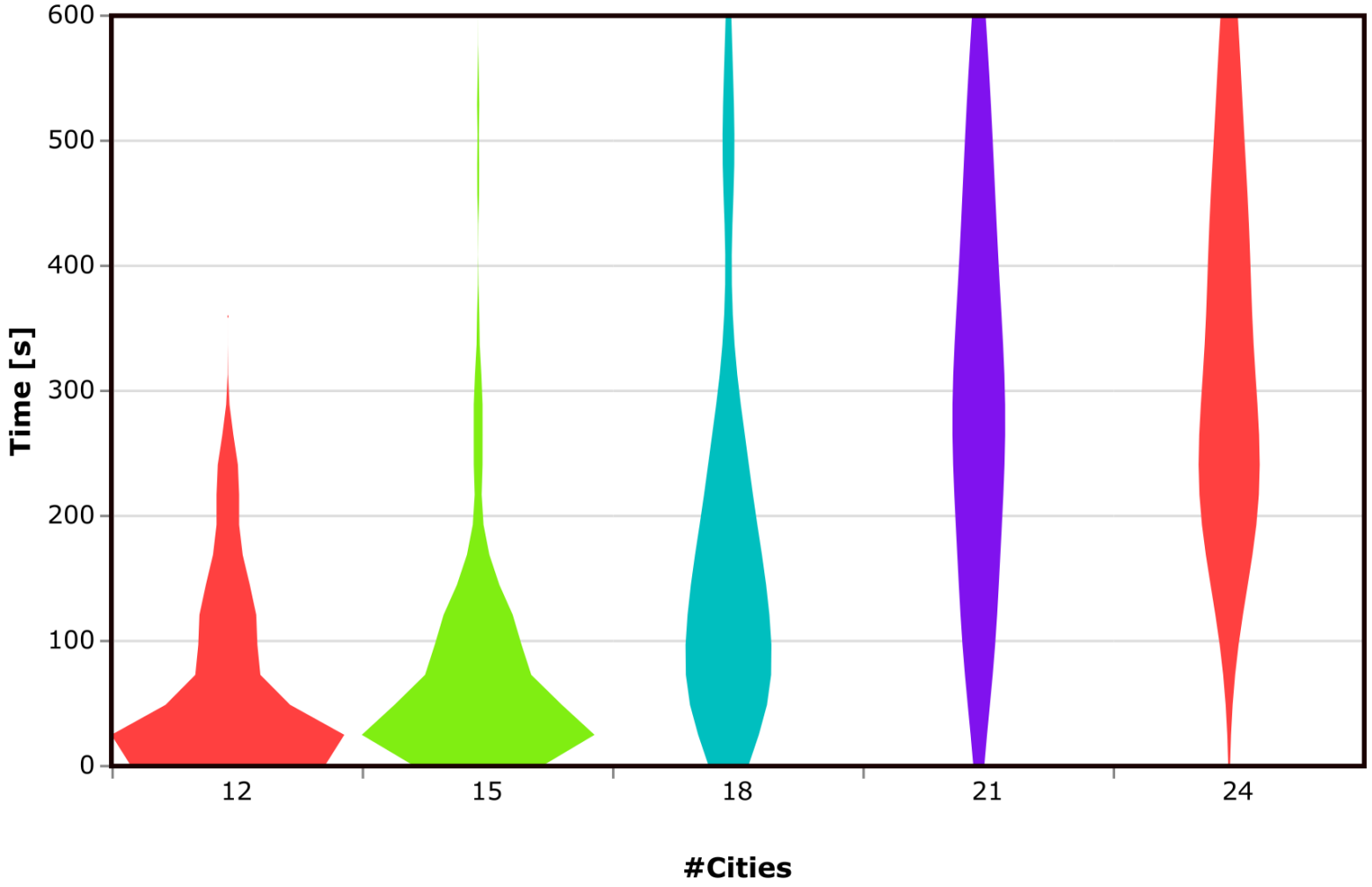
- Metropolis Hastings to sample configurations of the form $|n_1, n_2, \ldots, n_N\rangle$
- Probabilities of accepting new configurations are given by a trial wavefunction represented by a neural network

$$|\Psi\rangle \approx \sum_{\boldsymbol{n}} \psi_{\boldsymbol{\theta}}(\boldsymbol{n})|\boldsymbol{n}\rangle$$

Trial wavefunction, $\boldsymbol{\theta}$ are variational parameters or neural network weights

- Variational parameters are determined by minimising the energy of the system (i.e. distance of the tour).

Experiments with different structural parameters of VMC and neural network



Energy convergence