Ground States of Quantum Lattice Models via Reinforcement Learning

Willem Gispen and Austen Lamacraft

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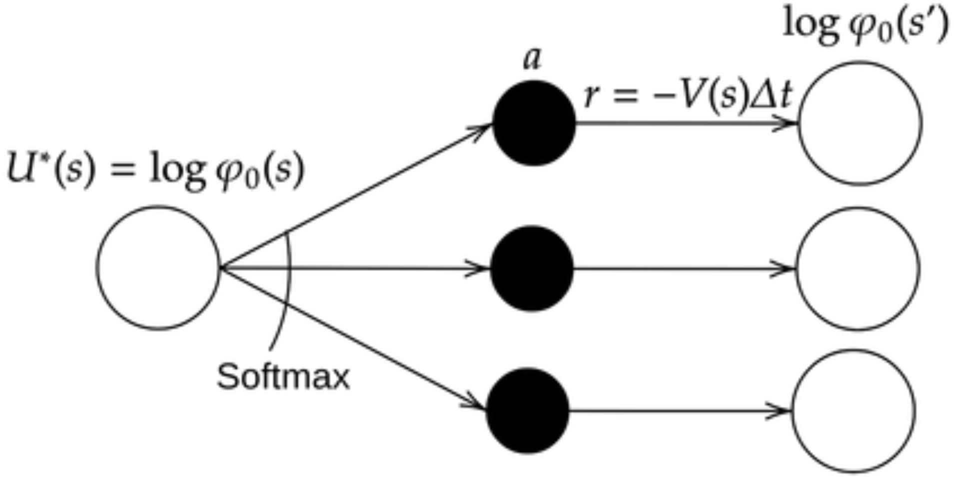
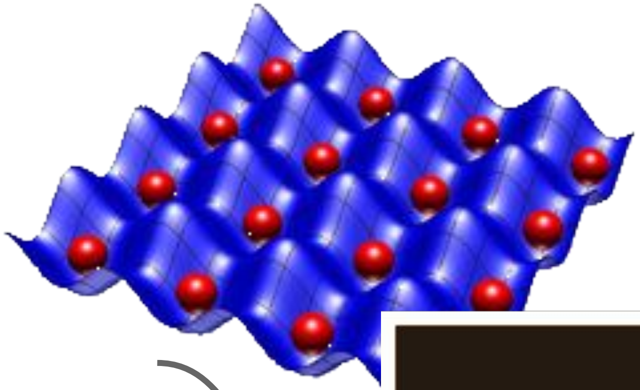
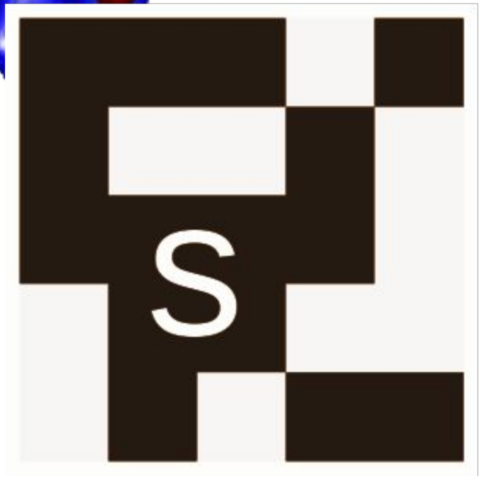


Quantum lattice models



Lattice models provide a useful simplification of e.g. strongly correlated many-body systems



Ground state

$$\mathbf{s} \mapsto \varphi_0(\mathbf{s})$$

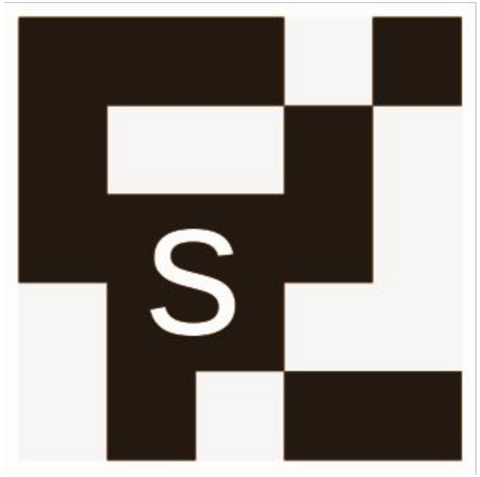
$$H\varphi_0 = E_0\varphi_0$$

Even for a spin-½ lattice model, the ground state of N particles is an eigenfunction with 2^N possible inputs!

Neural quantum states

Existing deep learning approaches:

- use a convolutional neural network for representation
- optimize the *variational energy* with Monte Carlo (VMC)



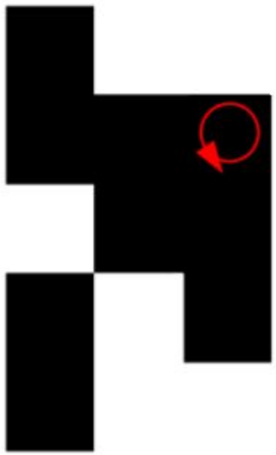
$$\overset{CNN}{\longmapsto} \varphi(\mathbf{s})$$

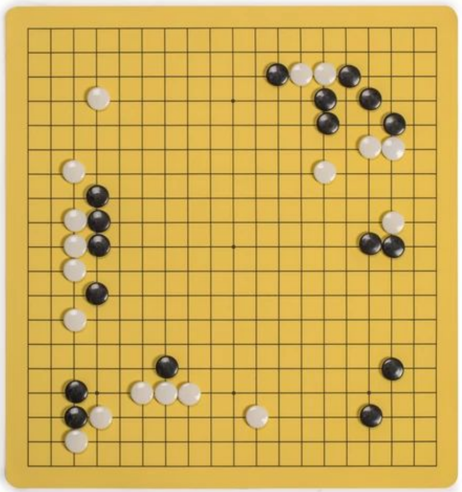
$$\langle H \rangle = \mathbb{E}_{\mathbf{s} \sim |\varphi|^{\mathbf{2}}} \left[\frac{H\varphi}{\varphi} \right]$$

Outline

In three steps, we show a novel optimization method for neural quantum states:

1. Stochastic dynamics of φ_0
2. Reinforcement learning reformulation
3. Application to neural quantum states





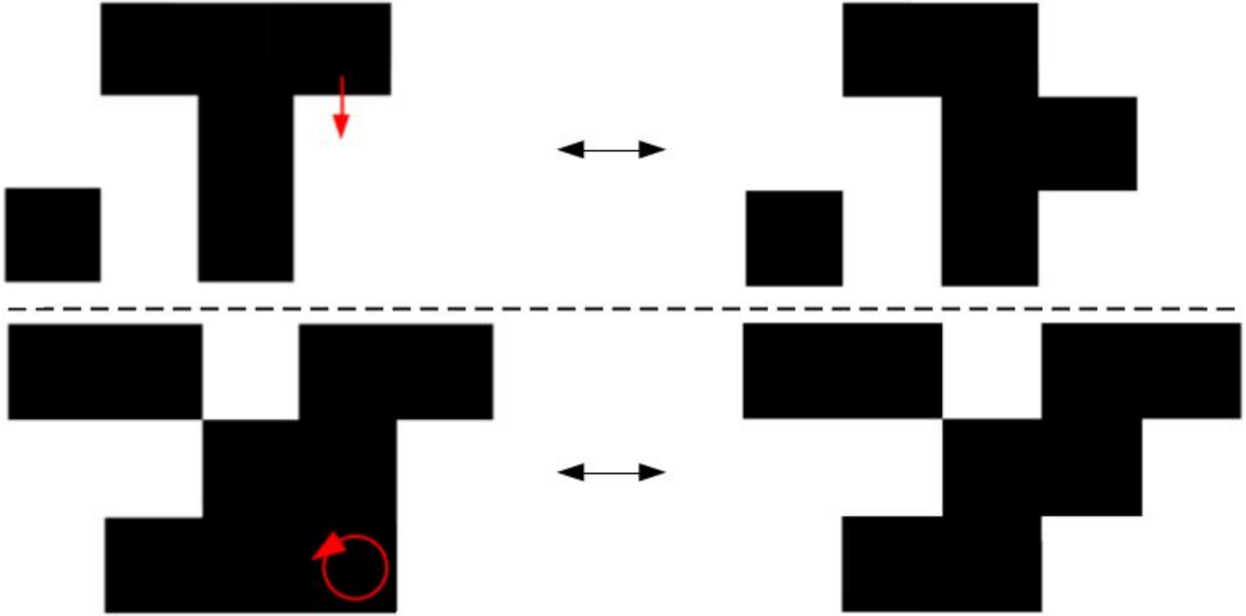
Stochastic dynamics of φ_0

Stoquastic Hamiltonians H can be decomposed into a kinetic and potential energy. The kinetic part Γ describes stochastic changes of the configuration.

$$H = -\Gamma + V$$

XY

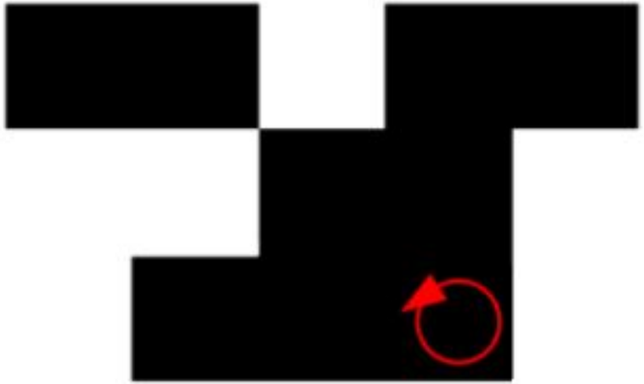
Ising



Stochastic dynamics of φ_0

Dynamics in imaginary time (converges to ground state as $t \to \infty$)

$$\partial_t \varphi(t) = -H\varphi(t)$$



for a stoquastic Hamiltonian

$$H_{\mathbf{ss}'} = -\Gamma_{\mathbf{ss}'} + V(\mathbf{s})\delta_{\mathbf{ss}'}$$

we have the Feynman-Kac representation

$$\varphi(\mathbf{s_t}, t) = \mathbb{E}_\Gamma \left[\exp\left(-\int_t^{t+T} V(\mathbf{s_{t'}})dt' \right) \varphi(\mathbf{s_{t+T}}, t+T) \right]$$

Reinforcement learning formulation

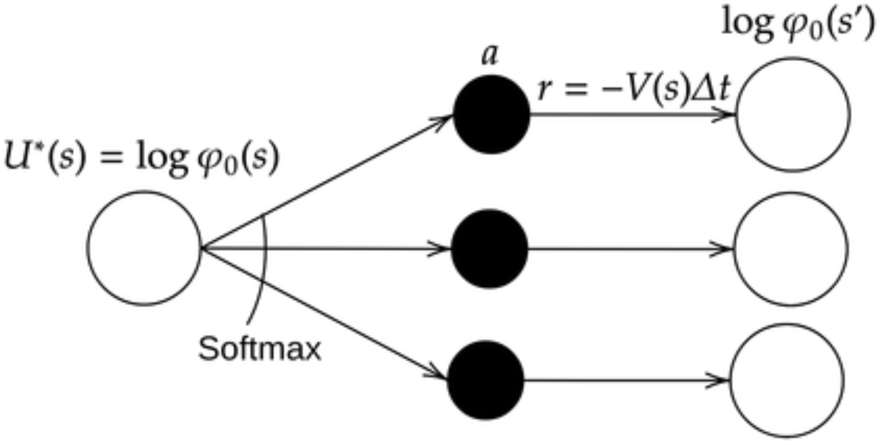
Todorov: maximum entropy RL can be linearized

Reverse transformation:

Feynman-Kac (ground state)

$$\varphi(\mathbf{s_0}, 0) = \mathbb{E}_{\mathbb{P}}\left[e^{-\int V(\mathbf{s_t})dt}\varphi(\mathbf{s_T}, T)\right]$$

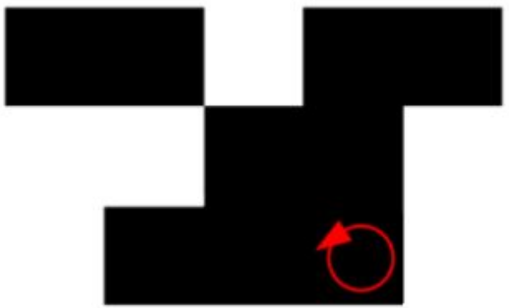
Soft Bellman (RL)

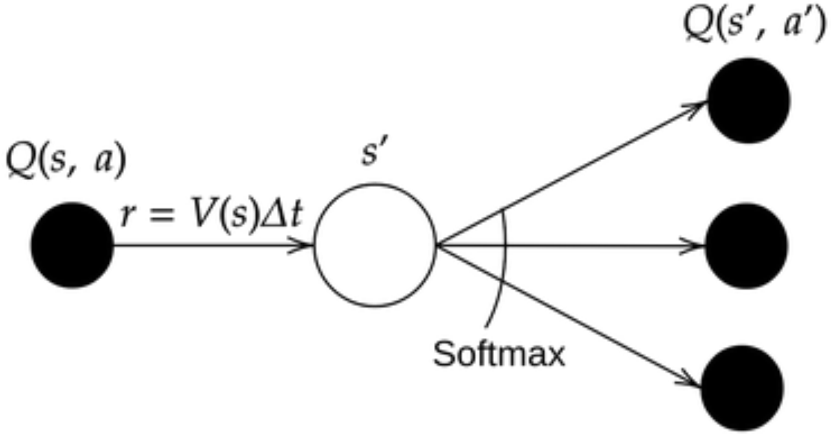


Application: neural quantum states

Method:

1. Represent action-value $Q(s,a)$ with CNN
2. Optimize: solve soft Bellman with soft Q-learning (Haarnoja et al)
3. Result: ground state approximation $\log \varphi(\mathbf{s}) = \mathrm{Softmax}(Q(\mathbf{s},\mathbf{a}))$
4. Follow policy to sample φ





Application: neural quantum states

Method:

1. Represent $Q(s, a)$ with CNN
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3. Result: $\log \varphi(\mathbf{s}) = \mathrm{Softmax}(Q(\mathbf{s}, \mathbf{a}))$
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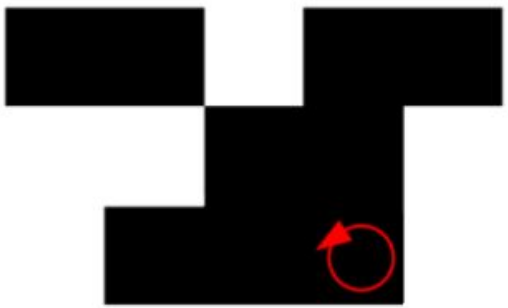
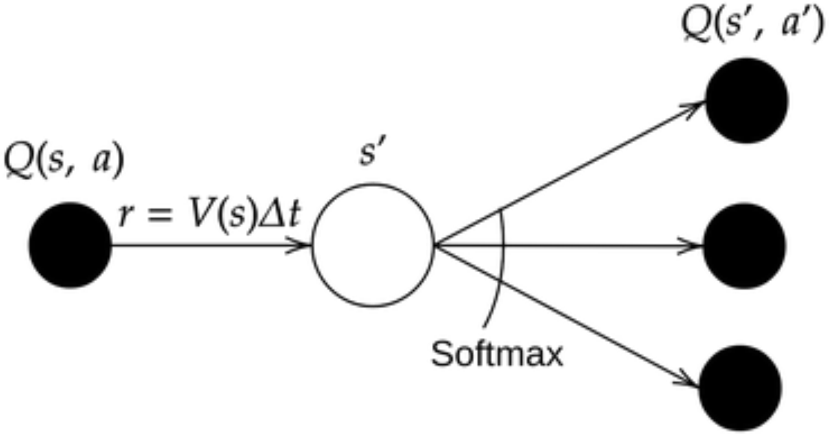
Pros/cons:

1. Larger CNN
2. Faster update steps
3. -
4. Higher acceptance rate





Experiments

Proof of principle

- test case: 6x6 Ising model
- 0.1% error in ground state energy
- only 20 min training time (12 GB GPU)
- $\mathcal{O}(\sqrt{N})$ faster sampling of ground state

Code: github.com/WillemGispen/Lattice-Quarl

More in the papers!

Three different RL formulations:

- Continuous time (this talk)
- Discrete and infinite time horizon
- Discrete time and terminal states

Last year:

- Continuous state spaces
- Atomic and molecular systems

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Ground States of Quantum Lattice Models via Reinforcement Learning

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- Quantum mechanics ⟷ reinforcement learning
- New optimization methods for neural quantum states
- Faster optimization steps and sampling