Accelerated Monte Carlo simulations with restricted Boltzmann machines

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Motivation

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Quantum Monte Carlo zoo 1

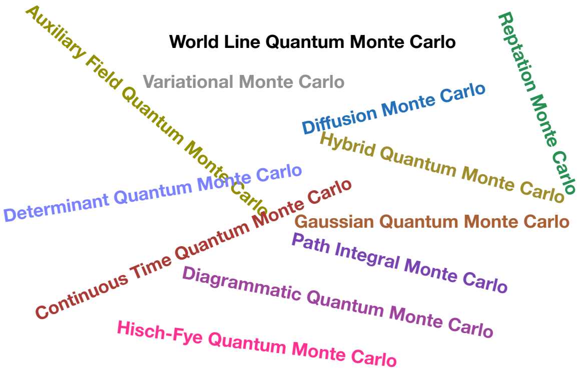

Figure: Various quantum Monte Carlo algorithms

Ref.: Quantum Monte Carlo Methods, 2016

Quantum Monte Carlo zoo 2

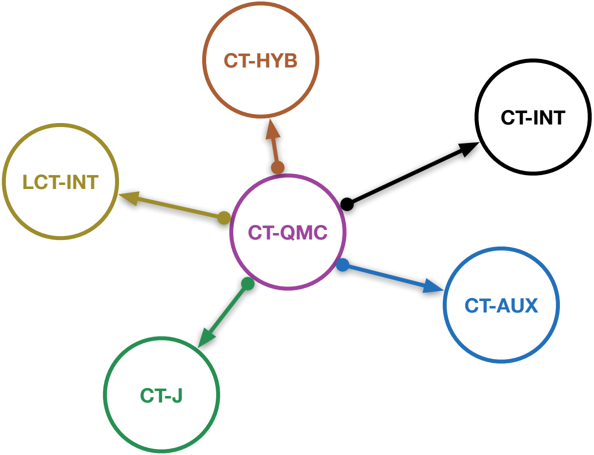

Figure: Various continuous time quantum Monte Carlo algorithms

Ref.: Rev. Mod. Phys. 83, 349 (2011)

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Troubles

In my opinions, the applications of quantum Monte Carlo methods are mainly hampered by the following three problems:

How to visit the configuration space efficiently?

Critical slowing down

Negative sign problem (for fermionic system)

Machine learning + Many-body physics 1

Detecting phase transitions in classic or quantum models

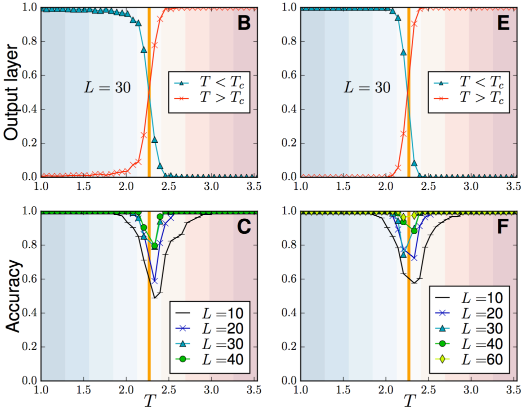

Figure: Detecting phase transitions in Ising model with ANN

Ref.: Nat. Phys. 13, 431 (2017)

Machine learning + Many-body physics 2

Representation of quantum many-body states

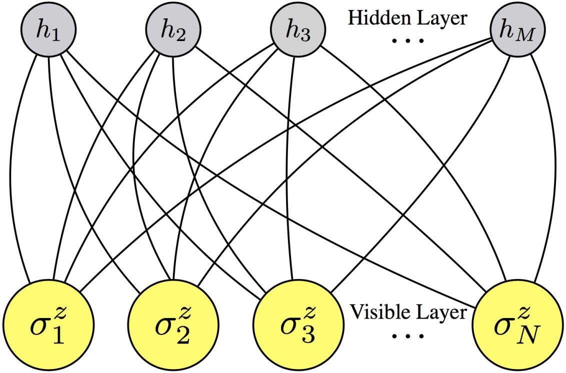

Figure: Artificial neural network encoding a many-body quantum state

Ref.: Science 355, 602 (2017)

Machine learning + Many-body physics 3

Solve the inverse problems

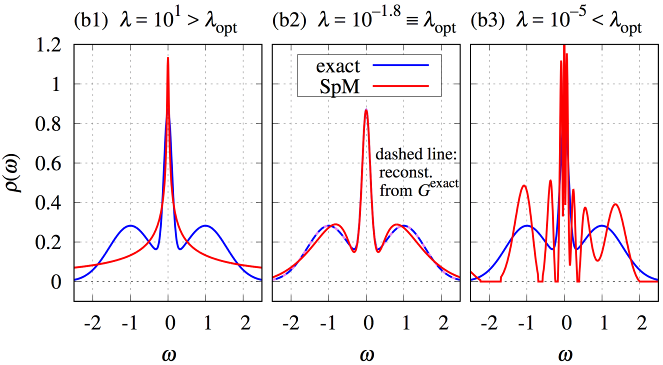

Figure: Sparse modeling approach to analytical continuation of $G(\tau)$

Ref.: Phys. Rev. E 95, 061302 (2017)

Our ideas 1

Is it possible to use ML tools to accelerate QMC?

- Supposed that it is difficult (not easy) to sample the target distributions by Monte Carlo directly.
- With the available data, we train a restricted Boltzmann machine (RBM) which can be viewed as a proxy (approximation) of the statistical distributions.
- We simulate the trained RBM, and then use it to propose new (local or non-local) Monte Carlo updates. The role played by the RBM in the Monte Carlo simulation is just like a recommender system in e-commerce platforms.

Our ideas 2

How to visit the configuration space efficiently?

- The acceptance ratio is increased.

Critical slowing down

- The autocorrelation time is reduced.

Negative sign problem (for fermionic system)

- NO SOLUTION!

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Method

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Falicov-Kimball model 1: Hamiltonian

Hamiltonian:

$$\hat{H}_{\mathrm{FK}} = \sum_{i,j} \hat{c}_i^{\dagger} \mathcal{K}_{ij} \hat{c}_j + U \sum_{i=1}^{N} \left(\hat{n}_i - \frac{1}{2} \right) \left(x_i - \frac{1}{2} \right) \tag{1}$$

Probability distribution:

$$p_{\mathrm{FK}}(\mathbf{x}) = e^{-F_{\mathrm{FK}}(\mathbf{x})} / Z_{\mathrm{FK}} \tag{2}$$

"Free energy":

$$-F_{\mathrm{FK}}(\mathbf{x}) = \frac{\beta U}{2} \sum_{i=1}^{N} x_i + \ln \det \left(1 + e^{-\beta \mathcal{H}} \right) \tag{3}$$

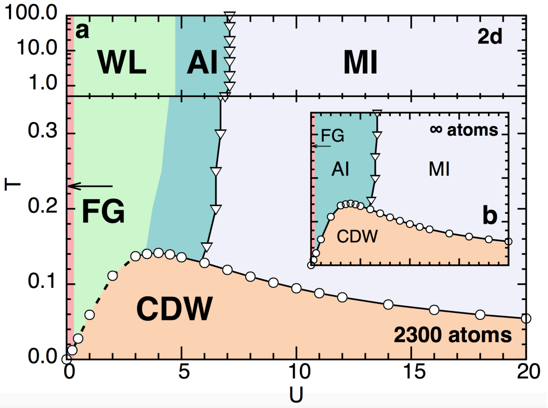
$x_i \in \{0, 1\}$: occupation number of the localized fermion at site i.

$\hat{n}_i \equiv \hat{c}_i^{\dagger} \hat{c}_i$: occupation number operator of the mobile fermion.

$\mathcal{K}$ is the kinetic energy matrix of the mobile fermions.

Falicov-Kimball model 2: Phase diagram

Ref.: Phys. Rev. Lett. 117, 146601 (2016)



CDW: charge density wave insulator

AI: Anderson insulator

MI: Mott insulator

FG: Fermi gas

WL: weakly localized

Falicov-Kimball model 3: Lattice QMC

Bit-flip update:

$$x_i \longrightarrow 1 - x_i \tag{4}$$

Detailed balance condition:

$$\frac{T(\mathbf{x} \rightarrow \mathbf{x}')}{T(\mathbf{x}' \rightarrow \mathbf{x})} \frac{A(\mathbf{x} \rightarrow \mathbf{x}')}{A(\mathbf{x}' \rightarrow \mathbf{x})} = \frac{p_{\mathrm{FK}}(\mathbf{x}')}{p_{\mathrm{FK}}(\mathbf{x})} \tag{5}$$

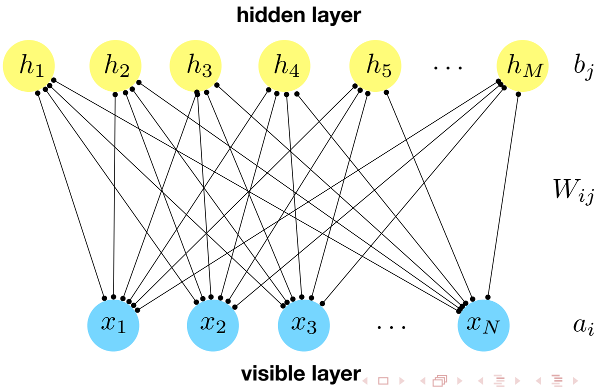
Cons:

- Scaling: $O(N^4)$
- Long autocorrelation times

RBM 1: Architecture

The RBM is a classical statistical mechanics system defined by the following energy function

$$E\left(\mathbf{x},\mathbf{h}\right) = -\sum_{i=1}^{N} a_i x_i - \sum_{j=1}^{M} b_j h_j - \sum_{i=1}^{N}\sum_{j=1}^{M} x_i W_{ij} h_j, \qquad (6)$$



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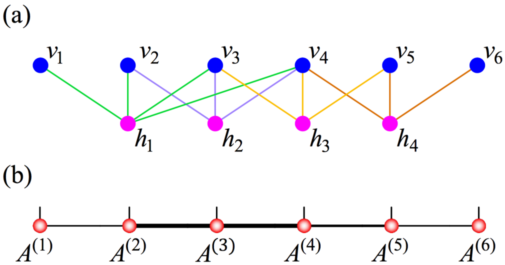
RBM 2: Recent applications

Connecting RBM with tensor networks states



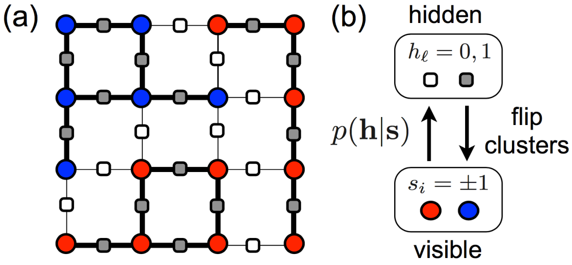
$$\Psi_{\mathsf{RBM}}(v) = \sum_h e^{-E(v,h)} = \prod_{i,j} e^{a_i v_i}\left(1 + e^{b_j + \sum_i v_i W_{ij}}\right) \qquad (7)$$

$$\Psi_{\mathsf{MPS}}(v) = \mathsf{Tr}\left(\prod_{i=1}^{n_v} A^{(i)}[v_i]\right) \qquad (8)$$

Ref.: arXiv:1701.04831

RBM 3: Recent applications

Searching new cluster updates



Ref.: arXiv:1702.08586

Numerical recipes 1: Collecting data

Collecting training data set $\{\mathbf{x}\}$ by traditional Monte Carlo method in a preliminary calculation.

Numerical recipes 2: Training RBM

Joint probability distribution of the visible and hidden variables

$$p(\mathbf{x}, \mathbf{h}) = e^{-E(\mathbf{x}, \mathbf{h})}/Z \tag{9}$$

Marginal distribution

$$p(\mathbf{x}) = \sum_{\mathbf{h}} p(\mathbf{x}, \mathbf{h}) = e^{-F(\mathbf{x})}/Z \tag{10}$$

"Free energy" of RBM

$$-F(\mathbf{x}) = \sum_{i=1}^{N} a_i x_i + \sum_{j=1}^{M} \ln\left(1 + e^{b_j + \sum_{i=1}^{N} x_i W_{ij}}\right) \tag{11}$$

Numerical recipes 3: Training RBM (cont.)

"Free energy" of RBM

$$-F(\mathbf{x}) = \sum_{i=1}^{N} a_i x_i + \sum_{j=1}^{M} \ln\left(1 + e^{b_j + \sum_{i=1}^{N} x_i W_{ij}}\right) \quad (12)$$

"Free energy" of Falicov-Kimball model

$$-F_{\mathrm{FK}}(\mathbf{x}) = \frac{\beta U}{2} \sum_{i=1}^{N} x_i + \ln\det\left(1 + e^{-\beta \mathcal{H}}\right), \quad (13)$$

We use $F(\mathbf{x})$ to approximate $F_{\mathrm{FK}}(\mathbf{x})$, and setup the parameters a_i, b_i, and W_{ij} of RBM.

Numerical recipes 4: Training RBM (cont.)

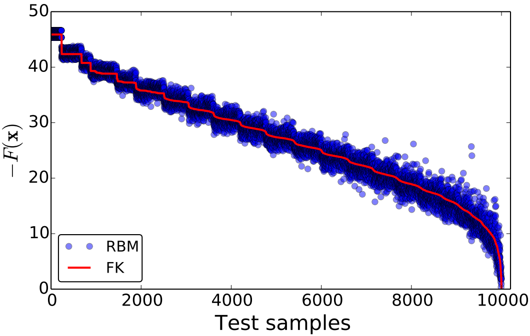
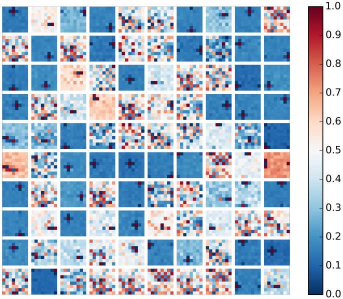


Figure: Fitting of the log probability of the RBM to the one of the Falicov-Kamball model.

Numerical recipes 5: Training RBM (cont.)



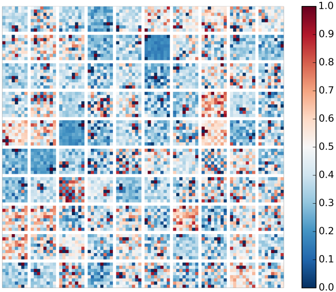


Figure: Connection weights W_{ij} of the RBM. (left) $T/t = 0.15$. (right) $T/t = 0.13$.

Numerical recipes 6: Simulating RBM

We simulate the trained RBM using the standard blocked Gibbs sampling approach. The conditional probabilities of the hidden variables and visible variables read:

$$p(\mathbf{h}|\mathbf{x}) = \prod_{j=1}^{M} p(h_j|\mathbf{x}) \tag{14}$$

$$p(\mathbf{x}|\mathbf{h}) = \prod_{i=1}^{N} p(x_i|\mathbf{h}) \tag{15}$$

$$p(h_j = 1|\mathbf{x}) = \sigma\left(b_j + \sum_{i=1}^{N} x_i W_{ij}\right) \tag{16}$$

$$p(x_i = 1|\mathbf{h}) = \sigma\left(a_i + \sum_{j=1}^{M} W_{ij} h_j\right) \tag{17}$$

Numerical recipes 7: Simulating RBM (cont.)

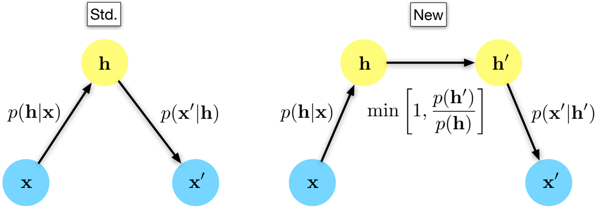


Figure: Two strategies of proposing Monte Carlo updates using the RBM.

Numerical recipes 8: RBM + MC

We use the trained RBM to propose new updates (instead of local bit-flip updates), and then apply the Metropolis algorithm to update the Markov chain.

$$A(\mathbf{x} \to \mathbf{x}') = \min\left[1, \frac{p(\mathbf{x})}{p(\mathbf{x}')} \cdot \frac{p_{\mathrm{FK}}(\mathbf{x}')}{p_{\mathrm{FK}}(\mathbf{x})}\right]. \quad (18)$$

Ideally, the acceptance ratio is one if the RBM fits the Falicov-Kimball model perfectly.

Results

Preliminary results

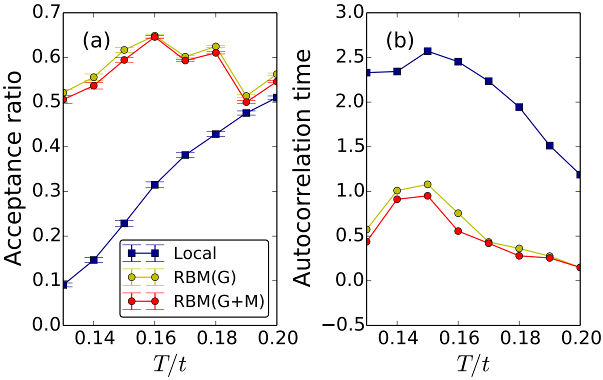


Figure: (a) The acceptance ratio and (b) the total energy autocorrelation time of the Falicov-Kimball model.

Discussions

Discussion 1

Why does it work?

- The trained RBM captures the target distribution correctly.
- It is more efficient to explore the configuration space.
- non-local updates vs. local updates

Discussion 2

Is this method general?

No! Since the limitation of RBM architecture, the MC algorithm must have binary degree of freedoms.

- Ising and Z_2 gauge fields models
- Determinant quantum Monte Carlo
- CT-AUX
- HF-QMC
- etc.

Discussion 3

Is this idea general?

Sure. We can consider RBM as an efficient recommender system to accelerate Monte Carlo simulations.

Similar works:

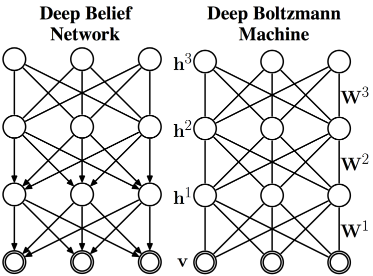
- Using classic gas model to accelerate CT-INT
  Ref.: Phys. Rev. E 95, 031301 (2017)
- Using effective Ising model to accelerate DQMC and CT-AUX
  Ref.: Phys. Rev. B 95, 041101 (2017), Phys. Rev. B 95, 241104 (2017), arXiv:1612.03804, arXiv:1705.06724

Discussion 4

Is there space to improve it?

Sure.

- Self-guiding or online training approach
- Deep Boltzmann machines or deep belief networks



Take-home messages

- It is possible to design special recommender systems to accelerate some Monte Carlo simulations.
- The RBM is a good recommender system for the Monte Carlo simulation for Falicov-Kimball model.

Ref.: Phys. Rev. B 95, 035105 (2017)

Future works:

- Exploring reliable and efficient recommender systems for CT-HYB, which is the core computational engine in dynamical mean-field theory.

Ref.: Phys. Rev. E 95, 031301 (2017)