Differentiable Monte Carlo for spin models

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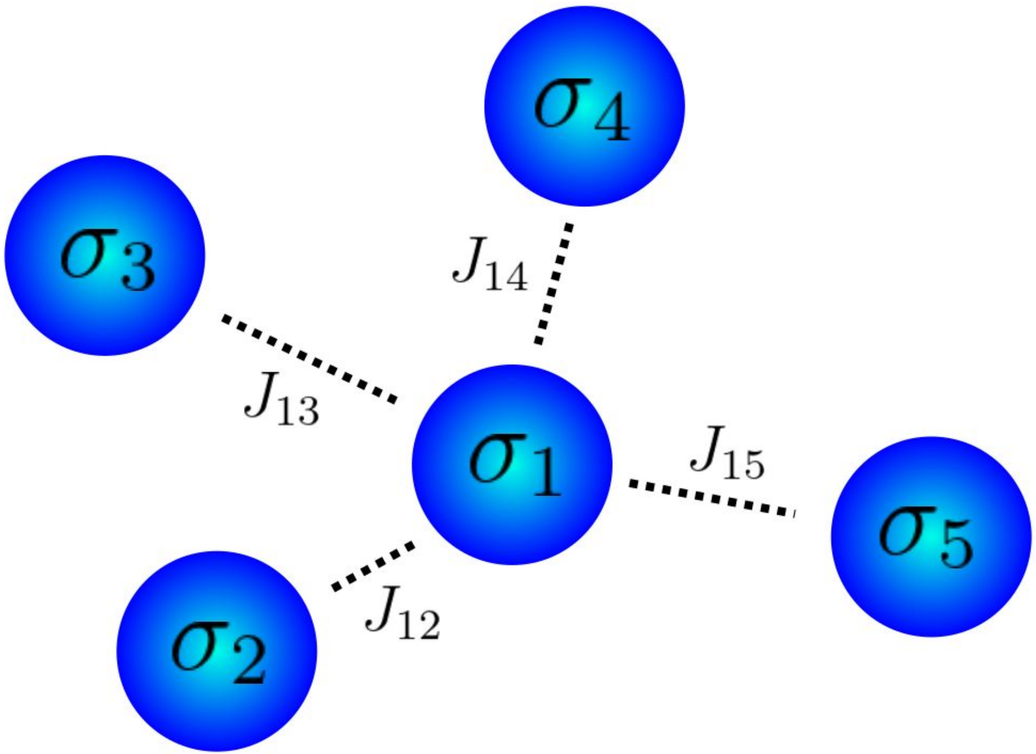
Spin Models



- Materials
- Biological cells
- Machine learning
- Combinatorial problems

$$\mathcal{H} = \sum_{i,j} J_{ij}\sigma_i\sigma_j$$

$$\sigma \in \{-1, 1\}$$

Monte Carlo simulation

Metropolis-Hastings algorithm

- Select random spin σ_i
- Flip its value $\sigma_i \to -\sigma_i$
- Calculate energy difference ΔE
- If ΔE < 0, accepts the flip
- Else accepts the flip with probability $p = e^{-\Delta E/k_B T}$

Differentiable Monte Carlo

Differentiable Monte Carlo

- Select random spin σ_i
- Flip its value $\sigma_i^{'} = -\sigma_i$
- Calculate energy difference ΔE
- Calculate the probability of flip $p = e^{-\Delta E / k_B T}$
- Calculate the weight $q = (1 + e^{-\alpha(p-r)})^{-1}$
- Change the spin value to $\sigma_i \leftarrow q\sigma_i^{'} + (1-q)\sigma_i$
- Optimize or discretize the spin values

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We have standard MC at $\alpha \to \infty$

Results

Finding the state with lowest energy

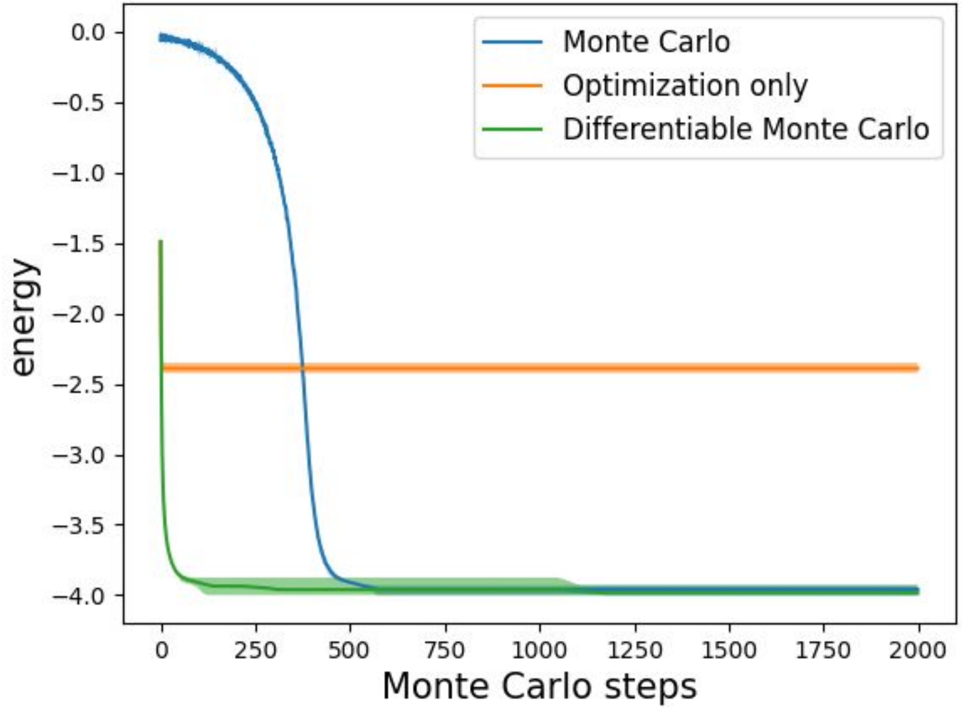
$$\mathcal{L} = \sum J_{i,j}\sigma_i\sigma_j$$

$$\sigma \leftarrow \sigma - \eta \frac{\partial \mathcal{L}}{\partial \sigma}$$

Finding the state with lowest energy

ferromagnetic Ising

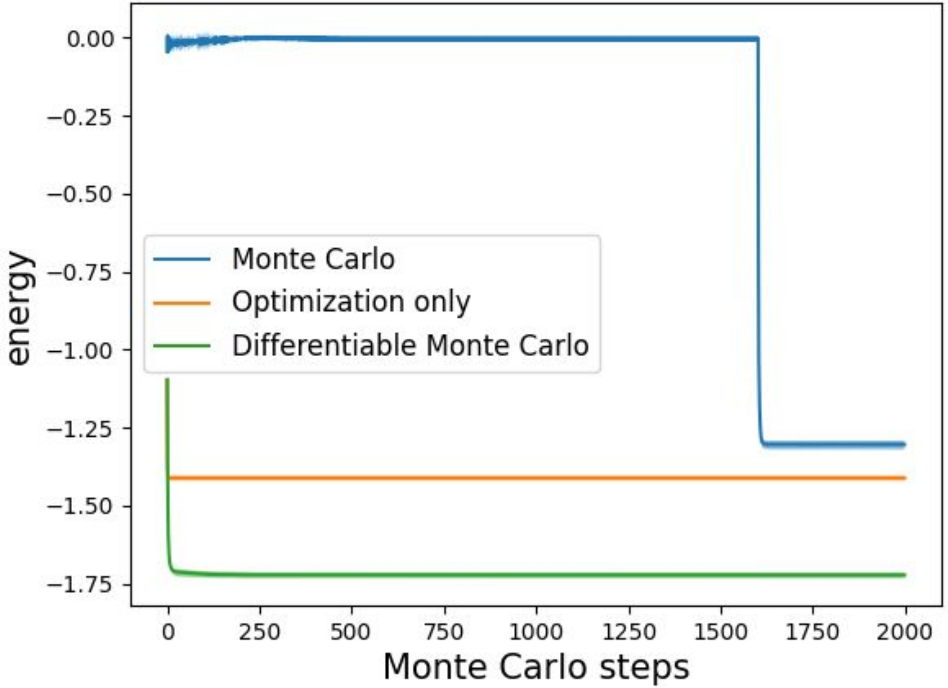
$$J_{ij} = -1 \ \forall \ \{i, j\}$$



Finding the state with lowest energy

spin glass

$$J_{ij} \in [-1, 1]$$



State preparation

$$\mathcal{L} = \frac{1}{N}\sum_i (\hat{\sigma}_i - \sigma_i)^2$$

$$J \leftarrow J - \eta \frac{\partial \mathcal{L}}{\partial J}$$

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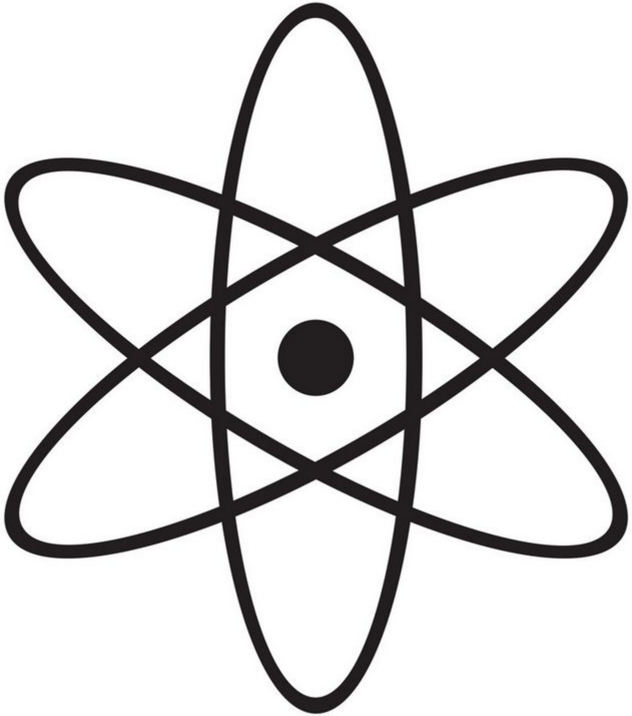
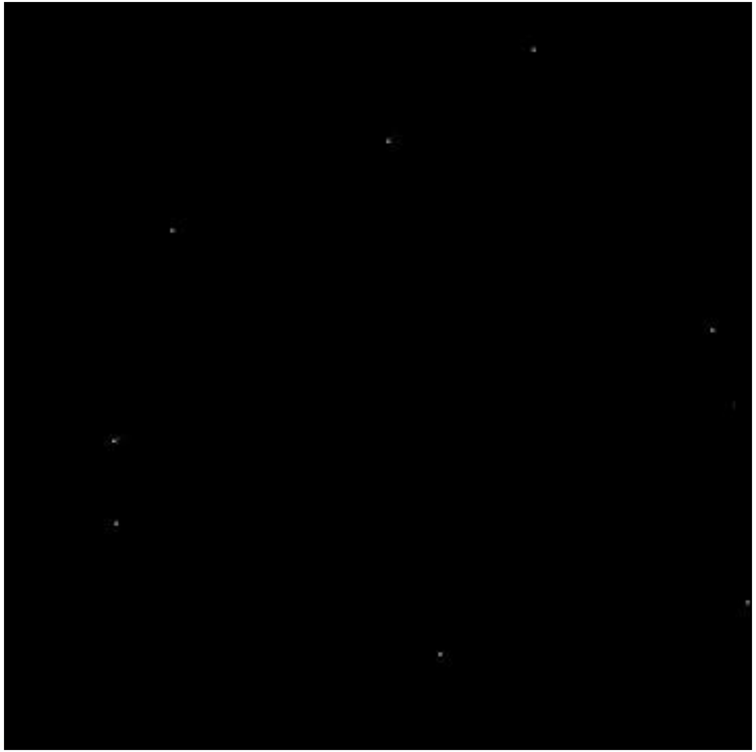
State preparation

Target

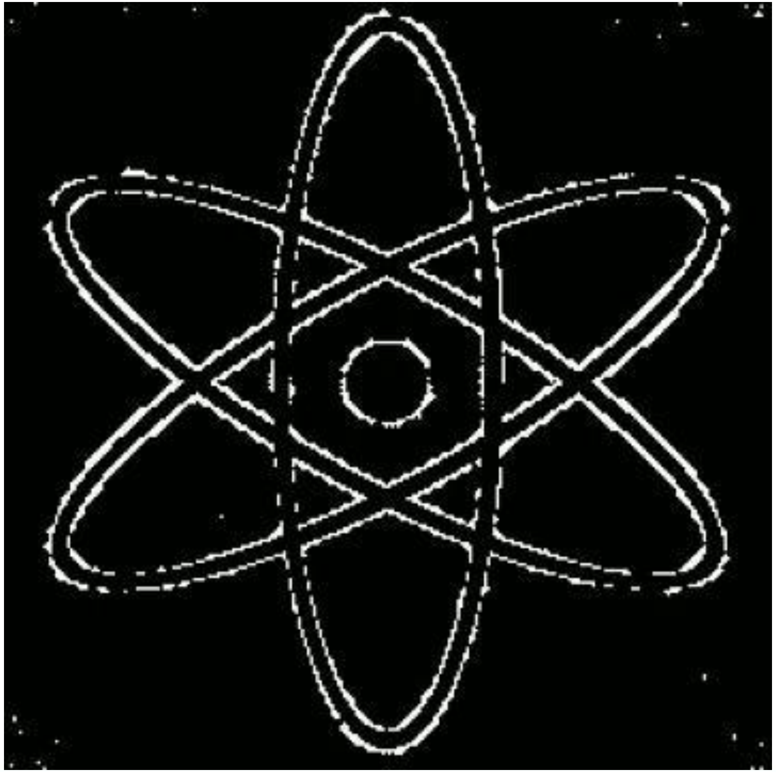


Training



State preparation

Simulation



Conclusions and future scope

- We presented Differentiable Monte Carlo, a method that can optimize spins or exchange parameters with Monte Carlo simulation;
- We applied DMC to optimize spins values in order to get the state of lowest energy;
- We applied DMC to optimize the exchange parameters in order for the spins to reach a specific distribution;

- We presented Differentiable Monte Carlo, a method that can optimize spins or exchange parameters with Monte Carlo simulation;
- We applied DMC to optimize spins values in order to get the state of lowest energy;
- We applied DMC to optimize the exchange parameters in order for the spins to reach a specific distribution;

- Apply DMC to combinatorial problems: vehicle routing, travelling salesman, etc;
- Apply DMC to machine learning: Boltzmann machine;
- Extend DMC to quantum spin models;
- Investigate material properties (e.g. topological materials) with DMC.

Thank you!

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