

Monte Carlo de cadena de Markov de muchas configuraciones (MCMCMC)

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Propuesta general

• Reproducir los resultados de Šimkovic y Ross en su artículo "Many-Configurations Markov-Chain Monte Carlo" (MCMCMC) [arXiv:2102.05613v1] en el que proponen una generalización del método de Monte Carlo de cadena de Markov (MCMC) y lo aplican a los modelos de Sherrington-Kirkpatrick y Fermi-Hubbard.

Many-Configuration Markov-Chain Monte Carlo

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We propose a minimal generalization of the celebrated Markov-Chain Monte Carlo algorithm which allows for an arbitrary number of configurations to be visited at every Monte Carlo step. This is advantageous when a parallel computing machine is available, or when many biased configurations can be evaluated at little additional computational cost. As an example of the former case, we report a significant reduction of the thermalization time for the paradigmatic Sherrington-Kirkpatrick spin-glass model. For the latter case, we show that, by leveraging on the exponential number of biased configurations automatically computed by Diagrammatic Monte Carlo, we can speed up computations in the Fermi-Hubbard model by two orders of magnitude.

Objetivos específicos

- Implementar los algoritmos de MCMC y MCMCMC para los modelos de Sherrington-Kirkpatrick y de Fermi-Hubbard
- Comparar el desempeño de MCMC vs. MCMCMC en el tiempo de termalización y la velocidad computacional para alcanzar un error deseado

Modelos matemáticos

Sherrington-Kirkpatrick: vidrios de espín

$$H = \frac{1}{\sqrt{L}} \sum_{j \le k} J_{jk} S_j S_k$$

$$\frac{\langle E \rangle}{L} = \frac{\sum_{\{S_j\}} e^{-H/T} H/L}{\sum_{\{S_j\}} e^{-H/T}}$$

[Wikipedia]

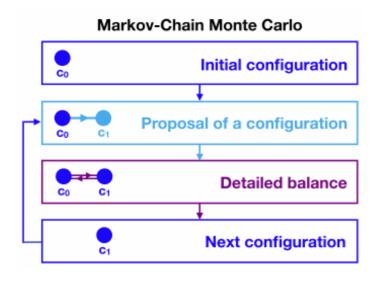
 Fermi-Hubbard 2D dopado: fermiones dopados en una red bidimensional

$$H = \sum_{k,\sigma} (\epsilon_k - \mu) c_{k\sigma}^{\dagger} c_{k\sigma} + U \sum_i n_{\uparrow i} n_{i\downarrow}$$

[Yamada, et. al., doi 10.1007/978-3-319-69953-0 14]

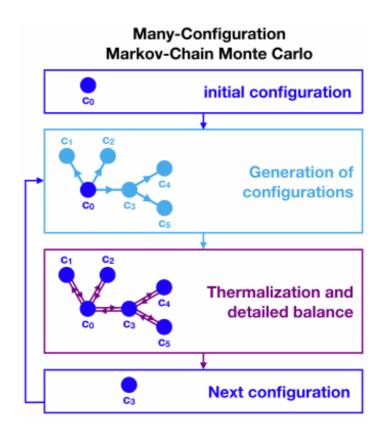
Método computacional

MCMC



VS

MCMCMC

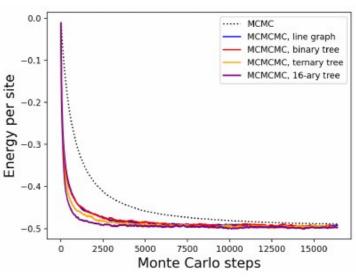


[arXiv:2102.05613v1]

Resultados a reproducir

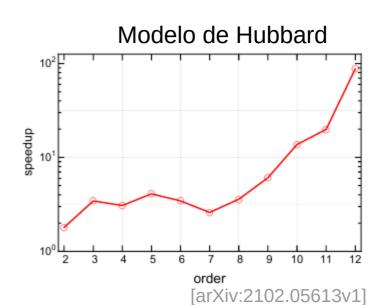
Termalización más rápida

Modelo Sh-K



[arXiv:2102.05613v1]

 Aceleración en el tiempo que que el Monte Carlo alcanza un error deseado



Referencias

- Fedor Šimkovic and Riccardo Rossi. Many-configuration markov-chain monte carlo, 2021. arXiv:2102.05613v1
- William H. Press, et al. Numerical Recipes The art of scientific computing, Third edition, Cambridge University Press, New York.
- Panchenko, Dmitry. "The Sherrington-Kirkpatrick model: an overview." Journal of Statistical Physics 149.2 (2012): 362-383.
- Hubbard, J. (1963). "Electron Correlations in Narrow Energy Bands". Proceedings of the Royal Society of London. 276 (1365): 238–257.