Extracting partition function zeros from Fukui-Todo simulations

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Introduction

Since its introduction by Lee and Yang in 1952 [1] and extension by Fisher in 1965 [2], the partition-function-zero approach has become established as a powerful tool to understand and analyse phase transitions at fundamental and precise levels. Despite extensive literature on its theory and applications (see for example the review [3] and references therein) only a few models permit exact computation or analytical estimation of zeros and their critical properties. Instead, the vast majority of cases necessitate computer simulations.

Introduced in 2009, the Fukui-Todo (FT) cluster algorithm is one of the most advanced approaches to Monte-Carlo simulations and it has proved especially important for systems with long-range interactions [4]. Its strength is that it performs in $O(N)$ time for long-range systems, an order of magnitude faster than the O(N^2) operations per sweep delivered by earlier, benchmark algorithms. However, its distinct feature of bypassing sample-by-sample computation of system energy has thus far hindered attempts to harness the power of the partition-function-zero approach.

Model

To demonstrate a method, we apply the algorithm to the q state Potts model. We consider each vertex i, j of an arbitrary graph as occupied by a spin s that can be in one of q discrete states $s_i = 1, \ldots, q$. Each edge or bond l represents an interaction between them. The corresponding Hamiltonian reads

$$H = -\sum_{\langle ij \rangle} J_{ij}\delta_{s_i s_j} = -\sum_{l} J_l \sigma_l,$$

where the first sum is over pairs of spins with J_{ij} the associated coupling constant.

The thermodynamic properties of the system are encoded in its partition function,

$$Z(\beta) = \sum_{\{s\}} e^{-\beta H}, \tag{1}$$

where β is a measure of inverse temperature and the sum is over all possible spin configurations.

Fukui-Todo algorithm

The FT algorithm utilises an extended representation of the Fortuin-Kasteleyn partition function. Each bond is assigned a variable that can take any non negative integer value $k_l \in \mathbb{N}_0$ and these values are distributed in a Poissonian manner [4]:

$$f(k_l; \lambda_l) = \frac{e^{-\lambda_l}\lambda_l^{k_l}}{k_l!},$$

where $\lambda_l = \beta J_l$. Bonds with $k_l = 0$ are considered as inactive and $k_l \geq 1$ as active. In this extended phase space the partition function is

$$Z_{\mathrm{FT}} = \sum_{\{s\}} \prod_{\ell=1}^{N_\mathrm{b}} \sum_{k_\ell=0}^{\infty} \Delta(\sigma_\ell, k_\ell) V_\ell(k_\ell) \tag{2}$$

where

$$\Delta(\sigma_l, k_l) = \begin{cases} 0 & \text{if } k_l \geq 1 \text{ and } \sigma_l = 0 \\ 1 & \text{otherwise} \end{cases} \qquad V_l(k_l) = \frac{(\beta J_l)^{k_l}}{k_l!}.$$

Summing over k_l in Eq.(2) delivers a partition function identical to (1).

The FT algorithm takes advantage of the Poisson process for independent events in that only one random variable needs to be generated and then distributed among the bonds with mean $\lambda_{\mathrm{tot}} = \beta \sum_l J_l$. Generating a random number from Poisson distribution takes $O(\lambda_{\mathrm{tot}})$ time, which is $O(N)$ for models with converging energy per spin. The second step, distributing these random numbers, can be performed in $O(1)$ time so that the full Monte-Carlo update in the FT approach takes $O(N)$ time.

Extracting the zeros through FT reweighting

From Eq. (2) it is easy to derive the relation between the partition functions at different temperatures [5]

$$Z_{\mathrm{FT}}(\beta') = Z_{\mathrm{FT}}(\beta)\Big\langle \left(\frac{\beta'}{\beta}\right)^{K} \Big\rangle_{\beta}. \tag{3}$$

Because K is distributed according to the Poisson distribution the average in Eq. (3) is convergent and, assuming that it is equivalent to the average over the simulation data, it transforms into $1/M \times \sum_{i=1}^{M} \left(\beta'/\beta\right)^{K_i}$, where the summation extends over all M measurements. Because the partition function $Z(\beta) > 0$ is strictly positive, one only has to find $\beta' \in \mathbb{C}$ such that

$$\frac{1}{M}\sum_{i=1}^{M}\left(\frac{\beta'}{\beta}\right)^{K_i} = 0. \tag{4}$$

This allows zeros at complex $\beta' = \beta_r + i\beta_i$ to be extracted from simulations performed at real temperatures β.

The minimal value $K_{\mathrm{min}} = \min\{K_i\}$ can be subtracted from each term in the sum changing it to the form

$$\sum_{i=1}^{M}\left(\frac{\beta'}{\beta}\right)^{K_i - K_{\mathrm{min}}} = 0. \tag{5}$$

Here K_{min} is the minimum value of K over each simulation with a given graph, temperature β and the number of states q. Since the ratio of the temperatures is non-zero, dividing each of the terms in the sum by a non-zero value does not change the location of the roots of this equation.

The solution of Eq. (5) can be estimated with the help of graphical representation.

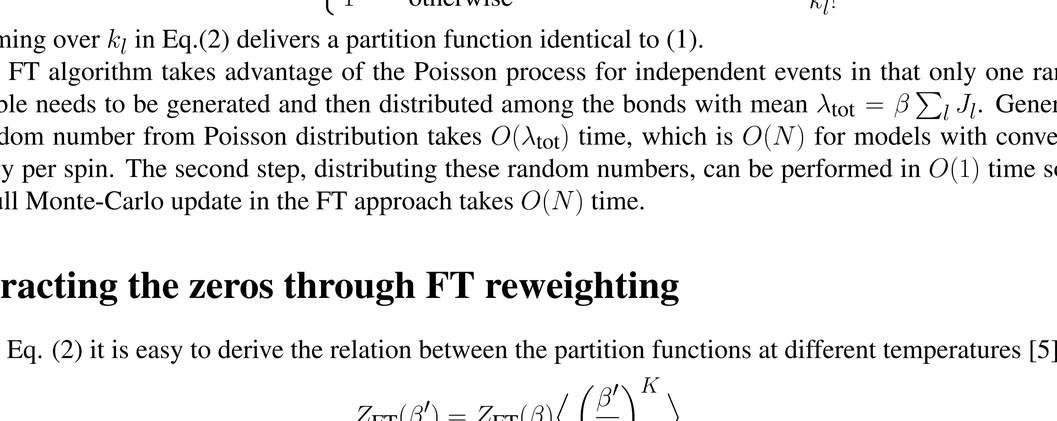

Figure 1: Blue and yellow lines represent the points where the real and imaginary parts of Eq. (4) (left plot) and Eq. (5) (right plot) change the sign. Subtracting the minimal value K_{min} allows to significantly "clean" the plot and better locate the intersection points, which are the Fisher zeros. This example is shown for the two dimensional Ising model $(q = 2, d = 2)$ on a square lattice with the system size 48×48.

Results

Having introduced the approach, we next need to calibrate it against previous approaches to substantiate claims as to its efficacy. The 2D Potts model is often used as a test bed in such circumstances because some results are known exactly. For $q \leq 4$ this model displays second-order phase transitions, while for $q > 4$ transitions are discontinuous. We consider $q = 2, 3, 6$ to straddle the two regimes. In the second order case, finite-size scaling of Fisher zero yields the correlation-length critical exponent ν: [6]

$$\begin{aligned} \mathrm{Re}\,\beta &= \beta_c + A \cdot L^{-1/\nu} \\ \mathrm{Im}\,\beta &= B \cdot L^{-1/\nu}. \end{aligned} \tag{6}$$

In the $q = 2$ (Ising) and $q = 3$ cases, $\nu = 1$ and $\nu = 5/6$, respectively. Formally identifying ν with $1/d$ in the first-order case, can be used to discriminate between the two types of phase transition so that ν is effectively 1/2 in our case of two dimensions.

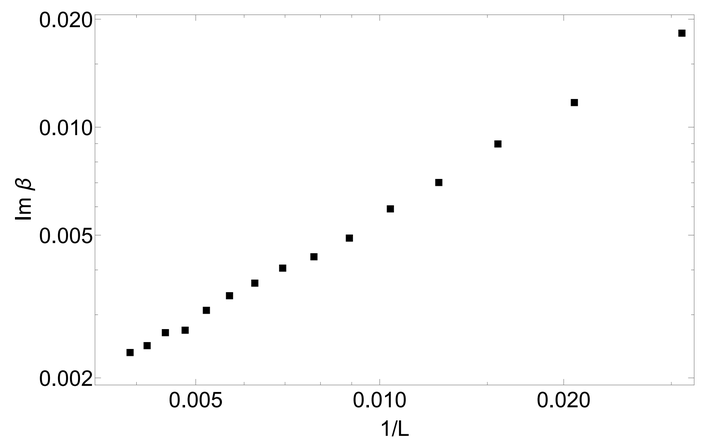

Figure 2: Imaginary parts of the coordinates of the first Fisher zero as a function of the inverse system size for the two dimensional Ising model $(q = 2, d = 2)$ on a square lattice of size L.

Having coordinates of the first Fisher zero for various system sizes allows using the FFS ansatz (6) to extract the values of the critical exponent ν from the scaling of the imaginary part and critical temperature T_c from the scaling of the real part. Resulting estimates are listed in Tab. 1.

q	M	L	T_c (exact)	T_c (our result)	ν (exact)	ν (our result)	ν (from literature)
2	500000	32-256	0.28365	0.28373(9)	1	1.042(7)	1.0016(25)(Nam 2008), 1.03(4)(Zheng 1998), 1.003(10)(Lee 1990), 1.00(4)(Tomita 2001)
3	500000	32-256	0.24874	0.24875(2)	0.8333	0.8359(9)	0.838(3)(Huang 2010), 0.81(2)(Schulke 1996), 0.824(4)(Nam 2008), 0.83(2)(Qian 2016), 0.8197(17)(Caparica 2015), 0.818(18)(Kim 1998)
6	200000	32-192	0.201902	0.201898(1)	0.5	0.535(2)	0.515(5)(Iino 2019)

Table 1: Comparing our results with exact values and results from other methods in the literature. The first column indicates three different numbers of states that were considered. The second and the third columns give exact critical temperature and the one obtained within our approach correspondingly. The last three columns are comparing exact value of the correlation length critical exponent with our results and those known in the literature.

Conclusions

We have presented a simple way to extract Fisher zeros from simulational data obtained within the Fukui-Todo algorithm. The advantage of the former is that it delivers more precise scaling than that coming from response functions. The advantage of the latter is that it requires $O(N)$ time even for long-range models. Combining these two approaches was hitherto impaired because the FT algorithm does not measure energy in each MC sample. Our results are in a good agreement with exact values and competitive with simulational results for response functions in the literature. However, early evidence suggests that our approach is computationally more efficient as it harnesses advantages of two powerful schemes widely used in statistical physics.

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