Lightning-quick introduction to dynamical mean field theory

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Last updated: December 10, 2022

Abstract

This is a very short introduction to the philosophy and algorithm of dynamical mean field theory (DMFT). I brought these points together and wrote this up mostly to cement my own understanding of the topic.

1 Introduction to single site DMFT

Dynamical mean field theory is a method of solving a lattice model by mapping it to a self-consistent impurity model with less degrees of freedom. Local observables on the lattice model are then calculated by solving the self-consistent impurity model. The mapping to a self-consistent impurity model holds only in a certain limit where the lattice self-energy becomes local: $\Sigma(k,\omega) = \Sigma(\omega)$.

2 Refresher on (static) mean field theory

The Curie-Weiss version of mean field theory involves replacing the spatial fluctuations in the Hamiltonian or the energy by an effective static field. The static field has to be determined self-consistently. To see what this means, we take the canonical example of the Ising model. Its Hamiltonian is given by

$$H = J\sum_{\langle ij\rangle} S_i^z S_j^z = J\sum_i S_i^z \sum_{j\in \text{NN of } i} S_j^z \tag{1}$$

In order to introduce the mean-field, we replace the spins S_j^z of the nearest-neighbour sites by their average value $\left\langle S_j^z\right\rangle \equiv m_j$:

$$H_{\text{MF}} = J\sum_i S_i^z \sum_{j\in \text{NN of } i} m_j \tag{2}$$

Because of translation symmetry, we expect the average local magnetisation to be independent of the position j: $m_j \equiv m_{\text{loc}}$. If z is the coordination number of the lattice, we get

$$H_{\text{MF}} = J\sum_i S_i^z zm = h_{\text{MF}}\sum_i S_i^z, \tag{3}$$

where we have defined the static mean field $h_{\text{MF}} \equiv Jzm_{\text{loc}}$. This mean field Hamiltonian is solvable, in terms of h_{MF}. The mean-field itself, however, is still unknown. To determine it, we will use the fact that if our approach is to be internally consistent, the average magnetisation $\langle S_i^z\rangle$ obtained from the mean-field Hamiltonian H_{MF} should be equal to that defined before, m_{loc}. This is again demanded on grounds of translation invariance. Since H_{MF} just consists of decoupled spins, the local Hamiltonian has two solutions: $S_i^z = \pm\frac{1}{2}$ with energies $\pm\frac{h_{\text{MF}}}{2}$. The local partition function Z_{MF} and hence the magnetisation at site i is then obtained easily:

$$Z_{\text{MF}} = 2\cosh\left(\beta h_{\text{MF}}/2\right), m = \frac{1}{Z_{\text{MF}}}\sum_{S_i^z=\pm\frac{1}{2}} S_i^z e^{-\beta h_{\text{MF}} S_i^z} = \tanh\left(\beta h_{\text{MF}}/2\right) \tag{4}$$

The self-consistency equation takes the form

$$m_{\text{loc}} = m = \tanh\left(\beta Jzm_{\text{loc}}/2\right) \tag{5}$$

This equation now has to be solved numerically, to obtain the value of the local magnetisation m_{loc}.

Even though this approach to obtaining the local magnetisation works for the Ising model, it is not very general; for a more complicated Hamiltonian, it will not be possible to solve it analytically and obtain an explicit self-consistency equation. We will therefore re-implement mean-field theory on the Ising model but now using a different approach, one that can be generalised to other models. This new approach involves the following steps:

1. Assume some initial guess value of m_{loc}.
2. Assume the mean-field form of the Hamiltonian, H_{MF} in terms of the chosen m_{loc}.
3. Solve this Hamiltonian to obtain a local magnetisation m.
4. Take this as the updated value of m_{loc}: $m_{\text{loc}} = m$, and construct a new Hamiltonian H_{MF} using the updated m_{loc}.
5. Restart from step 3.

The idea is that we start with a guess value of the environment local magnetisation m_{loc} and solve the Hamiltonian with this mean-field to obtain a value for the local magnetisation, m. These values will most probably not satisfy $m = \tanh \beta J z m_{\text{loc}}/2$, because we guess the value of m_{loc}. In order to get closer to the self-consistent value, we *update* m_{loc} by setting it equal to the value of m computed in the last step. We then solve the Hamiltonian with this updated value of m_{loc} to obtain a new value of m, and these values will be closer to the self-consistent value. We keep doing this until we converge to the self-consistent value. This is shown in Fig. 1.

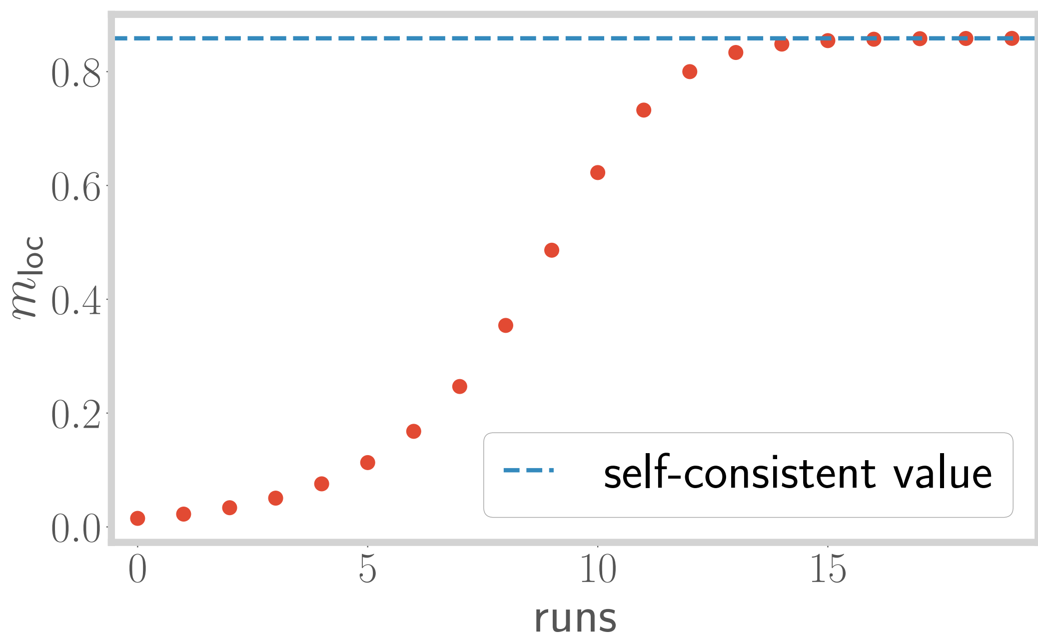

Figure 1: Convergence of the local magnetisation to the self-consistent value after repeatedly solving the Hamiltonian and updating it with the solution.

The more general approach to applying the mean field approximation can therefore be formalised as follows:

- Figure out what the self-consistency equation is. It will be of the following generic form: y = f(y).
- Replace the fluctuations by an effective local mean field $f(y)$, in order to obtain a simpler problem (the simplified Hamiltonian H_{MF}).
- Solve the simpler problem at a particular local site i by starting with some guess value of $f(y)$, to calculate the mean field y' from it.
- Create an updated Hamiltonian by setting $y = y'$.
- Solve this new Hamiltonian to obtain yet another updated y', and keep repeating this until y does not change.