Computational Statistical Physics

Part I: Statistical Physics and Phase Transitions

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Renormalization group

Self-similarity

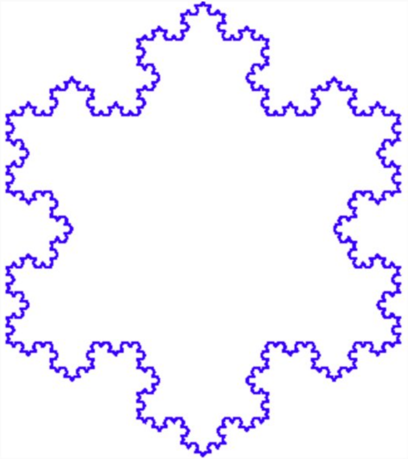

Figure 1: The Koch snowflake as an example of a self-similar pattern.

Renormalization and free energy

To build some intuition for renormalization approaches, we consider a scale transformation of the characteristic length L of our system with that leads to a rescaled characteristic length $\tilde{L} = L/l$

Moreover, we consider the partition function of an Ising system. A scale transformation with $\tilde{L} = L/l$ leaves the partition function

$$Z = \sum_{\{\sigma\}} e^{-\beta H} \tag{1}$$

and the corresponding free energy invariant.

Renormalization and free energy

Free energy density of the system also stays invariant under scale transformations. Since the free energy F is an *extensive* quantity[1], it scales with the system size and

$$F(\epsilon, H) \quad = l^{-d} \tilde{F}\left(\tilde{\epsilon}, \tilde{H}\right) \text{ with } \quad \epsilon = T - T_c, \tag{2}$$

where $\tilde{F}$ is the renormalized free energy.

[1] *Extensive* quantities such as volume or the total mass of a gas are proportional to the system size. *Intensive* quantities are not dependent on the system size, e.g., the energy density or the temperature.

Renormalization and free energy

We can rescale previous equation by setting

$$\tilde{\epsilon} = l^{y_T} \epsilon \quad \text{and} \quad \tilde{H} = l^{y_H} H \tag{3}$$

and obtain in terms of the renormalized free energy

$$\tilde{F}\left(\tilde{\epsilon}, \tilde{H}\right) = \tilde{F}\left(l^{y_T} \epsilon, l^{y_H} H\right). \tag{4}$$

Renormalization and free energy

Since renormalization also affects the correlation length

$$\xi \sim |T - T_c|^{-\nu} = |\epsilon|^{-\nu} \tag{5}$$

we can relate the critical exponent ν to y_T.

The renormalized correlation length $\tilde{\xi} = \xi/l$ scales as

$$\tilde{\xi} \sim \tilde{\epsilon}^{-\nu}. \tag{6}$$

Renormalization and free energy

And due to

$$l^{y_T}\epsilon = \tilde{\epsilon} \sim \epsilon l^{\frac{1}{\nu}}, \tag{7}$$

we find $y_T = 1/\nu$.

The critical point is a fixed point of the transformation since $\epsilon = 0$ at T_c and ϵ does not change indepedent of the value of the scaling factor.

Majority rule

A straightforward example which can be regarded as renormalization of spin systems is the *majority rule*. Instead of considering all spins in a certain neighborhood separately, one just takes the direction of the net magnetization of these regions as new spin value, i.e.,

$$\tilde{\sigma}_{\tilde{i}} = \text{sign}\left(\sum_{\text{region}} \sigma_i\right). \tag{8}$$

Majority rule

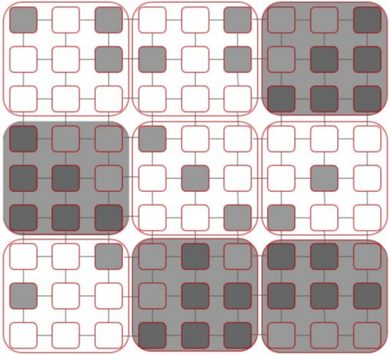

Figure 2: An illustration of the majority rule renormalization.

Decimation of the one-dimensional Ising model

Another possible rule is *decimation* which eliminates certain spins, generally in a regular pattern.

The spins only interact with their nearest neighbors and the coupling constant $K = J/(k_B T)$ is the same for all spins.

Decimation of the one-dimensional Ising model

Figure 3: An example of a one-dimensional Ising chain.

Decimation of the one-dimensional Ising model

To further analyze this system, we compute its partition function Z and obtain

$$
\begin{aligned}
Z &= \sum_{\{\sigma\}} e^{K \sum_i \sigma_i} = \sum_{\sigma_{2i}=\pm 1} \prod_{2i} \left[\sum_{\sigma_{2i+1}=\pm 1} \prod_{2i+1} e^{K(\sigma_{2i}\sigma_{2i+1} + \sigma_{2i+1}\sigma_{2i+2})} \right] \\
&= \sum_{\sigma_{2i}=\pm 1} \prod_{2i} \left\{ 2\text{cosh}\left[K\left(\sigma_{2i} + \sigma_{2i+2}\right)\right]\right\} \\
&= \sum_{\sigma_{2i}=\pm 1} \prod_{2i} z\left(K\right) e^{K' \sigma_{2i}\sigma_{2i+2}} \\
&= \left[z\left(K\right)\right]^{\frac{N}{2}} \sum_{\sigma_{2i}=\pm 1} \prod_{2i} e^{K' \sigma_{2i}\sigma_{2i+2}},
\end{aligned}
\tag{9}
$$

where we used in the third step that the $\cosh(\cdot)$ function only depends on even spins.

Decimation of the one-dimensional Ising model

According to Eq. (9), the relation

$$Z(K,N) = [z\,(K)]^{\frac{N}{2}}\, Z(K',N/2) \tag{10}$$

holds as a consequence of the decimation method. The function $z(K)$ is the spin-independent part of the partition function and K' is the renormalized coupling constant.

Decimation of the one-dimensional Ising model

We compute the relation
$z(K)\, e^{K' s_{2i} s_{2i+2}} = 2\cosh\left[K\left(s_{2i} + s_{2i+2}\right)\right]$ explicitly and find

$$z(K)\, e^{K' s_{2i} s_{2i+2}} = \begin{cases} 2\cosh(2K) & \text{if } s_{2i} = s_{2i+2}, \\ 2 & \text{otherwise .} \end{cases} \qquad (11)$$

Decimation of the one-dimensional Ising model

Dividing and multiplying the latter two expressions yields

$$e^{2K'} = \cosh(2K) \quad \text{and} \quad z^2(K) = 4\cosh(2K). \tag{12}$$

And the renormalized coupling constant K' in terms of K is given by

$$K' = \frac{1}{2}\ln\left[\cosh(2K)\right]. \tag{13}$$

Decimation of the one-dimensional Ising model

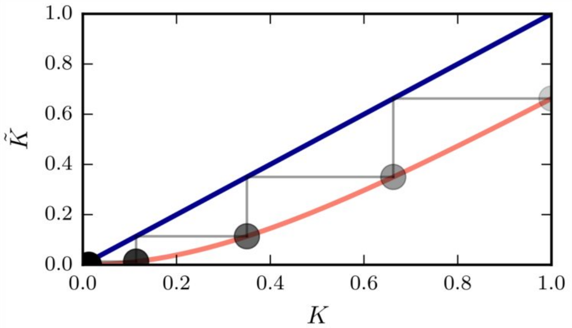

Figure 4: An illustration of the fixed point iteration defined by Eq. 13.

Decimation of the one-dimensional Ising model

Given the partition function, we now compute the free energy according to $F = -k_B T N f(K) = -k_B T \ln(Z)$, with $f(K)$ being the free energy density. Taking the logarithm of Eq. 10, we get:

$$\ln[Z(K,N)] = N f(K) = \frac{1}{2} N \ln[z(K)] + \frac{1}{2} N f(\tilde{K}) \tag{14}$$

Based on the previous equation, we can derive the following recursive relation for the free energy density

$$f(\tilde{K}) = 2 f(K) - \ln[2 \ \cosh \ (2K)^{\frac{1}{2}}] \tag{15}$$

Decimation of the one-dimensional Ising model

There exists one *stable fixed point* at $K^* = 0$ and another *unstable one* at $K^* \to \infty$. Every fixed point $(K^* = \tilde{K})$ implies that Eq. 15 can be rewritten due to $f(\tilde{K}) = f(K^*)$.

The case of $K^* = 0$ corresponds to the high-temperature limit where the free energy approaches the value

$$F = -k_B T N f(K^*) = -k_B T N \ln(2). \qquad (16)$$

In this case, the entropy dominates the free energy.

Decimation of the one-dimensional Ising model

For $K^* \to \infty$, the system approaches the low temperature limit and the free energy is given by

$$F = -k_B T N f(K^*) = -k_B T N K = -NJ, \qquad (17)$$

i.e., the free energy of the system is given by its internal energy.

Generalization

In general, multiple coupling constants are necessary, e.g., in the two-dimensional Ising model. Thus, we have to construct a renormalized Hamiltonian based on multiple renormalized coupling constants, i.e.,

$$\tilde{H} = \sum_{\alpha=1}^{M} \tilde{K}_\alpha \tilde{O}_\alpha \text{ with } \tilde{O}_\alpha = \sum_i \prod_{k \in c_\alpha} \tilde{\sigma}_{i+k} \tag{18}$$

where c_α is the configuration subset over which we renormalize and

$$\tilde{K}_\alpha \left(K_1, \ldots, K_M\right) \quad \text{with} \quad \alpha \in \{1, \ldots, M\} \, .$$

Generalization

At T_c there exists a fixed point $K_\alpha^* = \tilde{K}_\alpha\left(K_1^*, \ldots, K_M^*\right)$. A first ansatz to solve this problem is the linearization of the transformation. Thus, we compute the Jacobian $T_{\alpha,\beta} = \frac{\partial \tilde{K}_\alpha}{\partial K_\beta}$ and obtain

$$\tilde{K}_\alpha - K_\alpha^* = \sum_\beta T_{\alpha,\beta}\big|_{K^*}\left(K_\beta - K_\beta^*\right) \tag{19}$$

Generalization

To analyze the behavior of the system close to criticality, we consider eigenvalues $\lambda_1, \ldots, \lambda_M$ and eigenvectors $\phi_1, \ldots, \phi_M$ of the linearized transformation defined by Eq. (19). The eigenvectors fulfill $\tilde{\phi}_\alpha = \lambda_\alpha \phi_\alpha$ and the fixed point is unstable if $\lambda_\alpha > 1$.

Generalization

The largest eigevalue dominates the iteration and we can identify the scaling field $\tilde{\epsilon} = l^{y_T}\epsilon$ with the eigenvector of the transformation, and the scaling factor with eigenvalue $\lambda_T = l^{y_T}$. Then, we compute the exponent ν according to

$$\nu = \frac{1}{y_T} = \frac{\log(l)}{\log(\lambda_T)}. \tag{20}$$

Monte Carlo renormalization group

Since we are dealing with generalized Hamiltonians with many interaction terms, we compute the thermal average using the operators O_α, i.e.,

$$\langle O_\alpha \rangle = \frac{\sum_{\{\sigma\}} O_\alpha e^{\sum_\beta K_\beta O_\beta}}{\sum_{\{\sigma\}} e^{\sum_\beta K_\beta O_\beta}} = \frac{\partial F}{\partial K_\alpha} \tag{21}$$

where F is the free energy.

Monte Carlo renormalization group

Using the fluctuation-dissipation theorem, we can also numerically calculate the response functions:

$$\chi_{\alpha,\beta} = \frac{\partial \langle O_\alpha \rangle}{\partial K_\beta} = \langle O_\alpha O_\beta \rangle - \langle O_\alpha \rangle \langle O_\beta \rangle ,$$

$$\tilde{\chi}_{\alpha,\beta} = \frac{\partial \left\langle \tilde{O}_\alpha \right\rangle}{\partial K_\beta} = \left\langle \tilde{O}_\alpha O_\beta \right\rangle - \left\langle \tilde{O}_\alpha \right\rangle \langle O_\beta \rangle .$$

Monte Carlo renormalization group

Using the chain rule, one can calculate with equation (21) that

$$\tilde{\chi}^{(n)}_{\alpha,\beta} = \frac{\partial \left\langle \tilde{O}^{(n)}_{\alpha} \right\rangle}{\partial K_\beta} = \sum_\gamma \frac{\partial \tilde{K}_\gamma}{\partial K_\beta} \frac{\partial \left\langle \tilde{O}^{(n)}_{\alpha} \right\rangle}{\partial K_\gamma} = \sum_\gamma T_{\gamma,\beta} \chi^{(n)}_{\alpha,\gamma}.$$

It is thus possible to derive a value of $T_{\gamma,\beta}$ from the correlation functions by solving a set of M coupled linear equations. At point $K = K^*$, we can apply this method in an iterative manner to compute critical exponents as suggested by Eq. 20.

Monte Carlo renormalization group

There are many error sources in this technique, that originate from the fact that we are using a combination of several tricks to obtain our results:

- Statistical errors,
- Truncation of the Hamiltonian to the M^{th} order,
- Finite number of scaling iterations,
- Finite size effects,
- No precise knowledge of K^*.