7.9: Appendix I- Equivalence of the Mean Field Descriptions

In both the variational density matrix and mean field Hamiltonian methods as applied to the Ising model, we obtained the same result $m=\tanh\big((m+h)/\theta\big)$. What is perhaps not obvious is whether these theories are in fact the same, if their respective free energies agree. Indeed, the two free energy functions,

`\begin{split} f\nd_\ssr{A}(m,h,\theta)&=-\half\,m^2 -h m + \theta\> \bigg\{\bigg({1+m\over 2}\bigg) \ln \bigg({1+m\over 2}\bigg) +\bigg({1- m\over 2}\bigg) \ln \bigg({1-m\over 2}\bigg) \bigg\}\\ f\nd_\ssr{B}(m,h,\theta)&`

where `f\ns_\ssr{A}` is the variational density matrix result and `f\ns_\ssr{B}` is the mean field Hamiltonian result, clearly are different functions of their arguments. However, it turns out that upon minimizing with respect to m in each cast, the resulting free energies obey `f\nd_\ssr{A}(h,\theta)=f\nd_\ssr{B}(h,\theta)`. This agreement may seem surprising. The first method utilizes an approximate (variational) density matrix applied to the exact Hamiltonian $\hat{H}$. The second method approximates the Hamiltonian as `\HH\ns_\ssr{MF}`, but otherwise treats it exactly. The two Landau expansions seem hopelessly different:

`\begin{split} f\nd_\ssr{A}(m,h,\theta)&=-\theta\,\ln 2 - hm +\half\, (\theta-1) \,m^2 + \frac{\theta}{12}\,m^4 + \frac{\theta}{30}\,m^6 + \ldots\vph\\ f\nd_\ssr{B}(m,h,\theta)&=-\theta\,\ln 2 + \half m^2 - {(m+h)^2\over 2\,\t`

We shall now prove that these two methods, the variational density matrix and the mean field approach, are in fact equivalent, and yield the *same* free energy $f(h,\theta)$.

Let us generalize the Ising model and write

$$\hat{H}=-\sum_{i<j} J_{ij}\,\varepsilon(\sigma_i,\sigma_j)-\sum_i \Phi(\sigma_i)\ . \tag{7.9.1}$$

Here, each 'spin' σ_i may take on any of K possible values, $\{s_1,\ldots,s_K\}$. For the $S=1$ Ising model, we would have $K=3$ possibilities, with $s_1=-1$, $s_2=0$, and $s_3=+1$. But the set $\{s_\alpha\}$, with $\alpha\in\{1,\ldots,K\}$, is completely arbitrary[20]. The 'local field' term $\Phi(\sigma)$ is also a completely arbitrary function. It may be linear, with $\Phi(\sigma)=H\sigma$, for example, but it could also contain terms quadratic in σ, or whatever one desires.

The symmetric, dimensionless interaction function $\varepsilon(\sigma,\sigma')=\varepsilon(\sigma',\sigma)$ is a real symmetric $K\times K$ matrix. According to the singular value decomposition theorem, any such matrix may be written in the form

$$\varepsilon(\sigma,\sigma')=\sum_{p=1}^{N_s} A_p\,\lambda_p(\sigma)\,\lambda_p(\sigma')\ , \tag{7.9.2}$$

where the $\{A_p\}$ are coefficients (the singular values), and the $\big\{\lambda_p(\sigma)\big\}$ are the singular vectors. The number of terms N_s in this decomposition is such that $N_s\le K$. This treatment can be generalized to account for continuous σ.

Variational Density Matrix

The most general single-site variational density matrix is written

$$\varrho(\sigma)=\sum_{\alpha=1}^K x_\alpha\,\delta_{\sigma,s_\alpha}\ . \tag{7.9.3}$$

Thus, x_α is the probability for a given site to be in state α, with $\sigma=s_\alpha$. *The* $\{x_\alpha\}$ are the K variational parameters, subject to the single normalization constraint, $\sum_\alpha x_\alpha=1$. We now have

$$\begin{aligned} f&=\frac{1}{N\hat{J}(0)}\bigg\{\textsf{Tr}\,(\varrho\hat{H})+k_BT\ \textsf{Tr}\,(\varrho\ln\varrho)\bigg\}\\ &=-\frac{1}{2}\sum_p\sum_{\alpha,\alpha'} A_p\,\lambda_p(s_\alpha)\,\lambda_p(s_{\alpha'})\,x_\alpha\,x_{\alpha'}-\sum_\alpha\varphi(s_\alpha)\,x_\alpha+\theta\sum_\alpha x_\alpha\ln x_\alpha\ , \end{aligned}$$

where $\varphi(\sigma)=\Phi(\sigma)/\hat{J}(0)$. We extremize in the usual way, introducing a Lagrange undetermined multiplier ζ to enforce the constraint. This means we extend the function $f\big(\{x_\alpha\}\big)$, writing

$$f^*(x_1,\ldots,x_K,\zeta)=f(x_1,\ldots,x_K)+\zeta\left(\sum_{\alpha=1}^K x_\alpha-1\right)\ , \tag{7.9.4}$$

and freely extremizing with respect to the $(K+1)$ parameters $\{x_1,\ldots,x_K,\zeta\}$. This yields K nonlinear equations,

$$0=\frac{\partial f^*}{\partial x_\alpha}=-\sum_p\sum_{\alpha'} A_p\,\lambda_p(s_\alpha)\,\lambda_p(s_{\alpha'})\,x_{\alpha'}-\varphi(s_\alpha)+\theta\,\ln x_\alpha+\zeta+\theta\ , \tag{7.9.5}$$

for each α, and one linear equation, which is the normalization condition,

$$0=\frac{\partial f^*}{\partial\zeta}=\sum_\alpha x_\alpha-1\ . \tag{7.9.6}$$

We cannot solve these nonlinear equations analytically, but they may be recast, by exponentiating them, as

$$x_\alpha=\frac{1}{Z}\,\exp\left\{\frac{1}{\theta}\left[\sum_p\sum_{\alpha'} A_p\,\lambda_p(s_\alpha)\,\lambda_p(s_{\alpha'})\,x_{\alpha'}+\varphi(s_\alpha)\right]\right\}\ , \tag{7.9.7}$$

with

$$Z=e^{(\zeta/\theta)+1}=\sum_\alpha\exp\left\{\frac{1}{\theta}\left[\sum_p\sum_{\alpha'} A_p\,\lambda_p(s_\alpha)\,\lambda_p(s_{\alpha'})\,x_{\alpha'}+\varphi(s_\alpha)\right]\right\}\ . \tag{7.9.8}$$

From the logarithm of x_α, we may compute the entropy, and, finally, the free energy:

$$f(\theta)=\frac{1}{2}\sum_p\sum_{\alpha,\alpha'} A_p\,\lambda_p(s_\alpha)\,\lambda_p(s_{\alpha'})\,x_\alpha\,x_{\alpha'}-\theta\ln Z\ , \tag{7.9.9}$$

which is to be evaluated at the solution of [nonla], $\big\{x^*_\alpha(h,\theta)\big\}$

Mean Field Approximation

We now derive a mean field approximation in the spirit of that used in the Ising model above. We write

$$\lambda_p(\sigma)=\big\langle\lambda_p(\sigma)\big\rangle+\delta\lambda_p(\sigma)\ , \tag{7.9.10}$$

and abbreviate $\labar_p=\big\langle\lambda_p(\sigma)\big\rangle$, the thermodynamic average of $\lambda_p(\sigma)$ on any given site. We then have

$$\begin{aligned}\lambda_p(\sigma)\,\lambda_p(\sigma') &= \labar_p^2 + \labar_p\,\delta\lambda_p(\sigma) + \labar_p\,\delta\lambda_p(\sigma') + \delta\lambda_p(\sigma)\,\delta\lambda_p(\sigma') \\ &= -\labar_p^2 + \labar_p\,\big(\lambda_p(\sigma) + \lambda_p(\sigma')\big) + \delta\lambda_p(\sigma)\,\delta\lambda_p(\sigma')\,.\end{aligned}$$

The product $\delta\lambda_p(\sigma)\,\delta\lambda_p(\sigma')$ is of second order in fluctuations, and we neglect it. This leads us to the mean field Hamiltonian,

\HH\ns_\ssr{MF}=+\half N \jhz\sum_p A_p\,\labar_p^2 -\sum_i \bigg[\jhz\sum_p A_p\,\labar_p\,\lambda_p(\sigma_i) + \RPhi(\sigma_i)\bigg]\ .

The free energy is then

$$f\big(\{\labar_p\},\theta\big) = \frac{1}{2}\sum_p A_p\,\labar_p^2 - \theta\,\ln\sum_\alpha \exp\left\{\frac{1}{\theta}\left[\sum_p A_p\,\labar_p\,\lambda_p(s_\alpha) + \varphi(s_\alpha)\right]\right\}\,. \tag{7.9.11}$$

The variational parameters are the mean field values $\{\labar_p\}$.

The single site probabilities $\{x_\alpha\}$ are then

$$x_\alpha = \frac{1}{Z}\,\exp\left\{\frac{1}{\theta}\left[\sum_p A_p\,\labar_p\,\lambda_p(s_\alpha) + \varphi(s_\alpha)\right]\right\}\,, \tag{7.9.12}$$

with Z implied by the normalization $\sum_\alpha x_\alpha = 1$. These results reproduce exactly what we found in Equation [nonla], since the mean field equation here, $\partial f/\partial\labar_p = 0$, yields

$$\labar_p = \sum_{\alpha=1}^K \lambda_p(s_\alpha)\,x_\alpha\,. \tag{7.9.13}$$

The free energy is immediately found to be

$$f(\theta) = \frac{1}{2}\sum_p A_p\,\labar_p^2 - \theta\,\ln Z\,, \tag{7.9.14}$$

which again agrees with what we found using the variational density matrix.

Thus, whether one extremizes with respect to the set $\{x_1,\ldots,x_K,\zeta\}$, or with respect to the set $\{\labar_p\}$, the results are the same, in terms of all these parameters, as well as the free energy $f(\theta)$. Generically, both approaches may be termed 'mean field theory' since the variational density matrix corresponds to a mean field which acts on each site independently[21].