Information Geometry of Mean Field Approximation for Quantum Boltzmann Machines

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Abstract. Mean field theory(MFT), originated in statistical physics, has been widely used both in classical and quantum settings. In particular, mean field approximation(MFA) which is based on the MFT has been extensively used for the classical Boltzmann machine(CBM) and also several authors have discussed its properties in view of information geometry(IG). In this paper, we apply MFA to the quantum Boltzmann machine(QBM) and discuss its properties using the information geometrical concepts. The quantum relative entropy as a quantum divergence function is used for approximation, where e-(exponential) and m-(mixture) projections play an important role. We derive the naive mean field equations for QBMs from the viewpoint of IG. Finally, we outline the formulation which leads to the higher-order MFAs.

Keywords: classical Boltzmann machine, quantum Boltzmann machine, information geometry, mean field theory, Kullback-Leibler(KL) divergence, quantum relative entropy, quantum exponential family

1 IG of MFA for CBMs

Let us consider a CBM (see [1]) where $x = (x_1, \cdots, x_n)$; $x_i = \pm 1$ denotes the values of n spin variables. The equilibrium distribution is given by

$$q = \exp\Big\{\sum_i h_i x_i + \sum_{i<j} w_{ij} x_i x_j - \psi(q)\Big\}, \qquad (1)$$

where $\psi(q)$ is the normalization constant. Here, h_i, w_{ij} are parameters and we assume $w_{ij} = w_{ji}$ and $w_{ii} = 0$.

Let $\mathcal{S}$ be the manifold of CBMs of the form (1), where (w_{ij}, h_i) together form a coordinate system and specify each distribution in $\mathcal{S}$. Let E_q be the expectation with respect to $q \in \mathcal{S}$. Then, the expectations $\eta_{ij} := E_q[x_i x_j]$ and $m_i := E_q[x_i]$ jointly form another coordinate system for $\mathcal{S}$. We know that $\{m_i\}$ are related to $\{w_{ij}, h_i\}$ by $m_i = \frac{\partial \psi(q)}{\partial h_i}$, but the partition function $\exp(\psi(q))$ is difficult to calculate for a large system. Our objective is to obtain a good approximation of m_i for a given $q \in \mathcal{S}$.

Let $\mathcal{M}$ be the set of product distributions in $\mathcal{S}$ specified by $w_{ij} = 0$, whose elements are written as

$$p = \exp\Big\{\sum_i \bar{h}_i x_i - \psi(p)\Big\}.$$

This is a submanifold of $\mathcal{S}$ having $\bar{h}_i$ as its coordinates. The expectations $\bar{m}_i := E_p[x_i]$ form another coordinate system of $\mathcal{M}$. For a given $p \in \mathcal{M}$, it is easy to obtain $\bar{m}_i = E_p[x_i]$ because x_i's are independent. We can calculate $\bar{m}_i$ to be $\bar{m}_i = E_p[x_i] = \tanh(\bar{h}_i)$. The simple idea behind the MFA for a $q \in \mathcal{S}$ is to use quantities obtained in the form of expectation with respect to some relevant $p \in \mathcal{M}$.

Let us now define the KL divergence on $\mathcal{S}$ for $q, p \in \mathcal{S}$ as $D(q\|p) \stackrel{\text{def}}{=} \sum_x q(x)[\log q(x) - \log p(x)]$. Given $q = q(\cdot, w, h) \in \mathcal{S}$, its e- and m- projections (see [5]) to $\mathcal{M}$ are defined by

$$p^{*(e)} \stackrel{\text{def}}{=} \arg\min_{p\in\mathcal{M}} D(p\|q) \quad \text{and} \quad p^{*(m)} \stackrel{\text{def}}{=} \arg\min_{p\in\mathcal{M}} D(q\|p)$$

respectively. While the m-projection of q to $\mathcal{M}$ gives the true values of expectations, that is $m_i = \bar{m}_i$ or $E_q[x_i] = E_p[x_i]$ for $p = p^{*(m)}$, the e-projection of q to $\mathcal{M}$ gives the naive MFA ([3], [4]). It is well known that the naive mean field equations for CBMs are given by

$$\bar{m}_i = \tanh\Big(\sum_j w_{ij}\bar{m}_j + h_i\Big),$$

where $\bar{m}_i = E_p[x_i]$ for $p = p^{*(e)}$.

2 IG of MFA for QBMs

2.1 The manifold of QBMs and its submanifold of product states

The equilibrium states of an n-element QBM defined in [2] can be represented as

$$\rho = \exp\Big[\sum_{i,s} h_{is}\sigma_{is} + \sum_{i<j}\sum_{s,t} w_{ijst}\sigma_{is}\sigma_{jt} - \psi(\rho)\Big], \qquad (2)$$

where $\sigma_{is} = I^{\otimes(i-1)} \otimes \sigma_s \otimes I^{\otimes(n-i)}$ and $\psi(\rho)$ is the normalization constant. Here, I is the identity matrix and σ_s for $s = x, y, z$ being the Pauli matrices. Furthermore, h_{is}, w_{ijst} are parameters and we assume that $w_{ijst} = w_{jits}$ and $w_{iist} = 0$.

Let $\mathcal{S}$ be the manifold of QBMs of the form (2), which is a quantum exponential family (QEF) in the sense given in [2], where (w_{ijst}, h_{is}) form a coordinate system to specify each QBM in $\mathcal{S}$. The expectations $\eta_{ijst} := \mathrm{Tr}[\rho\,\sigma_{is}\sigma_{jt}]$ and $m_{is} := \mathrm{Tr}[\rho\,\sigma_{is}]$ form another coordinate system for $\mathcal{S}$. Our objective is to obtain a good approximation of m_{is} for a given QBM ρ.

Now consider the subset $\mathcal{M}$ of $\mathcal{S}$ such that $w_{ijst} = 0$. Then $\mathcal{M}$ consists of all the product density operators of the form

$$\tau = \exp\Big\{\sum_{i,s} \bar{h}_{is}\sigma_{is} - \psi(\tau)\Big\}, \qquad (3)$$

where $\psi(\tau) = \sum_i \log\{\exp(\|\bar{h}_i\|) + \exp(-\|\bar{h}_i\|)\}$ with $\|\bar{h}_i\| := \sqrt{\sum_s (\bar{h}_{is})^2}$. This is a submanifold of $\mathcal{S}$ specified by $w_{ijst} = 0$ and $\bar{h}_{is}$ as its coordinates. Moreover,

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it forms a QEF. The expectation coordinates of $\mathcal{M}$ are related to $\{\bar{h}_{is}\}$ by

$$\bar{m}_{is} = \mathrm{Tr}[\tau\sigma_{is}] = \frac{\partial\psi(\tau)}{\partial\bar{h}_{is}} = \frac{\bar{h}_{is}}{||\bar{h}_i||}\tanh(||\bar{h}_i||) \quad (4)$$

$$\text{or} \quad \bar{h}_{is} = \frac{\bar{m}_{is}}{||\bar{m}_i||}\tanh^{-1}(||\bar{m}_i||). \quad (5)$$

2.2 The e,m-projection and MFA

We introduce a quantum divergence function on $\mathcal{S}$ of QBMs. The divergence in this case is considered to be the quantum relative entropy from $\rho \in \mathcal{S}$ to $\sigma \in \mathcal{S}$, which is defined as $D(\rho\|\sigma) \stackrel{\text{def}}{=} \mathrm{Tr}[\rho(\log\rho - \log\sigma)]$. Now consider the tangent space $T_\tau(\mathcal{S})$ of $\mathcal{S}$ at τ. For $\forall\partial \in T_\tau(\mathcal{S})$, we have the relations

$$\partial D(\rho\|\tau) = \mathrm{Tr}[(\tau-\rho)\partial\log\tau] \quad (6)$$

$$\text{and} \quad \partial D(\tau\|\rho) = \mathrm{Tr}[(\log\tau - \log\rho)\partial\tau], \quad (7)$$

where ∂ operates on τ as the partial differentiation.

If we take τ to be the m-projection $\tau = \arg\min_{\tau'\in\mathcal{M}} D(\rho\|\tau')$ of ρ to $\mathcal{M}$, we have from (6), $\partial D(\rho\|\tau) = 0 \quad (\forall\partial \in T_\tau(\mathcal{M}))$. That is

$$\mathrm{Tr}[\tau\frac{\partial}{\partial\bar{h}_{is}}\log\tau] = \mathrm{Tr}[\rho\frac{\partial}{\partial\bar{h}_{is}}\log\tau] \quad (\forall i, \forall s),$$

which implies that $\mathrm{Tr}[\tau\sigma_{is}] = \mathrm{Tr}[\rho\sigma_{is}]$ or $\bar{m}_{is} = m_{is}$. This means that if we use the m-projection the expectation values do not change. On the other hand, if we take τ to be the e-projection $\tau = \arg\min_{\tau'\in\mathcal{M}} D(\tau'\|\rho)$ of ρ to $\mathcal{M}$, we have from (7) $\partial D(\tau\|\rho) = 0 \quad (\forall\partial \in T_\tau(\mathcal{M}))$. This leads to $0 = \bar{h}_{kr} - \sum_{i,s} w_{iksr}\bar{m}_{is} - h_{kr}$ where we define $\bar{m}_{is} := \mathrm{Tr}[\tau\sigma_{is}]$. Therefore we have

$$\bar{h}_{kr} = h_{kr} + \sum_{i,s} w_{iksr}\bar{m}_{is}. \quad (8)$$

Both (4) (or (5)) and (8) together give the naive mean field equation for QBMs. This equation may have several solutions $\{\bar{h}_{kr}\}$ for a given set of $\{h_{kr}, w_{iksr}\}$.

3 Plefka expansion & higher-order MFAs

We briefly outline the steps which lead to the higher-order approximations using a Taylor expansion of the quantum relative entropy. The formulation follows [4] in the classical case. Let us consider the manifold $\mathcal{S}$ of QBMs and its submanifold $\mathcal{M}$ of product states as in the previous sections. For a given QBM $\rho \in \mathcal{S}$, we have its coordinates (w_{ijst}, h_{is}) and the dual coordinates (η_{ijst}, m_{is}). In addition to the potential function $\psi(\rho)$ given in (2), we introduce its dual by

$$\phi(\rho) \stackrel{\text{def}}{=} \sum_{i,s} h_{is}m_{is} + \sum_{i<j}\sum_{s,t} w_{ijst}\eta_{ijst} - \psi(\rho) = \mathrm{Tr}\,\rho\log\rho.$$

Now let us define two types of subsets of $\mathcal{S}$ as

$$\mathcal{F}(w) = \{\rho \mid w_{ijst} = \text{constant} \quad \forall i,j,s,t\}$$

and

$$\mathcal{A}(m) = \{\rho \mid m_{is} = \text{constant} \quad \forall i,s\}.$$

Note that $\{\mathcal{F}(w)\}_w$ and $\{\mathcal{A}(m)\}_m$ form mutually dual foliations of $\mathcal{S}$ (see [5]). Obviously, $\mathcal{F}(\mathbf{0})$ is the submanifold $\mathcal{M}$ of product states. On each $\mathcal{F}(w)$, we can define a pair of dual potentials $\tilde{\psi} = \psi$ and $\tilde{\phi} = \sum_{is} h_{is}m_{is} - \psi$. For any two density operators $\tau, \rho \in \mathcal{F}(w)$, the quantum relative entropy of τ and ρ can be expressed in terms of the dual potentials $\tilde{\phi}$ and $\tilde{\psi}$ as

$$D(\tau\|\rho) = \tilde{\phi}(\tau) + \tilde{\psi}(\rho) - \sum_{i,s} h_{is}(\rho)\, m_{is},$$

where $m_{is} = m_{is}(\tau)$. Note that, since we have $\rho = \arg\min_{\tau\in\mathcal{F}(w)} D(\tau\|\rho)$, the condition that $\frac{\partial}{\partial m_{is}}D(\tau\|\rho) = 0$ or equivalently $\frac{\partial}{\partial m_{is}}(\tilde{\phi}(\tau) - \sum_{is} h_{is}(\rho)\, m_{is}) = 0$ determines the expectations m_{is} for ρ, though this differentiation is impossible when n is large. Here, we have

$$\tilde{\phi}(\tau) = \tilde{\phi}(\tau_0) - \sum_{i<j}\sum_{s,t} w_{ijst}m_{is}m_{jt} + O(||w||^2)$$

or equivalently $D(\tau\|\rho) = D(\tau_0\|\rho) + O(||w||^2)$, where τ_0 is the unique element of $\mathcal{F}(\mathbf{0}) \cap \mathcal{A}(m)$ which is the m-projection of τ to $\mathcal{F}(\mathbf{0}) = \mathcal{M}$. Then the differentiation becomes tractable if we neglect the term $O(||w||^2)$, which is nothing but the essence of naive MFA discussed in the previous section. More precise approximations of $\{m_{is}\}$ may be derived by considering the higher-order expansion

$$\{\tilde{\phi}(\tau_0) - \sum_{i<j}\sum_{s,t} w_{ijst}m_{is}m_{jt}\} - \tilde{\phi}(\tau) = D(\tau_0\|\rho) - D(\tau\|\rho)$$

$$= \frac{1}{2}\sum_{IJ} g_{IJ}(\tau_0)w_Iw_J + \frac{1}{6}\sum_{IJK} h_{IJK}(\tau_0)w_Iw_Jw_K + \cdots, \quad (9)$$

where the indices I, J, K represent quadruplets of indices such as (i,j,s,t). This is the idea due to Plefka [6],[7], and we call (9) the Plefka expansion following [4]. Now, applying the Pythagorean theorem for the mutually dual foliations [5], we have $D(\tau_0\|\rho) - D(\tau\|\rho) = D(\tau_0\|\tau)$, from which it immediately follows that $\{g_{IJ}\}$ are components of the BKM-Fisher metric and that $\{h_{IJK}\}$ are represented in terms of the coefficients of e,m-connections evaluated at τ_0. Finally, we note that MFAs have recently been given for a quantum spin glass in [7] from a viewpoint of statistical physics. Understanding this work in our geometrical framework will be significant.

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