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GIBBS MEASURES ASSOCIATED WITH THE FULLY VISIBLE BOLTZMANN MACHINE

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RESUME

In this work, we have undertaken a rigorous study of Boltzmann machines and the associated Gibbs measures they induce. Beginning from the machine's energy function, we have detailed the construction of the corresponding Gibbs measures and derived the requisite consistency (Kolmogorov) conditions. We have further identified precise criteria under which these consistency conditions hold and have evaluated their implications for the coherence and validity of statistical models built upon Boltzmann-machine architectures.

Key words: Boltzmann machine, Gibbs measure, Cayley tree, energy function, consistency conditions, statistical models.

1. Preliminaries

There is a substantial body of work on Gibbs measures for the Ising model [3], but relatively little has been done on the energy function in Boltzmann machines (the Boltzmann model). In this paper, we investigate the Gibbs measure for such models.

The interplay between statistical physics and machine learning has led to significant advancements in probabilistic modeling, with Gibbs measures and Boltzmann machines standing at the forefront of this synergy. This paper explores the mathematical foundations of Gibbs measures in Boltzmann machines [8], their algorithmic implementations, and their applications in generative modeling, unsupervised learning, and optimization.

We formalize the connection between statistical mechanics and energy-based models, analyze sampling techniques, and discuss modern variants such as quantum Boltzmann machines. We also address challenges related to the intractability of the partition function and the scalability of these models.

Gibbs measures, originating from statistical mechanics, provide a rigorous framework for describing systems in thermal equilibrium, where the probability distribution of states follows the Boltzmann law. In machine learning, Boltzmann machines leverage this framework to model high-dimensional data distributions through stochastic interactions between units.

A Boltzmann Machine is a stochastic, energy-based neural network that operates on principles from statistical mechanics and is primarily used for unsupervised learning tasks. The network consists of binary units (neurons) that can exist in states $s_i \in \{0, 1\}$ or $\{-1, +1\}$, connected through symmetric weights $w_{ij} = w_{ji}$ with no self-connections ($w_{ii} = 0$). Each unit has an associated bias term a_i representing its activation tendency.

The system's behavior is governed by an energy function:

$$E(\mathbf{s}) = - \sum_{i < j} w_{ij} s_i s_j - \sum_i a_i s_i, \quad (1.1)$$

where lower energy states are more probable. In the machine-learning context, this model is called a fully visible Boltzmann machine.

The probability distribution over states follows the Boltzmann distribution:

$$P(\mathbf{s}) = \frac{1}{Z} e^{-E(\mathbf{s})/T}, \quad (1.2)$$

where Z is the partition function, that is $Z = \sum_{\mathbf{s}} e^{-E(\mathbf{s})/T}$ that normalizes probabilities and T represents the temperature parameter controlling the system's stochasticity.

The Cayley tree $\Gamma^k = (V, L)$ of order $k \geq 1$ is an infinite tree, i.e. graph without cycles, each vertex of which has exactly $k + 1$ edges. Here V is the set of vertices of Γ^k and L is the set of its edges.

Consider models where the spin takes values in the set $\{0, 1\}$, and is assigned to the vertices of the tree. For $A \subset V$ a configuration σ_A on A is an arbitrary function $\sigma_A : A \rightarrow \{0, 1\}$. Let $\Omega_A = \{0, 1\}^A$ be the set of all configurations on A . A configuration σ on V is defined as a function $x \in V \mapsto \sigma(x) \in \{0, 1\}$; the set of all configurations is $\Omega := \{0, 1\}^V$. We consider all elements of V are numerated (in any order) by the numbers: $0, 1, 2, 3, \dots$. Namely, we can write $V = \{x_0, x_1, x_2, \dots\}$.

Ω can be considered as a metric space with respect to the metric $\rho : \Omega \times \Omega \rightarrow \mathbb{R}^+$ given by

$$\rho(\{\sigma(x_n)\}_{x_n \in V}, \{\sigma'(x_n)\}_{x_n \in V}) = \sum_{n: \sigma(x_n) \neq \sigma'(x_n)} 2^{-n}$$

(or any equivalent metric the reader might prefer, this metric taken from [2]), and let \mathcal{B} be the σ -field of Borel subsets of Ω .

For each $m \geq 0$ let $\pi_m : \Omega \rightarrow \{0, 1\}^{m+1}$ be given by $\pi_m(\sigma_0, \sigma_1, \sigma_2, \dots) = (\sigma_0, \dots, \sigma_m)$ and let $\mathcal{C}_m = \pi_m^{-1}(\mathcal{P}(\{0, 1\}^{m+1}))$, where $\sigma_i := \sigma(x_i)$ and $\mathcal{P}(\{0, 1\}^{m+1})$ is the family of all subsets of $\{0, 1\}^{m+1}$ (Cartesian product of $\{0, 1\}$). Then \mathcal{C}_m is a field and each of the sets in \mathcal{C}_m is open and closed set in the metric space (Ω, ρ) ; also $\mathcal{C}_m \subset \mathcal{C}_{m+1}$. Let $\mathcal{C} = \bigcup_{m \geq 0} \mathcal{C}_m$; then \mathcal{C} is a field (the field of **cylinder sets**) and each of the sets in \mathcal{C} is both an open and closed. Denote $\mathcal{S}(\mathcal{C})$ - the smallest sigma field containing \mathcal{C} . Every element of $\mathcal{S}(\mathcal{C})$ is called “**measurable cylinder**”.

Let λ be the Lebesgue measure on $\{0, 1\}$. The set of all configurations on A the a priori measure λ_A is introduced as the $|A|$ -fold product of the measure λ . Here and further on $|A|$ denotes the cardinality of A . Below, W_m stands for a ‘sphere’ and V_m for a ‘ball’ on the tree, of radius $m = 1, 2, \dots$, centered at a fixed vertex x^0 (an origin):

$$W_m = \{x \in V : d(x, x^0) = m\}, \quad V_m = \{x \in V : d(x, x^0) \leq m\},$$

and

$$L_m = \{(x, y) \in L : x, y \in V_m\}.$$

Here distance $d(x, y)$, $x, y \in V$, is the length of (i.e. the number of edges in) the shortest path connecting x with y . Ω_{V_n} is the set of configurations in V_n (and Ω_{W_n} that in W_n ; see below). Furthermore, $\sigma|_{V_n}$ and $\omega|_{W_{n+1}}$ denote the restrictions of configurations $\sigma, \omega \in \Omega$ to V_n and W_{n+1} , respectively.

2. Gibbs measures for the fully visible Boltzmann machine

Let $h : x \in V \mapsto h_x = (h_{t,x} : t \in \{0, 1\}) \in \mathbb{R}^{\{0,1\}}$ be mapping of $x \in V \setminus \{x^0\}$. Given $n = 1, 2, \dots$, consider the probability distribution $\mu^{(n)}$ on Ω_{V_n} defined by

$$\mu^{(n)}(\sigma_n) = Z_n^{-1} \exp \left(-\beta H(\sigma_n) + \sum_{x \in W_n} h_{\sigma_n(x), x} \right). \quad (2.1)$$

Here, as before, $\sigma_n : x \in V_n \mapsto \sigma(x)$ and Z_n is the corresponding partition function:

$$Z_n = \int_{\Omega_{V_n}} \exp \left(-\beta H(\tilde{\sigma}_n) + \sum_{x \in W_n} h_{\tilde{\sigma}_n(x), x} \right) \lambda_{V_n}(d\tilde{\sigma}_n). \quad (2.2)$$

Let $\Lambda \in \mathcal{N}$ and $\Delta \subset \Lambda$, where \mathcal{N} is the set of all finite subsets of V . For any $\Lambda \in \mathcal{N}$, \mathcal{B}_Λ is the minimal σ -field on the configuration space Ω_Λ . If μ_Λ is a measure on \mathcal{B}_Λ , the projection of μ_Λ on \mathcal{B}_Δ is measure $\pi_\Delta(\mu_\Lambda)$ on \mathcal{B}_Δ defined by

$$[\pi_\Delta(\mu_\Lambda)](B) = \mu_\Lambda\{\sigma \in \Omega_\Lambda : \sigma|_\Delta \in B\}, \quad B \in \mathcal{B}_\Delta.$$

Similarly, if μ is a measure on \mathcal{B} , the projection of μ on \mathcal{B}_Λ is defined by

$$[\pi_\Delta(\mu)](B) = \mu\{\sigma \in \Omega : \sigma_\Lambda \in B\} = \mu(\sigma|_\Lambda = \sigma_\Lambda : \sigma_\Lambda \in B), \quad B \in \mathcal{B}_\Lambda.$$

Define a **finite-dimensional distribution** of a probability measure μ in the volume V_n as

$$\mu_n(\sigma_n) = Z_n^{-1} \exp \left\{ -\beta H_n(\sigma_n) + \sum_{x \in W_n} h_x \sigma(x) \right\}, \quad (2.3)$$

where $\beta = 1/T$, $T > 0$ is temperature, Z_n^{-1} is the normalizing factor, $\{h_x \in \mathbb{R}, x \in V\}$ is a collection of real numbers, and

$$H_n(\sigma_n) = - \sum_{\langle x_i, x_j \rangle \in L_n} w_{ij} \sigma(x_i) \sigma(x_j) - \sum_i a_i \sigma(x_i) \quad (2.4)$$

is the Hamiltonian of the Boltzmann model.

We say that the probability distributions (2.3) are **compatible** if for all $n \geq 1$ and $\sigma_{n-1} \in \Phi^{V_{n-1}}$:

$$\sum_{\omega_n \in \Phi^{W_n}} \mu_n(\sigma_{n-1} \vee \omega_n) = \mu_{n-1}(\sigma_{n-1}). \quad (2.5)$$

Here $\sigma_{n-1} \vee \omega_n$ is the concatenation of the configurations. In this case, according to the Kolmogorov theorem, there exists a unique measure μ on Φ^V such that, for all n and $\sigma_n \in \Phi^{V_n}$,

$$\mu(\{\sigma|_{V_n} = \sigma_n\}) = \mu_n(\sigma_n). \quad (2.6)$$

Such a measure is called a **splitting Gibbs measure** corresponding to the Hamiltonian (2.4) and function $h_x, x \in V$.

The following statement describes conditions on h_x guaranteeing compatibility of $\mu_n(\sigma_n)$.

Theorem 2.1. *Probability distributions $\mu_n(\sigma_n)$, $n = 1, 2, \dots$, in (2.3) are compatible iff for any $x \in V$ the following equation holds:*

$$h_x = \sum_{y \in S(x)} f(h_y, \theta). \quad (2.7)$$

Here, $\theta = e^{\beta w_{ij}}$, $f(h, \theta) = \ln \frac{1+\theta e^h}{1+e^h}$, and $S(x)$ is the set of direct successors of x on Cayley tree of order k .

Proof. *Necessity.* Suppose that (2.5) holds; we want to prove (2.7). Substituting (2.3) in (2.5), obtain that for any configurations $\sigma_{n-1}: x \in V_{n-1} \mapsto \sigma_{n-1}(x) \in \{0, 1\}$:

$$\frac{Z_{n-1}}{Z_n} \sum_{\omega_n \in \Omega_{W_n}} \exp \left(\sum_{x \in W_{n-1}} \sum_{y \in S(x)} (\beta w_{ij} \sigma_{n-1}(x) \omega_n(y) + \beta a_i \omega_n(y) + h_y \omega_n(y)) \right) = \exp \left(\sum_{x \in W_{n-1}} h_x \sigma_{n-1}(x) \right), \quad (2.8)$$

where $\omega_n: x \in W_n \mapsto \omega_n(x)$, a_i is a constant corresponding to y vertex and w_{ij} is a weight between configurations at the x and y vertexes.

From (2.8) we get:

$$\frac{Z_{n-1}}{Z_n} \sum_{\omega_n \in \Omega_{W_n}} \prod_{x \in W_{n-1}} \prod_{y \in S(x)} \exp(\beta w_{ij} \sigma_{n-1}(x) \omega_n(y) + \beta a_i \omega_n(y) + h_y \omega_n(y)) = \prod_{x \in W_{n-1}} \exp(h_x \sigma_{n-1}(x)).$$

Rewrite now the last equality for $\sigma_{n-1}(x) = 1$ and $\sigma_{n-1}(x) = 0$, then dividing first of them by the second one we get

$$\prod_{y \in S(x)} \frac{\sum_{u \in \{0,1\}} \exp(\beta w_{ij} u + h_y u)}{\sum_{u \in \{0,1\}} \exp(h_y u)} = \exp(h_x),$$

which implies (2.7) where one has to use the following formula:

$$f(h, \theta) = \ln \frac{1 + \theta e^h}{1 + e^h}. \quad (2.9)$$

Sufficiency. Suppose that (2.7) holds. It is equivalent to the representations

$$\prod_{y \in S(x)} \sum_{u \in \{-1, 1\}} \exp(\beta w_{ij} t u + \beta a_i u + h_y u) = a(x) \exp(th_x), \quad t \in \{0, 1\} \quad (2.10)$$

for some function $a(x) > 0$, $x \in V$. We have

$$\text{LHS of (2.5)} = \frac{1}{Z_n} \exp(-\beta H(\sigma_{n-1})) \times \prod_{x \in W_{n-1}} \prod_{y \in S(x)} \sum_{u \in \{0, 1\}} \exp(\beta w_{ij} \sigma_{n-1}(x) u + \beta a_i u + h_y u). \quad (2.11)$$

Substituting (2.10) into (2.11) and denoting $A_{n-1} = \prod_{x \in W_{n-1}} a(x)$, we get

$$\text{RHS of (2.10)} = \frac{A_{n-1}}{Z_n} \exp(-\beta H(\sigma_{n-1})) \prod_{x \in W_{n-1}} \exp(h_x \sigma_{n-1}(x)). \quad (2.12)$$

Since $\mu^{(n)}, n \geq 1$ is a probability measure, we should have

$$\sum_{\sigma_{n-1} \in \Omega_{V_{n-1}}} \sum_{\omega_n \in \Omega_{W_n}} \mu^{(n)}(\sigma_{n-1}, \omega_n) = 1.$$

Hence from (2.12) we get $Z_{n-1} A_{n-1} = Z_n$, and (2.5) holds. \square

From Theorem 2.1 it follows that for any $h = \{h_x, x \in V\}$ satisfying the functional equation (2.7) there exists a unique positive measure μ and vice versa. This result is equivalent to the fact that (2.7) is not easy.

In next sections we shall give several solutions to (2.7).

Remark 2.1. Note that if there is more than one solution to equation (2.7) then there is more than one Gibbs measure corresponding to these solutions. One says that a phase transition occurs for the Boltzmann model, if equation (2.7) has more than one solution. The number of the solutions of equation (2.7) depends on the parameter $\beta = \frac{1}{T}$. The phase transition usually occurs for low temperature. If it is possible to find an exact value T^* in which a critical value of temperature does occur for all $T \leq T^*$, then T^* is called a critical value of temperature.

Finding the exact value of the critical temperature for some models means to exactly solve the models.

3. Periodic Gibbs measures of the Boltzmann model

Since the set of vertices V has the group representation G_k . Without loss of generality we identify V with G_k , i.e., we sometimes replace V with G_k .

In this section we study periodic solutions of (2.7).

Definition 3.1. Let K be a subgroup of $G_k, k \geq 1$. We say that a function $h = (h_x \in R : x \in G_k)$ is K -periodic if $h_{yx} = h_x$ for all $x \in G_k$ and $y \in K$. A G_k -periodic function h is called translation-invariant.

Definition 3.2. A Gibbs measure is called K -periodic if it corresponds to K -periodic function h .

Observe that a translation-invariant Gibbs measure is G_k -periodic. Firstly, we shall find all translation-invariant solutions h_x to the functional equation (2.7), ferromagnetic Boltzmann model. Note that such solutions are constant functions, $h_x = h, \forall x \in G_k$. In this case from (2.7) we get

$$h = kf(h, \theta), \quad \theta > 0. \quad (3.1)$$

The following properties of the function $f(h, \theta)$ are obvious:

1. $\lim_{x \rightarrow \infty} f(x, \theta) = \ln \theta, \lim_{x \rightarrow -\infty} f(x, \theta) = 0$;
2. $\frac{d}{dx} f(x, \theta) < 0$ if $\theta < 1$, $\frac{d}{dx} f(x, \theta) = 0$ if $\theta = 1$, $\frac{d}{dx} f(x, \theta) > 0$ if $\theta > 1$.

From these properties it follows that equation (3.1) has unique solution h^* that $h^*(h^* < 0)$, if $\theta < 1$, $h^* = 0$, if $\theta = 1$ and $h^*(h^* > 0)$ if $\theta > 1$.

There are as many Gibbs measures as there are solutions to equation (2.7), and it follows that there is a unique Gibbs measure. Namely,

Lemma 3.1. *For the ferromagnetic Boltzmann model on the Cayley tree of order $k \geq 2$ the following statement is true. If $T \in R$ then there is unique translation-invariant Gibbs measure μ_0 .*

We now give a complete description of periodic Gibbs measures for the Boltzmann model, i.e., a characterization of such measures with respect to any normal subgroup of finite index in G_k . Let K be a subgroup of index r in G_k , and let $G_k/K = \{K_0, K_1, \dots, K_{r-1}\}$ be the quotient group, with the coset $K_0 = K$. Denote $q_i(x) = |S_1(x) \cap K_i|$, $i = 0, 1, \dots, r-1$; $N(x) = |\{j : q_j(x) \neq 0\}|$, where $S_1(x) = \{y \in G_k : \langle x, y \rangle\}$, $x \in G_k$ and $|\cdot|$ is the number of elements in the set. Denote $Q(x) = (q_0(x), q_1(x), \dots, q_{r-1}(x))$.

We note (see Theorem 1.5[3]) that for every $x \in G_k$ there is a permutation π_x of the coordinates of the vector $Q(e)$ (where e is the identity of G_k) such that

$$\pi_x Q(e) = Q(x). \quad (3.2)$$

It follows from this equality that $N(x) = N(e)$ for all $x \in G_k$. Each K -periodic collection is given by $\{h_x = h_i \text{ for } x \in K_i, i = 0, 1, \dots, r-1\}$. By Theorem 2.1 and (3.2), $h_n, n = 0, 1, \dots, r-1$, satisfies

$$h_n = \sum_{j=1}^{N(e)} q_{i_j}(e) f(h_{\pi_n(i_j)}, \theta) - f(h_{\pi_n(i_{j_0})}, \theta), \quad (3.3)$$

where $i_j = 1, \dots, N(e)$, $N(e) = |\{i_1, \dots, i_{N(e)}\}|$.

From monotonicity of $f(h, \theta)$ with respect to h , one gets:

Lemma 3.2. $f(h, \theta) = f(u, \theta)$ if and only if $h = u$.

Let $G_k^{(2)}$ be the subgroup in G_k consisting of all words of even length. Clearly, $G_k^{(2)}$ is a subgroup of index 2.

Theorem 3.1. *Let K be a normal subgroup of finite index in G_k . Then each K -periodic Gibbs measure for the Boltzmann model is either translation-invariant or $G_k^{(2)}$ -periodic.*

Proof. We see from (3.3) that

$$f(h_{\pi_n(i)}, \theta) = f(h_{\pi_n(i')}, \theta),$$

for any $i, i' \in Q(e), n = 0, 1, \dots, r-1$. Hence by Lemma 3.2 we have

$$h_{\pi_n(i_1)} = h_{\pi_n(i_2)} = \dots = h_{\pi_n(i_{N(e)})}.$$

Therefore,

$$\begin{aligned} h_x &= h_y = h \text{ if } x, y \in S_1(z), z \in G_k^{(2)}, \\ h_x &= h_y = l \text{ if } x, y \in S_1(z), z \in G_k \setminus G_k^{(2)}. \end{aligned}$$

Thus the measures are translation-invariant (if $h = l$) or $G_k^{(2)}$ -periodic (if $h \neq l$). This completes the proof of the theorem. \square

Let K be a normal subgroup of finite index in G_k .

What condition on K will guarantee that each K -periodic Gibbs measure is translation-invariant? We put $I(K) = K \cap \{a_1, \dots, a_{k+1}\}$, where $a_i, i = 1, \dots, k+1$ are generators of G_k .

Theorem 3.2. *If $I(K) \neq \emptyset$, then each K -periodic Gibbs measure for the Boltzmann model is translation-invariant.*

Proof. Take $x \in K$. We note that the inclusion $xa_i \in K$ holds if and only if $a_i \in K$. Since $I(K) \neq \emptyset$, there is an element $a_i \in K$. Therefore K contains the subset $Ka_i = \{xa_i : x \in K\}$. By Theorem 3.1 we have $h_x = h$ and $h_{xa_i} = l$. Since x and xa_i belong to K , it follows that $h_x = h_{xa_i} = h = l$. Thus each K -periodic Gibbs measure is translation-invariant. \square

Theorems 3.1 and 3.2 reduce the problem of describing K -periodic Gibbs measures with $I(K) \neq \emptyset$ to describing the fixed points of $kf(h, \theta)$ which describes translation-invariant Gibbs measures.

If $I(K) = \emptyset$, this problem is reduced to describing the solutions of the system:

$$\begin{cases} u = kf(v, \theta), \\ v = kf(u, \theta). \end{cases} \quad (3.4)$$

Evidently, roots of the equation

$$u = g(u) = kf(kf(u, \theta), \theta), \quad (3.5)$$

describe the $G_k^{(2)}$ -periodic Gibbs measures. Using properties of function f one can easily note that: The system of equations (3.4) has a unique solution $h_0 = (h_*, h_*)$ if $\theta \in R$; We denote by μ_0 the Gibbs measures which correspond to these solution. Note that the measure μ_0 are translation-invariant. By an argument analogous to that of Lemma 3.1., we obtain the following result:

Theorem 3.3. *For the ferromagnetic Boltzmann model all periodic Gibbs measures are translation-invariant.*

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REZYUME

Ushbu ishda Boltzmann mashinalari va ular bilan bogʻliq Gibbs oʻlchovlari nazariy jihatdan chuqur oʻrganildi. Avvalo, mashinaning energiya funksiyasidan boshlab, unga mos Gibbs oʻlchovlarini qurish jarayoni bosqichma-bosqich tushuntirildi. Shuningdek, bu oʻlchovlarning mavjudligi uchun zarur boʻlgan muvofiqlik (Kolmogorov) shartlari keltirib chiqarildi. Keyin esa ushbu shartlarning bajarilishi uchun aniq mezonlar aniqlanib, ularning Boltzmann mashinasi tuzilishiga asoslangan statistik modellarning izchilligi va haqiqiylikiga qanday taʼsir qilishi tahlil qilindi.

Kalit soʻzlar: Boltzmann mashinasi, Gibbs oʻlchovi, Keli daraxti, energiya funksiyasi, muvofiqlik shartlari, statistik modellar.

РЕЗЮМЕ

В данной работе мы провели строгое исследование машины Больцмана и связанных с ней мер Гиббса. Начиная с энергетической функции машины, мы подробно описали построение соответствующих мер Гиббса и вывели необходимые условия согласованности (условия Колмогорова). Далее мы установили точные критерии, при которых выполняются эти условия согласованности, и оценили их влияние на согласованность и достоверность статистических моделей, построенных на архитектуре машины Больцмана.

Ключевые слова: машина Больцмана, мера Гиббса, дерево Кэли, энергетическая функция, условия согласованности, статистические модели.