

1 1D Case

Definition 1.1 (Potts chain). *A Potts chain is a chain of spins s_i with $i \in \mathbb{Z}$ and each s_i can assume any integer value from 1 to the vocabulary size V .*

Later on, to highlight links with Natural Language Processing (NLP) we will use interchangeably the word spins and tokens.

Definition 1.2 (Windowed Hamiltonian). *A windowed Hamiltonian H_i is an Hamiltonian that acts only on the spins inside his finite window of interaction \mathcal{W}_i . Without loss of generality, we are going to assume that the lowest energy state has a value of zero*

Definition 1.3 (Pseudo-Convolutional Hamiltonian). *A pseudo-convolutional Hamiltonian $H = \sum_i H_i$ is an Hamiltonian that can be written as the sum of several windowed Hamiltonians H_i all with the same window width \mathcal{W} . For sake of simplicity we are going to assume that there exists an upper bound to the highest energy of every windowed Hamiltonian $E_i^{max} < E^{max}$*

Pseudo-convolutional Hamiltonians, in matrix form, are band matrices, meaning that after a certain distance from the diagonal, all of their elements are equal to zero. An example of a band matrix is the matrix B in equation 1

$$B = \begin{bmatrix} B_{11} & B_{12} & 0 & \cdots & \cdots & 0 \\ B_{21} & B_{22} & B_{23} & \ddots & \ddots & \vdots \\ 0 & B_{32} & B_{33} & B_{34} & \ddots & \vdots \\ \vdots & \ddots & B_{43} & B_{44} & B_{45} & 0 \\ \vdots & \ddots & \ddots & B_{54} & B_{55} & B_{56} \\ 0 & \cdots & \cdots & 0 & B_{65} & B_{66} \end{bmatrix} \quad (1)$$

Definition 1.4 (Stored Pattern). *A stored pattern \mathcal{P} is a particular sequence of spins $(\dots, s_{-1}, s_0, s_1, \dots)$ such that the energy of the pseudo-convolutional Hamiltonian H associated to this pattern is equal to zero. If more than one stored pattern is present, they can be numbered as $\mathcal{P}^n = (\dots, s_{-1}^n, s_0^n, s_1^n, \dots)$.*

Theorem 1.1. *Let H be a pseudo-convolutional Hamiltonian with $N > 1$ stored patterns. At non-zero temperature the system will be unable to converge to single stored pattern*

Proof. Suppose that our Potts chain starts out equal to our first stored pattern $\mathcal{C} = \mathcal{P}^1$. Now we want to know if the formation of a single domain barrier is thermodynamically favorable.

$$\Delta F = \Delta E - T\Delta S < 0 \quad (2)$$

For that to be true, the Free energy of the system must decrease upon the formation of a domain barrier.

Upon the formation of a domain barrier, The windowed Hamiltonians that intersect it will have a non zero, positive energy. Therefore $\Delta E > 0$, however, we know that the energy of each window Hamiltonian is smaller than E^{\max} and no more that $\mathcal{W} - 1$ windows can be affected by a domain wall, therefore

$$0 \leq \Delta E \leq (\mathcal{W} - 1)E^{\max} \quad (3)$$

At the same time we know that in a sequence long L there can be $L - 1$ possible places where a domain wall can appear, and for each of this possible places it can lead to any of the $N - 1$ other patterns saved, therefore there are $(L - 1)(N - 1)$ possible configurations where the system has a single domain wall. This means that the change of the entropy of the system is

$$\Delta S = \log[(N - 1)(L - 1)] \quad (4)$$

Putting equations 3 and 4 all together we have that

$$\Delta F \leq (\mathcal{W} - 1)E^{\max} - T \log[(N - 1)(L - 1)] \quad (5)$$

In the thermodynamic limit ($L \rightarrow \infty$) we have that the right hand side of the equation becomes eventually negative, therefore the domain barriers are inevitable \square

Definition 1.5 (Auto-Regressive Model). *During inference time, given some input tokens $\{s_i | i_{\text{first}} \leq i \leq i_{\text{last}}\}$ an auto-regressive model M return a V -dimensional (p_1, \dots, p_V) vector with an estimate of the probability for the next token in the sequence to predict $i_{\text{pred}} = i_{\text{last}} + 1$.*

$$M(s_{i_{\text{first}}}, \dots, s_{i_{\text{last}}}) = (p_1, \dots, p_V) \quad (6)$$

Theorem 1.2. *It is possible to associate pseudo-convolutional Hamiltonian to any auto-regressive model*

Proof. Through Boltzmann's equation it's possible to turn a probability distribution of equation 6 to some energy levels

$$p_c = \frac{1}{Z} e^{-\frac{E_c}{T}} \quad \text{with } c = 1 \dots V \quad (7)$$

Without loss of generality, we can assume $T = 1$ and set the energy associated with every prediction turns out to be

$$E_c = -\log p_c + \text{const} \quad \text{with } c = 1 \dots V \quad (8)$$

Where we can set the constant in such a way that the lowest energy state has a energy equal to zero.

We can now define a windowed Hamiltonian

$$H_{i_{\text{pred}}}(s_{i_{\text{first}}}, \dots, s_{i_{\text{last}}}, s_{i_{\text{pred}}}) = -\log [M(s_{i_{\text{first}}}, \dots, s_{i_{\text{last}}}) \cdot s_{i_{\text{pred}}}] + \text{const} \quad (9)$$

And the full pseudo-convolutional Hamiltonian can now be seen as the sum of all the $H = \sum H_{i_{\text{pred}}}$ of the sequence.

The generation process can now be seen as sampling from the Boltzmann distribution given from

$$p_{\text{sequence}} = \frac{1}{Z} e^{-\frac{1}{T} H(\text{sequence})} \quad (10)$$

□

Corollary 1.2.1. *Autoregressive models with fixed window size are incapable of generating infinite length, coherent output*

Proof. From theorem 1.2 we know that autoregressive models can be modelled by pseudo-convolutional Hamiltonians, which we know that from Theorem 1.1 are not able to converge to any single pattern □

2 2D Case

We have seen before that in 1D case a Windowed Hamiltonian cannot lead us to a coherent phase and how this applies to auto-regressive models.

All the definitions given before are now generalized to 2-dimensions, I will later write them down.

Theorem 2.1. *Let H be a pseudo-convolutional Hamiltonian acting on a Potts grid with $N > 2$ stored patterns. At thermal equilibrium, there exists a critical temperature T_c below which the system will converge to a single stored pattern*

Proof. The following proof will be a generalization of the Peierls argument. We now start with a $L \times L$ grid of V -dimensional Potts spins with $N > 1$ saved patterns. Suppose that our Potts chain starts out equal to our first stored pattern $\mathcal{C} = \mathcal{P}^1$. Now we want to know if the formation of a single domain barrier like in figure 1 is thermodynamically favorable.

We now imagine starting in a state of a large 2D system with the spins on the boundary frozen in the pattern \mathcal{P}^1 configuration. We again wish to compute the free energy difference of inserting a domain wall at the origin that has a different sign. Now our domain wall boundary consists not just of a pair of points, but of some perimeter of length P . Each spin with its window intersecting the boundary creates an energy penalty of at least E^{\min} and at most E^{\max} . The number of such spins is linearly proportional to the perimeter length P and the area of the window of at most \mathcal{W}^2 (and at least just one element) so the total change in energy is

$$PE^{\min} \leq \Delta E \leq \mathcal{W}^2 PE^{\max} \quad (11)$$

We can give an upper bound on the number of domain barrier is $(N-1)P^2 3^P$. This is because the domain is a connected component, so the boundary is a self-avoiding curve. The curve has perimeter P , so it must fit inside a box of

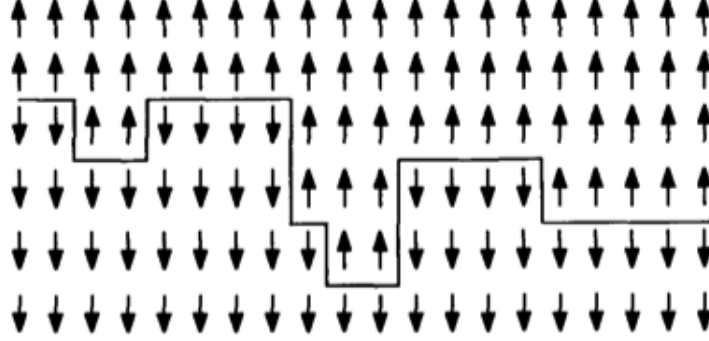


Figure 1: A Domain wall in 2D

side-length P centered at the origin. Each step along the perimeter of this curve has at most 3 choices for where to step next (or else it would backtrack and self-intersect). Since the total length is P and there are at most P^2 starting points at which to begin the curve, there are at most $P^2 3^P$ such domain walls. Furthermore any domain wall can appear between the starting pattern \mathcal{P}^1 and any other stored pattern, therefore the number of configuration is multiplied by $(N - 1)$

$$\Delta S \leq \log(N - 1) + 2 \log P + P \log 3 \quad (12)$$

Therefore

$$\Delta F \geq P E^{\min} - T P \log 3 \quad (13)$$

This means that for

$$T \leq E^{\min} / \log 3 \quad (14)$$

We have an ordered phase that converges to one of the stored patterns. \square

2.1 Some problems with this proof

The problem with this proof is that we assume that the free energy is actually minimized. This is true at thermal equilibrium, otherwise you could extract energy from the system. However some energy landscapes are so rugged that the free energy cannot be completely minimized.

This means that even though the lowest free energy configuration is ordered, the system might never be able to reach it because it can take a very long, or infinite amount of time to reach it.

3 More complex Topologies

As you have seen from the two examples, determining whether or not an ordered phase can exist boils down to a counting problem.

1. Start with the system being equal to one of the patterns stored
2. Create a domain wall
3. Estimate the energy gained by the system
4. Count the number of such domain walls
5. See if the free energy increases or decreases as the size of the domain walls goes to infinity

This can be applied to systems with very different topologies, we are now going to explore that

Definition 3.1 (Graph Hamiltonian). *Let G be the adjacency matrix of a graph, then a Graph Hamiltonian H is a Hamiltonian that can be written as*

$$H = H * G \quad (15)$$

where the $(*)$ operator represents the element-wise multiplication

Definition 3.2 (Entropy Scaling). *Let H be a Graph Hamiltonian, and P be the perimeter length, or surface area of a domain wall, as the perimeter length increases, the number of possible configurations of domain barrier increases, thus increasing the entropy of the system ΔS . We say that the Entropy gained scales as f_S if*

$$\Delta S = O(f_S(P))$$

Definition 3.3 (Energy Scaling). *Let H be a Graph Hamiltonian, and P be the perimeter length, or surface area of a domain wall, as the perimeter length increases, the the Higher and Lower bound of the energy gained ΔE scale as respectively $O(f_E^{high}(P))$ and $O(f_E^{low}(P))$. If $f_E^{high} = f_E^{low} \equiv f_E$ we say that the energy gained scales as f_E*

$$\Delta E = O(f_E(P))$$

Theorem 3.1. *If $O(f_S) = O(f_E) = O(f)$ there exists a ordered phase*

Proof.

$$\Delta F = \Delta E - T\Delta S = \lim_{P \rightarrow \infty} O(f(P)) - TO(f(P)) \quad (16)$$

If we now do $\lim_{T \rightarrow 0}$ the term on the right disappears, therefore the change in free energy is negative and a coherent phase is favored \square

Theorem 3.2. *Let H be a Graph Hamiltonian with $N > 1$ stored patterns. At thermal equilibrium, the ability to converge to a ordered phase doesn't depend on N*

Proof. The change in entropy due to the creation of a domain barrier can always be written as

$$\Delta S = \log[(N-1)N_{\text{barriers}}] = \log N_{\text{barriers}} + \log(N-1) \quad (17)$$

Where N_{barriers} is the number of barriers of a certain shape. In the thermodynamic limit, the term proportional to the number of barriers increases, while the one proportional to the number of patterns stored stays constant, therefore can be ignored as it doesn't change the entropy scaling \square

Theorem 3.3. *Let $H = \sum_i H_i$, if there exists two energies E_{\max}, E_{\min} which are the biggest and smallest non-zero energy level of all the windowed Hamiltonians H_i . At thermal equilibrium, the ability to converge to a ordered phase doesn't depend from the energy levels and the window sizes*

Proof. The proof will be similar to the steps done to reach equation 11. Let \mathcal{W} be the biggest window size, and 1 the smallest of any H_i , and let P be the perimeter length of our domain wall. The energy gain by creating such a domain wall is bounded by

$$PE^{\min} \leq \Delta E \leq \mathcal{W}PE^{\max} \quad (18)$$

In both cases we have that

$$E = O(P) \quad (19)$$

\square

As an example on determining whether or not, a coherent phase can exist we focus on the Connected Tree of Spins

Definition 3.4 (Connected Tree of Spins). *ADD IMAGES*

A connected tree of spins is a tree structure where each node has C children and all the spins on the same level have next-neighbor interactions.

Theorem 3.4. *The Ising model on a connected tree does have a condensed phase*

Proof. REWRITE THIS PROOF BETTER AND WITH IMAGES

The Hamiltonian is

$$H = -J \sum_{\langle i,j \rangle} s_i s_j \quad (20)$$

Where $\langle i,j \rangle$ means that is summed over all the couple of nodes connected in the tree.

The energy Δ required to create a perimeter of length P is equal to

$$\Delta E = 2JP$$

Similar to Peierls argument, the number of turn a perimeter can take, in this geometry is either 2 or 3, and the number of starting positions is $L^{\log L}/(\log L)!$, so

$$\Delta S \leq P \log 3 + \dots \quad (21)$$

By the end we have that

$$\Delta F \geq 2JP - TP \log 3 \quad (22)$$

This means that for low enough temperature we have a condensed phase \square

4 The role of disorder

The problem with the theorems stated so far is that some of this systems can exhibit spin-glass like behavior, this is due to the intrinsic quenched disorder present in machine learning algorithms.

For example the actual form of the Free energy is

$$F = -T \int e^{-\lambda l(\theta|\mathcal{D})} \log \left[\int e^{-H(\{s_i\}|\theta)/T} Ds_i \right] D\theta \quad (23)$$

This systems, under certain conditions exhibit glassy behaviors.

5 Local Hopfield Networks

We are now going to focus on Hopfield networks to study the stability of this systems as a function of the topology and the number of stored patterns.

Definition 5.1 (Hopfield Network). *An Hopfield network is a system described by the Hamiltonian*

$$H = - \sum_{\mu}^N F \left(\sum_i^L X_i^{\mu} \sigma_i \right) \quad (24)$$

where N is the number of patterns stored and L is the sequence length

Definition 5.2 (Local Hopfield Network). *The Hamiltonian of a windowed Hopfield networks is a sum over many Hopfield networks, each of which interacts inside its own window*

$$H = - \sum_j^L \sum_{\mu}^N F \left(\sum_{\langle i,j \rangle} X_i^{\mu} \sigma_i \right) \quad (25)$$

Theorem 5.1. *a Local Hopfield network with an energy function that is the sum of several sub-Hopfield networks with window size of W has a storage capacity of any given sub-network*

Proof.

$$\Delta E = \sum_{\langle j,k \rangle} \sum_{\mu}^N F \left(X_k^{\mu} X_k^{\nu} + \sum_{\langle i,j \rangle \neq k} X_i^{\mu} X_i^{\nu} \right) - F \left(-X_k^{\mu} X_k^{\nu} + \sum_{\langle i,j \rangle \neq k} X_i^{\mu} X_i^{\nu} \right) \quad (26)$$

Now we are going to define the average local change in energy.

$$\Delta E_{\text{loc}}(j) \equiv \sum_{\mu}^N F \left(X_k^{\mu} X_k^{\nu} + \sum_{\langle i,j \rangle \neq k} X_i^{\mu} X_i^{\nu} \right) - F \left(-X_k^{\mu} X_k^{\nu} + \sum_{\langle i,j \rangle \neq k} X_i^{\mu} X_i^{\nu} \right) \quad (27)$$

for each j we have a sub-Hopfield network, and when averaging the j dependence goes away. And from [1, 2] we have that

$$\langle \Delta E_{\text{loc}} \rangle = \begin{cases} 2nW^{n-1} & \text{if } F(x) = x^n \\ e^{\alpha W} & \text{if } F(x) = e^x \end{cases} \quad (28)$$

this means that

$$\langle \Delta E \rangle = \sum_{\langle j,k \rangle} \langle \Delta E \rangle_{\text{loc}} = W \langle \Delta E \rangle_{\text{loc}} \quad (29)$$

Therefore we have that

$$\langle \Delta E \rangle = \begin{cases} 2nW^n & \text{if } F(x) = x^n \\ We^{\alpha W} & \text{if } F(x) = e^x \end{cases} \quad (30)$$

Now we calculate the variances, first the change in energy can be written as

$$\Delta E^2 = \sum_{\langle j_1,k \rangle} \sum_{\langle j_2,k \rangle} \Delta E_{\text{loc}}(j_1) \Delta E_{\text{loc}}(j_2) \quad (31)$$

Now we calculate the average of the term inside the sum.

When we flip a bit in one window, the change in energy in the other window will be the same¹. This means that

$$\langle \Delta E_{\text{loc}}(j_1) \Delta E_{\text{loc}}(j_2) \rangle = \langle \Delta E_{\text{loc}}^2(j_1) \rangle = \langle \Delta E_{\text{loc}}^2 \rangle \quad (32)$$

Therefore we have that

$$\langle \Delta E^2 \rangle = W^2 \langle \Delta E_{\text{loc}}^2 \rangle \quad (33)$$

and the variance is

$$\Sigma^2 = W^2 \left(\langle \Delta E_{\text{loc}}^2 \rangle - \langle \Delta E_{\text{loc}} \rangle^2 \right) = W^2 \Sigma_{\text{loc}} \quad (34)$$

¹Not actually true, but the change in energy will be very similar most of the times $\Delta E_{\text{loc}}(j_1) \approx \Delta E_{\text{loc}}(j_2)$

The probability to have an error P is

$$\begin{aligned}
P &= \int_{\Delta E}^{\infty} \frac{1}{\sqrt{2\pi\Sigma^2}} e^{-\frac{x^2}{2\Sigma^2}} dx = \\
&= \int_{W\Delta E_{\text{loc}}}^{\infty} \frac{1}{\sqrt{2\pi W^2\Sigma_{\text{loc}}^2}} e^{-\frac{x^2}{2W^2\Sigma_{\text{loc}}^2}} dx = \\
&= \int_{\Delta E_{\text{loc}}}^{\infty} \frac{1}{\sqrt{2\pi\Sigma_{\text{loc}}^2}} e^{-\frac{z^2}{2\Sigma_{\text{loc}}^2}} dz = \\
&= P_{\text{loc}}
\end{aligned} \tag{35}$$

Where in the last passage we defined $z = x/W$.

This means that a Hopfield network with an energy function that is the sum of several sub-Hopfield networks with window size of W has a storage capacity of any given sub-network \square

References

- [1] D. Krotov and J. J. Hopfield, “Dense associative memory for pattern recognition,” *Advances in neural information processing systems*, vol. 29, 2016.
- [2] M. Demircigil, J. Heusel, M. Löwe, S. Upgang, and F. Vermet, “On a model of associative memory with huge storage capacity,” *Journal of Statistical Physics*, vol. 168, pp. 288–299, 2017.