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## 1 Notation

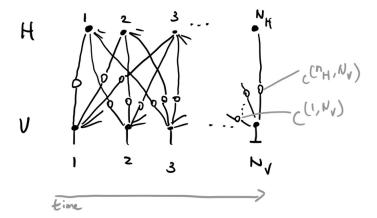
Firstly, define  $N_H$  and  $N_V$  to be the number of hidden and visible units respectively.  $H_h$  is a vector of weights for the hidden units, where  $h = 1, 2, \ldots, N_H$ . Similarly,  $V_v$  is a vector of weights for the visible units, where  $v = 1, 2, \ldots, N_V$ .  $W_{hv}$  is a matrix of weights.  $C_{kl}^{(hv)}$  is the coupling matrix between the hth hidden unit and the vth visible unit. For simplicity, we will assume that C is a  $d \times d$  matrix.

#### 1.0.1 Note on the coordination number

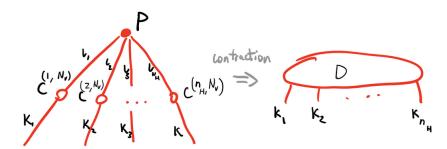
 $n_V^{(h)}$  is the coordination number for visible units of the  $h^{\rm th}$  hidden unit. This is the number of connected visible units. Similarly,  $n_H^{(v)}$  is the coordination number for hidden units of the  $v^{\rm th}$  visible unit.

Throughout this section, we are operating on the last visible unit (the  $N_V^{\rm th}$  unit), which is connected to  $n_H^{(N_V)}$  hidden units. Since it is clear which visible unit we are referring to, the superscript will be omitted.

In the general case,  $n_H = N_H$  as the hidden and visible units form a complete bipartite graph. In the Snake RBM case, each visible unit is connected to exactly one hidden unit so  $n_H = 1$ .



# 2 Imposing the causality condition on RBMs

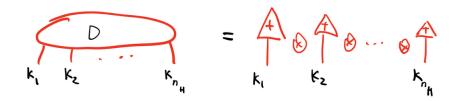


Let  $D_{k_1k_2...k_{n_H}}$  be the contraction of the red network, and  $|+\rangle$  to be a vector of 1s.

If the causality condition were to hold, then,

$$D = \bigotimes_{n_H} |+\rangle \,. \tag{1}$$

This is represented visually as



The RHS is then a tensor of 1s. This amounts to an a set of equations where each element of D must equal 1.

### 2.1 Preliminary steps

Let P be the contraction of the vectorised identity with the copy tensor, and let  $k = \sqrt{d}$ . The index at which a one appears in the vectorised identity is given by a sequence  $S = (s_1, s_2, \ldots, s_k)$  where  $s_i = k(i-1) + i$  for  $1 \le i \le k$ .

$$P_{l_1 l_2 \dots l_{n_H}} = \begin{cases} 1 & l_1 = l_2 = \dots = l_{n_H} \text{ and } l_1 \in S \\ 0 & \text{otherwise} \end{cases}$$

### 2.2 Defining the coupling matrices

 $C_{kl}^{(hv)}$  is a  $d \times d$  coupling matrix between the hth hidden and vth visible unit. In our notation, we extend k and l to range over [1, d], so a more useful definition could be as follows.

$$C_{kl}^{(hv)} = e^{W_{h,v}(k-1)(l-1) + \frac{H_h(k-1)}{N_H} + \frac{V_v(l-1)}{N_V}}$$
(2)

# 2.3 Equation for elements of the contracted tensor

In fact, we can solve for specific elements of the D tensor.

$$D_{k_1 k_2 \dots k_{n_H}} = \sum_{l_1 l_2 \dots l_{n_H}} P_{l_1 l_2 \dots l_{n_H}} C_{k_1 l_1}^{(1, N_V)} C_{k_2 l_2}^{(2, N_V)} \cdots C_{k_{n_H} l_{n_H}}^{(n_H, N_V)}$$
(3)

$$= \sum_{s \in S} P_{ss...s} C_{k_1 s}^{(1,N_V)} C_{k_2 s}^{(2,N_V)} \cdots C_{k_{n_H} s}^{(n_H,N_V)}$$

$$\tag{4}$$

$$= \sum_{s \in S} C_{k_1 s}^{(1, N_V)} C_{k_2 s}^{(2, N_V)} \cdots C_{k_{n_H} s}^{(n_H, N_V)}$$
(5)

$$= \sum_{s \in S} \prod_{h=1}^{n_H} C_{k_h,s}^{(h,N_V)} \tag{6}$$

$$= \sum_{s \in S} \prod_{h=1}^{n_H} e^{W_{h,N_V}(k_h-1)(s-1) + \frac{V_{N_V}(s-1)}{N_V} + \frac{H_h(k_h-1)}{N_H}}$$
(7)

#### 2.3.1 A special case with no solutions

Using the general equation (7), we can solve for the very first element of the tensor,  $D_{1,1,\dots,1}$ . (Here, let  $k_1 = k_2 = \dots = k_{n_H} = 1$ .)

$$D_{1,1,\dots,1} = \sum_{s \in S} \prod_{h=1}^{n_H} e^{(s-1)\frac{V_{N_V}}{N_V}}$$
(8)

$$= \sum_{s \in S} e^{(s-1)\frac{n_H V_{N_V}}{N_V}} \tag{9}$$

Suppose that d=4 (the case that  $C^{(hv)}$  is a  $2\times 2$  matrix), then S=(1,4).

$$D_{1,1,\dots,1} = \sum_{s \in \{1,4\}} e^{(s-1)\frac{n_H V_{N_V}}{N_V}}$$
 (10)

$$=e^{0} + e^{\frac{3n_{H}V_{N_{V}}}{N_{V}}} \tag{11}$$

But requiring  $D_{1,1,\dots,1}=1$  implies  $\exp(\frac{3n_H V_{N_V}}{N_V})=0$ , which has no solution.

In fact, the number of terms in the summation in (7) is equal to the length of  $S = \sqrt{d}$ .

### 2.4 Interpreting results for Uniform RBMs

Up until now, we have been considering the general case of fully-connected RBMs. Consider the special subset of RBMs where all coupling matrices are identical. That is, for all  $1 \le h_1, h_2 \le n_H$ , and  $1 \le v_1, v_2 \le N_V$ ,

$$C_{kl}^{(h_1v_1)} = C_{kl}^{(h_2v_2)} (12)$$

It immediately follows from the definition of the coupling matrices, that all entries of W, H, and V are also identical. So the subscripts for the indices can be ommitted. This means that (6) can be simplified.

$$D_{k_1 k_2 \dots k_{n_H}} = \sum_{s \in S} \prod_{h=1}^{n_H} C_{k_h, s}^{(h, N_V)}$$
 (6 revisited)

$$= \sum_{s \in S} \prod_{h=1}^{n_H} e^{W(k_h - 1)(s - 1) + \frac{V(s - 1)}{N_V} + \frac{H(k_h - 1)}{N_H}}$$
(13)

# 2.5 Interpreting results for minimally-connected RBMs

Consider a subset of RBMs that are connected in a minimal way... We will call this the  $Snake\ RBM$ . "Snake RBM" has this form.



Solving the Snake RBM amounts to solving the following simplified equation.