Simulating Recurrent Neural Networks on Graphic Processing Units

Summer Project

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Introduction

Introduction

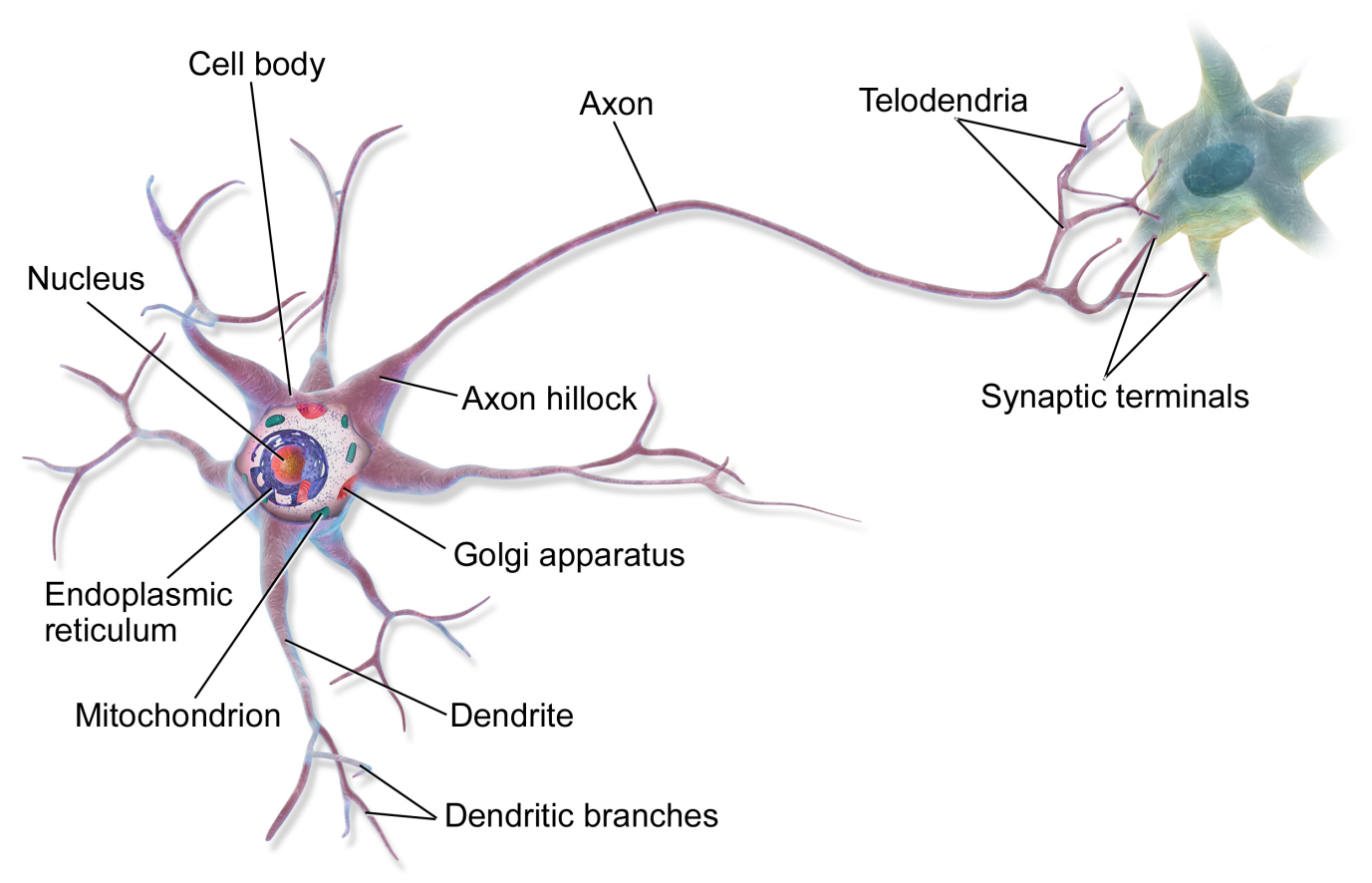


Figure 1: Anatomy of a neuron[1]

[1] By BruceBlaus - Own work, CC BY 3.0, https://commons.wikimedia.org/w/index.php?curid=28761830

Feedforward Neural Network

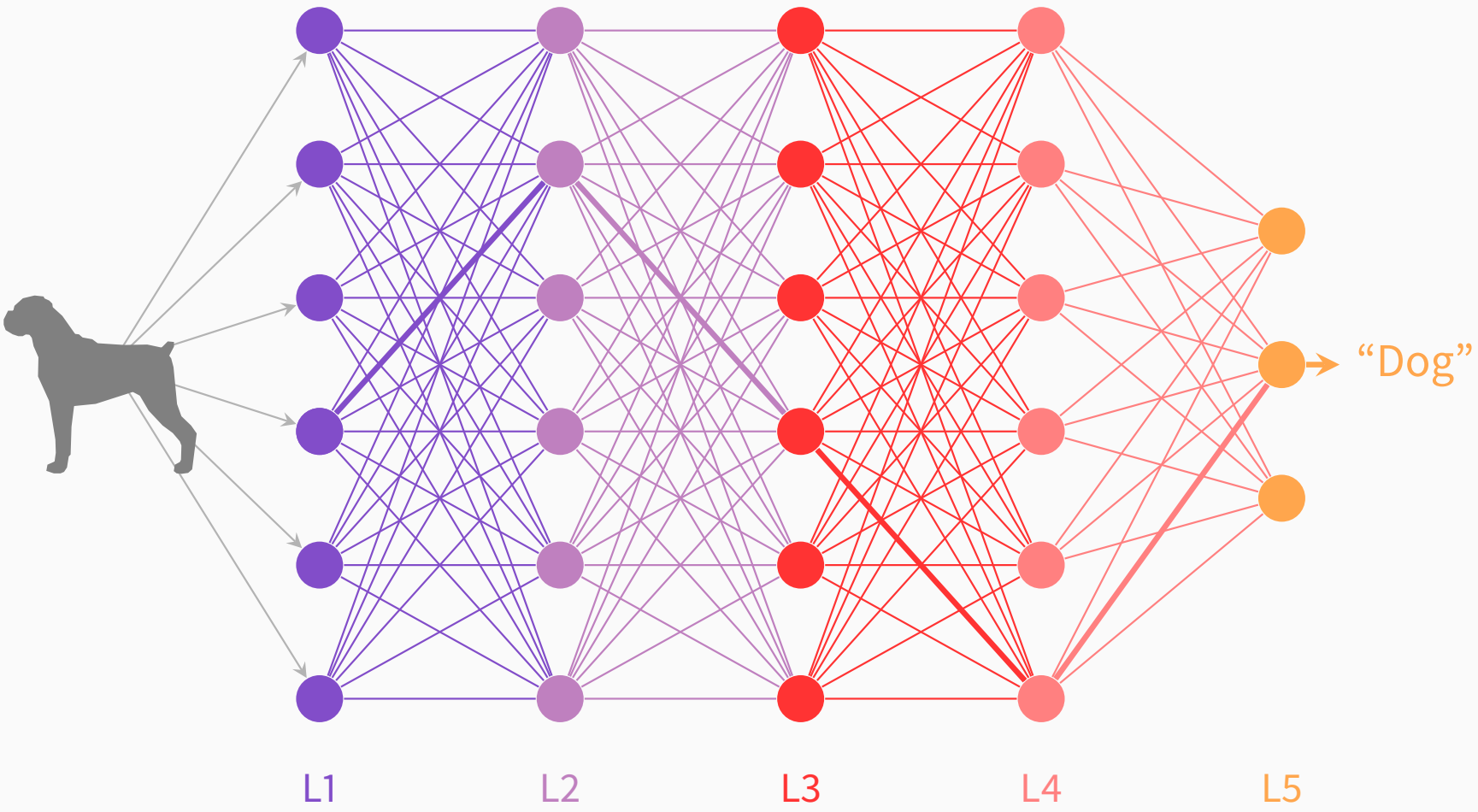
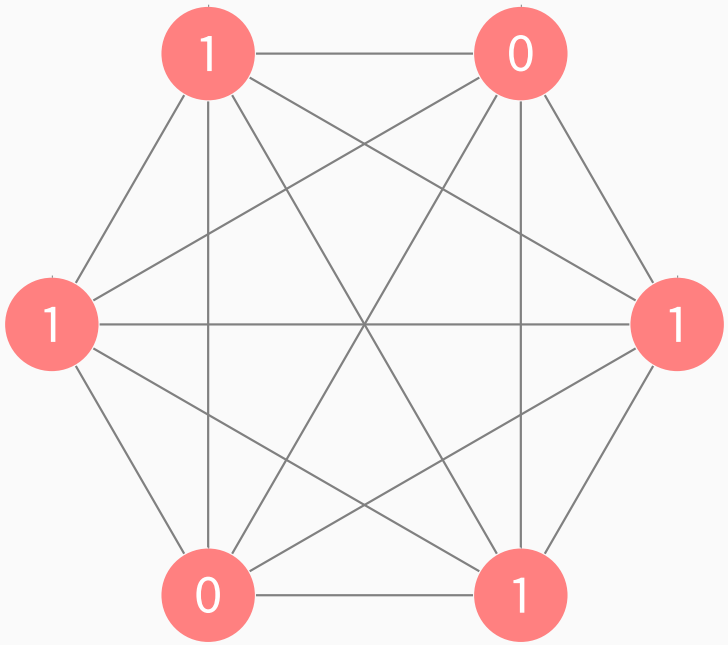


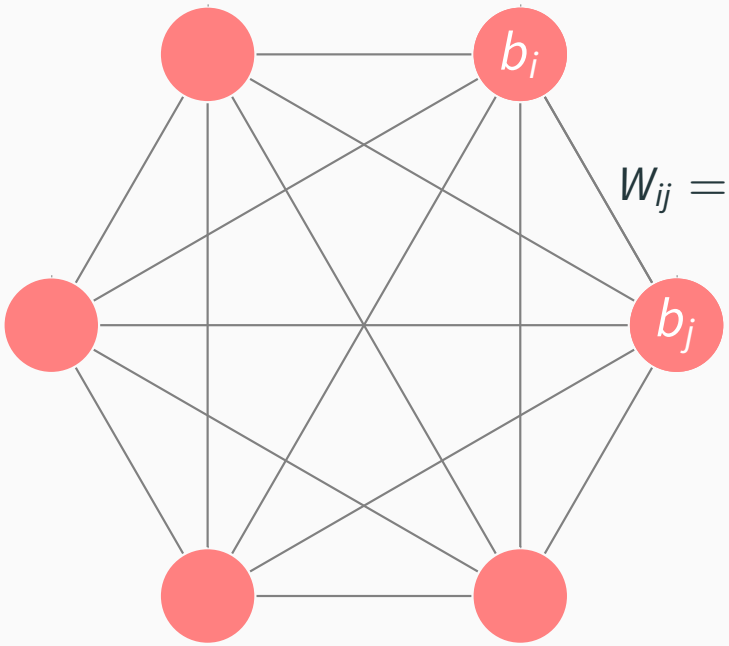
Figure 2: Feedforward Neural Network

Recurrent Neural Networks

Boltzmann Machines



Boltzmann Machines



Energy configuration, $E = -\sum_{i<j} W_{ij} x_i x_j - \sum_i b_i x_i$

Energy gap, $\Delta E_i = E(x_i = 0) - E(x_i = 1) = \sum_j W_{ij} x_j + b_i$

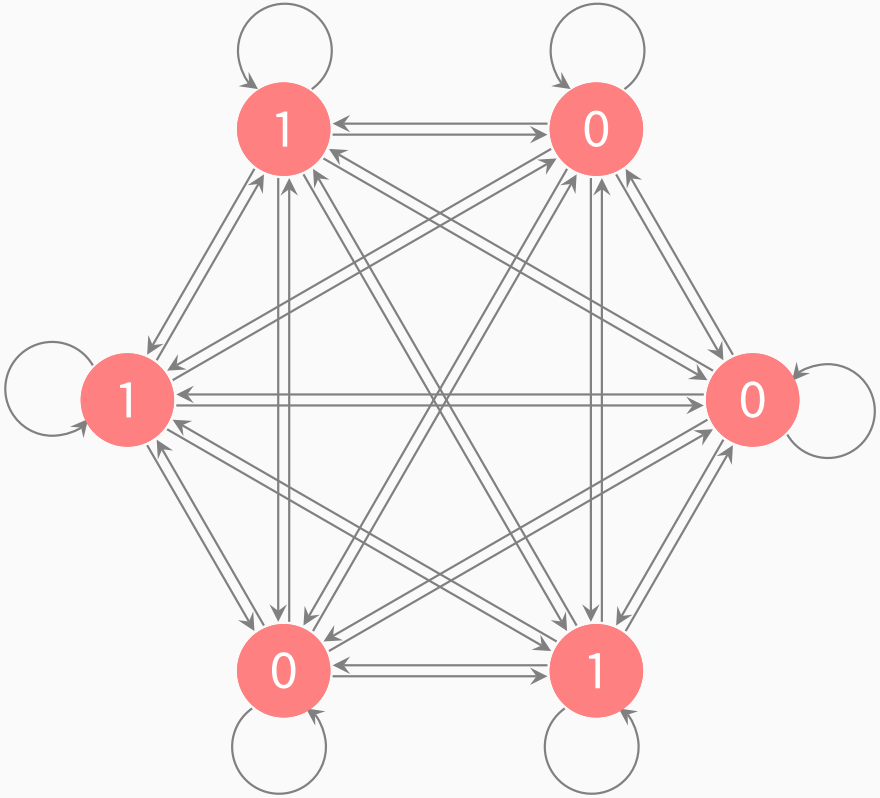
$$p_i := \mathbb{P}(x_i = 1) = \frac{1}{1 + e^{-\Delta E_i / \tau}}$$

Algorithm 1 Boltzmann Machine Simulation.

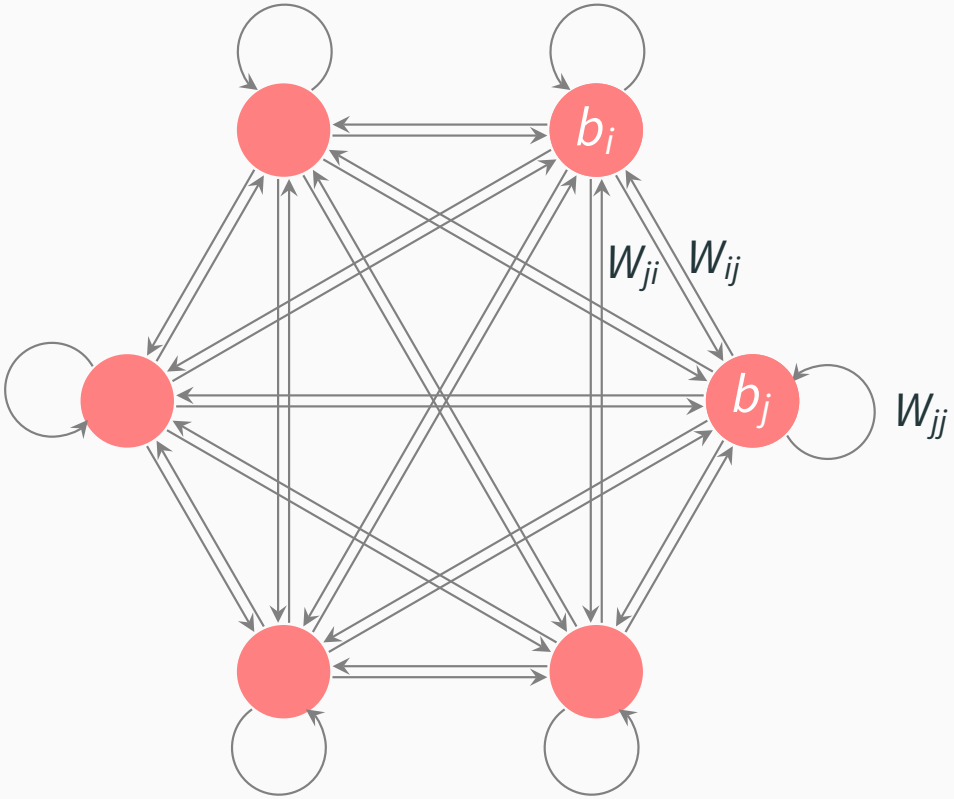
1: Initialize $\boldsymbol{W}, \boldsymbol{b}$
2: Initialize $\boldsymbol{x}^{(0)}$
3: **for** i from 1 to N **do**
4: Random $k \in \{1, \ldots, d\}$, where d is the number of neurons
5: Compute $p_k = \frac{1}{1+e^{-\Delta E_k / \tau}}$
6: Sample from the Bernoulli distribution with $p = p_k$
7: $\boldsymbol{x}^{(i)} \leftarrow \text{update}(\boldsymbol{x}^{(i-1)})$
8: **end for**

where update($x^{(i-1)}$) updates the chosen neuron k with the outcome of the sample from the Bernoulli distribution.

McCulloch-Pitts Machines



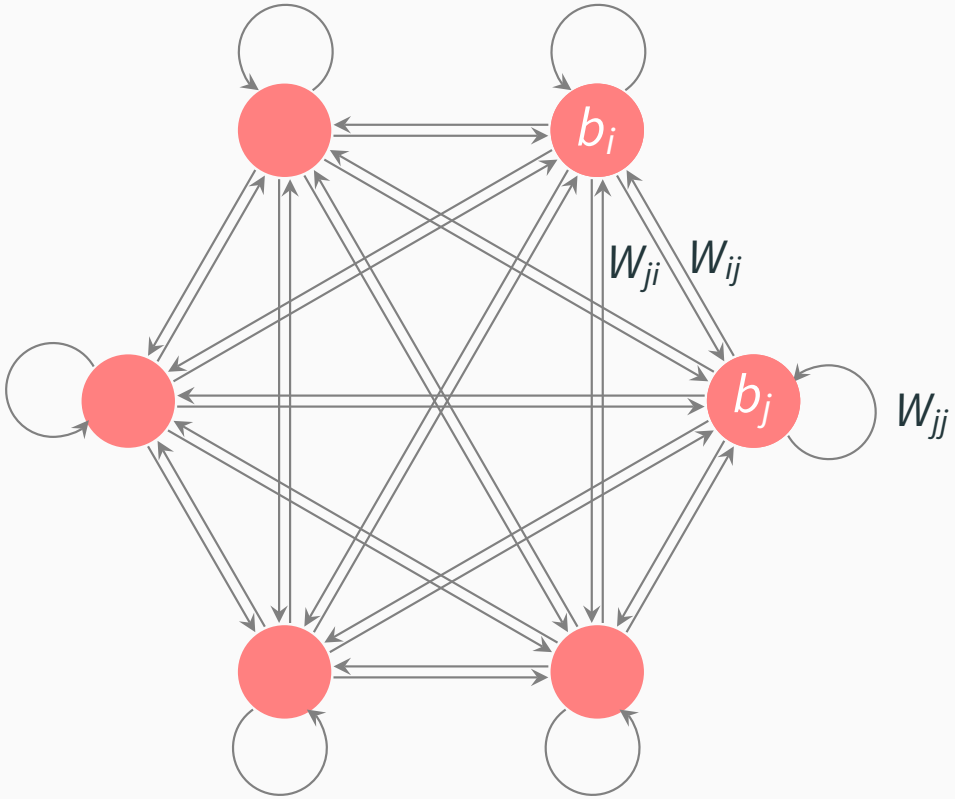
McCulloch-Pitts Machines



$$\text{Transition Energy, } E(y, x|\theta) = -\sum_{ji \in E} W_{ji} y_j x_i - \sum_{j \in V} b_j x_j - \sum_{i \in V} b_i x_i$$

$$\Gamma_{yx} = \exp\left(-\frac{1}{2\tau} E(y, x|\theta) + \frac{1}{2\tau} E(x, x|\theta)\right)$$

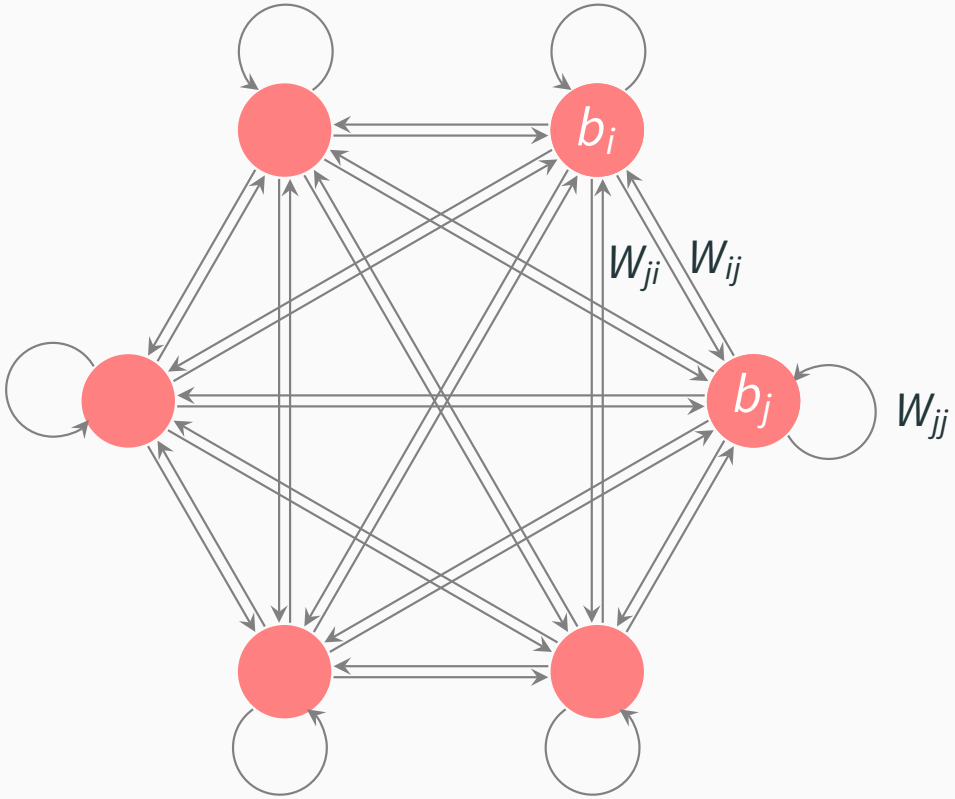
McCulloch-Pitts Machines



$$\lambda_j := \Gamma_{yx} = \exp\left(\frac{1}{2\tau} s_j z_j\right)$$

where $s_j = 1 - 2x_j$, $z_j = \sum_j W_{ji} x_i + b_j$ and x, y differ by the jth unit.

McCulloch-Pitts Machines



Transition probability from x to y, $p_{yx} = \dfrac{\lambda_j}{\sum_{j'} \lambda_{j'}}$

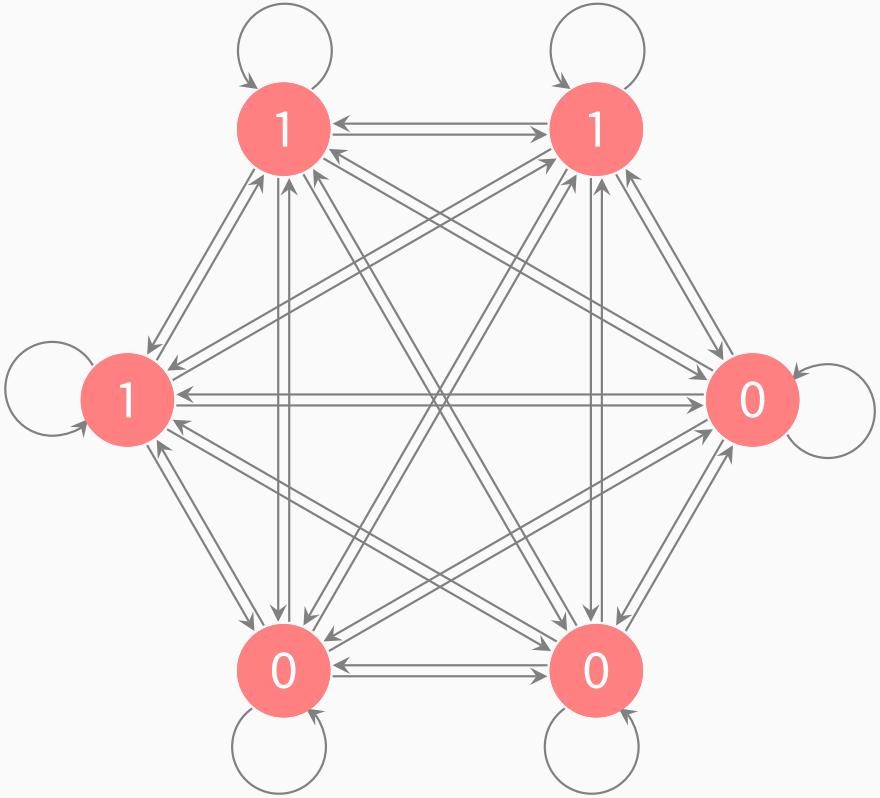
Sample holding times, $T_{yx} \sim Exp(a_x)$, where $a_x = \sum_j \lambda_j$

Algorithm 2 CTMC Simulation.

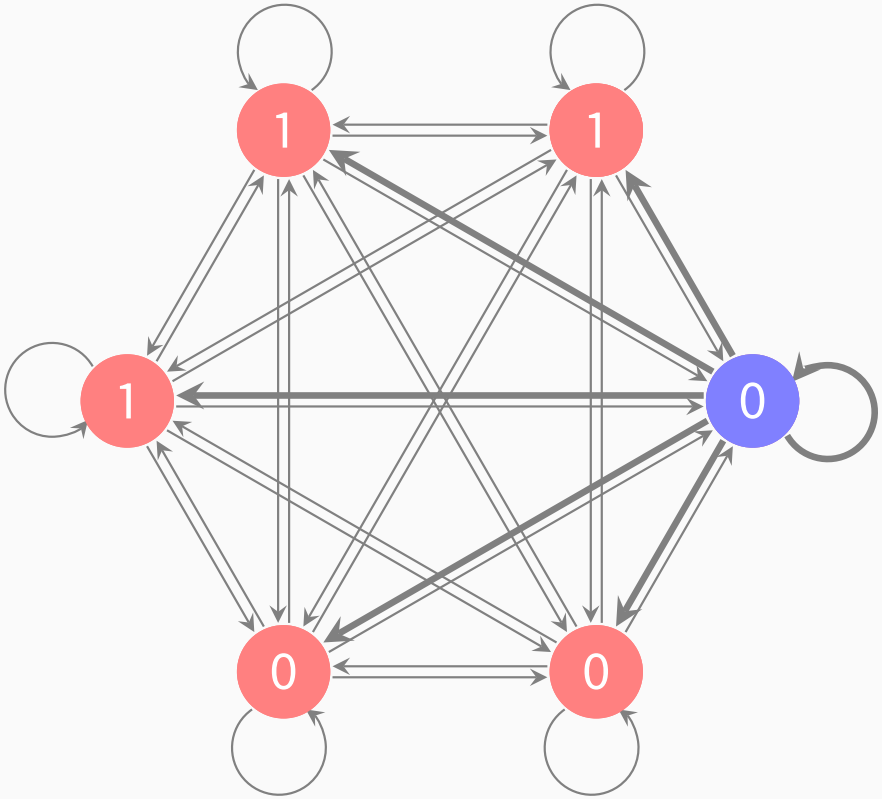
1: Initialize $\boldsymbol{W}, \boldsymbol{b}$
2: Initialize $\boldsymbol{x}^{(0)}$
3: **for** i from 1 to N **do**
4: Compute Γ_{yx}, p_{yx} for each $\boldsymbol{y} \neq \boldsymbol{x}$
5: Compute $a_x = \sum \Gamma_{yx}$
6: $\boldsymbol{x}^{(i)} \leftarrow \text{flip}(\boldsymbol{x}^{(i-1)})$
7: Sample holding time $T_i \sim \text{Exp}(a_x)$
8: **end for**

where $\text{flip}(x^{(i-1)})$ flips the state of the transiting neuron.

McCulloch-Pitts Machines

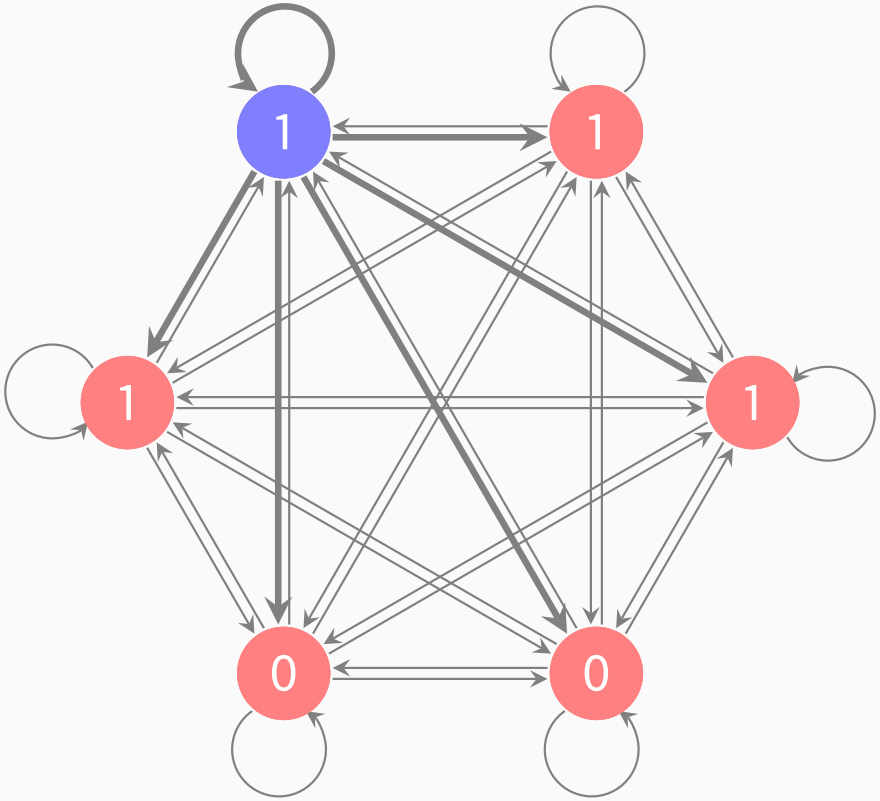


McCulloch-Pitts Machines



$(T_0, (1, 0, 0, 0, 1, 1))$

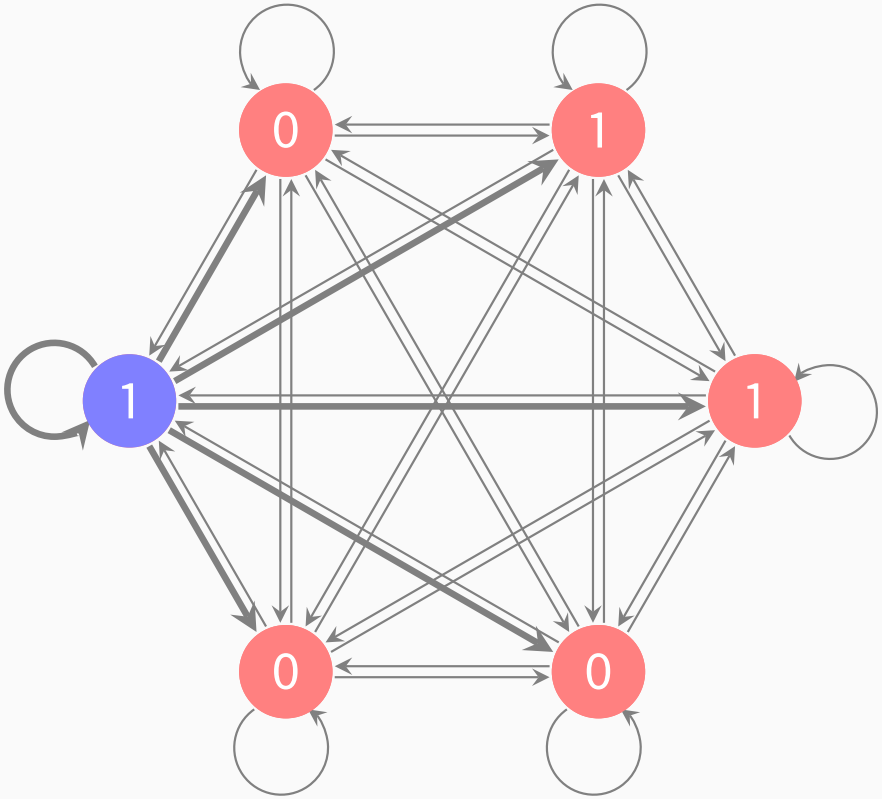
McCulloch-Pitts Machines



$(T_0, (1, 0, 0, 0, 1, 1))$

$(T_1, (1, 0, 0, 1, 1, 1))$

McCulloch-Pitts Machines



$$(T_0, (1, 0, 0, 0, 1, 1))$$

$$(T_1, (1, 0, 0, 1, 1, 1))$$

$$(T_2, (1, 0, 0, 1, 1, 0))$$

Simulating on GPUs

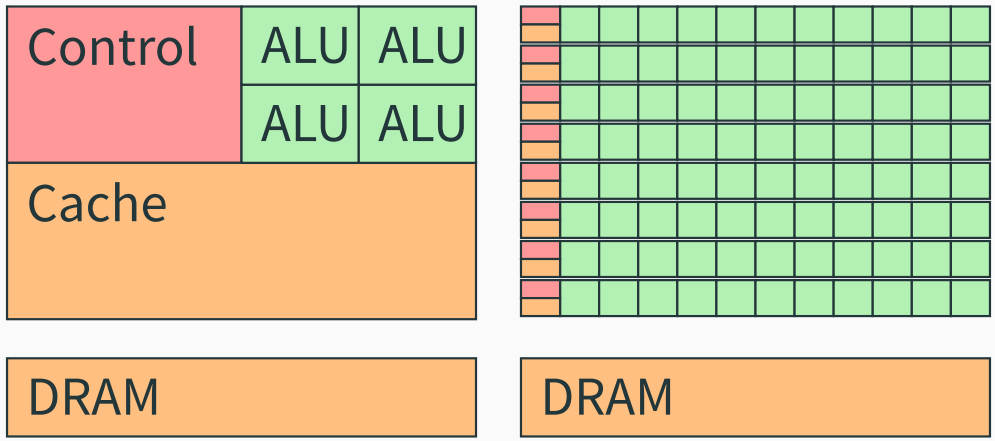
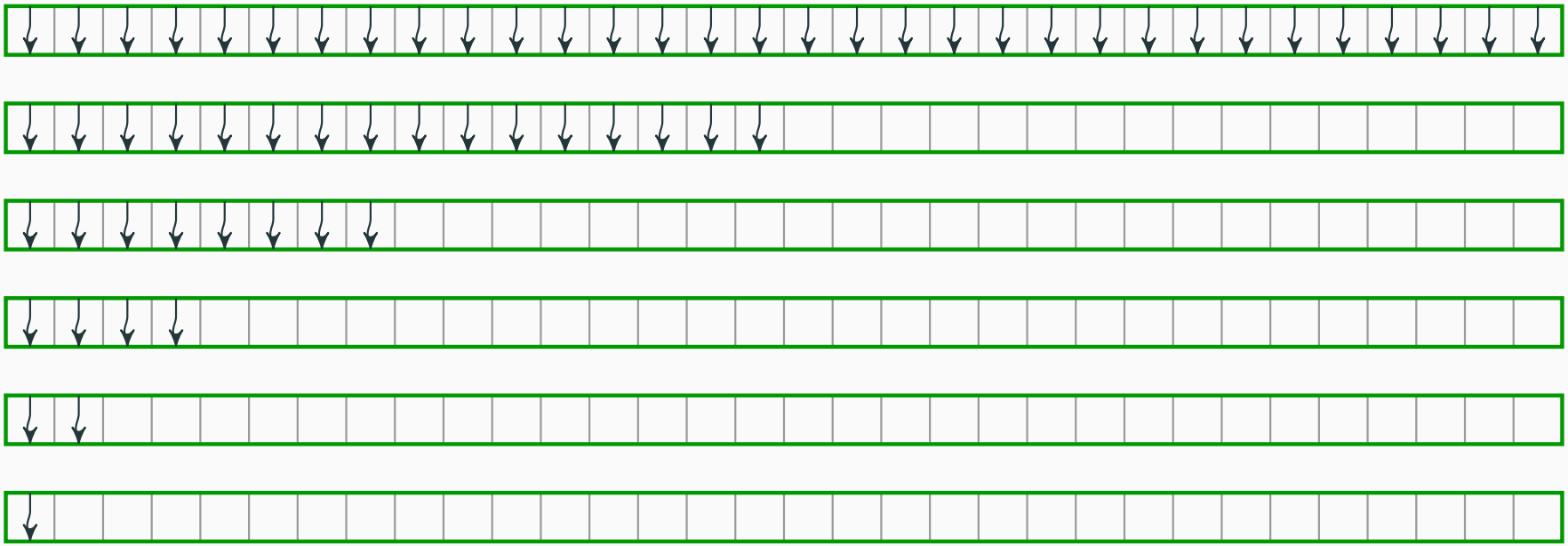


Figure 3: Comparison between the amount of transistors devoted to different functions inside a CPU and a GPU.

GPU Algorithm: Reduction



Reduction

```
mod = SourceModule("""
        __global__ void reduce_kernel(float *d_out, float *d_in)
        {
            int myId = threadIdx.x + blockDim.x * blockIdx.x;
            int tid = threadIdx.x;
            // do reduction in global memory
            for (unsigned int s = blockDim.x / 2; s > 0; s >>= 1)
            {
                if (tid < s)
                {
                    d_in[myId] += d_in[myId + s];
                }
                __syncthreads(); // make sure all adds at one stage are
                    done
            }
            // only thread 0 writes result for this block back to global
                memory
            if (tid == 0)
            {
                d_out[blockIdx.x] = d_in[myId];
            }
        }
        """, arch='sm_60')
```

Importance to Simulating on GPUs

- Faster matrix multiplication
- Larger neural networks
- Larger function space
- Energy efficiency

References

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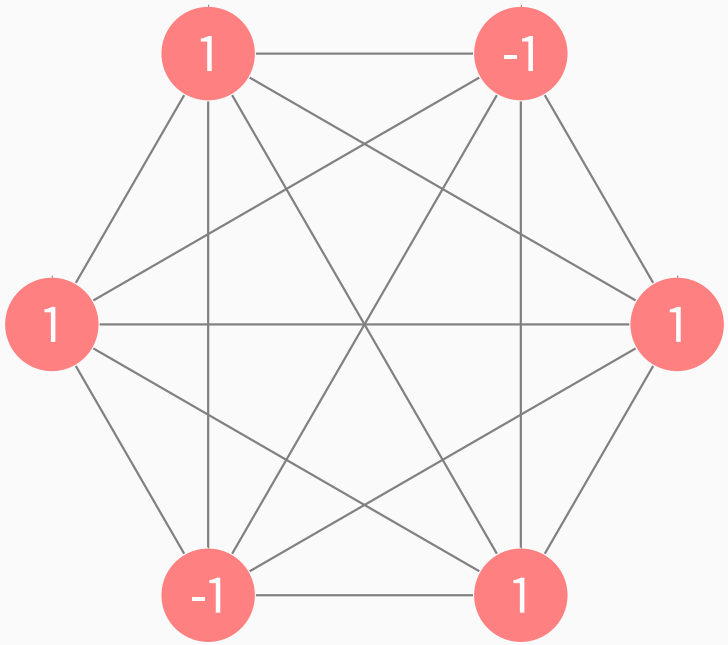
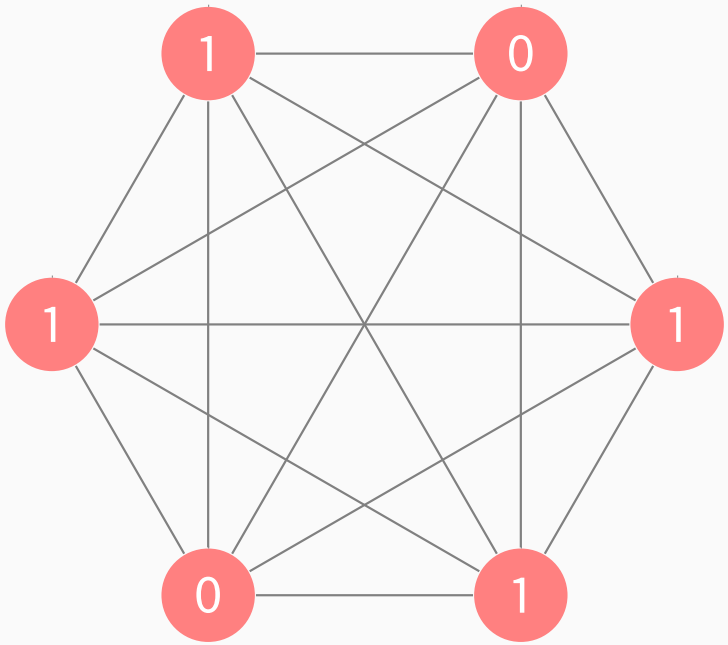
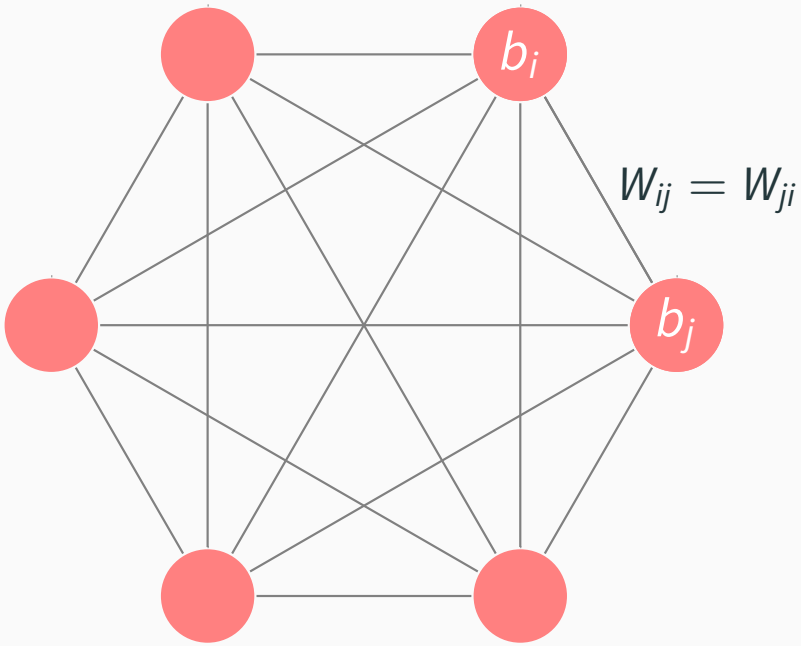
Hopfield Networks



Hopfield Networks



Hopfield Networks

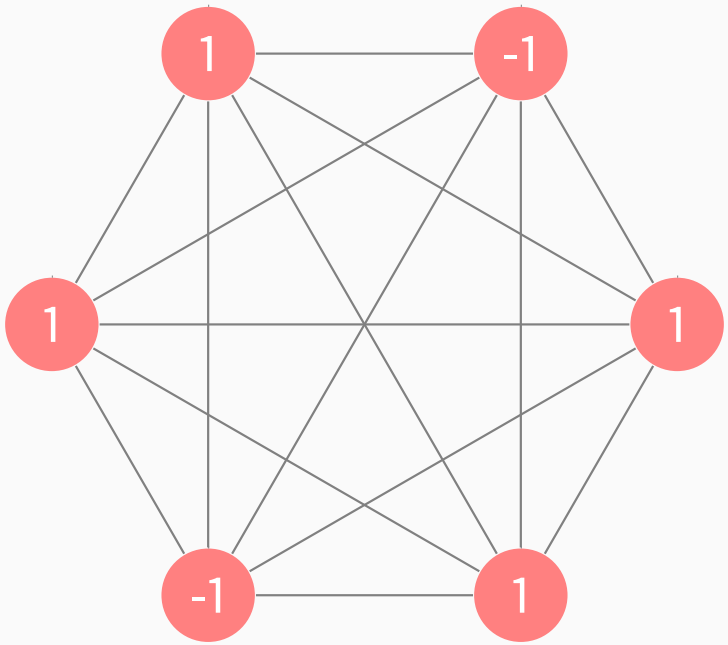


$$\text{Energy configuration, } E = -\sum_{i<j} W_{ij} x_i x_j - \sum_i b_i x_i$$

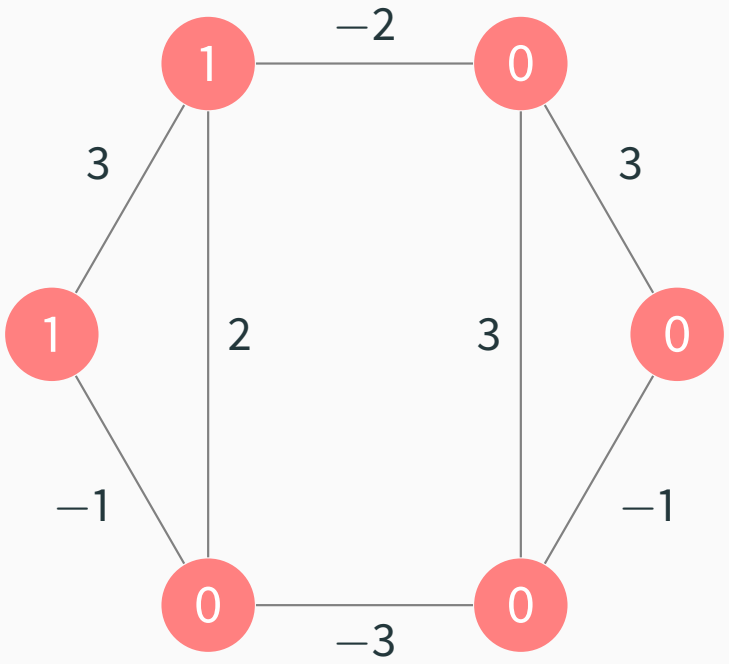
$$\text{Energy gap, } \Delta E_i = E(x_i = 0) - E(x_i = 1) = \sum_j W_{ij} x_j + b_i$$

$$\text{Update rule, } x_i := \begin{cases} 1 & \sum_j W_{ij} x_j + b_i \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

Hopfield Networks

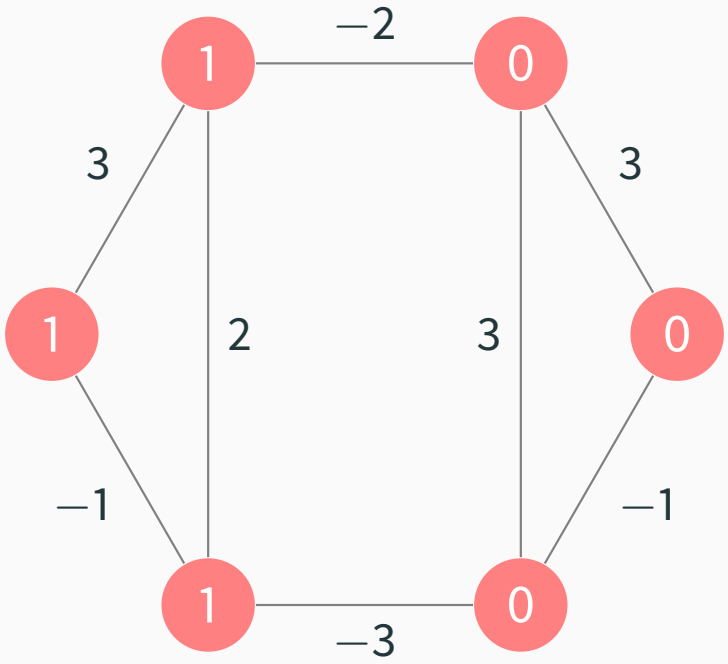


Hopfield Networks



(1, 0, 0, 0, 0, 1)

Hopfield Networks



(1, 0, 0, 0, 0, 1)

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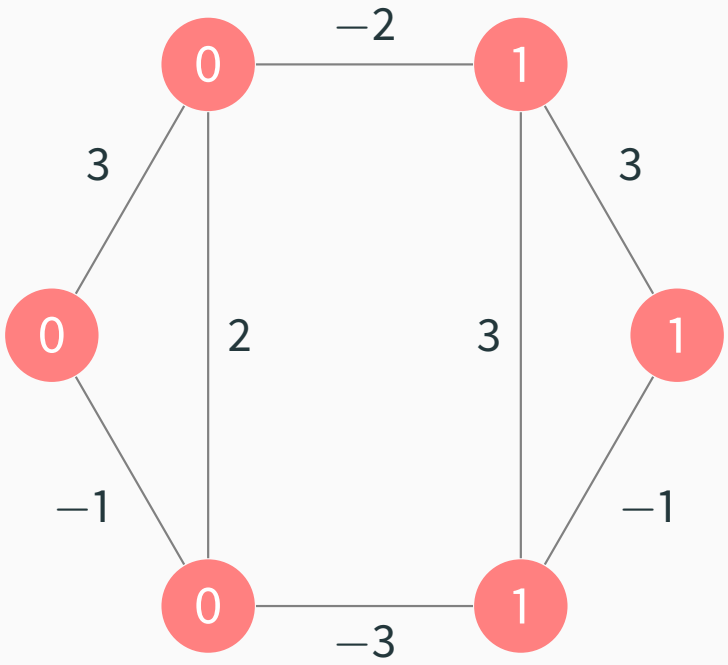
Hopfield Networks



(1, 0, 0, 0, 0, 1)

(1, 1, 0, 0, 0, 1)

(0, 0, 1, 1, 1, 0)