Restricted Boltzmann Machines (RBM's)

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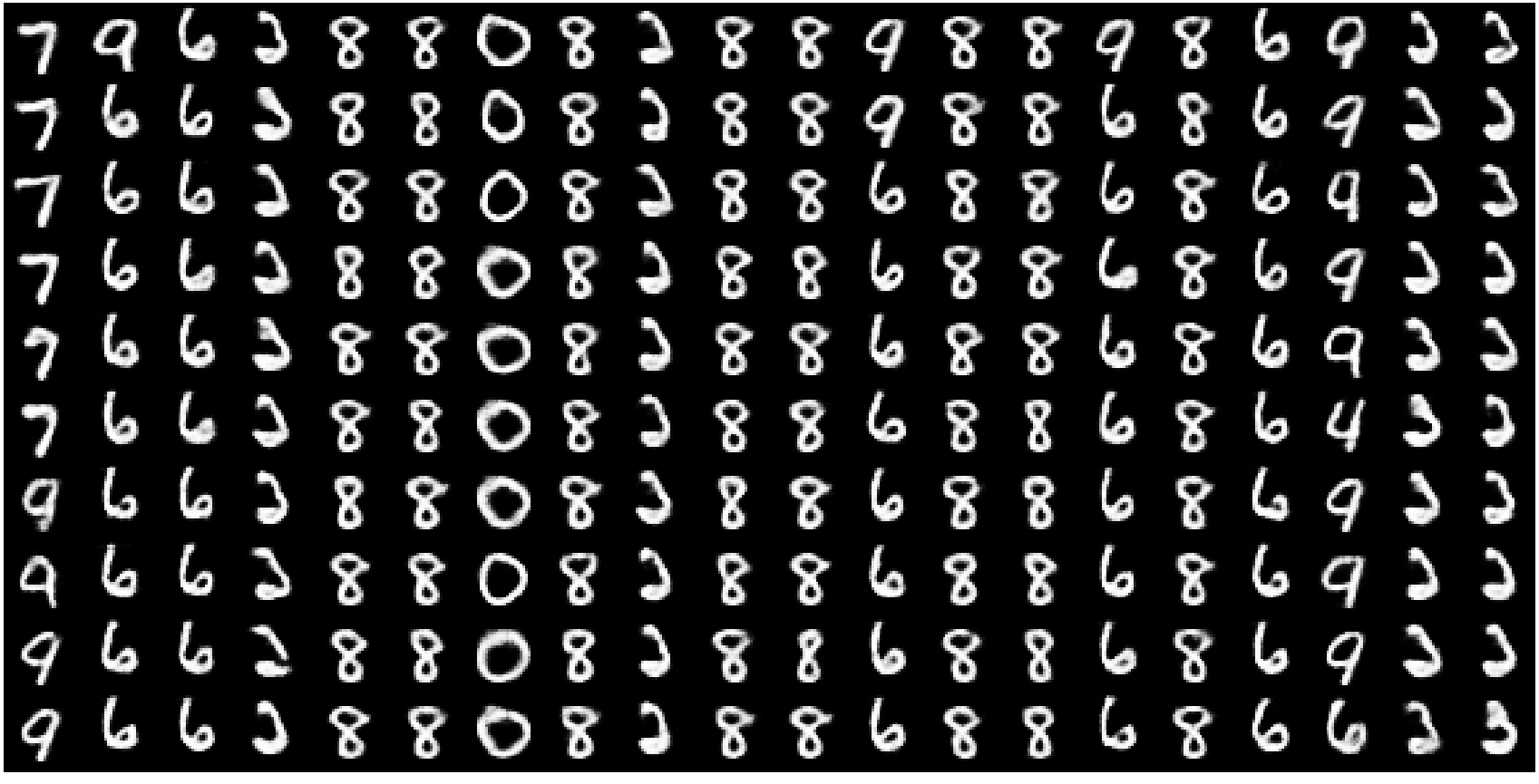
Why do we need this

We want to understand high-dimensional data with rich structure.
"Understanding" $\rightarrow$ Density estimation (true $p(\boldsymbol{x})$ under data)

- generative models
- Missing value imputation (given partial $\boldsymbol{x}$)
- Denoising (return original $\boldsymbol{x}$ given damaged $\tilde{\boldsymbol{x}}$)
- ...

$\rightarrow$ Density estimation (true $p(\boldsymbol{x})$ under data)

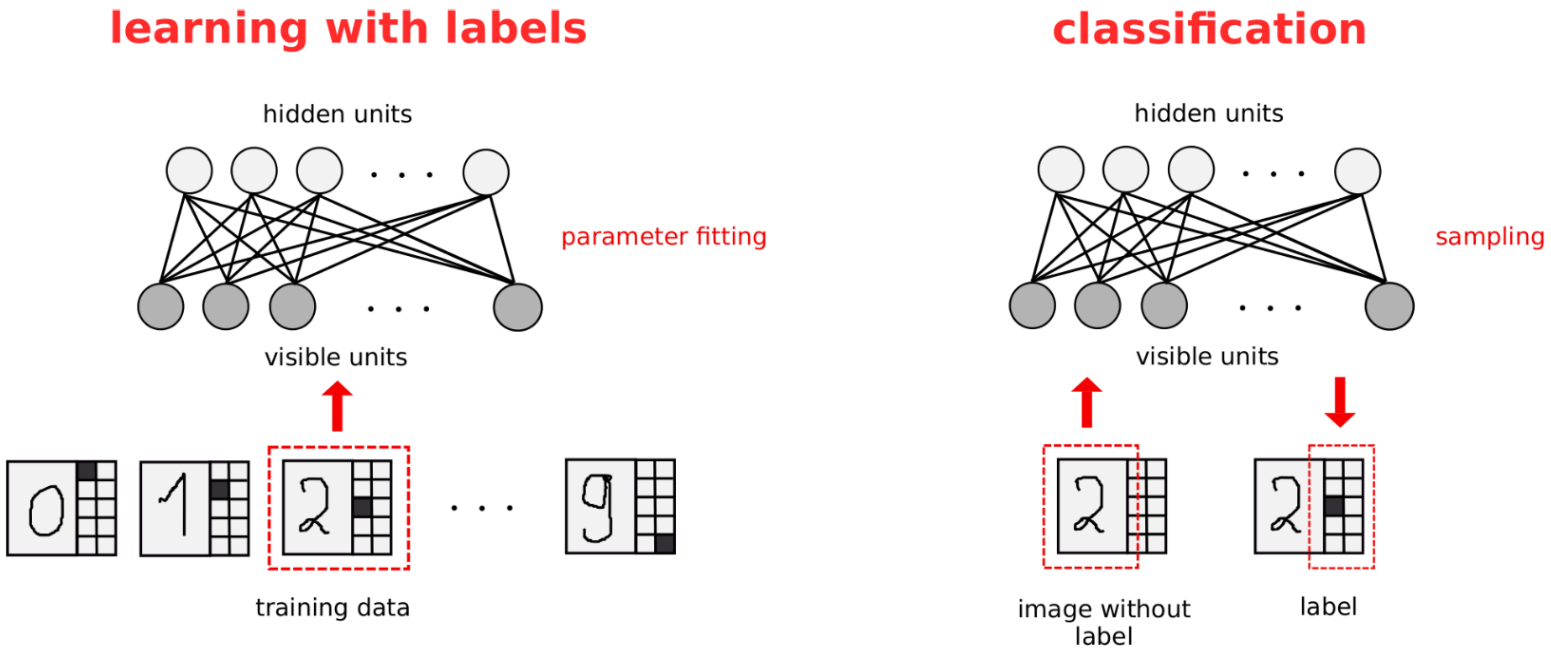
- generative models



[7]

$\rightarrow$ Density estimation (true $p(\boldsymbol{x})$ under data)

- Missing value imputation (given partial $\boldsymbol{x}$)
  $\rightarrow$ classification is actually special case!



$\rightarrow$ Density estimation (true $p(\boldsymbol{x})$ under data)

- Denoising (return original $\boldsymbol{x}$ given damaged $\tilde{\boldsymbol{x}}$)

[14] note: this result uses more advanced concepts based on RBMs

Why this is hard

This requires modelling the underlying probability distribution.

$\rightarrow$ fundamentally problematic

Naive approach to represent probabilitiy distribution has space complexity $\mathcal{O}(n^k)$ (where n is the cardinality of the state space of the probality distribution, k is the number of random variables)

Idea: use conditional structure of probability distribution to reduce complexity

$\rightarrow$ motivation for so called **graphical models**

Graphical models

$G = (V, E)$, V nodes, E edges, defines an **undirected Graph**.

clique is a subset of V in which all nodes are pairwise connected. Call a clique **maximal**, if no node can be added without violating the definition of a clique.

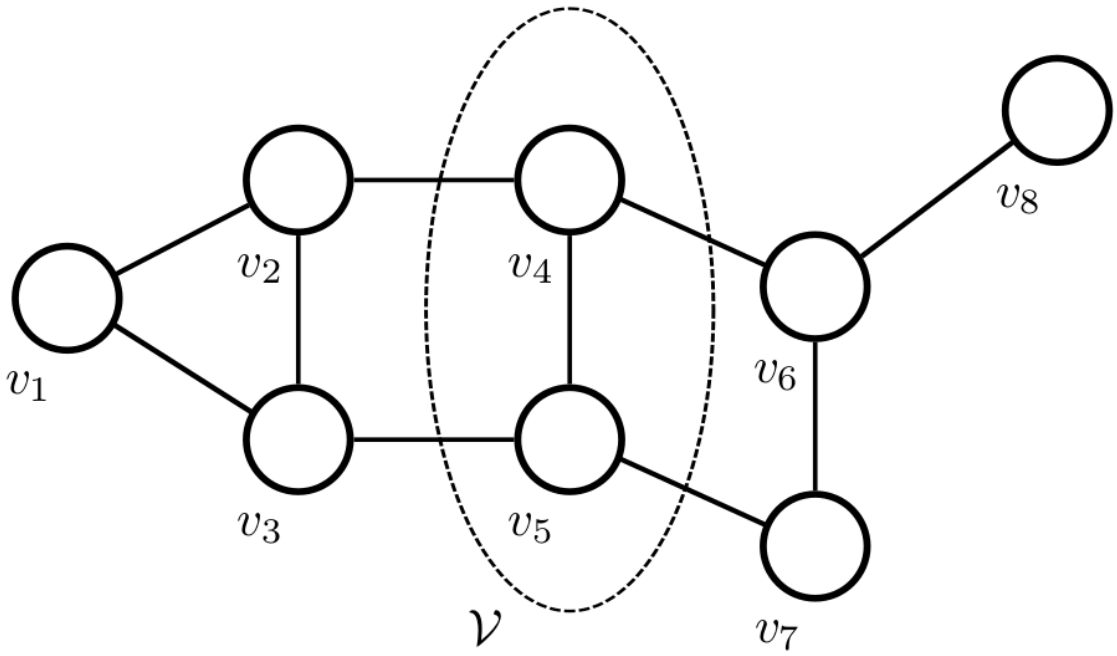


Figure 1: Undirected graph, $\{v_4, v_5\}$ clique, also maximal [6]

Graphical Models

$\rightarrow$ each node $v \in V$ corresponds to random variable X_v

$\rightarrow$ edges encode direct probabilistic interaction

Markov random fields

The set $\boldsymbol{X} = (X_v)_{v \in V}$ is called a **Markov random field (MRF)** iff

$$\forall \boldsymbol{x} : \forall v \in V : p\left(x_v | (x_w)_{w \in V \setminus \{v\}}\right) = p\left(x_v | (x_w)_{w \in \mathcal{N}_v}\right) \tag{1}$$

$$\mathcal{N}_v = \{w \in V : \{w, v\} \in E\} \text{ neighborhood of } v$$

In other words, in a Markov random field all X_v are conditionally independent of all other variables given their neighborhood.

Markov random fields

Theorem (Hammersley-Clifford) [15]

For a Markov random field the following equivalence holds

1) the distribution p is strictly positive

2) p factorizes over the Graph G, i.e.

$$p(\boldsymbol{x}) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}) \tag{2}$$

where the product runs over all maximal cliques.

The $\psi_C(\boldsymbol{x})$ are often referred to as **clique potentials**.

Energy based models and Gibbs distribution

Rewrite (2):

$$p(\boldsymbol{x}) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}) = \frac{1}{Z} e^{\sum_{C \in \mathcal{C}} \ln \psi_C(\boldsymbol{x})} = \frac{1}{Z} e^{-E(\boldsymbol{x})} \tag{3}$$

$\rightarrow$ **Energy based model (EBM)** (alt.: harmony based model)

underlying distribution: **Boltzmann distribution / Gibbs distribution**

$\rightarrow$ + latent variables = **Boltzmann machine**

Problem

general MRFs virtually **untrainable**

Problem

general MRFs virtually **untrainable**

$\rightarrow$ in the most general case (fully connected) no benefit for graphical model!

$\rightarrow$ hard to do something clever without relying on some structure

Restricted Boltzmann machines (Harmonium)

Constraining structure $\rightarrow$ **bipartite graph**

one layer of visible & one layer of hidden/latent variables

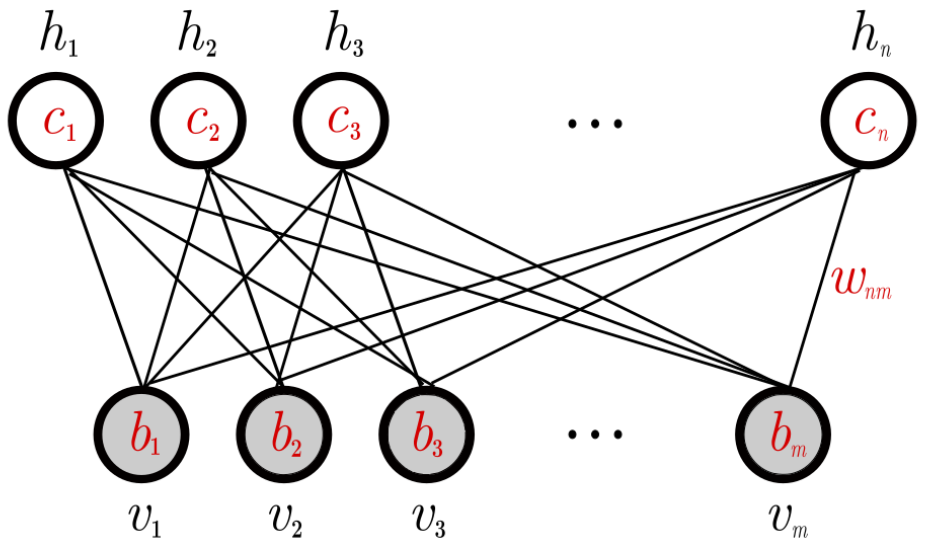
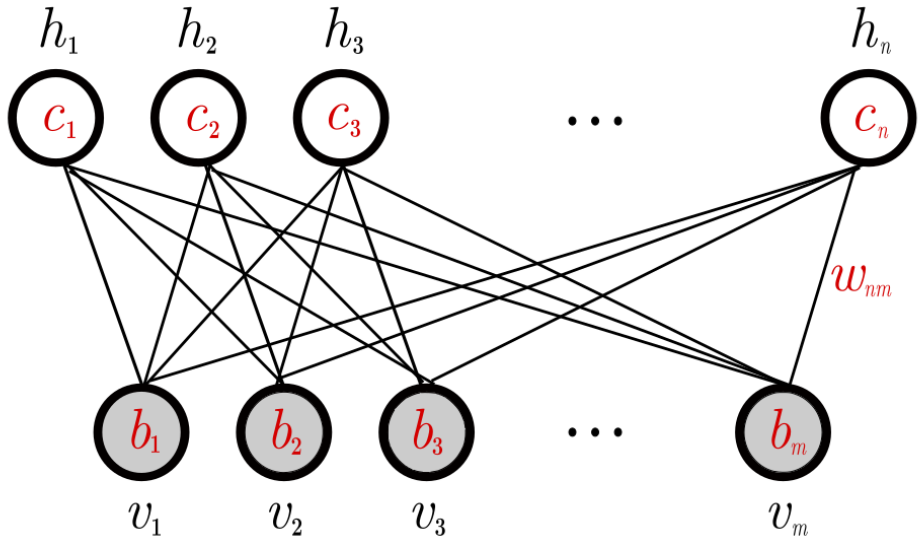
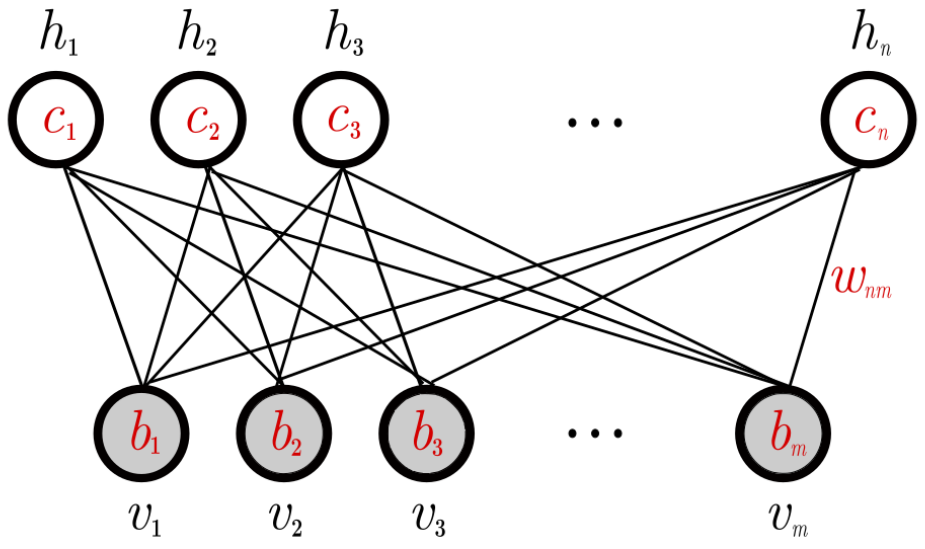


Figure 2: Restricted Boltzmann machine



binary random variables $(\boldsymbol{V}, \boldsymbol{H}) \rightarrow (\boldsymbol{v}, \boldsymbol{h}) \in \{0,1\}^{m+n}$

$$E(\boldsymbol{v}, \boldsymbol{h}) = -\sum_{i=1}^{n}\sum_{j=1}^{m} w_{ij} h_i v_j - \sum_{j=1}^{m} b_j v_j - \sum_{i=1}^{n} c_i h_i \tag{4}$$



takeaway: RBMs are Boltzmann machines with structure & energy constraint

Properties of RBMs

no connections inside each layer

$$p(\boldsymbol{h}|\boldsymbol{v}) = \prod_{i=1}^{n} p\left(h_i|\boldsymbol{v}\right)$$
$$p(\boldsymbol{v}|\boldsymbol{h}) = \prod_{j=1}^{m} p\left(v_j|\boldsymbol{h}\right) \tag{5}$$

Properties of RBMs

universal approximators for distributions on $\{0,1\}^m$

$\rightarrow$ additionally quite a few other results about universal approximator properties [11] [13]

Sampling from RBMs

How to access what we learn

Calculating partition function of RBM's intractable

$\rightarrow$ **Markov chain Monte Carlo** (MCMC) methods provide ways to sample from $p(\boldsymbol{v}, \boldsymbol{h})$ without knowing Z

Markov Chains

A **Markov chain** is a family of random variables $X = \left\{X^k | k \in \mathbb{N}_0\right\}$ that, $\forall k \geq 0$ and $\forall j, i, i_0, \ldots, i_{k-1} \in \Omega$ satisfies

$$\Pr\left(X^{(k+1)} = j | X^{(k)} = i, \ldots, X^{(0)} = i_0\right) = \Pr\left(X^{(k+1)} = j | X^{(k)} = i\right) \tag{6}$$

Markov Chains

Transition matrix $\mathbf{P} = \left(\Pr\left(X^{(k+1)} = j | X^{(k)} = i\right)\right)_{i,j\in\Omega} = (p_{ij})_{i,j\in\Omega}$

stationary distribution π for which $\pi^{\mathrm{T}} = \pi^{\mathrm{T}}\mathbf{P}$

Detailed balance condition $\pi(i)p_{ij} = \pi(j)p_{ji}$ sufficient for stationarity of π

Markov Chains

irreducible (can get from any state in Ω to any other in finite number of transitions)

$$\forall s_i, s_j \in \Omega : \exists n \in \mathbb{N} : P\left(X_n = s_i | X_0 = s_j\right) > 0$$

aperiodic (every state can reoccur at irregular times)

$$\gcd\left\{n > 0 : \Pr\left(X_n = i | X_0 = i\right) > 0\right\} = 1$$

$\Rightarrow$ Markov chain over finite Ω converges to its stationary distribution

Gibbs sampling

Idea

Construct Markov chain by updating each variable based on its conditional distribution given state of the others

Gibbs sampling - Metropolis-Hastings

MRF $\boldsymbol{X} = (X_1, \ldots, X_N)$ w.r.t. $G = (V, E)$ and $p(\boldsymbol{x}) = \frac{1}{Z} e^{-E(\boldsymbol{x})}$, then produce new state as follows:

1. Pick $X_i, i \in V$ at random with strictly positive $q(i)$
2. Transition between $\boldsymbol{x}$ and $\boldsymbol{y}$, $\boldsymbol{x} \neq \boldsymbol{y}$ with $p_{\boldsymbol{xy}} =$
$$\begin{cases} q(i)p\left(y_i | \left(x_v\right)_{v \in \mathcal{N}_i}\right), & \text{if } \exists i \in V \text{ so that } \forall v \in V \text{ with } v \neq i : x_v = y_v \\ 0, & \text{else} \end{cases}$$
and stay in $\boldsymbol{x}$ with $p_{\boldsymbol{xx}} = \sum_{i \in V} q(i)p\left(x_i | \left(x_v\right)_{v \in \mathcal{N}_i}\right)$

Gibbs sampling

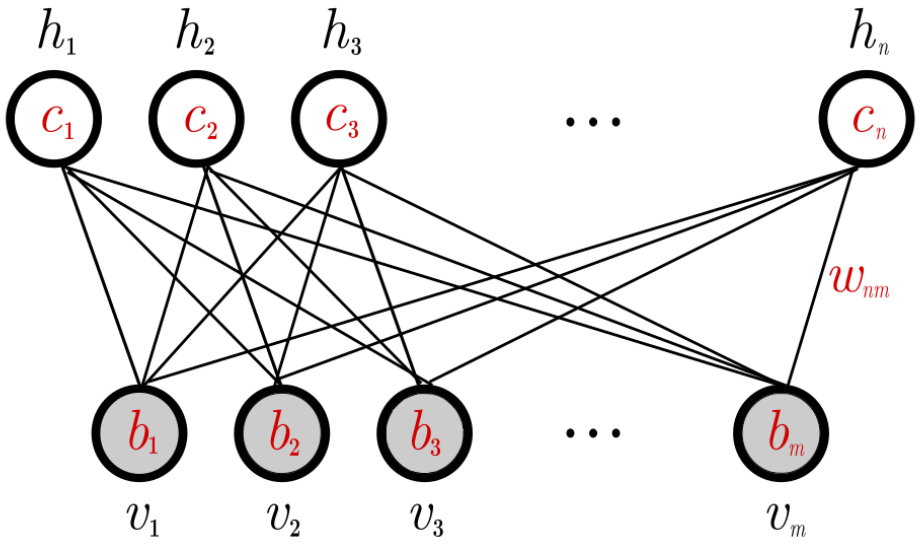
$p(\boldsymbol{x}) = \frac{1}{Z} e^{-E(\boldsymbol{x})}$ and conditional probabilities strictly positive

$\rightarrow$ Chain irreducible and aperiodic

$\rightarrow$ Chain converges to stationary distribution

$\rightarrow$ $p(\boldsymbol{x}) = \frac{1}{Z} e^{-E(\boldsymbol{x})}$ stationary distribution (detailed balance)

k-step Block Gibbs sampling in RBM's



no intralayer connections in RBM's

$\rightarrow$ sample states of all variables in one layer jointly

Algorithm 1 Block Gibbs sampling in RBM's

Input RBM $(V_1, \ldots, V_m, H_1, \ldots, H_n)$, Gibbs steps k
Output sample $(\boldsymbol{v}^{(k)}, \boldsymbol{h}^{(k)})$ after k Gibbs steps
$\boldsymbol{v}^{(0)} \leftarrow$ random_vector
for $t = 0, \ldots, k-1$ **do**
    for $i = 1..n$ **do**
        Sample $h_i^{(t)} \sim p\left(h_i | \boldsymbol{v}^{(t)}\right)$
    end for
    for $j = 1..m$ **do**
        Sample $v_j^{(t+1)} \sim p\left(v_j | \boldsymbol{h}^{(t)}\right)$
    end for
end for

Training RBMs

What to minimize

Gibbs sampling helps once we have parameters

But how to learn them?

$\rightarrow$ minimize distance between (unknown) data distribution q and RBM-distribution p in terms of **Kullback-Leibler divergence**

KL and log-likelihood

Minimizing

$$\mathrm{KL}(q\|p) = \sum_{\boldsymbol{x}\in\Omega} q(\boldsymbol{x}) \ln \frac{q(\boldsymbol{x})}{p(\boldsymbol{x})} = \sum_{\boldsymbol{x}\in\Omega} q(\boldsymbol{x}) \ln q(\boldsymbol{x}) - \sum_{\boldsymbol{x}\in\Omega} q(\boldsymbol{x}) \ln p(\boldsymbol{x}) \quad (7)$$

$\Longleftrightarrow$

Maximizing **log-likelihood**

$$\ln \mathcal{L}(\boldsymbol{\theta}|S) = \ln \prod_{i=1}^{\ell} p\left(\boldsymbol{x}_i|\boldsymbol{\theta}\right) = \sum_{i=1}^{\ell} \ln p\left(\boldsymbol{x}_i|\boldsymbol{\theta}\right) \quad (8)$$

over training data $S = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_\ell\}$ w.r.t. parameters $\boldsymbol{\theta}$

Unsupervised RBM learning

$\rightarrow$ Learning $=$ gradient ascent on log-likelihood with learning rate $\eta \in \mathbb{R}^+$,

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} + \eta \frac{\partial}{\partial \boldsymbol{\theta}^{(t)}} \left(\ln \mathcal{L} \left(\boldsymbol{\theta}^{(t)} | S \right) \right) \tag{9}$$

Unsupervised RBM learning

For single training example $\boldsymbol{v}$,

$$\ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v}) = \ln \sum_{\boldsymbol{h}} e^{-E(\boldsymbol{v},\boldsymbol{h})} - \ln \sum_{\boldsymbol{v},\boldsymbol{h}} e^{-E(\boldsymbol{v},\boldsymbol{h})}$$

$$\Rightarrow \frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial \boldsymbol{\theta}} = \frac{\partial}{\partial \boldsymbol{\theta}} \left(\ln \sum_{\boldsymbol{h}} e^{-E(\boldsymbol{v},\boldsymbol{h})} \right) - \frac{\partial}{\partial \boldsymbol{\theta}} \left(\ln \sum_{\boldsymbol{v},\boldsymbol{h}} e^{-E(\boldsymbol{v},\boldsymbol{h})} \right)$$

$$= -\frac{1}{\sum_{\boldsymbol{h}} e^{-E(\boldsymbol{v},\boldsymbol{h})}} \sum_{\boldsymbol{h}} e^{-E(\boldsymbol{v},\boldsymbol{h})} \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial \boldsymbol{\theta}} + \frac{1}{\sum_{\boldsymbol{v},\boldsymbol{h}} e^{-E(\boldsymbol{v},\boldsymbol{h})}} \sum_{\boldsymbol{v},\boldsymbol{h}} e^{-E(\boldsymbol{v},\boldsymbol{h})} \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial \boldsymbol{\theta}}$$

$$\frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial \boldsymbol{\theta}} = -\sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) \frac{\partial E(\boldsymbol{v}, \boldsymbol{h})}{\partial \boldsymbol{\theta}} + \sum_{\boldsymbol{v}, \boldsymbol{h}} p(\boldsymbol{v}, \boldsymbol{h}) \frac{\partial E(\boldsymbol{v}, \boldsymbol{h})}{\partial \boldsymbol{\theta}} \qquad (10)$$

The first term in (10) is referred to as **positive phase** the second as **negative phase**.

Positive and negative phase

Positive phase

$-\sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial \boldsymbol{\theta}}$

$\rightarrow$ finds hidden configurations that work well with $\boldsymbol{v}$ and lowers their energies

Negative Phase

$\sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial \boldsymbol{\theta}}$

$\rightarrow$ finds joint configuration that are the "best competitors" and raises their energies

Positive phase in RBM's

$\rightarrow$ generally very easy for RBM's exploiting independence property (5):

$$p(\boldsymbol{h}|\boldsymbol{v}) = \prod_{i=1}^{n} p\left(h_i|\boldsymbol{v}\right)$$

$$p(\boldsymbol{v}|\boldsymbol{h}) = \prod_{j=1}^{m} p\left(v_j|\boldsymbol{h}\right)$$

For example, positive Phase w.r.t. w_{ij} (and similarly for b_i, c_j):

Let $\boldsymbol{h}_{-i}$ denote state of all hidden variables but the i-th one, then

$$-\sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v})\frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} = \sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) h_i v_j = \sum_{\boldsymbol{h}} \prod_{k=1}^{n} p\left(h_k|\boldsymbol{v}\right) h_i v_j$$

$$= \sum_{h_i}\sum_{\boldsymbol{h_{-i}}} p\left(h_i|\boldsymbol{v}\right) p\left(\boldsymbol{h}_{-i}|\boldsymbol{v}\right) h_i v_j = \sum_{h_i} p\left(h_i|\boldsymbol{v}\right) h_i v_j \sum_{\boldsymbol{h_{-i}}} p\left(\boldsymbol{h}_{-i}|\boldsymbol{v}\right)$$

$$= p\left(H_i = 1|\boldsymbol{v}\right) v_j \tag{11}$$

$\rightarrow$ saves us from exponential sum in number of hidden variables

Negative phase in RBM's

We're not so lucky here!

$\rightarrow$ same trick gets rid only of either $\sum_{\boldsymbol{v}}$ or $\sum_{\boldsymbol{h}}$ in $\sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}}$

For example, getting rid of $\sum_{\boldsymbol{h}}$ leaves:

$$\sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} = -\sum_{\boldsymbol{v}} p(\boldsymbol{v}) \sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) h_i v_j$$

$$= -\sum_{\boldsymbol{v}} p(\boldsymbol{v}) p\left(H_i = 1|\boldsymbol{v}\right) v_j \tag{12}$$

$\rightarrow$ sum remains exponential either in hidden or visible variables

$$\frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial w_{ij}} = -\sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) \frac{\partial E(\boldsymbol{v}, \boldsymbol{h})}{\partial w_{ij}} + \sum_{\boldsymbol{v}, \boldsymbol{h}} p(\boldsymbol{v}, \boldsymbol{h}) \frac{\partial E(\boldsymbol{v}, \boldsymbol{h})}{\partial w_{ij}}$$

$$\frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial w_{ij}} = -\sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} + \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}}$$

$$= p\left(H_i = 1|\boldsymbol{v}\right) v_j + \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}}$$

$$\begin{aligned}
\frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial w_{ij}} &= -\sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} + \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} \\
&= p\left(H_i = 1|\boldsymbol{v}\right) v_j + \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} \\
&= p\left(H_i = 1|\boldsymbol{v}\right) v_j - \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) h_i v_j
\end{aligned}$$

$$\frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial w_{ij}} = -\sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} + \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}}$$

$$= p\left(H_i = 1|\boldsymbol{v}\right) v_j + \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}}$$

$$= p\left(H_i = 1|\boldsymbol{v}\right) v_j - \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) h_i v_j$$

$$= p\left(H_i = 1|\boldsymbol{v}\right) v_j - \sum_{\boldsymbol{v}} p(\boldsymbol{v}) p\left(H_i = 1|\boldsymbol{v}\right) v_j$$

$$\begin{aligned}
\frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial w_{ij}} &= -\sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} + \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} \\
&= p\left(H_i = 1|\boldsymbol{v}\right) v_j + \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} \\
&= p\left(H_i = 1|\boldsymbol{v}\right) v_j - \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) h_i v_j \\
&= p\left(H_i = 1|\boldsymbol{v}\right) v_j - \sum_{\boldsymbol{v}} p(\boldsymbol{v}) p\left(H_i = 1|\boldsymbol{v}\right) v_j \\
&= p\left(H_i = 1|\boldsymbol{v}\right) v_j - \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) h_i v_j
\end{aligned}$$

Training algorithms

For gradient ascent, need a way to compute second term:

$$\frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial w_{ij}} = p\left(H_i = 1|\boldsymbol{v}\right) v_j - \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) h_i v_j$$

$\rightarrow$ approximate this sum by MCMC methods

$$\sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) h_i v_j$$

$\rightarrow$ think of sum as expectation value

$\rightarrow$ Gibbs sampling $\rightarrow$ approximate as average over a few samples

Algorithm 2 Naive MCMC gradient estimation

Input RBM $(V_1, \ldots, V_m, H_1, \ldots, H_n)$, training batch S
Output Δw_{ij} for $i = 1, \ldots, n, j = 1, \ldots, m$
init: $\Delta w_{ij} = 0$ for $i = 1, \ldots, n, j = 1, \ldots, m$
for all $\boldsymbol{v} \in S$ **do**
    for l=1..ξ **do**
        $\boldsymbol{v}^{(0)} \leftarrow$ random_vector
        for $t = 0, \ldots, k-1$ **do**
            for $i = 1..n$ **do**
                Sample $h_i^{(t)} \sim p\left(h_i | \boldsymbol{v}^{(t)}\right)$
            end for
            for $j = 1..m$ **do**
                Sample $v_j^{(t+1)} \sim p\left(v_j | \boldsymbol{h}^{(t)}\right)$
            end for
        end for
    end for ▷ here ξ $(\boldsymbol{v}, \boldsymbol{h})$ pairs (approximately from $p(\boldsymbol{v}, \boldsymbol{h})$) $\rightarrow$ call these $(\boldsymbol{v}^l, \boldsymbol{h}^l)$
    for $i = 1, \ldots, n, j = 1, \ldots, m$ **do**
        $\Delta w_{ij} \leftarrow \Delta w_{ij} + p\left(H_i = 1 | \boldsymbol{v}\right) \cdot v_j - \frac{1}{\xi} \sum_{l=1..\xi} h_i^l v_j^l$
    end for
end for

Problem

requires running a lot of Gibbs chains (computationally expensive)

$\rightarrow$ take a step back, tackle the exponential sum again

$$\frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial w_{ij}} = -\sum_{\boldsymbol{h}} p(\boldsymbol{h}|\boldsymbol{v}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}} + \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) \frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial w_{ij}}$$

$$= p\left(H_i = 1|\boldsymbol{v}\right) v_j - \sum_{\boldsymbol{v}} p(\boldsymbol{v}) p\left(H_i = 1|\boldsymbol{v}\right) v_j$$

Contrastive divergence $CD - k$

- initialize Gibbs chain by data distribution $\rightarrow$ less time to burn in
- approximate the expectation value using a single sampled $\boldsymbol{v}^{(k)}$ (that is after k Gibbs steps)

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$$\approx p\left(H_i = 1|\boldsymbol{v}\right) v_j - p(H_i = 1|\boldsymbol{v}^{(k)}) v_j^{(k)}$$

Algorithm 3 k-step contrastive divergence [1]

Input RBM $(V_1, \ldots, V_m, H_1, \ldots, H_n)$, training batch S
Output $\Delta w_{ij}, \Delta b_j$ and Δc_i for $i = 1, \ldots, n, j = 1, \ldots, m$
init: $\Delta w_{ij} = \Delta b_j = \Delta c_i = 0$ for $i = 1, \ldots, n, j = 1, \ldots, m$
for all $\boldsymbol{v} \in S$ **do**
    $\boldsymbol{v}^{(0)} \leftarrow \boldsymbol{v}$
    for $t = 0, \ldots, k-1$ **do**
        for $i = 1..n$ **do**
            Sample $h_i^{(t)} \sim p\left(h_i | \boldsymbol{v}^{(t)}\right)$
        end for
        for $j = 1..m$ **do**
            Sample $v_j^{(t+1)} \sim p\left(v_j | \boldsymbol{h}^{(t)}\right)$
        end for
    end for
    for $i = 1, \ldots, n, j = 1, \ldots, m$ **do**
        $\Delta w_{ij} \leftarrow \Delta w_{ij} + p\left(H_i = 1 | \boldsymbol{v}^{(0)}\right) \cdot v_j^{(0)} - p\left(H_i = 1 | \boldsymbol{v}^{(k)}\right) \cdot v_j^{(k)}$
    end for
    for $j = 1..m$ **do**
        $\Delta b_j \leftarrow \Delta b_j + v_j^{(0)} - v_j^{(k)}$
    end for
    for $j = 1..n$ **do**
        $\Delta c_i \leftarrow \Delta c_i + p\left(H_i = 1 | \boldsymbol{v}^{(0)}\right) - p\left(H_i = 1 | \boldsymbol{v}^{(k)}\right)$
    end for
end for

Why does this even work?

- non-trivial and surprising when first introduced
- does not follow gradient of log-likelihood
  $\rightarrow$ important results give conditions for convergence and bounds on the expectation error, empirical observations support this further ([3, 4, 5, 17])

Why does this even work?

- non-trivial and surprising when first introduced
- does not follow gradient of log-likelihood
  $\rightarrow$ important results give conditions for convergence and bounds on the expectation error, empirical observations support this further ([3, 4, 5, 17])
- even more surprising: in practice, very often $k = 1$ [9]

Persistent contrastive divergence (PCD)

do not reinitialize Gibbs chains, but keep them permanently

$\rightarrow$ update step is small enough so distribution keeps close to previous step

Where to go from here?

- better training
  - fast persistent contrastive divergence (FPCD)
  - parallel tempering
- other models
  - Deep Belief Networks
  - Conditional Boltzmann machines
  - ...

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Error Bound CD-k

Let p denote the marginal distribution of the visible units of an RBM and let q be the empirical distribution defined by a set of samples $v_1, \ldots, v_l$. Then an upper bound on the expectation of the error of the CD-k approximation of the log-likelihood derivative w.r.t some RBM parameter Θ_a is given by

$$\left| E_{q\left(\boldsymbol{v}^{(0)}\right)} \left[E_{p\left(\boldsymbol{v}^{(k)} | \boldsymbol{v}^{(0)}\right)} \left[\frac{\partial \ln p\left(\boldsymbol{v}^{(k)}\right)}{\partial \theta_a} \right] \right| \leq \frac{1}{2} \left| q - p \right| \left(1 - e^{-(m+n)\Delta}\right)^k$$

with

$$\Delta = \max \left\{ \max_{l \in \{1,\ldots,m\}} \vartheta_l, \max_{l \in \{1,\ldots,n\}} \xi_l \right\}$$
$$\vartheta_l = \max \left\{ \left| \sum_{i=1}^{n} I_{\{w_{il} > 0\}} w_{il} + b_l \right|, \left| \sum_{i=1}^{n} I_{\{w_{il} < 0\}} w_{il} + b_l \right| \right\}$$
$$\xi_l = \max \left\{ \left| \sum_{j=1}^{m} I_{\{w_{lj} > 0\}} w_{lj} + c_l \right|, \left| \sum_{j=1}^{m} I_{\{w_{lj} < 0\}} w_{lj} + c_l \right| \right\}$$

RBMs and neural networks

Why is $p(H_i = 1|\boldsymbol{v})$ in positive phase computationally feasible?

$\rightarrow$ Z cancels out; explicit calculation shows:

$$p(H_i = 1|\boldsymbol{v}) = \text{sig}\left(\sum_{j=1}^{m} w_{ij} v_j + c_i\right)$$
$$p(V_j = 1|\boldsymbol{h}) = \text{sig}\left(\sum_{i=1}^{n} w_{ij} h_i + b_j\right)$$

Identify:

single variable $\rightarrow$ neuron

conditional probability $\rightarrow$ sigmoid activation function

RBM $\rightarrow$ **stochastic neural network**