The expressive power of mixture models and Restricted Boltzmann Machines

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Outline

- Mixture Models and RBMs
- Submodels of RBMs
- The number of modes
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- Submodels of RBMs
- The number of modes
Mixture models

Consider $n$ binary random variables. We want to study product distributions and their mixtures.

Definition
The $k$th mixture model $M_{n,k}$ consists of all convex combinations of $k$ product distributions.

$$p(x_1, \ldots, x_n) = \sum_{i=1}^{k} \lambda_i q_{i,1}(x_1) q_{i,2}(x_2) \cdots q_{i,n}(x_n).$$
Mixture models

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**Definition**
The $k$th mixture model $M_{n,k}$ consists of all convex combinations of $k$ product distributions.

$M_{n,k}$ is *(the closure of)* a graphical model with one hidden node of size $k$.

With this definition, the first mixture model is the *independence model*. 
Consider $n$ binary random variables.

**Definition**

The *Restricted Boltzmann Machine* $\text{RBM}_{n,m}$ is *(the closure of)* the graphical model of the complete bipartite graph $K_{n,m}$, where the group of $m$ nodes is hidden.
Relations between mixture models and RBMs

- \( \text{RBM}_{n,m} \) is a submodel of \( M_{n,2^m} \):

\[
p(v) = \sum_h p(v, h) = \sum_h p(v|h)p(h),
\]

where the conditionals \( p(v|h) \) are product distributions.

The mixture components \( p(h) \) belong to \( \text{RBM}_{m,n} \).

- For \( m = 1 \), equality holds: \( \text{RBM}_{n,1} = M_{n,2} \).

- \( \text{RBM}_{n,m} \) equals the \( m \)th Hadamard power of \( M_{n,2} \):
  - Hadamard product of functions = point-wise product
  - for probability distributions: renormalize afterwards

(Observation due to Cueto, Morton and Sturmfels 2009)
The expressive power

We want to describe, as precisely as possible, which probability distributions a model does or does not contain.

- Both RBMs and mixture models are semi-algebraic sets: They have an implicit description in terms of polynomial equations and inequalities.

Question
How does this semi-algebraic description look like?

This description would allow to easily check whether a given distribution belongs to the model.

... but it appears to be too difficult to compute.
The expressive power

Since a complete description seems out of reach, we can ask other questions:

**Easier problems**

- What is the dimension of the model?
- Find large subsets of the model that are easy to describe.
- Find large sets of probability distributions that are not contained in the model.
The dimension of a model

In many cases, the dimension of a parametrically defined semi-algebraic set is the expected dimension, i.e. the number of parameters (or the dimension of the ambient space).

- The dimension of binary mixture models was recently computed:

**Theorem (Catalisano, Geramita and Gimigliano 2011)**

The dimension of $M_{n,k}$ equals the expected dimension

$$\min\{nk + k - 1, 2^n - 1\}, \text{ unless } n = 4 \text{ and } m = 3.$$  

- For RBMs, the dimension is as expected in all known cases:

**Theorem (Cueto, Morton and Sturmfels 2009)**

The dimension of $\text{RBM}_{n,m}$ equals the expected dimension

$$\min\{nm + n + m, 2^n - 1\} \text{ for } k \leq 2^n - \lceil \log_2(n+1) \rceil \text{ and for } k \geq 2^n - \lceil \log_2(n+1) \rceil.$$
The role of dimension

It is wellknown that the dimension alone is not sufficient to decide, whether a model is *full*, i.e. contains all probability distributions:

- Zwiernik and Smith computed all inequalities of $M_{3,2}$. Montúfar proved that $M_{n,k}$ is full if and only if $k \geq 2^{n-1}$.

<table>
<thead>
<tr>
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<th>2</th>
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<td>7</td>
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<td>7</td>
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<tr>
<td>full?</td>
<td>no</td>
<td>no</td>
<td>no</td>
<td>yes</td>
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For $n = 3$:

- For RBMs with $n = 3$:

<table>
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<th>$m$</th>
<th>0</th>
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<tr>
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<td>3</td>
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<td>no</td>
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</table>
The model and its complement

The rest of the talk is about two projects that attack the following two problems:

**Problem 1**
Find large subsets of the model that are easy to describe.

We find “large” subsets of $\text{RBM}_{n,m}$. These subsets are related to mixtures of product distributions on disjoint supports and allow to estimate the maximal approximation error.

**Problem 2**
Find large sets of probability distributions that are not contained in the model.

We find “large” sets outside of $M_{n,k}$. Interestingly, these sets touch the uniform distribution, showing that the uniform distribution need not be an interior point of $M_{n,k}$, even if $M_{n,k}$ has the full dimension.
Outline

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- Submodels of RBMs
- The number of modes
Cubical sets

Idea:

- The RBM consists of mixtures of product distributions.
- Mixtures are difficult to describe...

... unless they have disjoint supports

Definition

A set $\mathcal{Y} \subseteq \{0, 1\}^n$ is **cubical**, if it corresponds to a face of the $n$-dimensional hypercube.

Cubical sets are **cylinder sets**, i.e. they are characterized by “sub-configurations.”
Cubical sets

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- Mixtures are difficult to describe...

... unless they have disjoint supports

Definition

A set $\mathcal{Y} \subseteq \{0, 1\}^n$ is **cubical**, if it corresponds to a face of the $n$-dimensional hypercube.

Cubical sets are the *support sets* of product distributions.
Mixtures on disjoint supports

**Theorem**

\[ \text{RBM}_{n,m} \text{ contains any mixture of one arbitrary product distribution and } m \text{ product distributions with pairwise disjoint cubical supports.} \]

**Corollary**

If \( m \geq 2^{n-1} - 1 \), then \( \text{RBM}_{n,m} \) is full.

**Proof of the Corollary.**

- Any distribution on an edge is a product distribution.
- The \( n \)-dimensional hypercube is covered by \( 2^{n-1} \) disjoint edges
- Hence any distribution is a mixture of \( 2^{n-1} \) product distributions supported on disjoint edges.
The approximation error

Now we can find upper bounds for the *approximation error*:

**Theorem**

Let \( m \leq 2^{n-1} - 1 \). Then the Kullback-Leibler divergence from any distribution on \( \{0, 1\}^n \) to \( \text{RBM}_{n,m} \) is upper bounded by

\[
\max_p D(p \| \text{RBM}_{n,m}) \leq n - \left\lceil \log(m + 1) \right\rceil - \frac{m + 1}{2\left\lceil \log(m+1) \right\rceil}
\]

The bound gives an idea about the value of additional hidden nodes.

**Idea of the proof:**

- Approximate a distribution \( p \) by a mixture of product distributions on disjoint supports.
- Where \( p \) puts more mass, the approximation must be better (choose smaller cubical sets).
Examples

**Theorem**

Let $m \leq 2^{n-1} - 1$. Then the Kullback-Leibler divergence from any distribution on $\{0, 1\}^n$ to $\text{RBM}_{n,m}$ is upper bounded by

$$\max_p D(p|| \text{RBM}_{n,m}) \leq n - \lfloor \log(m + 1) \rfloor - \frac{m + 1}{2^{\lfloor \log(m+1) \rfloor}}$$

\[ D(u_+|| \text{RBM}), \ n = 3 \]
\[ D(u_+|| \text{RBM}), \ n = 4 \]
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The number of modes

The set $Z_+$

**Question**
How to prove that $M_{n,k}$ is not full if $k < 2^{n-1}$?

Denote $Z_\pm$ the elements of $\{0, 1\}^n$ with *even/odd parity*.

**Lemma**
If $k < 2^{n-1}$, then $M_{n,k}$ does not contain the uniform distribution $u_+$ on $Z_+$. 
The number of modes

The set $Z_+$

![Diagram of $Z_+$]

**Lemma**

If $k < 2^{n-1}$, then $M_{n,k}$ does not contain the uniform distribution $u_+$ on $Z_+$.

**Proof.**

- If $u_+ = \sum_{i=1}^{N} \lambda_i p_i$, with $\lambda_i > 0$, then $Z_+ = \cup_i \text{supp}(p_i)$.
- If the $p_i$ are product measures, then $\text{supp}(p_i)$ is cubical.
- Only the one-element subsets of $Z_+$ are cubical.
The set $Z_+$

![Diagram showing the set $Z_+$]

**Note:** $M_{n,k}$ is full if and only if $M_{n,k}$ contains $u_+$.

**Conjecture**
The same is true for RBMs: $\text{RBM}_{n,m}$ is full if and only if $\text{RBM}_{n,m}$ contains $u_+$.

(true for $n = 3$)
The number of modes

Idea: Find a neighbourhood of $u_+$ which is not contained in $M_{n,k}$.

Definition
A *mode* of a distribution $p$ is a strict local maximum of $p$, where “local” refers to the neighbourhood structure on the cube.

- A single product distribution has (at most) one mode.
- $u_+$ has $2^{n-1}$ modes.
- If $p$ has $2^{n-1}$ modes, then the set of modes equals $Z_+$ or $Z_-$. 
The number of modes

**Idea:** Find a neighbourhood of $u_+$ which is not contained in $M_{n,k}$.

**Definition**

A *mode* of a distribution $p$ is a strict local maximum of $p$, where “local” refers to the neighbourhood structure on the cube.

- A single product distribution has (at most) one mode.
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- If $p$ has $2^{n-1}$ modes, then the set of modes equals $Z_+$ or $Z_-$. 

**Question**

How many modes can a mixture of $k$ product distributions have?
The number of modes

Let \( \alpha(n, k) \) denote the maximum number of modes that \( p \in M_{n,k} \) may have.

Properties:

- \( 2^{n-1} \geq \alpha(n, k) \geq \min\{k, 2^{n-1}\} \)
- \( \alpha(n, 1) = 1 \)
- \( \alpha(3, 2) = 2 \)
- \( \alpha(3, 3) = 3 \)

Corollary

\( M_{3,3} \) is not full.
Distributions with four modes

**Result**

\( \alpha(3, 3) = 3 \), and hence \( M_{3,3} \) is not full.

Note that there are distributions with four modes arbitrarily close to the uniform distribution.

**Corollary**

*The uniform distribution is not an interior point of \( M_{3,3} \), even though \( M_{3,3} \) is full-dimensional.*

*In particular, the uniform distribution is a singularity of \( M_{3,3} \).*

The set of distributions with four modes is a union of two polyhedral sets, containing distributions with four modes on \( \mathbb{Z}_\pm \).

Both polyhedral parts touch the uniform distributions.
Let $\alpha(n, k)$ denote the maximum number of nodes that $p \in M_{n,k}$ may have.

**Properties:**

- $2^{n-1} \geq \alpha(n, k) \geq \min\{k, 2^{n-1}\}$
- $\alpha(n, 1) = 1$
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**Properties:**

- $2^{n-1} \geq \alpha(n, k) \geq \min\{k, 2^{n-1}\}$
- $\alpha(n, 1) = 1$
- $\alpha(3, 2) = 2$
- $\alpha(3, 3) = 3$
- $\alpha(4, 2) = 3$

**This tells us:**

It is not sufficient to consider the number of modes:
For example, $\alpha(4, 7) = 8$, but $M_{4,7}$ is not full.
Summary

- Mixture models and RBM are important statistical models with many open problems.
- Mixtures of product distributions with disjoint supports can help to understand RBMs.
- Distributions with the maximal number of modes are difficult to approximate with mixture models and RBMs.

Open Problems:

- Compute $\alpha(n, k)$ for $n \geq 4$, $k \geq 2$.
- Is the uniform distribution always a singularity of $M_{n,k}$ (unless the model is full)?
- What about $\text{RBM}_{n,m}$?
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NIPS 2011

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arXiv 1008.0204

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