Restricted Boltzmann Machines: Learning, and Hardness of Inference

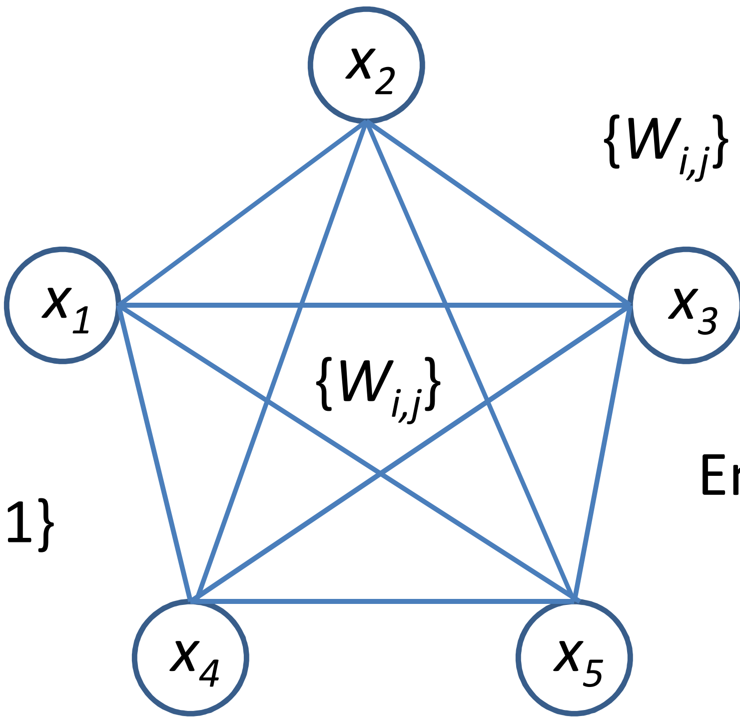
Presented by:
Nakul Verma

Recall: Hopfield Nets

- An energy based network of interconnected inputs (typically referred to as *neurons*) to encode memories.

n = 5

$\{W_{i,j}\}$ = connection weights



$x_i \in \{-1,1\}$

Energy of a configuration:

$$E[x;W] := -x^{\mathsf{T}}Wx/2$$

Goal: to ***encode*** memories -- that is, given *p* configurations $z^1,\ldots,z^p$, ***learn*** *W* such that each configuration z^i is (locally) a low energy state.

Hopfield Nets: limitations

- Not all memories can be encoded in this way!

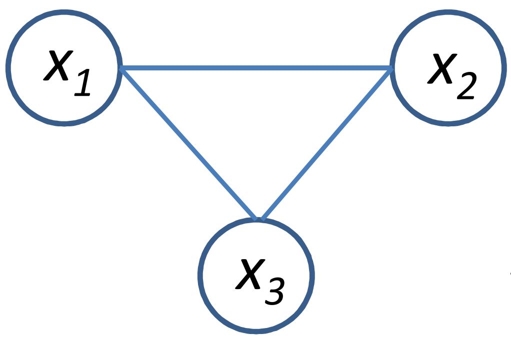
  Typically: Hopfield Nets cannot encode high-order correlations

Example

- Suppose $n = 3$ and we want to remember only two memories:

  learn patterns: $z^1 = \{1, -1, 1\}$ and $z^2 = \{1, 1, -1\}$

Want to learn: parameters W in a Hopfield Net, that assign locally low energy to these memories



What W should we choose?

Hopfield Nets: limitations

Memories to encode:
$z^1 = \{1, -1, 1\}$
$z^2 = \{1, 1, -1\}$

- Recall, we assigned the weights as

$$W := \sum_i z^i (z^i)^\mathsf{T}$$

It turns out that this assignment does **NOT** assign low energy (locally) to the given memory configurations.

Why? In this case, $W = z^1(z^1)^\mathsf{T} + z^2(z^2)^\mathsf{T} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & -2 \\ 0 & -2 & 2 \end{bmatrix}$

so, $E[z^1; W] = E[z^2; W] = -5$

BUT: for $x = \{-1, 1, -1\}$ (hamming distance 1 from z^2)

$$E[x; W] = -5$$

So, W is **not** locally energy minimizing!

Hopfield Nets: limitations

Question: Is there *any* symmetric W for which the memories z^1 and z^2 are (locally) energy minimizing configurations?

Unfortunately, the answer is still **NO**.

Solution:

Make use of hidden units (aka **Restricted Boltzmann Machines**)

Restricted Boltzmann Machines: An overview

- A **bipartite** network between input and hidden variables

- Was introduced as:

    ‘Harmoniums’ by Smolensky [Smo87]

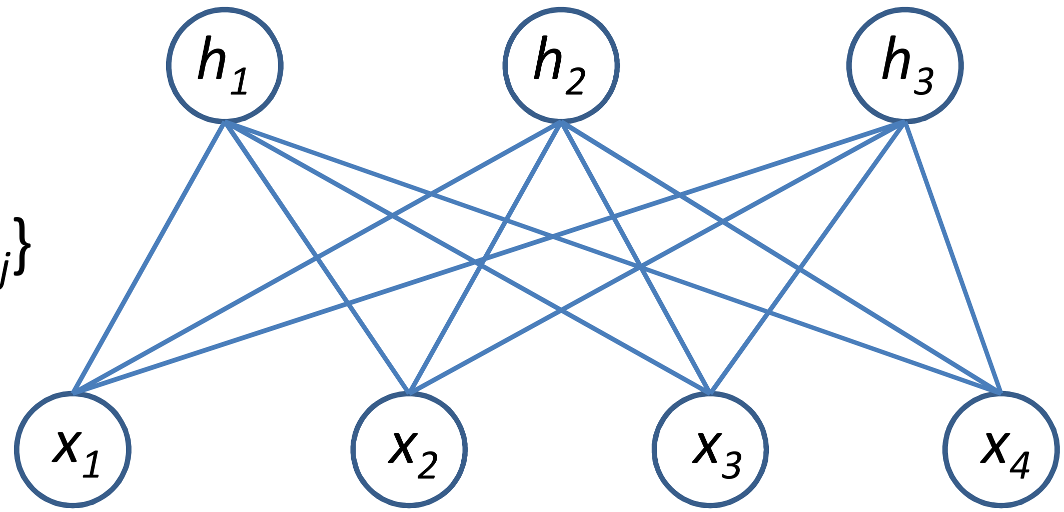
    ‘Influence Combination Machines’ by Freund and Haussler [FH91]

- Expressive enough to encode any distribution while being computationally efficient!

RBM: the structure

Hidden units:

weights $\{w_{i,j}\}$



$m = 3$

$h_i \in \{0, 1\}$

Input units:

$n = 4$

$x_j \in \{-1,+1\}$, or

$x_j \in (-\infty, \infty)$

Energy of a configuration:

$$E[x, h; W] := -x^\mathsf{T} W h \quad \text{(if } x \text{ binary)}$$

$$E[x, h; W] := -x^\mathsf{T} W h + \|x\|^2 \quad \text{(if } x \text{ real)}$$

Probability of a state:

$$P[x|W] \propto \sum_{h \in \{0,1\}^m} e^{-E(x,h;W)}$$

$$= \prod_{i=1}^{m} \left(1 + e^{-x \cdot W_{:i}}\right) \quad \text{(if } x \text{ binary)}$$

$$= e^{-\frac{1}{2}\|x\|^2} \prod_{i=1}^{m} \left(1 + e^{-x \cdot W_{:i}}\right) \quad \text{(if } x \text{ real)}$$

RBM: What can we do?

- **Can** encode ***any*** distribution over $\{-1,1\}^n$!

  well… given enough hidden units.

- **Can** estimate the right number of hidden units.

  will use a variant of projection pursuit method.

- **Cannot** efficiently estimate the $P[x|W]$

  cannot even approximate it!

Talk Outline

We will discuss each of the issues in detail.

- Universality [FH91].
- Learning the structure of RBM [FH91].
- Hardness of approximate inference [LS10].

Talk Outline

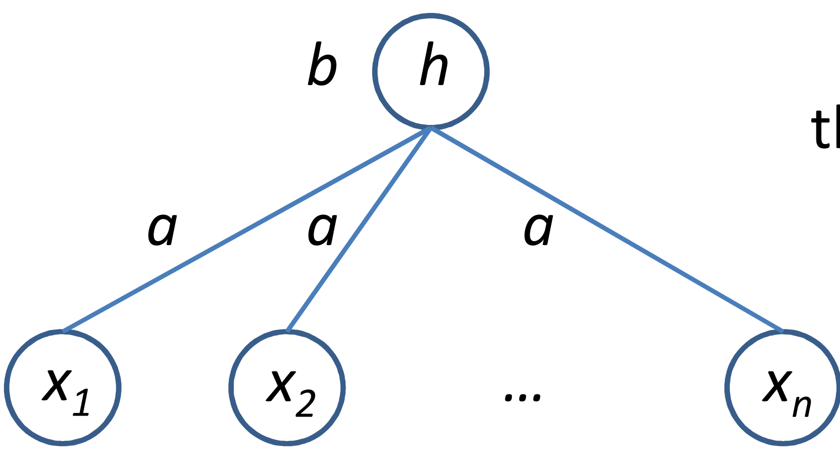
- Universality [FH91].
- Learning the structure of RBM [FH91].
- Hardness of approximate inference [LS10].

RBM: Universality [FH91]

- Pick a configuration, say, $x = \{1, 1, \dots, 1\}$. Suppose we want to learn weights W in an RBM that assigns $P[x|W] = p$.

- How can we do that?

Consider



$$E[x, h; a, b] := -(a \textstyle\sum_i x_i + b)h$$

$$P[x|a, b] \propto f(x; a, b) := 1 + e^{b + a \sum_i x_i}$$

if
$$a = \tfrac{1}{2}\ln(q-1) + \tfrac{1}{2}\ln(1/\epsilon)$$
$$b = -na + \ln(q-1)$$

then
$$f(x; a, b) = q \qquad \text{if } x = \{1, \dots, 1\}$$
$$1 \le f(x; a, b) \le 1 + \epsilon \qquad \text{o.w.}$$

RBM: Universality [FH91]

- Since we want $p = P[x|a,b] \approx \frac{q}{q+(2^n-1)}$ (for x = {1, … , 1})

  we want to set q to $\frac{p(2^n-1)}{1-p}$

- This can be easily generalized to different probability assignments for different configurations by adding additional hidden units.

- Therefore, in general, we can approximate any distribution by adding sufficiently many hidden units (2^n in the worst case)

Talk Outline

- Universality [FH91].
- Learning the structure of RBM [FH91].
- Hardness of approximate inference [LS10].

RBM: Learning the structure

- Recall that each hidden unit is able to encode at least one high-order interaction among the input variables.

- During learning, we want to have as few hidden units as possible while maintaining good representation.

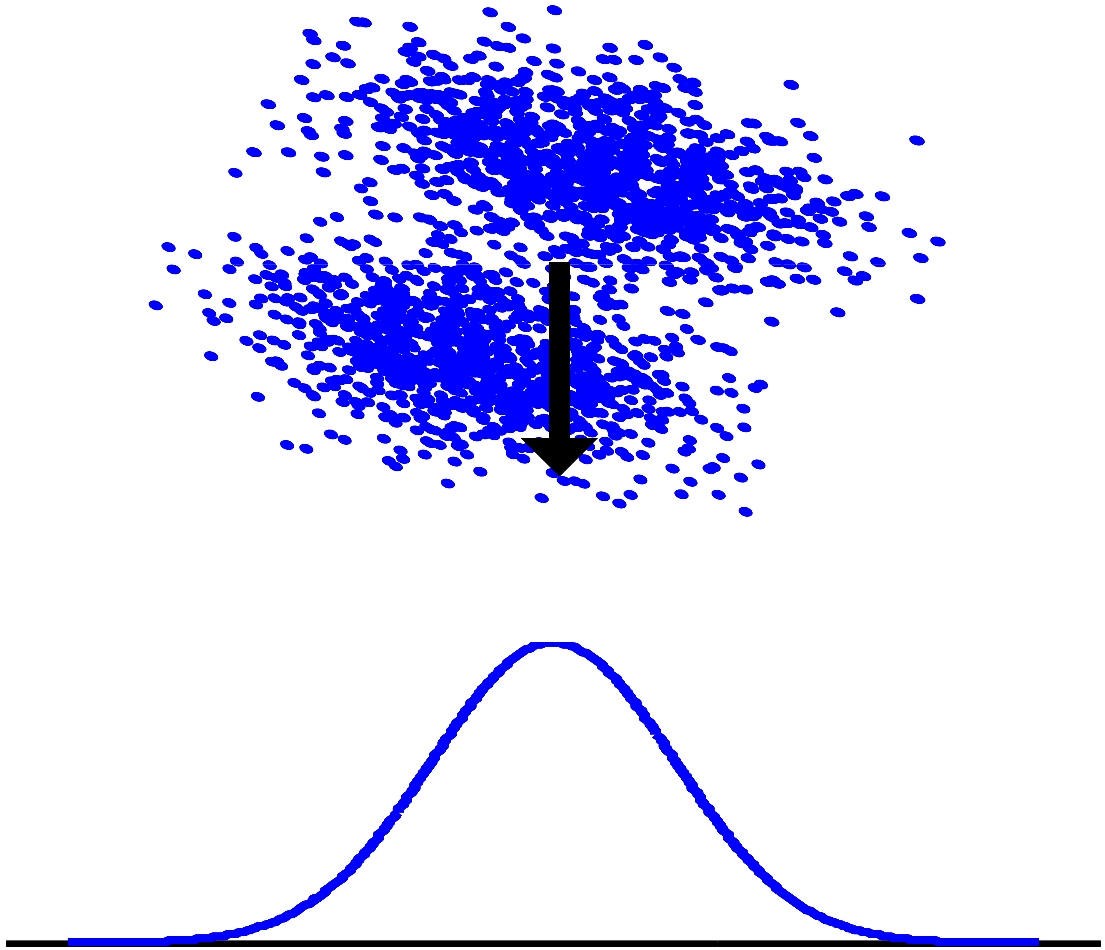
  Having too few units will give poor prediction, while having too many units will overfit the training data.

- Question: how can we estimate the right number of units?

  Solution: projection pursuit!

Detour: Projection Pursuit (PP)

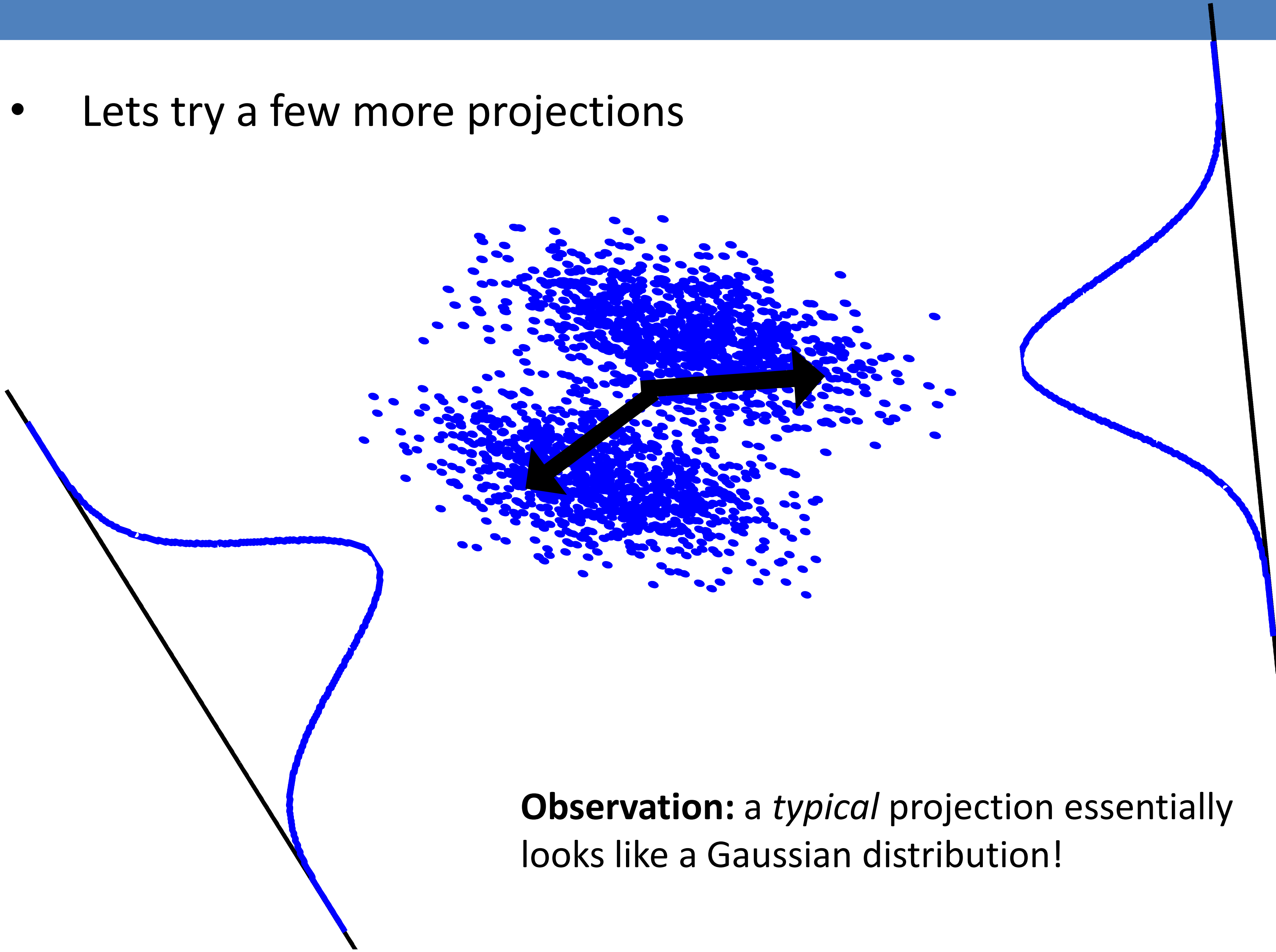
- A methodology for finding interesting characteristics of your underlying data distribution by observing 1D projections [FT74]



pick a projection direction, say, ⬇

Detour: Projection Pursuit (PP)

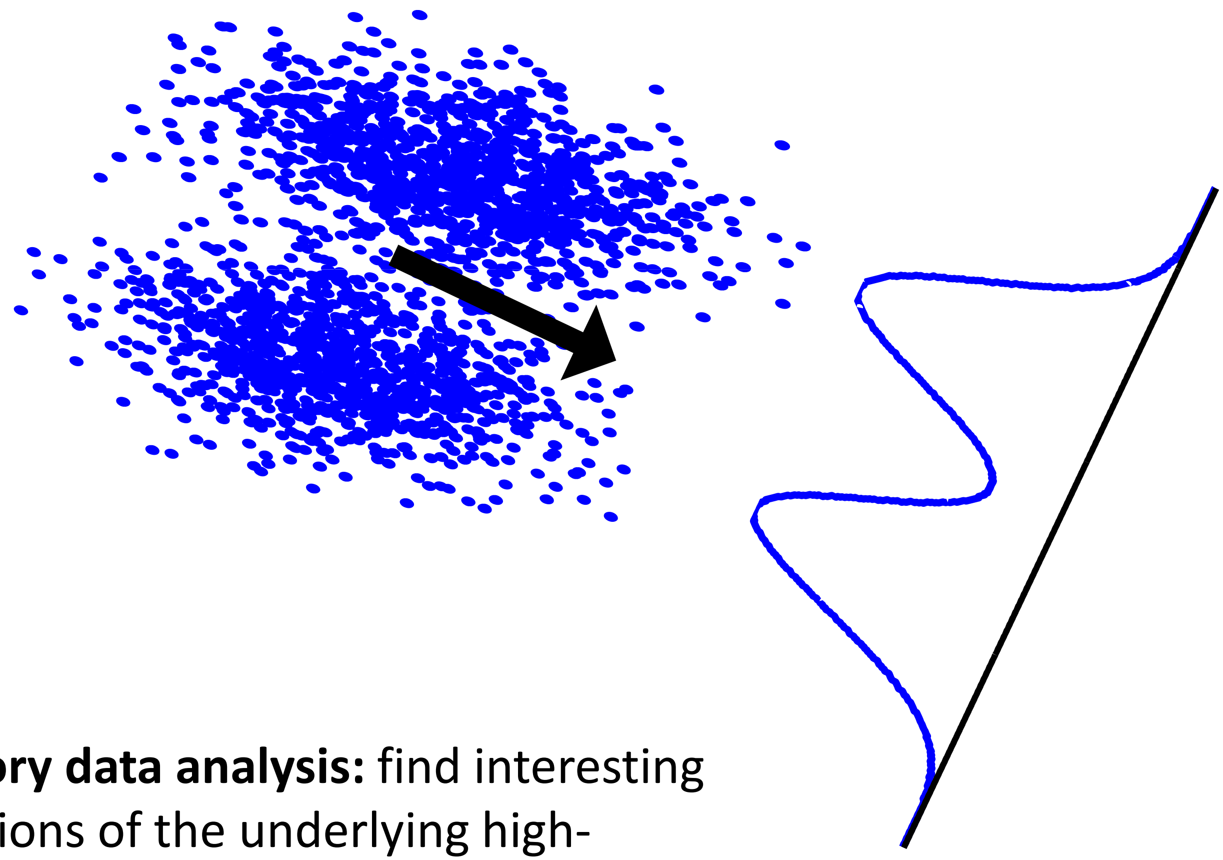
- Lets try a few more projections



Observation: a *typical* projection essentially looks like a Gaussian distribution!

Detour: Projection Pursuit (PP)

- Of course, there are specific directions that give a wealth of information about the underlying density.



PP goal for exploratory data analysis: find interesting (informative) projections of the underlying high-dimensional distribution.

Detour: PP for Density Estimation (PPDE)

- One can use the PP technique to develop **non-parametric density estimators** for the underlying distribution [FSS84].

How?

- Say we have an initial density estimate p_0
- We iteratively improve the estimate the by choosing a direction θ, and picking a univariate function *f* that best fits the (projected) data.

$$p_m(x) = p_0(x) \prod_{i=1}^{m} f_i(\theta_i \cdot x)$$

advantage over kernel density estimators: each time only estimating a 1D density, so the effects of the curse of dimensionality is mitigated

RBM: structure learning with PPDE [FH91]

- Recall: probability assigned to a (real-valued) state *x* by a RBM

$$P[x|W] \propto e^{-\frac{1}{2}\|x\|^2} \prod_{i=1}^{m} (1 + e^{-x \cdot W_{:i}})$$

This closely mimics the functional form of a PPDE!

$$p_m(x) = p_0(x) \prod_{i=1}^{m} f_i(\theta_i \cdot x)$$

- Thus, there is a natural iterative algorithm to estimate the number of hidden units in an RBM.

Each iteration corresponds to **adding a hidden unit** and estimating the parameters $W_{:i}$ using the input samples by an EM type procedure.

Repeat till no significant improvement in likelihood.

Talk Outline

- Universality [FH91].
- Learning the structure of RBM [FH91].
- Hardness of approximate inference [LS10].

RBM: Hardness of Inference [LS10]

- Recall the probably assigned to a particular state *x*

$$P[x|W] = \frac{1}{Z} \sum_{h \in \{0,1\}^m} e^{x^\top W h} = \frac{1}{Z} \prod_{i=1}^{m} \left(1 + e^{-x \cdot W_{:i}}\right)$$

where, the normalization $Z = \sum_{x \in \{-1,1\}^n, h \in \{0,1\}^m} e^{x^\top W h}$

Theorem: Given some *x, W* and approximation parameter *c* > 1, define $p = P[x|W]$.
If P ≠ NP then, returning a value $\hat{p}$ such that $\frac{1}{c} \cdot p \leq \hat{p} \leq c \cdot p$ is hard, even when $c = e^{Kn}$ (where *K* is a fixed constant).

RBM: Hardness of Inference [LS10]

It is equivalent to show that approximating the partition function *Z* to the same resolution is hard.

To this end, we shall use a recent result [AN04]

Lemma 1: If P ≠ NP then, exists $\epsilon > 0$ such that approximating

$$\|W\|_c := \max_{x, \in \{-1,+1\}^n, h \in \{0,1\}^n} x^\top W h$$

to within factor $1 + \epsilon$ is hard.

As a consequence, we have the following:

RBM: Hardness of Inference [LS10]

Lemma 2: If P ≠ NP then, exists $\alpha > 0$ such solving the following promise problem is hard. Let $f(n) \in \omega(n)$

Input: An *n* x *n* matrix W such that $\max_{i,j} |W_{ij}| \leq f(n)$ and either (i) $\|W\|_c > f(n)$; or (ii) $\|W\|_c \leq (1-\alpha)f(n)$

Output: Answer whether (i) or (ii) holds.

Proof sketch: Suppose (for contradiction), for every $\alpha > 0$, ALG_α efficiently solves the promise problem. Then, we can efficiently approximate $\|W\|_c$ for all $\epsilon > 0$ (contradicting Lemma 1).

How? Since $\max_{i,j} |W_{ij}| \leq \|W\|_c \leq n^2 \max_{i,j} |W_{ij}|$, maintain an interval [*l*,*b*] of possible values for $\|W\|_c$ and by repeatedly calling ALG_α do a binary search type pruning of the interval. ■

RBM: Hardness of Inference [LS10]

Lemma 3: If P ≠ NP then, exists $\alpha > 0$ such solving the following promise problem is hard. Let $f(n) \in \omega(n)$

Input: An *n* x *n* matrix W such that $\max_{i,j} |W_{ij}| \le f(n)$ and either

(i) $\sum_{x,h} e^{x^\mathsf{T} W h} > e^{f(n)}$; or

(ii) $\sum_{x,h} e^{x^\mathsf{T} W h} \le 4^n e^{(1-\alpha) f(n)}$

Output: Answer whether (i) or (ii) holds.

Proof sketch: By previous lemma, we know that $\max_{i,j} |W_{ij}| \le f(n)$ and either (a) $\max_{x,h}\{x^\mathsf{T} W h\} > f(n)$; or (b) $\max_{x,h}\{x^\mathsf{T} W h\} \le (1-\alpha) f(n)$

It is hard to determine (a) or (b).

Observe: (a) $\Rightarrow$ (i) and (b) $\Rightarrow$ (ii). So, for sufficiently large *n*, efficiently solving this problem, efficiently solves for the previous problem. ■

RBM: Hardness of Inference [LS10]

Theorem 4: Let $f(n) \in \omega(n)$ and *W a* matrix satisfying $\max_{i,j} |W_{ij}| \leq f(n)$
If P ≠ NP then, exists $\epsilon > 0$ such that approximating $\sum_{x,h} e^{x^\top W h}$
to a multiplicative factor of $e^{\epsilon f(n)}$ is hard.

Proof sketch: Let $\alpha > 0$ be from previous lemma.
Set $U = e^{f(n)}$, $L = 4^n e^{(1-\alpha) f(n)}$
If an algorithm can approximate $Z := \sum_{x,h} e^{x^\top W h}$ within factor $\sqrt{\frac{U}{L}}$
It can also distinguish $Z \geq U$ from $Z < L$

Note: an approx. better than this contradicts the previous lemma.

This gives us the approximation: $\sqrt{\frac{U}{L}} = e^{(\alpha/2) f(n) - (n/2) \ln 4}$ ■

Conclusion

- RBMs are simple yet powerful networks that can encode *any* distribution over $\{-1,1\}^n$!
- There is a simple PPDE-type algorithm that can estimate the right number of hidden units for the particular dataset.
- Approximate inference in RBMs is hard.

Questions/discussion

References

[AN04] Alon and Naor. Approximating the cut-norm via Grothendieck's inequality. *STOC* 2004.

[FH91] Freund and Haussler. Unsupervised learning of distributions on binary vectors using two layer networks. *NIPS* 1991.

[FSS84] Friedman, Stuetzle and Schroeder. Projection pursuit density estimation. *J. Amer. Stat. Assoc.* 1984.

[FT74] Friedman and Tukey. A projection pursuit algorithm for exploratory data analysis. *IEEE Trans. on Computers*, 1974.

[LS10] Long and Servedio. Restricted Boltzmann Machines are hard to approximately evaluate or simulate. *ICML* 2010.