## Model matters with restricted Boltzmann machines

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### What is this?

A Restricted Boltzman Machine (RBM) is an undirected probabilistic graphical model (for discrete or continuous random variables) with two layers, one hidden and one visible, with conditional independence within a layer (Smolensky 1986).

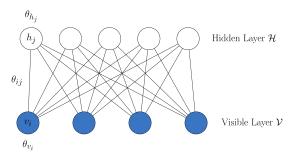


Figure 1: An example RBM, which consists of two layers. Hidden nodes are indicated by white circles and the visible nodes are indicated by blue circles

### How is it used?

Typically used for image classification. Each image pixel is a node in the visible layer. The output creates features, which are passed to a supervised learning algorithm.

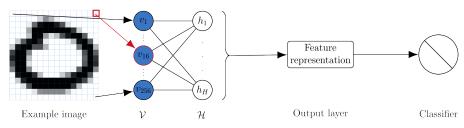


Figure 2: Image classification using a RBM. On the left, each image pixel comprises a node in the visible layer,  $\mathcal{V}$ . On the right, the output of the RBM is used to create features which are then passed to a supervised learning algorithm.

#### Joint distribution

Let  $\mathbf{x}=(h_1,\ldots,h_{n_H},v_1,\ldots,v_{n_V})$  represent the states of the visible and hidden nodes in an RBM. Each single "binary" random variable, visible or hidden, will take its values in a common coding set  $\mathcal{C}$ , with two possibilities for the coding set  $\mathcal{C}=\{0,1\}$  or  $\mathcal{C}=\{-1,1\}$ . A parametric form for probabilities corresponding to a potential vector of states of each node

$$f_{\theta}(\mathbf{x}) = \frac{\exp\left(\sum_{i=1}^{n_{V}}\sum_{j=1}^{n_{H}}\theta_{ij}v_{i}h_{j} + \sum_{i=1}^{n_{V}}\theta_{v_{i}}v_{i} + \sum_{j=1}^{n_{H}}\theta_{h_{j}}h_{j}\right)}{\gamma(\theta)}$$
(1)

where

$$\gamma(\boldsymbol{\theta}) = \sum_{\mathbf{x} \in \mathcal{C}^{n_H + n_V}} \exp\left(\sum_{i=1}^{n_V} \sum_{j=1}^{n_H} \theta_{ij} v_i h_j + \sum_{i=1}^{n_V} \theta_{v_i} v_i + \sum_{j=1}^{n_H} \theta_{h_j} h_j\right)$$

## Deep learning

- By stacking layers of RBMs in a deep architecture, proponents of the models claim the ability to learn "internal representations that become increasingly complex, which is considered to be a promising way of solving object and speech recognition problems" (Salakhutdinov and Hinton 2009, pp. 450).
- Stacking is achieved by treating a hidden layer of one RBM as the visible layer in a second RBM, etc.

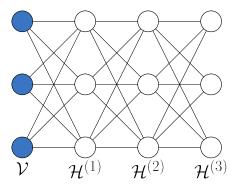


Figure 3: Three layer deep Boltzmann machine, with visible-to-hidden and hidden-to-hidden connections but no within-layer connections.

# Why do I care?

The model properties are largely unexplored in the literature and the commonly cited fitting methodology remains heuristic-based and abstruse (Hinton, Osindero, and Teh 2006).

We want to

- provide steps toward a thorough understanding of the model class and its properties from the perspective of statistical theory, and
- explore the possibility of a rigorous fitting methodology.

# Degeneracy, instability, and uninterpretability. Oh my!

The highly flexible nature of a RBM (having as it does  $n_H + n_V + n_H * n_V$  parameters) makes at least three kinds of potential model impropriety of concern, degeneracy, instability, and uninterpretability.

A model should "provide an explanation of the mechanism underlying the observed phenomena" (Lehmann 1990; G. E. P. Box 1967).

#### RBMs often

- fail to generate data with realistic variability and thus an unsatisfactory conceptualization of the data generation process.
- exhibit instability in the parameter space.

Such model impropriety issues have been documented in in RBMs (Li 2014), as well as other deep architectures (Szegedy et al. 2013; Nguyen, Yosinski, and Clune 2014).

## Near-degeneracy

## Definition (Model Degeneracy)

There is a disproportionate amount of probability placed on only a few elements of the sample space,  $C^{n_H+n_V}$ , by the model.

RBM models exhibit *near-degeneracy* when random variables in the neg-potential function

$$Q_{\theta}(x) = \sum_{i=1}^{n_{V}} \sum_{j=1}^{n_{H}} \theta_{ij} v_{i} h_{j} + \sum_{i=1}^{n_{V}} \theta_{v_{i}} v_{i} + \sum_{j=1}^{n_{H}} \theta_{h_{j}} h_{j},$$

have a mean vector  $\boldsymbol{\mu}(\boldsymbol{\theta})$  close to the boundary of the convex hull of  $\mathcal{T} = \{\boldsymbol{t}(x): x \in \mathcal{C}^{n_H+n_V}\}$  (Handcock 2003), where  $\boldsymbol{t}(\boldsymbol{x}) = \{v_1, \dots, v_{n_V}, h_1, \dots, h_{n_H}, v_1h_1, \dots, v_{n_V}h_{n_H}\}$  and the mean parameterization on the model parameters,  $\boldsymbol{\mu}(\boldsymbol{\theta})$  is

$$\mu(\theta) = \mathsf{E}_{\theta} t(\mathbf{X})$$

$$= \sum_{\mathbf{x} \in \mathcal{C}^{n_H + n_V}} \left\{ t(\mathbf{x}) \frac{\exp\left(\sum\limits_{i=1}^{n_V} \sum\limits_{j=1}^{n_H} \theta_{ij} v_i h_j + \sum\limits_{i=1}^{n_V} \theta_{v_i} v_i + \sum\limits_{j=1}^{n_H} \theta_{h_j} h_j\right)}{\sum\limits_{\mathbf{x} \in \mathcal{C}^{n_H + n_V}} \exp\left(\sum\limits_{i=1}^{n_V} \sum\limits_{j=1}^{n_H} \theta_{ij} v_i h_j + \sum\limits_{i=1}^{n_V} \theta_{v_i} v_i + \sum\limits_{j=1}^{n_H} \theta_{h_j} h_j\right)} \right\}$$

## Instability

## Definition (Instability)

Characterized by excessive sensitivity in the model, where small changes in the components of data outcomes, x, lead to substantial changes in probability.

Schweinberger (2011) introduced a concept of model deficiency related to *instability* considering only a class of exponential families of distributions.

To quantify *instability* in the RBM, it is useful to consider how a data model might be expanded to incorporate more visibles. For this, it becomes necessary to grow the number of model parameters in a sequence  $\theta_{n_V} \in \mathbb{R}^{n_V+n_H+n_V*n_H}, n_V \geq 1$  (one may also arbitrarily expand the number of hidden variables used).

### Unstable RBMs

#### Definition (S-unstable RBM)

A RBM model formulation is S-unstable if

$$\lim_{n_V \to \infty} \frac{1}{n_V} \mathsf{ELPR}(\boldsymbol{\theta}_{n_V}) = \infty.$$

where

$$\mathsf{ELPR}(\boldsymbol{\theta}_{n_{V}}) = \log \left[ \frac{\max\limits_{(v_{1}, \dots, v_{n_{V}}) \in \mathcal{C}^{n_{V}}} P_{\boldsymbol{\theta}_{n_{V}}}(v_{1}, \dots, v_{n_{V}})}{\min\limits_{(v_{1}, \dots, v_{n_{V}}) \in \mathcal{C}^{n_{V}}} P_{\boldsymbol{\theta}_{n_{V}}}(v_{1}, \dots, v_{n_{V}})} \right]$$
(2)

S-unstable RBM model sequences are undesirable for several reasons. Again, one is that small changes in data can lead to overly-sensitive changes in probability.

# One-pixel change

Consider, for example, the biggest log-probability ratio for a one-pixel (one component) change in data outcomes (visibles).

$$\Delta(\boldsymbol{\theta}_{n_V}) \equiv \max \left\{ \log \frac{P_{\boldsymbol{\theta}_{n_V}}(v_1, \dots, v_{n_V})}{P_{\boldsymbol{\theta}_{n_V}}(v_1^*, \dots, v_{n_V}^*)} \right\},$$

where  $(v_1,\ldots,v_{n_V})\&(v_1^*,\ldots,v_{n_V}^*)\in\mathcal{C}^{n_V}$  differ by exactly one component

#### Result

Let 
$$C>0$$
 and  $n_V\geq 1$ . If  $\frac{1}{n_V}\textit{ELPR}(\boldsymbol{\theta}_{n_V})>C$ , then  $\Delta(\boldsymbol{\theta}_{n_V})>C$ .

If the quantity (2) is too large, then a RBM model sequence will exhibit large probability shifts for very small changes in the data configuration.

## Tie to degeneracy

Unstable RBM model sequences are connected to degenerate model sequences (placing all probability on a small portion of their sample spaces). Define a modal set

$$M_{\epsilon, oldsymbol{ heta}_{n_V}} \equiv \left\{ oldsymbol{v} \in \mathcal{C}^{n_V} : \log P_{oldsymbol{ heta}_{n_V}}(oldsymbol{v}) > (1 - \epsilon) \max_{oldsymbol{v}^*} P_{oldsymbol{ heta}_{n_V}}(oldsymbol{v}^*) + \epsilon \min_{oldsymbol{v}^*} P_{oldsymbol{ heta}_{n_V}}(oldsymbol{v}^*) 
ight\}$$

of possible outcomes, for a given  $0<\epsilon<1$ .

#### Result

For an S-unstable RBM model, and for any given  $0 < \epsilon < 1$ ,  $P_{\theta_{n_V}}\left((v_1,\ldots,v_{n_V}) \in M_{\epsilon,\theta_{n_V}}\right) \to 1$  holds as  $n_V \to \infty$ .

As a consequence of unstable models, all probability will stack up on mode sets or potentially those few outcomes with the highest probability. Proofs of results 1-2 are provided later.

# Uninterpretability

## Definition (Uninterpretability)

Characterized by marginal mean-structure (controlled by main effect parameters  $\theta_{v_i}$ ,  $\theta_{h_j}$ ) not being maintained in the model due to dependence (interaction parameters  $\theta_{ij}$ ) (Kaiser 2007).

A measure of this is the magnitude of the difference between model expectations,  $E[\boldsymbol{X}|\boldsymbol{\theta}]$ , and expectations given independence,  $E[\boldsymbol{X}|\boldsymbol{\theta}^*]$ , where  $\boldsymbol{\theta}^*$  is defined to equal  $\boldsymbol{\theta}$  with all  $\theta_{ij}=0$  for  $i=1,\ldots,n_V, j=1,\ldots,n_H$ .

Using this, it is possible to investigate what parameters lead to uninterpretability in a model versus those that guarantee interpretability.

If  $|E[X|\theta] - E[X|\theta^*]|$  is large then the RBM with parameter vector  $\theta$  is uninterpetable.

# RBM quantities to compare

$$\mathsf{E}\left[\boldsymbol{X}|\boldsymbol{\theta}\right] = \sum_{\boldsymbol{x} \in \mathcal{C}^{n_H + n_V}} \boldsymbol{x} \frac{\exp\left(\sum\limits_{i=1}^{n_V}\sum\limits_{j=1}^{n_H} \theta_{ij} v_i h_j + \sum\limits_{i=1}^{n_V} \theta_{v_i} v_i + \sum\limits_{j=1}^{n_H} \theta_{h_j} h_j\right)}{\sum\limits_{\boldsymbol{x} \in \mathcal{C}^{n_H + n_V}} \exp\left(\sum\limits_{i=1}^{n_V}\sum\limits_{j=1}^{n_H} \theta_{ij} v_i h_j + \sum\limits_{i=1}^{n_V} \theta_{v_i} v_i + \sum\limits_{j=1}^{n_H} \theta_{h_j} h_j\right)}$$

$$\mathsf{E}\left[\boldsymbol{X}|\boldsymbol{\theta}^*\right] = \sum_{\boldsymbol{x} \in \mathcal{C}^{n_H + n_V}} \boldsymbol{x} \frac{\exp\left(\sum\limits_{i=1}^{n_V} \theta_{v_i} v_i + \sum\limits_{j=1}^{n_H} \theta_{h_j} h_j\right)}{\sum\limits_{\boldsymbol{x} \in \mathcal{C}^{n_H + V = n_V}} \exp\left(\sum\limits_{i=1}^{n_V} \theta_{v_i} v_i + \sum\limits_{j=1}^{n_H} \theta_{h_j} h_j\right)}$$

## Data coding to mitigate degeneracy

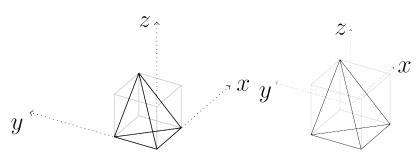


Figure 4: The convex hull of the "statistic space"  $\mathcal{T}=\{(v_1,h_1,v_1h_1):v_1,h_1\in\mathcal{C}\}$  in three dimensions for the toy RBM with one visible and one hidden node for  $\mathcal{C}=\{0,1\}$  (left) and  $\mathcal{C}=\{-1,1\}$  (right) data encoding. The convex hull of  $\mathcal{T}\subset\mathcal{C}^3$  does not fill the unit cube  $[0,1]^3$  (left), but does better with  $[-1,1]^3$  (right).

#### The center of the universe

- For the  $C = \{-1, 1\}$  encoding of hiddens  $(H_1, \ldots, H_{n_H})$  and visibles  $(V_1, \ldots, V_{n_V})$ , the origin is the center of the parameter space.
- At  $\theta = \mathbf{0}$ , RBM is equivalent to elements of X being distributed as iid Bernoulli $\left(\frac{1}{2}\right) \Rightarrow$  No near-degeneracy, instability, or uninterpretability!

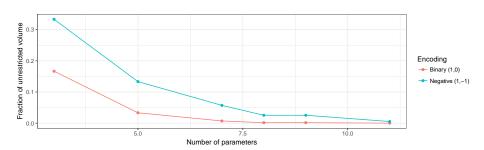


Figure 5: Relationship between volume of the convex hull of possible values of the RBM sufficient statistics and the cube containing it for different size models.

# Manageable (a.k.a. small) examples

- To explore the behavior of the RBM parameters  $\theta$  as it relates to near-degeneracy, instability, and uninterpretability, we consider models of small size. For  $n_H, n_V \in \{1, \ldots, 4\}$ , we sample 100 values of  $\theta$ .
  - **1** Split  $\theta$  into  $\theta_{interaction}$  and  $\theta_{main}$ , in reference to which sufficient statistics the parameters correspond to.
  - ② Allow the two types of terms to have varying average magnitudes,  $||\theta_{main}||/(n_H + n_V)$  and  $||\theta_{interaction}||/(n_H * n_V)$ .
  - Average magnitudes vary on a grid between 0.001 and 3 with 24 breaks, yielding 576 grid points.
- Calculate the three metrics of model impropriety,  $\mu(\theta)$ , ELPR( $\mathbf{x}$ )/ $n_V$ , and the coordinates of  $|\mathbf{E}[\mathbf{X}|\theta] \mathbf{E}[\mathbf{X}|\theta^*]|$ .
- In the case of near-degeneracy, we can go further and classify each model as near-degenerate or "viable" based on the distance of  $\mu(\theta)$  from the boundary of the convex hull of  $\mathcal T$

#### Simulation results

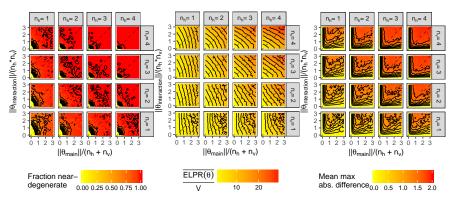


Figure 6: Results from the numerical experiment, here looking at the fraction of models that were near-degenerate (left), the sample mean value of  $\text{ELPR}(\theta)/n_V$  (middle), and the sample mean of the maximum component of the absolute difference between the model expectation vector,  $\text{E}[\boldsymbol{X}|\theta]$ , and the expectation vector given independence,  $\text{E}[\boldsymbol{X}|\theta^*]$  (right).

# Model fitting

- Typically, fitting a RBM via maximum likelihood (ML) methods will be infeasible mainly due to the intractibility of the normalizing term  $\gamma(\theta)$  in a model of any realistic size
  - Ad hoc methods are used instead, which aim to avoid this problem by using stochastic ML that employ a small number of MCMC draws.
- Computational concerns are not the only issues with fitting an RBM using ML, the RBM model, has the potential to re-create any distribution for the data.
  - Based on a random sample of visible variables, the model for the cell probabilities that has the highest likelihood over all possible model classes is the empirical distribution, and the parametrization of the RBM model itself ensures that this empirical distribution can be arbitrarily well approximated.
  - Whenever the empirical distribution contains empty cells, fitting steps for the RBM model will aim to chase parameters that necessarily diverge in magnitude in order to zero out the corresponding RBM cell probabilities.

# Bayesian methods

- We consider what might be done in a principled manner, testing on a  $n_V = n_H = 4$  case that already stretched the limits of what is computable in particular we consider Bayes methods.
- To avoid model impropriety for a fitted RBM, we want to avoid parts of the parameter space  $\mathbb{R}^{n_V+n_H+n_V*n_H}$  that lead to *near-degeneracy*, instability, and uninterpretability.
  - Shrink  $\theta$  toward  $\mathbf{0}$  by specifying priors that place low probability on large values of  $||\theta||$ , shrinking  $\theta_{interaction}$  more than  $\theta_{main}$ .
- We considered a test case with  $n_V=n_H=4$  and parameters given in in appendix. This parameter vector was chosen as a sampled value of  $\boldsymbol{\theta}$  that was not near the convex hull of the sufficient statistics for a grid point in figure 6 with <5% near-degeneracy. We simulated n=5,000 as a training set and fit the RBM using three Bayes methodologies.

# Fitting methodologies

**1** A "trick" prior (BwTPLV). Cancel out normalizing term in the likelihood, resulting full conditionals of  $\theta$  are multivariate Normal,  $h_j$  are carried along as latent variables.

$$\pi(\boldsymbol{\theta}) \propto \gamma(\boldsymbol{\theta})^n \exp\left(-\frac{1}{2\mathit{C}_1}\boldsymbol{\theta}'_{\textit{main}}\boldsymbol{\theta}_{\textit{main}} - \frac{1}{2\mathit{C}_2}\boldsymbol{\theta}'_{\textit{interaction}}\boldsymbol{\theta}_{\textit{interaction}}\right),$$

where  $C_2 < C_1$ . This is the method of Li (2014).

- ② A truncated Normal prior (BwTNLV). Independent spherical normal distributions as priors for  $\theta_{main}$  and  $\theta_{interaction}$ , with  $\sigma_{interaction} < \sigma_{main}$ , truncated at  $3\sigma_{main}$  and  $3\sigma_{interaction}$ , respectively. Simulation from the posterior using a geometric adaptive MH step (Zhou 2014),  $h_j$  are carried along in the MCMC implementation as latent variables.
- **3** A truncated Normal prior and marginalized likelihood (BwTNML). Marginalize out h in  $f_{\theta}(x)$ , and use the truncated Normal priors applied to the marginal probabilities for visible variables.

# Hyperparameters

Table 1: The values used for the hyperparameters for all three fitting methods. A rule of thumb is imposed which decreases prior variances for the model parameters as the size of the model increases and also shrinks  $\theta_{interaction}$  more than  $\theta_{main}$ . The common C defining  $C_1$  and  $C_2$  in the BwTPLV method is chosen by tuning.

Method	Hyperparameter	Value	
BwTPLV	$C_1$ $C_2$	$\frac{\frac{C}{n}\frac{1}{n_H+n_V}}{\frac{C}{n}\frac{1}{n_H*n_V}}$	
BwTNLV	$\sigma^2_{main}$ $\sigma^2_{interaction}$	$\frac{\frac{1}{n_H + n_V}}{\frac{1}{n_H * n_V}}$	
BwTNML	$\sigma^2_{main}$ $\sigma^2_{interaction}$	$\frac{\frac{1}{n_H + n_V}}{\frac{1}{n_H * n_V}}$	

## Mixing

The truncated Normal method (2) and the marginalized likelihood method (3) are drawing from the same stationary posterior distribution for images.

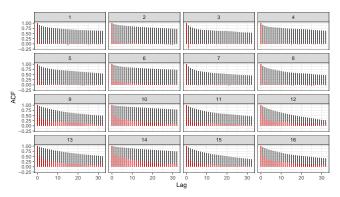


Figure 7: The autocorrelation functions (ACF) for the posterior probabilityies of all  $2^4 = 16$  possible outcomes for the vector of 4 visibles assessed at multiple lags for each method with BwTNLV in black and BwTNML in red.

## Effective sample size

We can use an overlapping blockmeans approach to get a crude estimate for the aysmptotic variance of the probability of each image and compare it to an estimate of the asymptotic variance assuming IID draws from the target distribution.

Table 2: The effective sample sizes for a chain of length M=1000 regarding all 16 probabilities for possible vector outcomes of visibles. BwTNLV would require at least 4.7 times as many MCMC iterations to achieve the same amount of effective information about the posterior distribution.

Outcome	BwTNLV	BwTNML	Outcome	BwTNLV	BwTNML
1	73.00	509.43	9	83.47	394.90
2	65.05	472.51	10	95.39	327.35
3	87.10	1229.39	11	70.74	356.56
4	72.64	577.73	12	81.40	338.30
5	71.67	452.01	13	105.98	373.59
6	66.49	389.78	14	132.61	306.91
7	84.30	660.37	15	82.15	365.30
8	75.46	515.09	16	98.05	304.57

# Posterior distributions of images

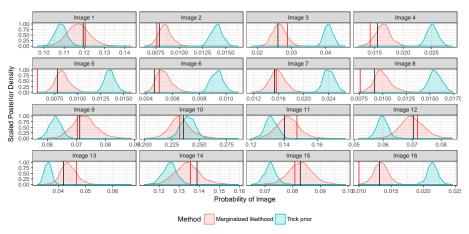


Figure 8: Posterior probabilities of  $16=2^4$  possible realizations of 4 visibles using two of the three Bayesian fitting techniques, BwTPLV and BwTNML. Black lines show true probabilities of each vector of visibles based on the parameters used to generate the training data while red lines show the empirical distribution.

# Wrapping up

- While RBMs are thought to be useful for classification, in the context of generative statistical models, RBMs are a poor fit due to near-degeneracy, S-instability, and wuninterpretability.
- Rigorous fitting methodology is difficult due to the dimension of the parameter space coupled with the size of the latent variable space.
- For a RBM model with enough hidden variables, any distribution for the visibles can be approximated arbitrarily well (Le Roux and Bengio 2008; Montufar and Ay 2011; and Montufar, Rauh, and Ay 2011).
  - The empirical distribution of a training set of vectors of visibles is the best fitting model for observed cell data.
  - There can be no "smoothed distribution" achieved in fitting a RBM model of sufficient size with a rigorous likelihood-based method.

We are skeptical that any model built using these structures (like a deep Boltzmann machine) can achieve useful prediction or inference in a principled way without limiting the flexibility of the fitted model.

## Future work

# **Appendices**

## Appendix: Proof of Result 1

We prove the contrapositive. Suppose that  $\Delta(\theta_{n_V}) \leq C$  holds for some C>0. Under the RBM model for visibles,  $P_{\theta_{n_V}}(\mathbf{v})>0$  holds for each outcome  $\mathbf{v}\in\mathcal{C}^{n_V}$ . Let  $\mathbf{v}_{min}\equiv\arg\min_{\mathbf{v}\in\mathcal{C}^{n_V}}P_{\theta_{n_V}}(\mathbf{v})$  and  $\mathbf{v}_{max}\equiv\arg\max_{\mathbf{v}\in\mathcal{C}^{N_V}}P_{\theta_{n_V}}(\mathbf{v})$ . Note there exists a sequence  $\mathbf{v}_{min}\equiv\mathbf{v}_0,\mathbf{v}_1,\ldots,\mathbf{v}_k\equiv\mathbf{v}_{max}$  in  $\mathcal{C}^{n_V}$  of component-wise switches to move from  $\mathbf{v}_{min}$  to  $\mathbf{v}_{max}$  in the sample space (i.e.  $\mathbf{v}_i,\mathbf{v}_{i+1}\in\mathcal{C}^{n_V}$ 

differ by exactly 1 component for i = 0, ..., k) for some integer  $k \in \{0, 1, ..., n_V\}$ . Then

$$\log \left[ \frac{P_{\theta_{n_{V}}}(\mathbf{v}_{max})}{P_{\theta_{n_{V}}}(\mathbf{v}_{min})} \right] = \left| \sum_{i=1}^{k} \log \left( \frac{P_{\theta_{n_{V}}}(\mathbf{v}_{i})}{P_{\theta_{n_{V}}}(\mathbf{v}_{i-1})} \right) \right|$$

$$\leq \sum_{i=1}^{k} \left| \log \left( \frac{P_{\theta_{n_{V}}}(\mathbf{v}_{i})}{P_{\theta_{n_{V}}}(\mathbf{v}_{i-1})} \right) \right|$$

 $< k\Delta(\theta_{n_V}) < n_V C$ 

using  $k \leq n_V$  and  $\Delta(\theta_{n_V}) \leq C.\square$ 

# Appendix: Proof of Result 2

Define  $\mathbf{v}_{max}$  and  $\mathbf{v}_{min}$  as in the proof of Proposition 1. Fix  $0<\epsilon<1$  Then,  $\mathbf{v}_{max}\in M_{\epsilon,\theta_{n_V}}$ , so  $P_{\theta_{n_V}}(M_{\epsilon,\theta})\geq P_{\theta_{n_V}}(\mathbf{v}_{max})$ . If  $\mathbf{v}\in\mathcal{C}^{n_V}\setminus M_{\epsilon,\theta_{n_V}}$ , then by definition  $P_{\theta_{n_V}}(\mathbf{v})\leq [P_{\theta_{n_V}}(\mathbf{v}_{max})]^{1-\epsilon}[P_{\theta_{n_V}}(\mathbf{v}_{min})]^{\epsilon}$  holds so that

$$\begin{split} 1 - P_{\boldsymbol{\theta}_{n_{V}}}(M_{\epsilon,\boldsymbol{\theta}_{n_{V}}}) &= P_{\boldsymbol{\theta}_{n_{V}}}(M_{\epsilon,\boldsymbol{\theta}_{n_{V}}}^{\mathcal{C}}) \\ &= \sum_{\boldsymbol{v} \in \mathcal{C}^{n_{V}} \setminus M_{\epsilon,\boldsymbol{\theta}_{n_{V}}}} P_{\boldsymbol{\theta}_{n_{V}}}(\boldsymbol{v}) \\ &\leq (2^{n_{V}})[P_{\boldsymbol{\theta}_{n_{V}}}(\boldsymbol{v}_{\textit{max}})]^{1 - \epsilon}[P_{\boldsymbol{\theta}_{n_{V}}}(\boldsymbol{v}_{\textit{min}})]^{\epsilon} \end{split}$$

Then,

$$\begin{split} \frac{1}{n_{V}}\log\left[\frac{P_{\theta_{n_{V}}}(\textit{M}_{\epsilon,\theta_{n_{V}}})}{1-P_{\theta_{n_{V}}}(\textit{M}_{\epsilon,\theta_{n_{V}}})}\right] \geq \frac{1}{n_{V}}\log\left[\frac{P_{\theta_{n_{V}}}(\textit{\textbf{v}}_{\textit{max}})}{(2^{n_{V}})[P_{\theta_{n_{V}}}(\textit{\textbf{v}}_{\textit{max}})]^{1-\epsilon}[P_{\theta_{n_{V}}}(\textit{\textbf{v}}_{\textit{min}})]^{\epsilon}}\right] \\ = \frac{\epsilon}{n_{V}}\log\left[\frac{P_{\theta_{n_{V}}}(\textit{\textbf{v}}_{\textit{max}})}{P_{\theta_{n_{V}}}(\textit{\textbf{v}}_{\textit{min}})}\right] - \log 2 \rightarrow \infty \end{split}$$

as  $n_V \to \infty$  by the definition of an unstable RBM model.

## Appendix: Parameters used

Table 3: Parameters used to fit a test case with  $n_V = n_H = 4$ . This parameter vector was chosen as a sampled value of  $\theta$  that was not near the convex hull of the sufficient statistics for a grid point in figure 6 with < 5% near-degeneracy.

Parameter	Value	Parameter	Value	Parameter	Value
$\theta_{v1}$	-1.1043760	$\theta_{11}$	-0.0006334	$\theta_{31}$	-0.0038301
$\theta_{v2}$	-0.2630044	$\theta_{12}$	-0.0021401	$\theta_{32}$	0.0032237
$\theta_{v3}$	0.3411915	$\theta_{13}$	0.0047799	$\theta_{33}$	0.0020681
$\theta_{v4}$	-0.2583769	$\theta_{14}$	0.0025282	$ heta_{34}$	0.0041429
$\theta_{h1}$	-0.1939302	$\theta_{21}$	0.0012975	$\theta_{41}$	0.0089533
$\theta_{h2}$	-0.0572858	$\theta_{22}$	0.0000253	$\theta_{42}$	-0.0042403
$\theta_{h3}$	-0.2101802	$\theta_{23}$	-0.0004352	$\theta_{43}$	-0.0000480
$\theta_{h4}$	0.2402456	$\theta_{24}$	-0.0086621	$\theta_{44}$	0.0004767

### References I

G. E. P. Box, W. J. Hill. 1967. "Discrimination Among Mechanistic Models." *Technometrics* 9 (1). [Taylor & Francis, Ltd., American Statistical Association, American Society for Quality]: 57–71.

Handcock, Mark S. 2003. "Assessing Degeneracy in Statistical Models of Social Networks." Center for Statistics; the Social Sciences, University of Washington. http://www.csss.washington.edu/.

Hinton, Geoffrey E, Simon Osindero, and Yee-Whye Teh. 2006. "A Fast Learning Algorithm for Deep Belief Nets." Neural Computation 18 (7). MIT Press: 1527–54.

Kaiser, Mark S. 2007. "Statistical Dependence in Markov Random Field Models." Statistics Preprints Paper 57. Digital Repository @ lowa State University. http://lib.dr.iastate.edu/stat\_las\_preprints/57/.

Le Roux, Nicolas, and Yoshua Bengio. 2008. "Representational Power of Restricted Boltzmann Machines and Deep Belief Networks." Neural Computation 20 (6). MIT Press: 1631–49.

Lehmann, E. L. 1990. "Model Specification: The Views of Fisher and Neyman, and Later Developments." Statistical Science 5 (2). Institute of Mathematical Statistics: 160–68.

Li, Jing. 2014. "Biclustering Methods and a Bayesian Approach to Fitting Boltzmann Machines in Statistical Learning." PhD thesis, Iowa State University; Graduate Theses; Dissertations. http://lib.dr.iastate.edu/etd/14173/.

Montufar, Guido, and Nihat Ay. 2011. "Refinements of Universal Approximation Results for Deep Belief Networks and Restricted Boltzmann Machines." *Neural Computation* 23 (5). MIT Press: 1306–19.

Montúfar, Guido F, Johannes Rauh, and Nihat Ay. 2011. "Expressive Power and Approximation Errors of Restricted Boltzmann Machines." In Advances in Neural Information Processing Systems, 415–23. NIPS.

Nguyen, Anh Mai, Jason Yosinski, and Jeff Clune. 2014. "Deep Neural Networks Are Easily Fooled: High Confidence Predictions for Unrecognizable Images." ArXiv Preprint ArXiv:1412.1897. http://arxiv.org/abs/1412.1897.

Salakhutdinov, Ruslan, and Geoffrey E Hinton. 2009. "Deep Boltzmann Machines." In International Conference on Artificial

#### References II

Intelligence and Statistics, 448-55. Al & Statistics.

Schweinberger, Michael. 2011. "Instability, Sensitivity, and Degeneracy of Discrete Exponential Families." *Journal of the American Statistical Association* 106 (496). Taylor & Francis: 1361–70.

Smolensky, Paul. 1986. "Information Processing in Dynamical Systems: Foundations of Harmony Theory." DTIC Document.

Szegedy, Christian, Wojciech Zaremba, Ilya Sutskever, Joan Bruna, Dumitru Erhan, Ian J. Goodfellow, and Rob Fergus. 2013. "Intriguing Properties of Neural Networks." ArXiv Preprint ArXiv:1312.6199. http://arxiv.org/abs/1312.6199.

Zhou, Wen. 2014. "Some Bayesian and Multivariate Analysis Methods in Statistical Machine Learning and Applications." PhD thesis, Iowa State University; Graduate Theses; Dissertations. http://lib.dr.iastate.edu/etd/13816/.