Deep Boltzmann Machines

Machine Learning Seminar

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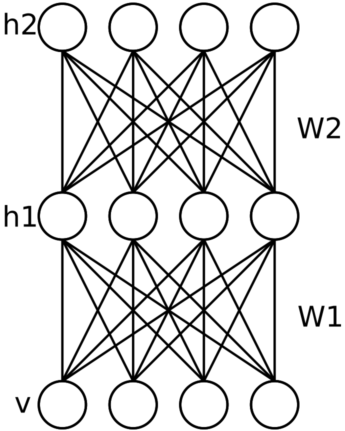
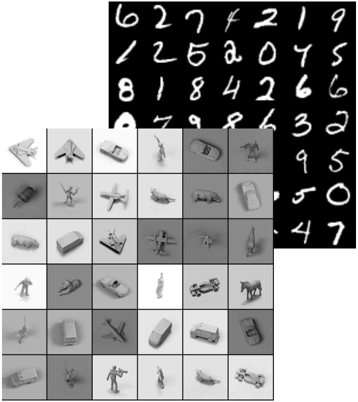
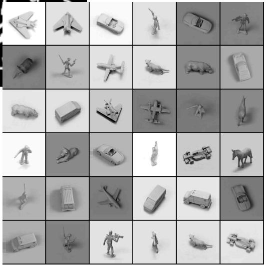




Motivation



- Unsupervised Pretraining helps
- Structure of data not to be found in its labels
- but in the data itself!

Outline

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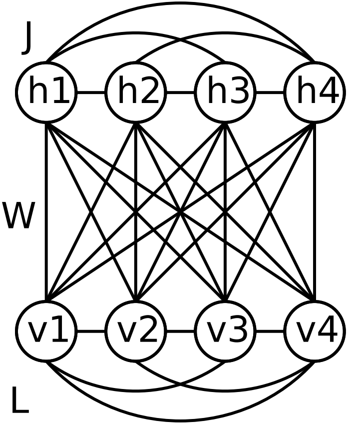
1. General Boltzmann Machines
2. Restricted Boltzmann Machines
3. Deep Boltzmann Machines
4. Neural Networks
5. Experimental Results
6. Conclusions

Boltzmann Machines
Definition



$$\mathbf{v} \in \{0,1\}^D$$

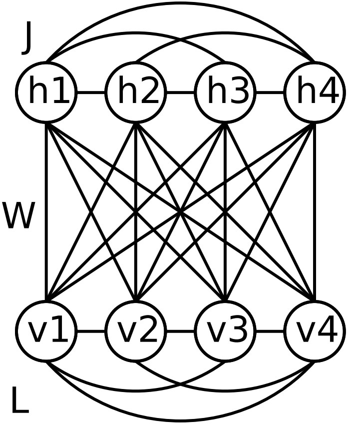
$$\mathbf{h} \in \{0,1\}^P$$

$$E(\mathbf{v},\mathbf{h};\theta) = -\frac{1}{2}\mathbf{v}^T\mathbf{L}\mathbf{v} - \frac{1}{2}\mathbf{h}^T\mathbf{J}\mathbf{h} - \mathbf{v}^T\mathbf{W}\mathbf{h}$$

$$p(\mathbf{v};\theta) = \frac{1}{Z(\theta)}\sum_{\mathbf{h}} \exp(-E(\mathbf{v},\mathbf{h};\theta))$$

$$\theta = \{\mathbf{W},\mathbf{L},\mathbf{J}\}$$

Boltzmann Machines
Gradients

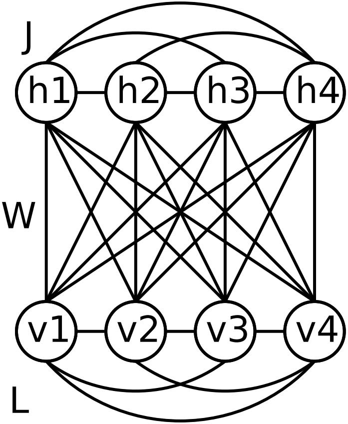


- Maximum Likelihood leads to the following gradients:

$$\Delta \mathbf{W} = \alpha(E_{P_{data}}[\mathbf{vh}^T] - E_{P_{model}}[\mathbf{vh}^T])$$

$$\Delta \mathbf{L} = \alpha(E_{P_{data}}[\mathbf{vv}^T] - E_{P_{model}}[\mathbf{vv}^T])$$

$$\Delta \mathbf{J} = \alpha(E_{P_{data}}[\mathbf{hh}^T] - E_{P_{model}}[\mathbf{hh}^T])$$



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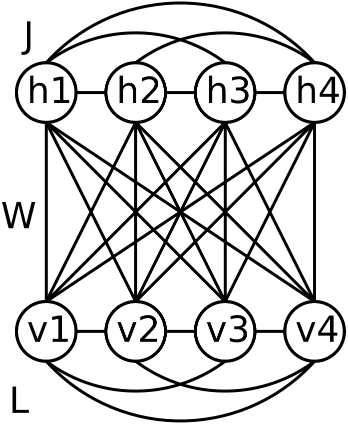
$$\Delta \mathbf{L} = \alpha(E_{P_{data}}[\mathbf{v}\mathbf{v}^T] - E_{P_{model}}[\mathbf{v}\mathbf{v}^T])$$

$$\Delta \mathbf{J} = \alpha(E_{P_{data}}[\mathbf{h}\mathbf{h}^T] - E_{P_{model}}[\mathbf{h}\mathbf{h}^T])$$

- $E_{P_{model}}[.]$ is the expectation over the distribution of the current model
  - approximated with samples

Boltzmann Machines

Gradients



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$$\Delta \mathbf{W} = \alpha(E_{P_{data}}[\mathbf{v}\mathbf{h}^T] - E_{P_{model}}[\mathbf{v}\mathbf{h}^T])$$

$$\Delta \mathbf{L} = \alpha(E_{P_{data}}[\mathbf{v}\mathbf{v}^T] - E_{P_{model}}[\mathbf{v}\mathbf{v}^T])$$

$$\Delta \mathbf{J} = \alpha(E_{P_{data}}[\mathbf{h}\mathbf{h}^T] - E_{P_{model}}[\mathbf{h}\mathbf{h}^T])$$

- $E_{P_{model}}[.]$ is the expectation over the distribution of the current model
  - approximated with samples
- $E_{P_{data}}[.]$ is the expectation over the completed data distribution
  - approximated e.g. with mean-field method

Boltzmann Machines
Difficulties

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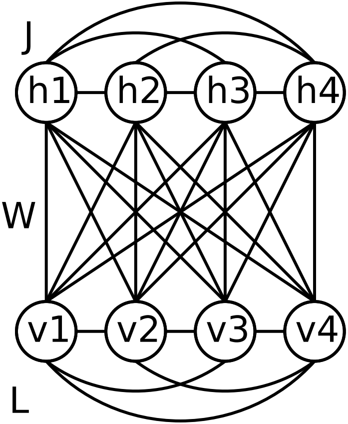
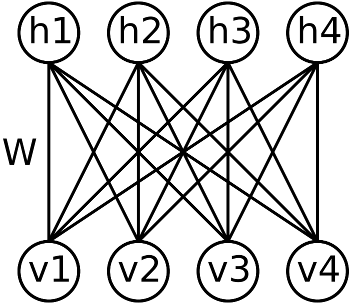


- cannot be trained directly
  - has to be approximated
- even inference is hard
  - e.g.: Gibbs sampling requires each node to be sampled independently
  - this takes a long time and is also an approximation

Restricted Boltzmann Machines



- most problems can be solved by setting $L = J = 0$.
- observing one layer makes the nodes of the other independent from each other.

Deep Boltzmann Machines

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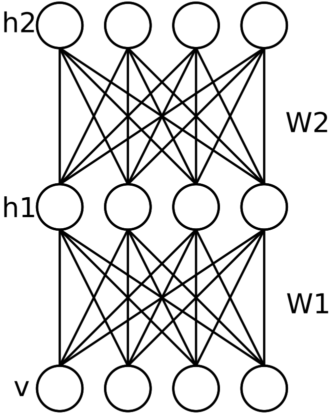
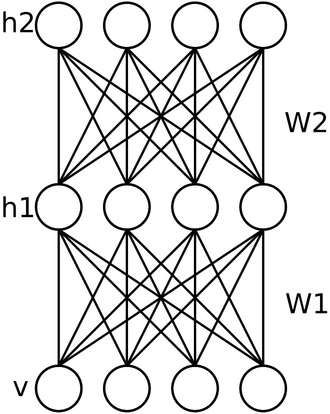


- Multiple RBMs stacked upon each other
- each layer captures complicated, higher-order correlations
- promising for object and speech recognition
- deals more robustly with ambigous inputs than e.g. deep belief networks
- may be trained the same way as a BM
  - is very slow
  - may get stuck in bad local optimum

Deep Boltzmann Machines

Two-Layer example



Model:

$$E(\mathbf{v}, \mathbf{h}^1, \mathbf{h}^2; \theta) = -\mathbf{v}^T \mathbf{W}^1 \mathbf{h}^1 - \mathbf{h}^{1T} \mathbf{W}^2 \mathbf{h}^2$$

$$p(\mathbf{v}; \theta) = \frac{1}{Z(\theta)} \sum_{\mathbf{h}^1, \mathbf{h}^2} \exp(-E(\mathbf{v}, \mathbf{h}^1, \mathbf{h}^2; \theta))$$

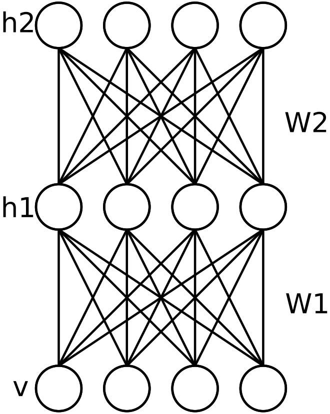
Conditional Probabilities:

$$p(h_j^1 | \mathbf{v}, \mathbf{h}^2) = \sigma(\sum_i W_{ij}^1 v_i + \sum_m W_{jm}^2 h_j^2)$$

$$p(h_m^2 | \mathbf{h}^1) = \sigma(\sum_j W_{im}^2 h_i^1)$$

$$p(v_i | \mathbf{h}^1) = \sigma(\sum_j W_{ij}^1 h_j^1)$$

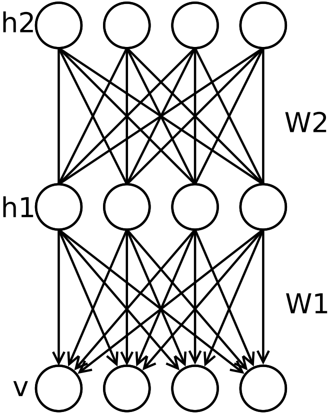
Deep Boltzmann Machines
Layer by Layer Pretraining



- Train each W_i individually by using the output of the lower RBM as input for the upper.
- The last RBM may be trained as it is.

Deep Boltzmann Machines

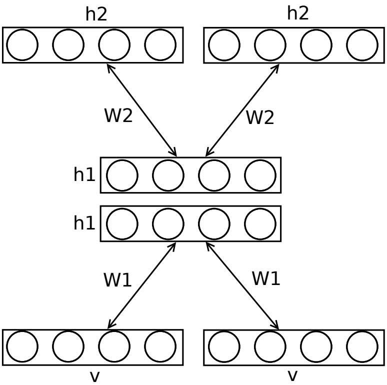
Deep Belief Networks



- Train each W_i individually by using the output of the lower RBM as input for the upper.
- The last RBM may be trained as it is.
- This results in a Deep Belief Network $p(\mathbf{v};\theta) = \sum_{\mathbf{h}^1} p(\mathbf{h}^1;\mathbf{W}^1)p(\mathbf{v}|\mathbf{h}^1;\mathbf{W}^1)$
- second RBM replaces $p(\mathbf{h}^1;\mathbf{W}^1)$ by $p(\mathbf{h}^1;\mathbf{W}^2) = \sum_{\mathbf{h}^2} p(\mathbf{h}^1,\mathbf{h}^2;\mathbf{W}^2)$
- if initialized correctly $p(\mathbf{h}^1;\mathbf{W}^2)$ is a better model

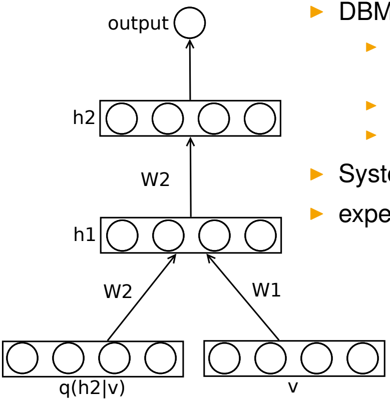
Deep Boltzmann Machines

Layer by Layer Pretraining



- modify RBMs s.th. learned weights are half
- conditionals for the bottom RBM:
  $p(h_j^1 = 1|\mathbf{v}) = \sigma(\sum_i W_{ij}^1 v_i + \sum_i W_{ij}^1 v_i)$
  $p(v_i = 1|\mathbf{h}^1) = \sigma(\sum_j W_{ij}^1 h_j^1)$
- conditionals for the top RBM:
  $p(h_j^1 = 1|\mathbf{h}^2) = \sigma(\sum_m W_{jm}^2 h_m^2 + \sum_m W_{jm}^2 h_m^2)$
  $p(h_m^2 = 1|\mathbf{h}^1) = \sigma(\sum_j W_{jm}^2 h_j^1)$
- after combining the distribution over $\mathbf{h}^1$ is:
  $p(h_j^1 = 1|\mathbf{v}, \mathbf{h}^2) = \sigma(\sum_i W_{ij}^1 v_i + \sum_m W_{jm}^2 h_m^2)$
- good initialization for mean-field method

Neural Networks



- DBM can be used to initialize a neural network
  - Weights of DBM become the weights of neural network
  - $q(\mathbf{h}|\mathbf{v})$ is the mean-field distribution of the posterior
  - neural network may be trained with backpropagation
- System may decide which of the input layers to use
- experiments show the use of both

Experimental Results

MNIST

Training Samples

2-layer DBM

3-layer DBM

- handwritten digits (28x28 Pixels)
- 60.000 Trainings images
- 10.000 Test images
- two DBMs were trained
  - 2-layer (500 and 1000 hidden units)
  - 3-layer (500, 500 and 1000 hidden units)
- error rates for discriminative models:
  - 2-layer DBN (baseline): 1,2%
  - 2-layer DBM: 0,95%
  - 3-layer DBM: 1,01%

Experimental Results

NORB

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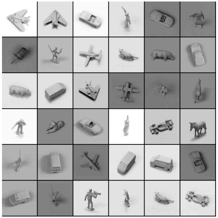
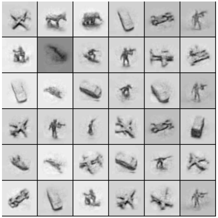


Training Samples



Generated Samples

- 24.300 stereo images (96x96 pixels)
  - 50 different 3D toy objects
  - 5 generic classes
  - 4.300 were used as test set
  - larger pixels around edges for dimensionality reduction
- trained DBMs:
  - preprocessing layer with 4000 units
  - two further layers with 4000 units
  - completely unsupervised
  - second DBM trained with additional 1.16M training instances
- error rates:
  - SVM (baseline): 11,6%
  - DBM: 10,8%
  - DBM (with additional training data): 7.1%

Conclusions

- DBMs find good features to model the data
- DBMs can be used for unsupervised learning
- Unsupervised Learning helps generalization
- labels do not carry much information

Sources

- R. Salakhutdinov, G. Hinton. 2009
  Deep Boltzmann Machines
- G. Hinton, S. Osindero, and Y. W. Teh. 2006
  A fast learning Algorithm for deep belief nets