

Neural Networks

Lecture 17

Boltzmann Machines as Probabilistic Models

Modeling binary data

- Given a training set of binary vectors, fit a model that will assign a probability to other binary vectors.
 - Useful for deciding if other binary vectors come from the same distribution.
 - This can be used for monitoring complex systems to detect unusual behavior.
 - If we have models of several different distributions it can be used to compute the posterior probability that a particular distribution produced the observed data.

$$p(\text{Model } i \mid \text{data}) = \frac{p(\text{data} \mid \text{Model } i)}{\sum_j p(\text{data} \mid \text{Model } j)}$$

A naïve model for binary data

For each component, j , compute its probability, p_j , of being on in the training set. Model the probability of test vector alpha as the product of the probabilities of each of its components:

$$p(\mathbf{s}^\alpha) = \prod_j \left(s_j^\alpha p_j + (1 - s_j^\alpha)(1 - p_j) \right)$$

↑ Binary vector alpha

↑ If component j of vector alpha is on

↑ If component j of vector alpha is off

A mixture of naïve models

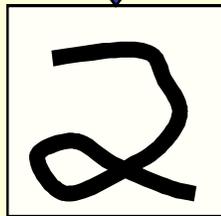
- Assume that the data was generated by first picking a particular naïve model and then generating a binary vector from this naïve model.
 - This is just like the mixture of Gaussians, but for binary data.

$$p(\mathbf{s}^\alpha) = \sum_{m \in \text{Models}} \pi_m \prod_j \left(s_j^\alpha p_j^m + (1 - s_j^\alpha)(1 - p_j^m) \right)$$

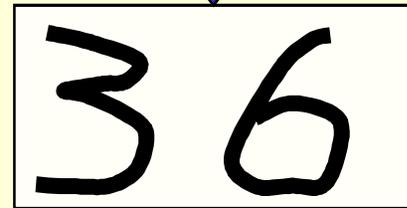
Limitations of mixture models

- Mixture models assume that the whole of each data vector was generated by exactly one of the models in the mixture.
 - This makes it easy to compute the posterior distribution over models when given a data vector.
 - But it cannot deal with data in which there are several things going on at once.

mixture of 10 models



mixture of 100 models



Dealing with compositional structure

- Consider a dataset in which each image contains N different things:
 - A distributed representation requires a number of neurons that is linear in N .
 - A localist representation (i.e. a mixture model) requires a number of neurons that is exponential in N .
 - Mixtures require one model for each possible combination.
- Distributed representations are generally much harder to fit to data, but they are the only reasonable solution.
 - Boltzmann machines use distributed representations to model binary data.

How a Boltzmann Machine models data

- It is **not** a causal generative model (like a mixture model) in which we first pick the hidden states and then pick the visible states given the hidden ones.
- Instead, everything is defined in terms of energies of joint configurations of the visible and hidden units.

The Energy of a joint configuration

binary state of unit i in joint configuration alpha, beta

$$E^{\alpha\beta} = - \sum_{i \in \text{units}} s_i^{\alpha\beta} b_i - \sum_{i < j} s_i^{\alpha\beta} s_j^{\alpha\beta} w_{ij}$$

Energy with configuration alpha on the visible units and beta on the hidden units

bias of unit i

indexes every non-identical pair of i and j once

weight between units i and j

Using energies to define probabilities

- The probability of a joint configuration over both visible and hidden units depends on the energy of that joint configuration compared with the energy of all other joint configurations.
- The probability of a configuration of the visible units is the sum of the probabilities of all the joint configurations that contain it.

$$p(\mathbf{v}^\alpha, \mathbf{h}^\beta) = \frac{e^{-E^{\alpha\beta}}}{\sum_{\gamma\delta} e^{-E^{\gamma\delta}}}$$

partition function

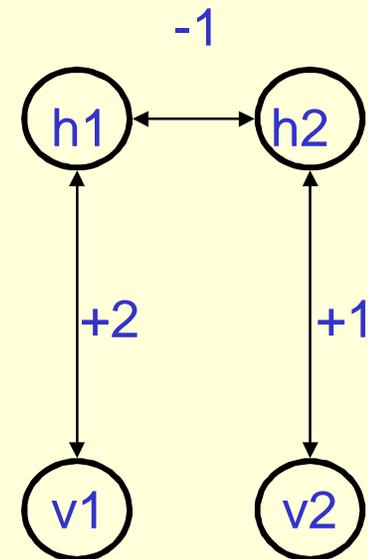
configuration alpha on the visible units

$$p(\mathbf{v}^\alpha) = \frac{\sum_{\beta} e^{-E^{\alpha\beta}}}{\sum_{\gamma\delta} e^{-E^{\gamma\delta}}}$$

An example of how weights define a distribution

| \mathbf{v} | \mathbf{h} | $-E$ | e^{-E} | $p(\mathbf{v}, \mathbf{h})$ | $p(\mathbf{v})$ |
|--------------|--------------|------|----------|-----------------------------|-----------------|
| 1 1 | 1 1 | 2 | 7.39 | .186 | 0.466 |
| 1 1 | 1 0 | 2 | 7.39 | .186 | |
| 1 1 | 0 1 | 1 | 2.72 | .069 | |
| 1 1 | 0 0 | 0 | 1 | .025 | |
| 1 0 | 1 1 | 1 | 2.72 | .069 | 0.305 |
| 1 0 | 1 0 | 2 | 7.39 | .186 | |
| 1 0 | 0 1 | 0 | 1 | .025 | |
| 1 0 | 0 0 | 0 | 1 | .025 | |
| 0 1 | 1 1 | 0 | 1 | .025 | 0.144 |
| 0 1 | 1 0 | 0 | 1 | .025 | |
| 0 1 | 0 1 | 1 | 2.72 | .069 | |
| 0 1 | 0 0 | 0 | 1 | .025 | |
| 0 0 | 1 1 | -1 | 0.37 | .009 | 0.084 |
| 0 0 | 1 0 | 0 | 1 | .025 | |
| 0 0 | 0 1 | 0 | 1 | .025 | |
| 0 0 | 0 0 | 0 | 1 | .025 | |

total =39.70



Getting a sample from the model

- If there are more than a few hidden units, we cannot compute the normalizing term (the partition function) because it has exponentially many terms.
- So use Markov Chain Monte Carlo to get samples from the model:
 - Start at a random global configuration
 - Keep picking units at random and allowing them to stochastically update their states based on their energy gaps.
 - Use simulated annealing to reduce the time required to approach thermal equilibrium.
- At thermal equilibrium, the probability of a global configuration is given by the Boltzmann distribution.

Getting a sample from the posterior distribution over distributed representations for a given data vector

- The number of possible hidden configurations is exponential so we need MCMC to sample from the posterior.
 - It is just the same as getting a sample from the model, except that we keep the visible units clamped to the given data vector.
 - Only the hidden units are allowed to change states
- Samples from the posterior are required for learning the weights.