Boltzmann Machines

Learning by Correlation
in a Hopfield-like Net

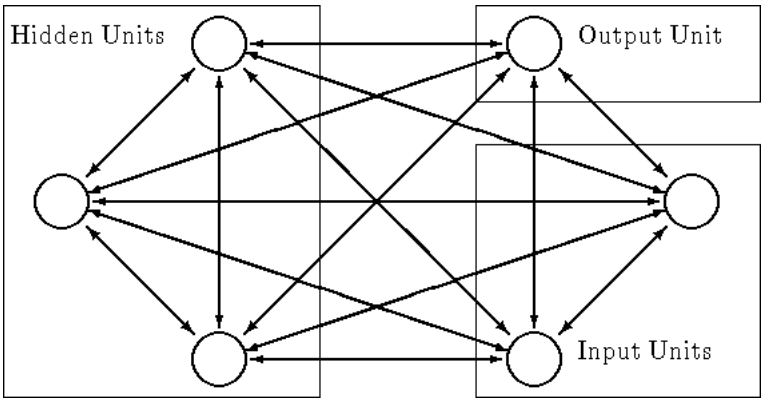
Boltzmann Machine

- Proposed by Ackley, Hinton, and Sejnowski, 1985.
- Extends Hopfield model with learning.
- Based on **probabilistic operation.**
- Learning is by **correlation** (sort of Hebbian in character).

Boltzmann Machine Structure

- The Boltzmann Machine is like a Hopfield network, in which
- the neurons are divided into two subsets:
  - **visible**, which are further divided into:
    - input
    - output
  - **hidden**
- As with the Hopfield model, the weights are symmetric.

Boltzmann Machine Structure



Boltzmann Machine Operation

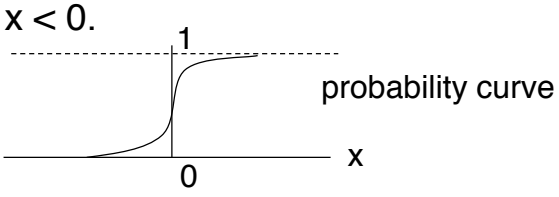
- There are two modes of operation:
  - clamped mode
  - free mode
- In **clamped** mode, the input and output of visible neurons are held fixed, while the hidden neurons are allowed to vary.
- In **free** mode, **only the inputs are held fixed** and all other neurons are allowed to vary.

Probabilistic Firing (used in Training)

- All neurons have output in {+1, -1}.
- The activation function determines not the exact next input, but rather the **probability** of the neuron's output being set to 1:
  - f(net) = probability that output is set to 1
  - where *net* is the weighted sum input
  - where f(x) = 1/(1 + exp(-2□x))
  - where □ is a parameter to be determined
  - so the higher the value of *net*, the more likely the neuron will be set to 1.

Probabilistic Firing

- f(x) = 1/(1 + exp(-2□x))
- Obviously this is a sigmoid:
  - With □ = 0, the probability of setting output 1 is 0.5, i.e. total randomness.
  - As □ increases, the probability of setting output to 1 approaches 1 if x > 0, and 0 if x < 0.



Controlling □

- In order to achieve a stable probability distribution for the network state, □ is gradually increased from 0 over time.

Controlling □

- We can think of the increase in □ as "cooling" the network.
- Thus, we can govern beta as □ = 1/T where T is the "temperature", which decreases with time (according to a *schedule*).
- The overall process is known as "**simulated annealing**".

Annealing Schedule

- The annealing schedule determines the temperature T as a function of the step of the algorithm.
- Example:

  $T = T_0/(1 + \log k)$

  where k is the step number and T_0 is an initial temperature.

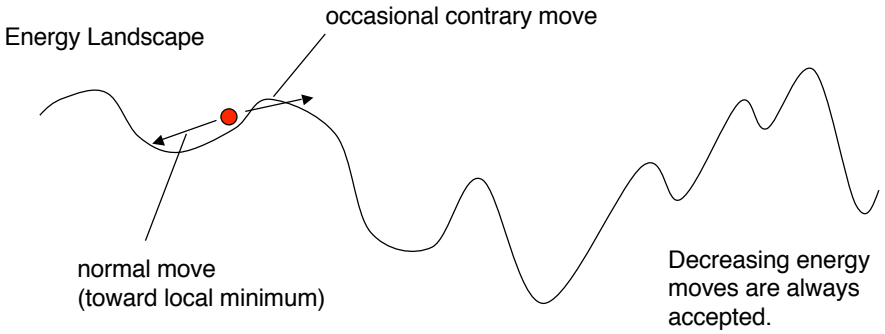
History of Simulated Annealing

- SA was first proposed in 1983 as a method for optimizing wire-routing on VLSI chips (an NP-hard problem)
- by Kirkpatrick, Gelatt, and Vecchi.
- This was a widely-celebrated result.
- SA is now used as a way to avoid local minima in a number of computational problems.

Role of Annealing in Stabilization

- Generally, move in direction of decreasing energy.
- **Occasionally, accept a move that increases energy.**
- This will be done with high probability at first, but lower probability as annealing progresses.

Role of Annealing in Stabilization



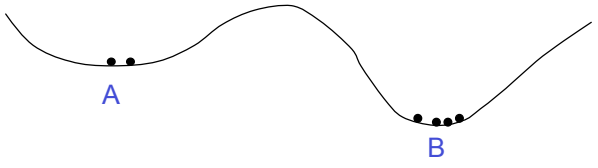
The probability of making a contrary move is inversely proportional to the energy increase and to the temperature (higher probability earlier in the annealing schedule).

How temperature affects transition probabilities (slide from Hinton)

High temperature transition probabilities

$p(A \to B) = 0.2$

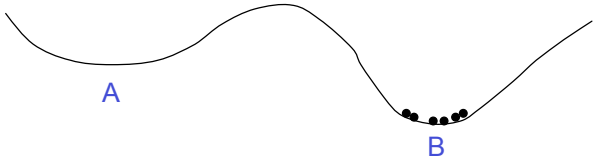
$p(A \to B) = 0.1$



Low temperature transition probabilities

$p(A \to B) = 0.001$

$p(A \to B) = 0.000001$

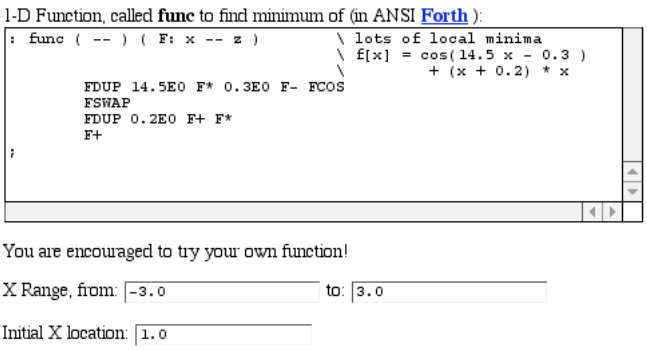


Annealing Advantage (as summarized by Hinton)

- At high temperature the ***transition*** probabilities for uphill jumps are much greater.
- At low temperature the ***equilibrium*** probabilities of low energy states are much better than the equilibrium probabilities of high energy ones.

Stand-alone demo of Simulated Annealing

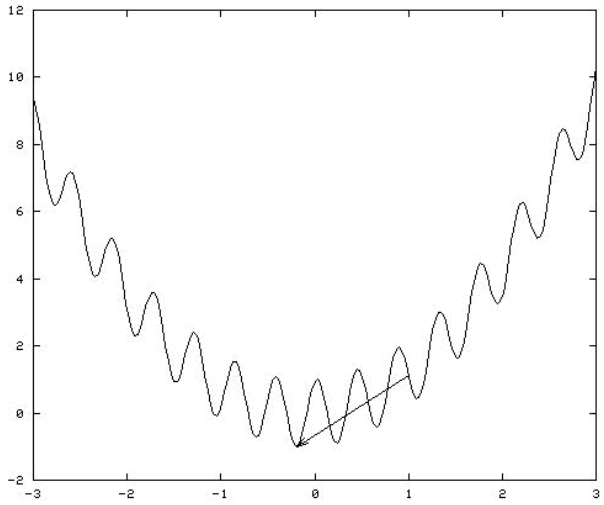
http://www.taygeta.com/annealing/demo1.html



Simulated Annealing Result

Initial x: 1
Estimated minimum x: -0.195065

Boltzman constant: 1.000000 Learning rate: 0.500000 Jump value: 100.000000 Dwell: 10 Dimension: 1 Current temperature: 0.093204 Current state: -0.195065



Energy-Based Simulation

- As we know from Hopfield theory, making a single transition according to the activation function will decrease the energy.
- So we can simply decide to “flip” a neuron based on whether the flip lowers the energy (defined as $-\sum\sum w_{ij} y_i y_j$).

Energy-Based Simulation

- To include the annealing temperature:
  - If a flip **lowers** the energy, do it.
  - If a flip **raises** the energy by ΔE, flip the output with probability $1/(1 + \exp(\Delta E/T))$.
    - This can be done by generating a random number η between 0 and 1, then setting the output of the neuron depending on whether

      $$\eta < \exp(\Delta E/T)$$

      the probability being greater or less than 1/2 depending on which case.

Energy-Based Simulation

- A similar technique was originally used in the famous Metropolis, Rosenbluth, Teller equation of state calculations in statistical mechanics
  (Ising or “spin-glass” model).

Energy-Based Simulation

- In order to compute ΔE, it is not necessary to fully compute the energy before and after. Instead could just use $\Delta E = \sum w_{ij} y_j$ where i is the neuron being flipped.

Code from a Boltzmann Machine

```
/* Change the value for only 1 node, on temperature t. At this
   temperature accept the change if it increases the energy, and accept it
   with some probability, if it decreases it. Probability depends on t */
void anneal_1_step(struct machine *p, double t)
{       int node, layer;
        double dE;

        select_node(p, &layer, &node);
        dE = energy_change(p, layer, node);

        if( accept_change(dE, t) )
                flip_state(p, layer, node);
}
```

Code from a Boltzmann Machine

```
/* Is a change of dE acceptable at temperature t? */
   accept_change(double dE, double t)
{      double prob, rand;
/* Always accept changes that decrease the energy */
       if( dE < 0 )
             return( 1 );

       /* If the change increases the energy, accept it with a
          certain probability */

       prob = 1 / (1 + exp(dE/t) );
       rand = get_rand(0.0, 1.0);
       return( rand < prob );
```

Code from a Boltzmann Machine

```
/* Simulated annealing over machine p. The temperature is constantly
   decreasing over a set of values. For each temperature a set of state
   changes are performed on randomly selected (non clamped!) nodes.
   Each state change is selected with a certain probability. If it decreases
   the total energy, it is selected; if not it is selected with a
   probability that is a function of the temperature
*/
void anneal(struct machine *p)
{      double temp = p->t0;
       int i, n;
       int node, layer;
       double dE;
```

Code from a Boltzmann Machine

```
/* Vary the temperature */
      while( temp >= p->tmin )
      {   /* For each temperature, perform a number of operations which
             is a function of the temperature of annealing. */
          n = get_num_changes(temp, p);
          for( i=0; i<n; i++ )
          {   select_node(p, &layer, &node);
              dE = energy_change(p, layer, node);
              if( accept_change(dE, temp) )
                  flip_state(p, layer, node);
          }
          temp *= p->beta;
      }
}
```

Boltzmann Distribution

- The name of the machine derives from the fact that, at steady state, if s and t are two states with energies E_s and E_t respectively, then the probabilities of being in those states P[s] vs. P[t] satisfy

$$P[s]/P[t] = \exp((E_t - E_s)/T)$$

where T is the temperature. This is known as the “Boltzmann distribution” or “Boltzmann-Gibbs distribution”.

Learning in the Boltzmann Machine

Multiple Simulations Per Sample

- Suppose we set the input and output neurons according to a specific **sample**.
- We then anneal the network.
  The final state reached is not necessarily unique, due to the probabilistic moves made along the way.
- We can observe, over **several** such simulations, which neurons' outputs are **correlated** at the ends, represented as a **correlation** $\rho_{ij} = E[y_i y_j]$, the expected (average) value of the product of the outputs of neurons i and j.

Learning Rule

- Let ρ_{ij}^{+} be the correlation value when the network is run in **clamped** mode, and ρ_{ij}^{-} be the correlation value when the network is run in **free** mode.
- The Boltzmann learning rule is

$$\Delta w_{ij} = \eta(\rho_{ij}^{+} - \rho_{ij}^{-})$$

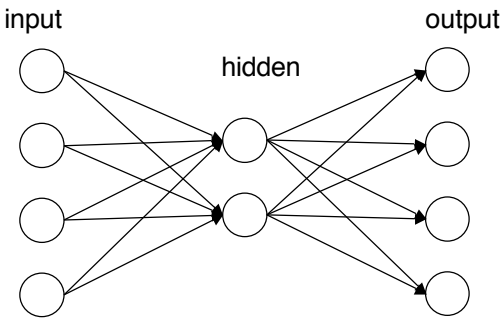
  where η is the learning rate.
- In other words, whether weights are changed depends on the difference between the correlations in clamped vs. free mode.

Batch Learning Algorithm (from Hinton)

- Clamped phase
  - For each data vector in the training set:
    - Clamp the data vector on the visible units.
    - Let the hidden units reach thermal equilibrium at a temperature of 1 (may use annealing to speed this up).
    - Sample $y_i\, y_j$ for all pairs of units.
- Free phase
  - Repeat many times to get good estimates
    For each data vector in the training set:
    - Do not clamp any of the [output?] units.
    - Let the whole network reach thermal equilibrium at a temperature of 1.
    - Sample $y_i\, y_j$ for all pairs of units.
- Weight updates
  - Update each weight by an amount proportional to the difference in $E[y_i\, y_j]$ in the two phases.

Boltzman Example

- Ackley, Hinton, and Sejnowski, 1985 presented the following example:
- 4 line one-hot encoder-decoder, 2 hidden units



Boltzman Example

- To prevent weights from growing too large, used a "noisy" **clamping** technique: each *on* bit of a clamped vector is set to *off* with prob. 0.15 and each *off* bit set to *on* with prob. 0.05.
- Network was **unclamped** and allowed to reach equilibrium. Statistics were gathered for the same number of annealings as in the clamped case.
- Annealing schedule: (time units @ temperature) 2@20, 2@15, 2@12, 4@10.
- 1 time unit = interval giving each neuron a chance to flip.

Additional Examples

- 4-2-4 encoder/decoder converged quickly
- 8-3-8: more difficult
- 40-10-40: converged in 98.6% of runs.

Boltzmann Simulators

- /cs/cs152/boltzmann
  - Simulates only the distribution, not learning.
  - It is analogous to a spin-glass simulation.
- /cs/cs152/boltz
  - Learning, weight-saving, etc.
  - An example, bxor, provides a demo of training a Boltzmann machine to implement xor. Run the shell script bxor.run (may have to run more than once for convergence).

Speedup Possibility

- Training of a Boltzmann machine is extremely slow.
- A possible speedup is to use the “mean-field” approximation to get the correlation values.
- This approach is due to Peterson and Anderson, 1987.

Mean-Field Theory

- If f is a function of two variables, then the expectation
  E[f(x, y)]
  can be *approximated* by
  f(E[x], E[y])
- This idea can be applied to the weight change rule of the Boltzmann machine, which entails computing

$$\rho_{ij} = E[y_i y_j] \approx E[y_i] E[y_j]$$

Mean-Field Theory

- For the Boltzmann distribution, the probability that node i takes value 1 at temperature T can be shown to be:

$$p_1 = 1/(1+\exp(-\sum w_{ij} E[y_j]/T))$$

- So the *expected* output of node i is

$$E[y_i] = 1*p_1 + (-1)*(1- p_1)$$

$$= \tanh(\sum w_{ij} E[y_j] / 2T)$$

Mean-Field Theory

- We now have n non-linear equations in n unknowns $E[y_j]$ which can be solved ***deterministically*** by using successive approximations (**without simulation**!, but we still have to anneal).

- We can then use these approximations to update the weights:

$$\Delta w_{ij} = \eta(E^+[y_i] E^+[y_j] - E^-[y_i] E^-[y_j])$$

where + and - designate clamped vs. free as before.

Cauchy Machine (Szu, 1986)

- Same topology as Boltzmann machine
- Learns arbitrary spatial patterns by Hebbian encoding and fast simulated annealing
- Claimed to find min. energy with probability 1.
- Probability of neuron being 1 is
  $p_1 = T/(T+(\Delta E)^2)$ vs.
  $p_1 = 1/(1+\exp(-\Delta E /T))$ for Boltzmann.
- Annealing schedule is
  $T = T_0/(1 + k)$ vs.
  $T = T_0/(1 + \log k)$ (typical) for Boltzmann.

Other Hopfield Machines

- BAM (Bi-directional Associative Memory) (Bart Kosko, USC)
- Stores input-output patterns
- Can retrieve either direction
  - Given input, find output
  - Given output, find input
- Hopfield net divided into two tiers with behavior activating one tier then the other.