Neural Networks

Hopfield Nets and Boltzmann Machines
Recap: Hopfield network

\begin{equation}
y_i = \Theta \left( \sum_{j \neq i} w_{ji} y_j + b_i \right)
\end{equation}

\begin{equation}
\Theta(z) = \begin{cases} 
+1 & \text{if } z > 0 \\
-1 & \text{if } z \leq 0 
\end{cases}
\end{equation}

- At each time each neuron receives a “field” \( \sum_{j \neq i} w_{ji} y_j + b_i \)
- If the sign of the field matches its own sign, it does not respond
- If the sign of the field opposes its own sign, it “flips” to match the sign of the field
Recap: Energy of a Hopfield Network

- The system will evolve until the energy hits a local minimum
- In vector form
  - Bias term may be viewed as an extra input pegged to 1.0

\[ y_i = \Theta \left( \sum_{j \neq i} w_{ji}y_j + b_i \right) \]

\[ \Theta(z) = \begin{cases} +1 & \text{if } z > 0 \\ -1 & \text{if } z \leq 0 \end{cases} \]

\[ E = - \sum_{i,j<i} w_{ij}y_iy_j - \sum_i b_iy_i \]

The system will evolve until the energy hits a local minimum

In vector form

- Bias term may be viewed as an extra input pegged to 1.0

\[ E = -\frac{1}{2} y^T W y - b^T y \]
Recap: Hopfield net computation

1. Initialize network with initial pattern
\[ y_i(0) = x_i, \quad 0 \leq i \leq N - 1 \]

2. Iterate until convergence
\[ y_i(t + 1) = \Theta \left( \sum_{j \neq i} w_{ji} y_j \right), \quad 0 \leq i \leq N - 1 \]

- Very simple
- Updates can be done sequentially, or all at once
- Convergence

\[ E = - \sum_i \sum_{j>i} w_{ji} y_j y_i \]

does not change significantly any more
Recap: Evolution

- The network will evolve until it arrives at a local minimum in the energy contour.

\[ E = -\frac{1}{2}y^TWy \]
Recap: Content-addressable memory

- Each of the minima is a “stored” pattern
  - If the network is initialized close to a stored pattern, it will inevitably evolve to the pattern

- This is a content addressable memory
  - Recall memory content from partial or corrupt values

- Also called associative memory
Examples: Content addressable memory

- Hopfield network reconstructing degraded images from noisy (top) or partial (bottom) cues.

Examples: Content addressable memory

Noisy pattern completion: Initialize the entire network and let the entire network evolve

Hopfield network reconstructing degraded images from noisy (top) or partial (bottom) cues.

- http://staff.itee.uq.edu.au/janetw/cmc/chapters/Hopfield/
Examples: Content addressable memory

Pattern completion: Fix the “seen” bits and only let the “unseen” bits evolve

Hopfield network reconstructing degraded images from noisy (top) or partial (bottom) cues.

- http://staff.itee.uq.edu.au/janetw/cmc/chapters/Hopfield/
Training a Hopfield Net to “Memorize” target patterns

• The Hopfield network can be trained to remember specific “target” patterns
  – E.g. the pictures in the previous example
• This can be done by setting the weights $W$ appropriately

Random Question:
Can you use backprop to train Hopfield nets?

Hint: Think unwrapping...
Training a Hopfield Net to “Memorize” target patterns

• The Hopfield network can be trained to remember specific “target” patterns
  – E.g. the pictures in the previous example

• A Hopfield net with $N$ neurons can designed to store up to $N$ target $N$-bit memories
  – But can store an exponential number of unwanted “parasitic” memories along with the target patterns

• **Training the network:** Design weights matrix $W$ such that the energy of ...
  – Target patterns is minimized, so that they are in energy wells
  – *Other untargeted* potentially parasitic patterns is maximized so that they don’t become parasitic
Training the network

\[ \hat{W} = \arg\min_w \sum_{y \in Y_P} E(y) - \sum_{y \notin Y_P} E(y) \]

Minimize energy of target patterns
Maximize energy of all other patterns
Optimizing $W$

$$E(y) = -\frac{1}{2} y^T W y$$
$$\hat{W} = \arg\min_W \sum_{y \in Y_P} E(y) - \sum_{y \notin Y_P} E(y)$$

- Simple gradient descent:

$$W = W + \eta \left( \sum_{y \in Y_P} yy^T - \sum_{y \notin Y_P} yy^T \right)$$

- Minimize energy of target patterns
- Maximize energy of all other patterns
Training the network

\[ W = W + \eta \left( \sum_{y \in Y_p} yy^T - \sum_{y \notin Y_p} yy^T \right) \]

*Minimize energy of target patterns*

*Maximize energy of all other patterns*
Simpler: Focus on confusing parasites

\[ W = W + \eta \left( \sum_{y \in Y_P} yy^T - \sum_{y \notin Y_P \& y = \text{valley}} yy^T \right) \]

- Focus on minimizing parasites that can prevent the net from remembering target patterns
  - Energy valleys in the neighborhood of target patterns
Simpler: Focus on confusing patterns

\[ w = w + \eta \left( \sum_{y \in Y_P} yy^T - \sum_{y \notin Y_P \& y=\text{valley}} yy^T \right) \]

- Lower energy at valid memories
- Initialize the network at valid memories and let it evolve a few steps
  - It will settle in a broad vicinity of the memory; raise it
Training the Hopfield network

\[ W = W + \eta \left( \sum_{y \in Y_P} yy^T - \sum_{y \notin Y_P \& y = \text{valley}} yy^T \right) \]

- Initialize \( W \)
- Compute the total outer product of all target patterns
  - More important patterns presented more frequently
- Initialize the network with each target pattern and let it evolve
  - And settle at a valley
- Compute the total outer product of valley patterns
- Update weights
Training the Hopfield network: SGD version

$$W = W + \eta \left( \sum_{y \in Y_P} yy^T - \sum_{y \notin Y_P \& y = \text{valley}} yy^T \right)$$

- Initialize $W$
- Do until convergence, satisfaction, or death from boredom:
  - Sample a target pattern $y_p$
    - Sampling frequency of pattern must reflect importance of pattern
  - Initialize the network at $y_p$ and let it evolve
    - And settle at a valley $y_v$
  - Update weights
    - $W = W + \eta (y_p y_p^T - y_v y_v^T)$
More efficient training

- Really no need to raise the entire surface, or even every valley
- Raise the *neighborhood* of each target memory
  - Sufficient to make the memory a valley
  - The broader the neighborhood considered, the broader the valley

![Energy vs. state graph](image)
Training the Hopfield network: SGD version

$$W = W + \eta \left( \sum_{y \in Y_p} yy^T - \sum_{y \notin Y_p \& y=\text{valley}} yy^T \right)$$

- Initialize $W$
- Do until convergence, satisfaction, or death from boredom:
  - Sample a target pattern $y_p$
    - Sampling frequency of pattern must reflect importance of pattern
  - Initialize the network at $y_p$ and let it evolve a few steps (2-4)
    - And arrive at a down-valley position $y_d$
  - Update weights
    - $W = W + \eta (y_p y_p^T - y_d y_d^T)$
Problem with Hopfield net

- Why is the recalled pattern not perfect?
A Problem with Hopfield Nets

- Many local minima
  - Parasitic memories

- May be escaped by adding some *noise* during evolution
  - Permit changes in state even if energy increases..
    - Particularly if the increase in energy is small
Recap – Analogy: Spin Glasses

The total energy of the system evolves to minimize the energy.

Dipoles stop flipping if flips result in an increase of energy.

Total field at current dipole:

\[
f(p_i) = \sum_{j \neq i} J_{ij} x_j + b_i
\]

Response of current dipole:

\[
x_i = \begin{cases} 
  x_i & \text{if } \text{sign}(x_i f(p_i)) = 1 \\
  -x_i & \text{otherwise}
\end{cases}
\]

The total energy of the system:

\[
E(s) = C - \frac{1}{2} \sum_i x_i f(p_i) = -\sum_i \sum_{j > i} J_{ij} x_i x_j - \sum_i b_i x_i
\]

The system evolves to minimize the energy.

- Dipoles stop flipping if flips result in an increase of energy.
Recap: Spin Glasses

- The system stops at one of its stable configurations
  - Where energy is a local minimum
Revisiting Thermodynamic Phenomena

- Is the system actually in a specific state at any time?
- No – the state is actually continuously changing
  - Based on the temperature of the system
    - At higher temperatures, state changes more rapidly
- What is actually being characterized is the *probability* of the state at equilibrium
  - The system “prefers” low energy states
  - Evolution of the system favors transitions towards lower-energy states
The Helmholtz Free Energy of a System

• A thermodynamic system at temperature $T$ can exist in one of many states
  – Potentially infinite states
  – At any time, the probability of finding the system in state $s$ at temperature $T$ is $P_T(s)$
• At each state $s$ it has a potential energy $E_s$
• The *internal energy* of the system, representing its capacity to do work, is the *expected value* of the PE:

$$U_T = \sum_s P_T(s) E_s$$
The Helmholtz Free Energy of a System

- The capacity to do work is counteracted by the internal disorder of the system, i.e. its entropy

\[ H_T = - \sum_s P_T(s) \log P_T(s) \]

- The *Helmholtz* free energy of the system measures the *useful* work derivable from it and combines the two terms

\[ F_T = U_T - kT H_T \]

\[ = \sum_s P_T(s) E_s + kT \sum_s P_T(s) \log P_T(s) \]
The Helmholtz Free Energy of a System

\[ F_T = \sum_s P_T(s) E_s + kT \sum_s P_T(s) \log P_T(s) \]

- A system held at a specific temperature \textit{anneals} by varying the rate at which it visits the various states, to reduce the free energy in the system, until a minimum free-energy state is achieved.

- The probability distribution of the states at steady state is known as the \textit{Boltzmann distribution}.
The Helmholtz Free Energy of a System

\[ F_T = \sum_s P_T(s) E_s + kT \sum_s P_T(s) \log P_T(s) \]

- Minimizing this w.r.t \( P_T(s) \), we get

\[ P_T(s) = \frac{1}{Z} \exp \left( \frac{-E_s}{kT} \right) \]

- Also known as the Gibbs distribution
- \( Z \) is a normalizing constant
- Note the dependence on \( T \)
- A \( T = 0 \), the system will always remain at the lowest-energy configuration with prob = 1.
Revisiting Thermodynamic Phenomena

• The evolution of the system is actually *stochastic*

• At equilibrium the system visits various states according to the Boltzmann distribution
  – The probability of any state is inversely related to its energy
    • and also temperatures: $P(s) \propto \exp\left(\frac{-E_s}{kT}\right)$

• The most likely state is the lowest energy state
Returning to the problem with Hopfield Nets

- Many local minima
  - Parasitic memories

- May be escaped by adding some noise during evolution
  - Permit changes in state even if energy increases..
    - Particularly if the increase in energy is small
The Hopfield net as a distribution

- Mimics the Spin glass system
- The stochastic Hopfield network models a **probability distribution** over states
  - Where a state is a binary string
  - Specifically, it models a Boltzmann distribution
  - The parameters of the model are the weights of the network

\[
E(S) = - \sum_{i < j} w_{ij}s_is_j - b_is_i
\]

\[
P(S) = \frac{\exp(-E(S))}{\sum_{S'} \exp(-E(S'))}
\]

- The probability that (at equilibrium) the network will be in any state is \( P(S) \)
  - It is a *generative* model: generates states according to \( P(S) \)
The field at a single node

- Let $S$ and $S'$ be otherwise identical states that only differ in the $i$-th bit
  - $S$ has $i$-th bit $= +1$ and $S'$ has $i$-th bit $= -1$

\[
\begin{align*}
P(S) &= P(s_i = 1 | s_{j \neq i}) P(s_{j \neq i}) \\
P(S') &= P(s_i = -1 | s_{j \neq i}) P(s_{j \neq i})
\end{align*}
\]

\[
\log P(S) - \log P(S') = \log P(s_i = 1 | s_{j \neq i}) - \log P(s_i = -1 | s_{j \neq i})
\]

\[
\log P(S) - \log P(S') = \log \frac{P(s_i = 1 | s_{j \neq i})}{1 - P(s_i = 1 | s_{j \neq i})}
\]
The field at a single node

- Let $S$ and $S'$ be the states with the $i$th bit in the $+1$ and $-1$ states

\[
\log P(S) = -E(S) + C
\]

\[
E(S) = -\frac{1}{2} \left( E_{\text{not } i} + \sum_{j \neq i} w_{ij} s_j + b_i \right)
\]

\[
E(S') = -\frac{1}{2} \left( E_{\text{not } i} - \sum_{j \neq i} w_{ij} s_j - b_i \right)
\]

- $\log P(S) - \log P(S') = E(S') - E(S) = \sum_{j \neq i} w_{ij} s_j + b_i$
The field at a single node

\[
\log \left( \frac{P(s_i = 1 | s_{j \neq i})}{1 - P(s_i = 1 | s_{j \neq i})} \right) = \sum_{j \neq i} w_{ij} s_j + b_i
\]

• Giving us

\[
P(s_i = 1 | s_{j \neq i}) = \frac{1}{1 + e^{-(\sum_{j \neq i} w_{ij} s_j + b_i)}}
\]

• The probability of any node taking value 1 given other node values is a logistic
Redefining the network

- First try: Redefine a regular Hopfield net as a stochastic system.
- Each neuron is now a stochastic unit with a binary state $s_i$, which can take value 0 or 1 with a probability that depends on the local field.
  - Note the slight change from Hopfield nets.
  - Not actually necessary; only a matter of convenience.

$$z_i = \sum_j w_{ij} s_j + b_i$$

$$P(s_i = 1|s_j \neq i) = \frac{1}{1 + e^{-z_i}}$$
The Hopfield net is a probability distribution over binary sequences
  – The Boltzmann distribution

The conditional distribution of individual bits in the sequence is a logistic

\[ z_i = \sum_j w_{ij} s_j + b_i \]

\[ P(s_i = 1|s_{j\neq i}) = \frac{1}{1 + e^{-z_i}} \]
**Running the network**

- Initialize the neurons
- Cycle through the neurons and randomly set the neuron to 1 or 0 according to the probability given above
  - Gibbs sampling: Fix N-1 variables and sample the remaining variable
  - As opposed to energy-based update (mean field approximation): run the test $z_i > 0$?
- After many many iterations (until “convergence”), *sample* the individual neurons

$$z_i = \sum_j w_{ij} s_j + b_i$$

$$P(s_i = 1 | s_{\neq i}) = \frac{1}{1 + e^{-z_i}}$$
1. Initialize network with initial pattern
   \[ y_i(0) = x_i, \quad 0 \leq i \leq N - 1 \]

2. Iterate \( 0 \leq i \leq N - 1 \)
   \[
   P = \sigma \left( \sum_{j \neq i} w_{ji} y_j \right)
   \]
   \[ y_i(t + 1) \sim Binomial(P) \]

Assuming \( T = 1 \)
Evolution of a stochastic Hopfield net

1. Initialize network with initial pattern

\[ y_i(0) = x_i, \quad 0 \leq i \leq N - 1 \]

2. Iterate \( 0 \leq i \leq N - 1 \)

\[ P = \sigma \left( \sum_{j \neq i} w_{ji} y_j \right) \]

\[ y_i(t + 1) \sim Binomial(P) \]

• When do we stop?
• What is the final state of the system
  – How do we “recall” a memory?
Evolution of a stochastic Hopfield net

1. Initialize network with initial pattern
   \[ y_i(0) = x_i, \quad 0 \leq i \leq N - 1 \]

2. Iterate \( 0 \leq i \leq N - 1 \)
   \[
   P = \sigma \left( \sum_{j \neq i} w_{ji} y_j \right)
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Assuming \( T = 1 \)
Evolution of a stochastic Hopfield net

1. Initialize network with initial pattern

\[ y_i(0) = x_i, \quad 0 \leq i \leq N - 1 \]

2. Iterate \( 0 \leq i \leq N - 1 \)

\[ P = \sigma \left( \sum_{j \neq i} w_{ji} y_j \right) \]

\[ y_i(t + 1) \sim \text{Binomial}(P) \]

• Let the system evolve to “equilibrium”
• Let \( y_0, y_1, y_2, \ldots, y_L \) be the sequence of values \((L \text{ large})\)
• Final predicted configuration: from the average of the final few iterations

\[ y = \left( \frac{1}{M} \sum_{t=L-M+1}^{L} y_t \right) > 0? \]

– Estimates the probability that the bit is 1.0.
– If it is greater than 0.5, sets it to 1.0
Evolution of the stochastic network

1. Initialize network with initial pattern

\[ y_i(0) = x_i, \quad 0 \leq i \leq N - 1 \]

2. For \( T = T_0 \) down to \( T_{\text{min}} \)

Noisy pattern completion: Initialize the entire network and let the entire network evolve

Pattern completion: Fix the “seen” bits and only let the “unseen” bits evolve

- Let the system evolve to “equilibrium”
- Let \( y_0, y_1, y_2, \ldots, y_L \) be the sequence of values (\( L \) large)
- Final predicted configuration: from the average of the final few iterations

\[
y = \left( \frac{1}{M} \sum_{t=L-M+1}^{L} y_t \right) > 0?
\]
Including a “Temperature” term

\[ z_i = \frac{1}{T} \sum_{j \neq i} w_{ij} y_j \]

\[ P(y_i = 1) = \sigma(z_i) \]

\[ P(y_i = 0) = 1 - \sigma(z_i) \]

• Including a temperature term in computing the local field
  – This is much more in accord with Thermodynamic models

• At \( T = \infty \) the energy “surface” will be flat. At \( T = 1 \) the surface will be the usual energy surface
  – This can be used to improve the likelihood of finding good (or optimal) minimum-energy states
Recap: Stochastic Hopfield Nets

- Including a temperature term in computing the local field
  - This is much more in accord with Thermodynamic models

- At $T = \infty$ the energy “surface” will be flat. At $T = 1$ the surface will be the usual energy surface
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\[ z_i = \frac{1}{T} \sum_{j \neq i} w_{ji} y_j \]

\[ P(y_i = 1) = \sigma(z_i) \]
Recap: Stochastic Hopfield Nets

• Including a temperature term in computing the local field:

\[ z_i = \frac{1}{T} \sum_{j \neq i} w_{ji} y_j \]

\[ P(y_i = 1) = \sigma(z_i) \]

The field quantifies the energy difference obtained by flipping the current unit.

If the difference is not large, the probability of flipping approaches 0.5.

• At \( T = \infty \) the energy “surface” will be flat. At \( T = 1 \) the surface will be the usual energy surface.

  – This can be used to improve the likelihood of finding good (or optimal) minimum-energy states.

At \( T = \infty \) the energy “surface” will be flat. At \( T = 1 \) the surface will be the usual energy surface.

  – This can be used to improve the likelihood of finding good (or optimal) minimum-energy states.
Recap: Stochastic Hopfield Nets

• Including a temperature term in computing the local field
  – This is much more in accord with thermodynamic models

If the difference is not large, the probability of flipping approaches 0.5

T is a “temperature” parameter: increasing it moves the probability of the bits towards 0.5
At T=1.0 we get the traditional definition of field and energy
At T = 0, we get deterministic Hopfield behavior

– This can be used to improve the likelihood of finding good (or optimal) minimum-energy states

\[ z_i = \frac{1}{T} \sum_{j \neq i} w_{ji} y_j \]

\[ P(y_i = 1) = \sigma(z_i) \]
Annealing

1. Initialize network with initial pattern
   \( y_i(0) = x_i, \quad 0 \leq i \leq N - 1 \)

2. For \( T = T_0 \) down to \( T_{\text{min}} \)
   i. For iter 1..\( L \)
      a) For \( 0 \leq i \leq N - 1 \)
         \[
         P = \sigma \left( \frac{1}{T} \sum_{j \neq i} w_{ji} y_j \right) \\
         y_i(t + 1) \sim \text{Binomial}(P)
         \]

- Let the system evolve to “equilibrium”
- Let \( y_0, y_1, y_2, \ldots, y_L \) be the sequence of values (\( L \) large)
- Final predicted configuration: from the average of the final few iterations
  
  \[
  y = \left( \frac{1}{M} \sum_{t=L-M+1}^{L} y_t \right) > 0?
  \]
Evolution of a stochastic Hopfield net

1. Initialize network with initial pattern
   \[ y_i(0) = x_i, \quad 0 \leq i \leq N - 1 \]

2. For \( T = T_0 \) down to \( T_{\text{min}} \)
   i. For iter 1..\( L \)
      a) For \( 0 \leq i \leq N - 1 \)
         \[
         P = \sigma \left( \frac{1}{T} \sum_{j \neq i} w_{ji} y_j \right)
         \]
         \[ y_i(t + 1) \sim \text{Binomial}(P) \]

• When do we stop?

• What is the final state of the system
  – How do we “recall” a memory?
Recap: Stochastic Hopfield Nets

- The probability of each neuron is given by a conditional distribution
- What is the overall probability of the entire set of neurons taking any configuration $y$?

$$z_i = \frac{1}{T} \sum_{j \neq i} w_{ji}y_j$$

$$P(y_i = 1|y_{j \neq i}) = \sigma(z_i)$$
The overall probability

\[ z_i = \frac{1}{T} \sum_{j \neq i} w_{ji} y_j \]

\[ P(y_i = 1|y_{j \neq i}) = \sigma(z_i) \]

- The probability of any state \( y \) can be shown to be given by the *Boltzmann distribution*

\[ E(y) = -\frac{1}{2} y^T W y \quad P(y) = C \exp \left( -\frac{E(y)}{T} \right) \]

- Minimizing energy maximizes log likelihood
The overall probability

\[ E(y) = -\frac{1}{2} y^T W y \quad P(y) = C \exp \left( \frac{-E(y)}{T} \right) \]

- Stop when the running average of the log probability of patterns stops increasing
  - I.e. when the (running average) of the energy of the patterns stops decreasing
The Hopfield net is a distribution

\[ z_i = \frac{1}{T} \sum_j w_{ji} s_j \]

\[ P(s_i = 1 | s_{j\neq i}) = \frac{1}{1 + e^{-z_i}} \]

- The Hopfield net is a probability distribution over binary sequences
  - The Boltzmann distribution
    \[ E(y) = -\frac{1}{2} y^T W y \]
    \[ P(y) = C \exp \left( -\frac{E(y)}{T} \right) \]
    - The parameter of the distribution is the weights matrix \( W \)
- The conditional distribution of individual bits in the sequence is a logistic
- We will call this a Boltzmann machine
The Boltzmann Machine

- The entire model can be viewed as a generative model
- Has a probability of producing any binary vector $y$:

$$E(y) = -\frac{1}{2}y^T Wy$$

$$P(y) = C \exp \left( -\frac{E(y)}{T} \right)$$

$$z_i = \frac{1}{T} \sum_j w_{ji} s_j$$

$$P(s_i = 1 | s_j \neq i) = \frac{1}{1 + e^{-z_i}}$$
Training the network

- **Training a Hopfield net**: Must learn weights to “remember” target states and “dislike” other states
  - “State” == binary pattern of all the neurons

- **Training Boltzmann machine**: Must learn weights to assign a desired probability distribution to states
  - (vectors $y$, which we will now call $S$ because I’m too lazy to normalize the notation)
  - This should assign more probability to patterns we “like” (or try to memorize) and less to other patterns
Training the network

- Must train the network to assign a desired probability distribution to states
- Given a set of “training” inputs $S_1, \ldots, S_N$
  - Assign higher probability to patterns seen more frequently
  - Assign lower probability to patterns that are not seen at all
- Alternately viewed: maximize likelihood of stored states

$$E(S) = -\sum_{i<j} w_{ij}s_is_j$$

$$P(S) = \frac{\exp(-E(S))}{\sum_{S'} \exp(-E(S'))}$$

$$P(S) = \frac{\exp(\sum_{i<j} w_{ij}s_is_j)}{\sum_{S'} \exp(\sum_{i<j} w_{ij}'s'_is'_j)}$$
Maximum Likelihood Training

\[ \log(P(S)) = \left( \sum_{i<j} w_{ij} s_i s_j \right) - \log \left( \sum_{S'} \exp \left( \sum_{i<j} w_{ij} s'_i s'_j \right) \right) \]

\[ \mathcal{L} = \frac{1}{N} \sum_{S \in \mathcal{S}} \log(P(S)) \] Average log likelihood of training vectors (to be maximized)

\[ = \frac{1}{N} \sum_S \left( \sum_{i<j} w_{ij} s_i s_j \right) - \log \left( \sum_{S'} \exp \left( \sum_{i<j} w_{ij} s'_i s'_j \right) \right) \]

- Maximize the average log likelihood of all “training” vectors \( \mathbf{S} = \{S_1, S_2, \ldots, SN\} \)
  - In the first summation, \( s_i \) and \( s_j \) are bits of \( S \)
  - In the second, \( s'_i \) and \( s'_j \) are bits of \( S' \)
Maximum Likelihood Training

\[ \mathcal{L} = \frac{1}{N} \sum_{s} \left( \sum_{i<j} w_{ij} s_i s_j \right) - \log \left( \sum_{s'} \exp \left( \sum_{i<j} w_{ij} s'_i s'_j \right) \right) \]

\[ \frac{d\mathcal{L}}{dw_{ij}} = \frac{1}{N} \sum_{s} s_i s_j \]

- We will use gradient ascent, but we run into a problem..
- The first term is just the average \( s_i s_j \) over all training patterns
- But the second term is summed over all states
  - Of which there can be an exponential number!
The second term

\[
\frac{d \log \left( \sum_{S_r} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right) \right)}{d w_{ij}} = \frac{1}{\sum_{S''} \exp \left( \sum_{i<j} w_{ij} s_i'' s_j'' \right)} \sum_{S_r} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right) s_i' s_j'
\]

\[
= \frac{1}{\sum_{S''} \exp \left( \sum_{i<j} w_{ij} s_i'' s_j'' \right)} \sum_{S_r} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right) s_i' s_j'
\]

\[
\frac{d \log \left( \sum_{S_r} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right) \right)}{d w_{ij}} = \sum_{S_r} \frac{\exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right)}{\sum_{S''} \exp \left( \sum_{i<j} w_{ij} s_i'' s_j'' \right)} s_i' s_j'
\]
The second term

\[
\frac{d \log \left( \sum_{s'} \exp \left( \sum_{i<j} w_{ij} s'_i s'_j \right) \right)}{dw_{ij}} = \frac{1}{\sum_{s''} \exp \left( \sum_{i<j} w_{ij} s''_i s''_j \right)} \sum_{s'} \exp \left( \sum_{i<j} w_{ij} s'_i s'_j \right) s'_i s'_j
\]

\[
\frac{d \log \left( \sum_{s'} \exp \left( \sum_{i<j} w_{ij} s'_i s'_j \right) \right)}{dw_{ij}} = \sum_{s'} \left( \frac{\exp \left( \sum_{i<j} w_{ij} s'_i s'_j \right)}{\sum_{s''} \exp \left( \sum_{i<j} w_{ij} s''_i s''_j \right)} \right) s'_i s'_j
\]

\[P(S')\]
The second term

\[
\frac{d\log \left( \sum_{s_r} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right) \right)}{dw_{ij}} = \frac{1}{\sum_{s''} \exp \left( \sum_{i<j} w_{ij} s_i'' s_j'' \right)} \frac{d \sum_{s_r} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right)}{dw_{ij}}
\]

\[
= \frac{1}{\sum_{s''} \exp \left( \sum_{i<j} w_{ij} s_i'' s_j'' \right)} \sum_{s_r} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right) s_i' s_j'
\]

\[
\frac{d\log \left( \sum_{s_r} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right) \right)}{dw_{ij}} = \sum_{s_r} \frac{\exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right)}{\sum_{s''} \exp \left( \sum_{i<j} w_{ij} s_i'' s_j'' \right)} s_i' s_j'
\]

\[
\frac{d\log \left( \sum_{s_r} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right) \right)}{dw_{ij}} = \sum_{s_r} P(S') s_i' s_j'
\]
**The second term**

\[
\frac{d \log \left( \sum_{S'} \exp \left( \sum_{i<j} w_{ij} s'_i s'_j \right) \right)}{dw_{ij}} = \sum_{S'} P(S') s'_i s'_j
\]

- The second term is simply the *expected value* of \(s_is_j\), over all possible values of the state.
- We cannot compute it exhaustively, but we can compute it by sampling!
Estimating the second term

\[
\frac{d \log \left( \sum_{S'} \exp\left( \sum_{i<j} w_{ij} s'_i s'_j \right) \right)}{dw_{ij}} = \sum_{S'} P(S') s'_i s'_j
\]

\[
\sum_{S'} P(S') s'_i s'_j \approx \frac{1}{M} \sum_{S' \in S_{samples}} s'_i s'_j
\]

• The expectation can be estimated as the average of samples drawn from the distribution

• Question: How do we draw samples from the Boltzmann distribution?
  – How do we draw samples from the network?
The simulation solution

- Initialize the network randomly and let it “evolve”
  - By probabilistically selecting state values according to our model
- After many many epochs, take a snapshot of the state
- Repeat this many many times
- Let the collection of states be

$$S_{simul} = \{S_{simul,1}, S_{simul,1=2}, \ldots, S_{simul,M}\}$$
The simulation solution for the second term

\[
\frac{d \log \left( \sum_{S_i} \exp \left( \sum_{i<j} w_{ij} s'_i s'_j \right) \right)}{dw_{ij}} = \sum_{S_i} P(S') s'_i s'_j
\]

\[
\sum_{S_i} P(S') s'_i s'_j \approx \frac{1}{M} \sum_{S_i \in S_{simul}} s'_i s'_j
\]

- The second term in the derivative is computed as the average of sampled states when the network is running “freely”
Maximum Likelihood Training

\[
\frac{d\langle \log(P(S)) \rangle}{dw_{ij}} = \frac{1}{N} \sum_s s_i s_j - \frac{1}{M} \sum_{s_t \in S_{simul}} s'_i s'_j
\]

\[
w_{ij} = w_{ij} + \eta \frac{d\langle \log(P(S)) \rangle}{dw_{ij}}
\]

- The overall gradient ascent rule
Overall Training

- Initialize weights
- Let the network run to obtain simulated state samples
- Compute gradient and update weights
- Iterate

\[
\frac{d\langle \log(P(S)) \rangle}{dw_{ij}} = \frac{1}{N} \sum_s s_i s_j - \frac{1}{M} \sum_{s' \in S_{simul}} s'_i s'_j
\]

\[
w_{ij} = w_{ij} + \eta \frac{d\langle \log(P(S)) \rangle}{dw_{ij}}
\]
Overall Training

\[
\frac{d\langle \log(P(S)) \rangle}{dw_{ij}} = \frac{1}{N} \sum_{s} s_i s_j - \frac{1}{M} \sum_{s' \in S_{\text{simul}}} s'_i s'_j
\]

\[
w_{ij} = w_{ij} + \eta \frac{d\langle \log(P(S)) \rangle}{dw_{ij}}
\]

Note the similarity to the update rule for the Hopfield network.
Adding Capacity to the Hopfield Network / Boltzmann Machine

• The network can store up to $N$ $N$-bit patterns
• How do we increase the capacity
Expanding the network

- Add a large number of neurons whose actual values you don’t care about!
• New capacity: $\sim (N + K)$ patterns
  – Although we only care about the pattern of the first $N$ neurons
  – We’re interested in $N$-bit patterns
Terminology:

- The neurons that store the actual patterns of interest: *Visible neurons*
- The neurons that only serve to increase the capacity but whose actual values are not important: *Hidden neurons*
- These can be set to anything in order to store a visible pattern
Training the network

• For a given pattern of *visible* neurons, there are any number of *hidden* patterns \(2^K\)

• Which of these do we choose?
  – Ideally choose the one that results in the lowest energy
  – But that’s an exponential search space!
The patterns

• In fact we could have *multiple* hidden patterns coupled with any visible pattern
  – These would be multiple stored patterns that all give the same visible output
  – How many do we permit

• Do we need to specify one or more particular hidden patterns?
  – How about *all* of them
  – What do I mean by this bizarre statement?
Boltzmann machine without hidden units

- This basic framework has no hidden units
- Extended to have hidden units

\[
\frac{d\langle \log(P(S)) \rangle}{dw_{ij}} = \frac{1}{N} \sum_s s_is_j - \frac{1}{M} \sum_{s' \in S_{simul}} s'_is'_j
\]

\[
w_{ij} = w_{ij} + \eta \frac{d\langle \log(P(S)) \rangle}{dw_{ij}}
\]
With hidden neurons

- Now, with hidden neurons the complete state pattern for even the *training* patterns is unknown
  - Since they are only defined over visible neurons
We are interested in the marginal probabilities over visible bits
- We want to learn to represent the visible bits
- The hidden bits are the “latent” representation learned by the network

\[ P(S) = \frac{\exp(-E(S))}{\sum_{S'} \exp(-E(S'))} \]

\[ P(S) = P(V, H) \]

\[ P(V) = \sum_H P(S) \]

\[ S = (V, H) \]
- \( V \) = visible bits
- \( H \) = hidden bits
With hidden neurons

We are interested in the marginal probabilities over visible bits
  - We want to learn to represent the visible bits
  - The hidden bits are the “latent” representation learned by the network

\[ P(S) = \frac{\exp(-E(S))}{\sum_{S', \exp(-E(S'))} P(S')} \]

\[ P(S) = P(V, H) \]

\[ P(V) = \sum_{H} P(S) \]

- \( S = (V, H) \)
  - \( V \) = visible bits
  - \( H \) = hidden bits

Must train to maximize probability of desired patterns of visible bits
Training the network

- Must train the network to assign a desired probability distribution to visible states.
- Probability of visible state sums over all hidden states.

\[ E(S) = - \sum_{i<j} w_{ij} s_i s_j \]

\[ P(S) = \frac{\exp \left( \sum_{i<j} w_{ij} s_i s_j \right)}{\sum_{S'} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right)} \]

\[ P(V) = \sum_H \frac{\exp \left( \sum_{i<j} w_{ij} s_i s_j \right)}{\sum_{S'} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right)} \]
Maximum Likelihood Training

\[
\log(P(V)) = \log \left( \sum_H \exp \left( \sum_{i<j} w_{ij}s_is_j \right) \right) - \log \left( \sum_{S'} \exp \left( \sum_{i<j} w_{ij}s'_is'_j \right) \right)
\]

\[
\mathcal{L} = \frac{1}{N} \sum_{V \in \mathcal{V}} \log(P(V))
\]

Average log likelihood of training vectors (to be maximized)

\[
= \frac{1}{N} \sum_{V \in \mathcal{V}} \log \left( \sum_H \exp \left( \sum_{i<j} w_{ij}s_is_j \right) \right) - \log \left( \sum_{S'} \exp \left( \sum_{i<j} w_{ij}s'_is'_j \right) \right)
\]

- Maximize the average log likelihood of all visible bits of “training” vectors \( \mathcal{V} = \{V_1, V_2, ..., V_N\} \)
  - The first term also has the same format as the second term
    - Log of a sum
      - Derivatives of the first term will have the same form as for the second term
Maximum Likelihood Training

\[ L = \frac{1}{N} \sum_{V \in V} \log \left( \sum_{H} \exp \left( \sum_{i<j} w_{ij} s_i s_j \right) \right) - \log \left( \sum_{s_l} \exp \left( \sum_{i<j} w_{ij} s_i' s_j' \right) \right) \]

\[
\frac{dL}{dw_{ij}} = \frac{1}{N} \sum_{V \in V} \sum_{H} \frac{\exp \left( \sum_{k<l} w_{kl} s_k s_l \right)}{\sum_H, \exp \left( \sum_{k<l} w_{kl} s_k' s_l' \right)} s_i s_j - \sum_{s_l, s''} \frac{\exp \left( \sum_{k<l} w_{kl} s_k s_l \right)}{\sum_{s''} \exp \left( \sum_{k<l} w_{ij} s_k s_l \right)} s_i s_j' \]

\[
\frac{dL}{dw_{ij}} = \frac{1}{N} \sum_{V \in V} \sum_{H} P(S|V) s_i s_j - \sum_{s_l} P(S') s_i s_j' \]

- We’ve derived this math earlier
- But now both terms require summing over an exponential number of states
  - The first term fixes visible bits, and sums over all configurations of hidden states for each visible configuration in our training set
  - But the second term is summed over all states
The simulation solution

\[
\frac{d\mathcal{L}}{dw_{ij}} = \frac{1}{N} \sum_{V \in V} \sum_{H} P(S|V)s_is_j - \sum_{s'} P(S')s'_is'_j
\]

\[
\sum_{H} P(S|V)s_is_j \approx \frac{1}{K} \sum_{H \in H_{simul}} s_is_j
\]

\[
\sum_{s'} P(S')s'_is'_j \approx \frac{1}{M} \sum_{s' \in S_{simul}} s'_is'_j
\]

- The first term is computed as the average sampled hidden state with the visible bits fixed.
- The second term in the derivative is computed as the average of sampled states when the network is running “freely”
More simulations

• Maximizing the marginal probability of $V$ requires summing over all values of $H$
  – An exponential state space
  – So we will use simulations again

\[ P(S) = \frac{\exp(-E(S))}{\sum_{S', \exp(-E(S'))}} \]

\[ P(V) = \sum_{H} P(S) \]
Step 1

- For each training pattern $V_i$
  - Fix the visible units to $V_i$
  - Let the hidden neurons evolve from a random initial point to generate $H_i$
  - Generate $S_i = [V_i, H_i]$
- Repeat K times to generate synthetic training
  $$S = \{S_{1,1}, S_{1,2}, \ldots, S_{1K}, S_{2,1}, \ldots, S_{N,K}\}$$
Step 2

- Now *unclamp* the visible units and let the entire network evolve several times to generate

$$S_{simul} = \{S_{simul,1}, S_{simul,1=2}, \ldots, S_{simul,M}\}$$
Gradients

\[
\frac{d \langle \log(P(S)) \rangle}{dw_{ij}} = \frac{1}{NK} \sum_S s_i s_j - \frac{1}{M} \sum_{S' \in S_{\text{simul}}} s'_i s'_j
\]

- Gradients are computed as before, except that the first term is now computed over the expanded training data.
Overall Training

- Initialize weights
- Run simulations to get clamped and unclamped training samples
- Compute gradient and update weights
- Iterate

\[
\frac{d\langle \log(P(S)) \rangle}{dw_{ij}} = \frac{1}{NK} \sum_{s} s_i s_j - \frac{1}{M} \sum_{s' \in S_{simul}} s'_i s'_j
\]

\[
w_{ij} = w_{ij} - \eta \frac{d\langle \log(P(S)) \rangle}{dw_{ij}}
\]
Boltzmann machines

- Stochastic extension of Hopfield nets
- Enables storage of many more patterns than Hopfield nets
- But also enables computation of probabilities of patterns, and completion of pattern
Boltzmann machines: Overall

\[ z_i = \sum_j w_{ji} s_i + b_i \]

\[ P(s_i = 1) = \frac{1}{1 + e^{-z_i}} \]

- **Training:** Given a set of training patterns
  - Which could be repeated to represent relative probabilities
- Initialize weights
- Run simulations to get clamped and unclamped training samples
- Compute gradient and update weights
- Iterate

\[
\frac{d\langle \log(P(S)) \rangle}{dw_{ij}} = \frac{1}{NK} \sum_S s_is_j - \frac{1}{M} \sum_{s' \in S_{simul}} s'_is'_j
\]

\[
w_{ij} = w_{ij} - \eta \frac{d\langle \log(P(S)) \rangle}{dw_{ij}}
\]
Boltzmann machines: Overall

• Running: Pattern completion
  – “Anchor” the known visible units
  – Let the network evolve
  – Sample the unknown visible units
    • Choose the most probable value
Applications

- Filling out patterns
- Denoising patterns
- *Computing conditional probabilities of patterns*
- **Classification!!**  
  – How?
Boltzmann machines for classification

• Training patterns:
  – \([f_1, f_2, f_3, \ldots, \text{class}]\)
  – Features can have binarized or continuous valued representations
  – Classes have “one hot” representation

• Classification:
  – Given features, anchor features, estimate a posteriori probability distribution over classes
    • Or choose most likely class
Boltzmann machines: Issues

- Training takes for ever
- Doesn’t really work for large problems
  - A small number of training instances over a small number of bits
Solution: *Restricted Boltzmann Machines*

- Partition visible and hidden units
  - Visible units ONLY talk to hidden units
  - Hidden units ONLY talk to visible units
- Restricted Boltzmann machine..
  - Originally proposed as “Harmonium Models” by Paul Smolensky
Solution: *Restricted Boltzmann Machines*

- Still obeys the same rules as a regular Boltzmann machine
- But the modified structure adds a big benefit.

\[ z_i = \sum_j w_{ji} s_i + b_i \]

\[ P(s_i = 1) = \frac{1}{1 + e^{-z_i}} \]
Solution: *Restricted* Boltzmann Machines

\[ z_i = \sum_j w_{ji} v_i + b_i \]

\[ P(h_i = 1) = \frac{1}{1 + e^{-z_i}} \]

\[ y_i = \sum_j w_{ji} h_i + b_i \]

\[ P(v_i = 1) = \frac{1}{1 + e^{-y_i}} \]
Recap: Training full Boltzmann machines: Step 1

- For each training pattern \( V_i \)
  - Fix the visible units to \( V_i \)
  - Let the hidden neurons evolve from a random initial point to generate \( H_i \)
  - Generate \( S_i = [V_i, H_i] \)
- Repeat K times to generate synthetic training
  \[ S = \{S_{1,1}, S_{1,2}, ..., S_{1,K}, S_{2,1}, ..., S_{N,K}\} \]
Sampling: Restricted Boltzmann machine

For each sample:
  – Anchor visible units
  – Sample from hidden units
  – No looping!!

\[ z_i = \sum_j w_{ji} v_i + b_i \]

\[ P(h_i = 1) = \frac{1}{1 + e^{-z_i}} \]
Now *unclamp* the visible units and let the entire network evolve several times to generate

\[ S_{\text{simul}} = \{ S_{\text{simul},1}, S_{\text{simul},1=2}, \ldots, S_{\text{simul},M} \} \]
Sampling: Restricted Boltzmann machine

• For each sample:
  – Iteratively sample hidden and visible units for a long time
  – Draw final sample of both hidden and visible units

\[
\begin{align*}
    z_i &= \sum_j w_{ji} v_i + b_i \\
    P(h_i = 1) &= \frac{1}{1 + e^{-z_i}}\\
    y_i &= \sum_j w_{ji} h_i + b_i \\
    P(v_i = 1) &= \frac{1}{1 + e^{-y_i}}
\end{align*}
\]
For each sample:
- Initialize $V_0$ (visible) to training instance value
- Iteratively generate hidden and visible units
  - For a very long time
Pictorial representation of RBM training

- Gradient (showing only one edge from visible node $i$ to hidden node $j$)

$$\frac{\partial \log p(v)}{\partial w_{ij}} = \langle v_i h_j \rangle^0 - \langle v_i h_j \rangle^{\infty}$$

- $\langle v_i, h_j \rangle$ represents average over many generated training samples
Recall: Hopfield Networks

• Really no need to raise the entire surface, or even every valley

• Raise the *neighborhood* of each target memory
  – Sufficient to make the memory a valley
  – The broader the neighborhood considered, the broader the valley
A Shortcut: Contrastive Divergence

- Sufficient to run one iteration!
  \[
  \frac{\partial \log p(v)}{\partial w_{ij}} = <v_i h_j>^0 - <v_i h_j>^1
  \]

- This is sufficient to give you a good estimate of the gradient
Restricted Boltzmann Machines

• Excellent generative models for binary (or binarized) data

• Can also be extended to continuous-valued data
  – “Exponential Family Harmoniums with an Application to Information Retrieval”, Welling et al., 2004

• Useful for classification and regression
  – How?
  – More commonly used to pretrain models
Continuous-values RBMs

Hidden units may also be continuous values

\[ z_i = \sum_j w_{ji} v_i + b_i \]

\[ P(h_i = 1) = \frac{1}{1 + e^{-z_i}} \]

\[ y_i = \sum_j w_{ji} h_i + b_i \]

\[ P(v_i) = r(y_i) \exp(y_i) \]
Other variants

- Left: “Deep” Boltzmann machines
- Right: Helmholtz machine
  - Trained by the “wake-sleep” algorithm
Topics missed..

- Other algorithms for Learning and Inference over RBMs
  - Mean field approximations
- RBMs as feature extractors
  - Pre training
- RBMs as generative models
- More structured DBMs
- ...