Associative Memories (II)
Stochastic Networks and Boltzmann Machines

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Deterministic Networks

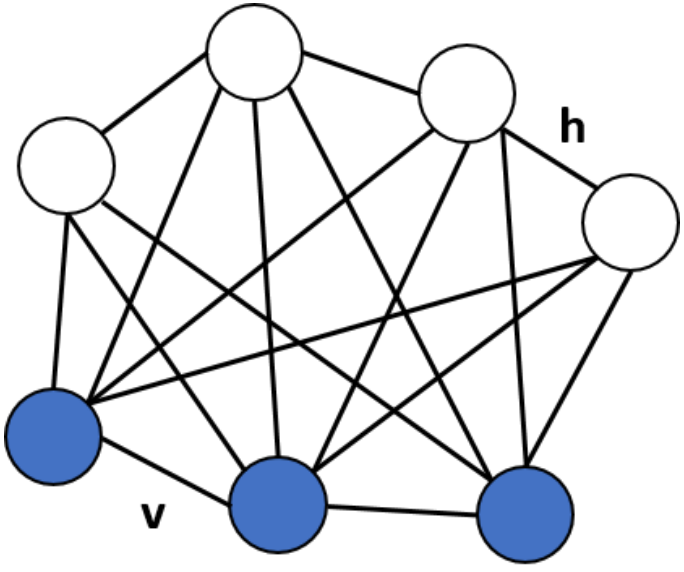
Consider the Hopfield network model introduced so far

- Neuron output is a deterministic function of its inputs
- Recurrent network of all visible units
- Learns to encode a set of fixed training patterns $\mathbf{V} = [\mathbf{v^1} \ldots \mathbf{v^P}]$

What models do we obtain if we relax the deterministic input-output mapping?

Stochastic Networks

- A network of units whose activation is determined by a stochastic function
  - The state of a unit at a given timestep is sampled from a given probability distribution
  - The network learns a probability distribution $P(\mathbf{V})$ from the training patterns



- Network includes both visible **v** and hidden **h** units
- Network activity is a sample from posterior probability given inputs (visible data)

Neural Sampling Hypothesis

The activity of each neuron can be sampled from the network distribution

- No distinction between input and output
- Natural way to deal with incomplete stimuli
- Stochastic nature of activation is coherent with neural response variability
- Spontaneous neural activity can be explained in terms of prior/marginal distributions

Probability and Statistics Refresher

On the blackboard

Stochastic Binary Neurons

- Spiking point neuron with binary output s_j
- Typically discrete time model with time into small Δt intervals
- At each time interval($t + 1 \equiv t + \Delta t$), the neuron can emit a spike with probability $p_j^{(t)}$

$$s_j^{(t)} = \begin{cases} 1, & \text{with probability } p_j^{(t)} \\ 0, & \text{with probability } 1 - p_j^{(t)} \end{cases}$$

The key is in the definition of the spiking probability (needs to be a function of local potential)

$$p_j^{(t)} \approx \sigma(x_j^{(t)})$$

General Sigmoidal Stochastic Binary Network

Network of N neurons with binary activation s_j

- Weight matrix $\mathbf{M} = [M_ij]_{i,j\in\{1,\dots,N\}}$
- Bias vector $\mathbf{b} = [b_j]_{j\in\{1,\dots,N\}}$

Local neuron potential x_j defined as usual

$$x_j^{(t+1)} = \sum_{i=1}^{N} M_{ij} s_i^{(t)} + b_j$$

A chosen neuron fires with spiking probability

$$p_j^{(t+1)} = P(s_j^{(t+1)} = 1 | \mathbf{s}^t) = \sigma(x_j^{(t+1)}) = \frac{1}{1 + e^{-x_j^{(t+1)}}}$$

Formulation highlights Markovian dynamics

Neurobiological Foundations

- Variability in transmitter release in synaptic vescicles $\approx$ Gaussian Distribution (Katz 1954)
- Assuming independent distributions and large number of synaptic connections
  - $\Rightarrow$ Central limit theorem
  - $\Rightarrow$ Local (membrane) potential $\approx$ Gaussian Distribution
- Conditional probability of neuron spiking is a Gaussian CDF $\approx$ scaled sigmoid

Network Dynamics (I)

How does the network state (activation of all neurons) evolve in time?

Assume neurons to be updated in parallel every Δt (Parallel dynamics)

$$P(\mathbf{s}^{(t+1)}|\mathbf{s}^{(t)}) = \prod_{j=1}^{N} P(s_j^{(t+1)}|\mathbf{s}^t) = T(\mathbf{s}^{(t+1)}|\mathbf{s}^{(t)})$$

Yielding a Markov process for state update

$$P(\mathbf{s}^{(t+1)} = \mathbf{s}') = \sum_{\mathbf{s}} T(\mathbf{s}'|\mathbf{s}) P(\mathbf{s}^{(t)} = \mathbf{s})$$

Network Dynamics (II)

- Parallel dynamics assumes a synchronization clock exist (biologically non plausible)
- Alternatively, one neuron at random can be chosen for update at each step (Glauber Dynamics)
- No fixed-point guarantees for $\mathbf{s}$ but it has a stationary distribution for the network at equilibrium state when its connectivity is symmetric

Given F_j as state flip operator for j-th neuron $\mathbf{s}^{(t+1)} = F_j \mathbf{s}^{(t)}$

$$T(\mathbf{s}^{(t+1)}|\mathbf{s}^{(t)}) = \frac{1}{N} P(s_j^{(t+1)}|\mathbf{s}^t)$$

While if $\mathbf{s}^{(t+1)} = \mathbf{s}^{(t)}$

$$T(\mathbf{s}^{(t+1)}|\mathbf{s}^{(t)}) = 1 - \frac{1}{N} \sum_j P(s_j^{(t+1)}|\mathbf{s}^t)$$

The Boltzmann-Gibbs Distribution

Symmetric connectivity enforces detailed balance condition

$$P(\mathbf{s})T(\mathbf{s}'|\mathbf{s}) = P(\mathbf{s}')T(\mathbf{s}|\mathbf{s}')$$

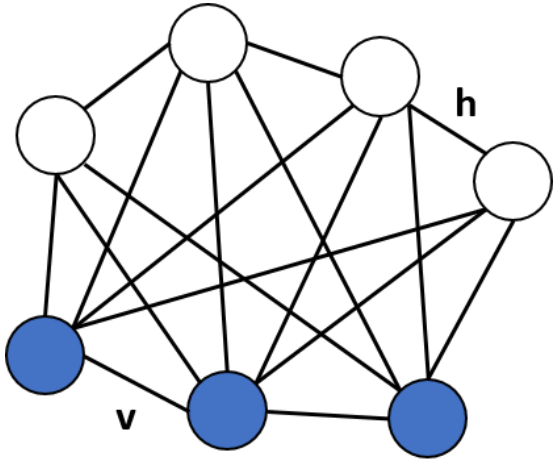
Ensures reversible transitions guaranteeing existence of equilibrium (Boltzmann-Gibbs) distribution

$$P_\infty(\mathbf{s}) = \frac{e^{-E(\mathbf{s})}}{Z}$$

where

- $E(\mathbf{s})$ is the energy function
- $Z = \sum_{\mathbf{s}} e^{-E(\mathbf{s})}$ is the partition function

Boltzmann Machines



A stochastic recurrent network where binary unit states are also random variables

- visible $\mathbf{v} \in \{0, 1\}$
- latent $\mathbf{h} \in \{0, 1\}$
- $\mathbf{s} = [\mathbf{vh}]$

Boltzmann-Gibbs distribution having linear energy function

$$E(\mathbf{s}) = -\frac{1}{2}\sum_{ij} M_{ij} s_i s_j - \sum_j b_j s_j = -\frac{1}{2}\mathbf{s}^T\mathbf{M}\mathbf{s} - \mathbf{b}^T\mathbf{s}$$

with symmetric and no self-recurrent connectivity

Learning

Ackley, Hinton and Sejnowski (1985)

Boltzmann machines can be trained so that the equilibrium distribution tends towards any arbitrary distribution across binary vectors given samples from that distribution

A couple of simplifications to start with

- Bias **b** absorbed into weight matrix **M**
- Consider only visible units $\mathbf{s} = \mathbf{v}$

Use probabilistic learning techniques to fit the parameters, i.e. maximizing the log-likelihood

$$\mathcal{L}(\mathbf{M}) = \frac{1}{L} \sum_{l=1}^{L} \log P(\mathbf{v}^l | \mathbf{M})$$

given the P visible training patterns $\mathbf{v}^l$

Gradient Approach

- First, the gradient for a single pattern

$$\frac{\partial P(\mathbf{v}|\mathbf{M})}{\partial M_{ij}} = -\langle v_i v_j \rangle + v_i v_j$$

with free expectations $\langle v_i v_j \rangle = \sum_{\mathbf{v}} P(\mathbf{v}) v_i v_j$

- Then, the log-likelihood gradient

$$\frac{\partial \mathcal{L}}{\partial M_{ij}} = -\langle v_i v_j \rangle + \langle v_i v_j \rangle_c$$

with clamped expectations $\langle v_i v_j \rangle_c = \frac{1}{L} \sum_{l=1}^{p} v_i^l v_j^l$

Something we have already seen..

It is Hebbian learning again!

$$\underbrace{\langle v_i v_j \rangle_c}_{\text{wake}} - \underbrace{\langle v_i v_j \rangle}_{\text{dream}}$$

- wake part is the usual Hebb rule applied to the empirical distribution of data that the machine *sees* coming in from the outside world
- dream part is an anti-hebbian term concerning correlation between units when generated by the internal dynamics of the machine

Can only capture quadratic correlation!

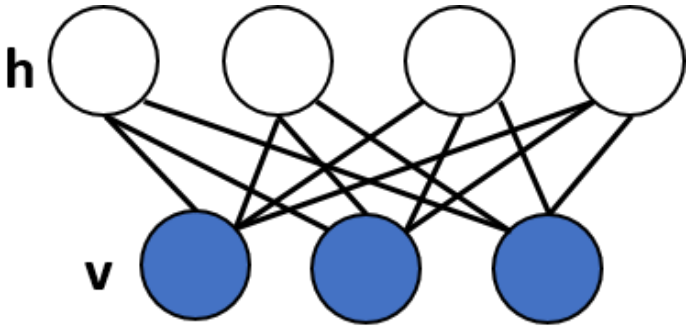
Learning with Hidden Units

- To efficiently capture higher-order correlations we need to introduce hidden units **h**
- Again log-likelihood gradient ascent (**s** = [**vh**])

$$\frac{\partial P(\mathbf{v}|\mathbf{M})}{\partial M_{ij}} = \sum_{\mathbf{h}} s_i s_j P(\mathbf{h}|\mathbf{v}) - \sum_{\mathbf{s}} s_i s_j P(\mathbf{s})$$
$$= \langle s_i s_j \rangle_c - \langle s_i s_j \rangle$$

- Expectations generally become intractable due to the partition function Z (exponential complexity)

Restricted Boltzmann Machines (RBM)



A special Boltzmann machine

- Bipartite graph
- Connections only between hidden and visible units

- Energy function, highlighting bipartition in hidden (**h**) and visible (**v**) units

$$E(\mathbf{v}, \mathbf{h}) = -\mathbf{v}^T \mathbf{M} \mathbf{h} - \mathbf{b}^T \mathbf{v} - \mathbf{c}^T \mathbf{h}$$

- Learning (and inference) becomes tractable due to graph bipartition which factorizes distribution

The RBM Catch

Hidden units are conditionally independent given visible units, and viceversa

$$P(h_j|\mathbf{v}) = \sigma(\sum_i M_{ij} v_i + c_j)$$

$$P(v_i|\mathbf{h}) = \sigma(\sum_j M_{ij} h_j + b_i)$$

They can be updated in batch!

Training Restricted Boltzmann Machines

Again by likelihood maximization, yields

$$\frac{\partial \mathcal{L}}{\partial M_{ij}} = \underbrace{\langle v_i h_j \rangle_c}_{\text{data}} - \underbrace{\langle v_i h_j \rangle}_{\text{model}}$$

A Gibbs sampling approach

Wake

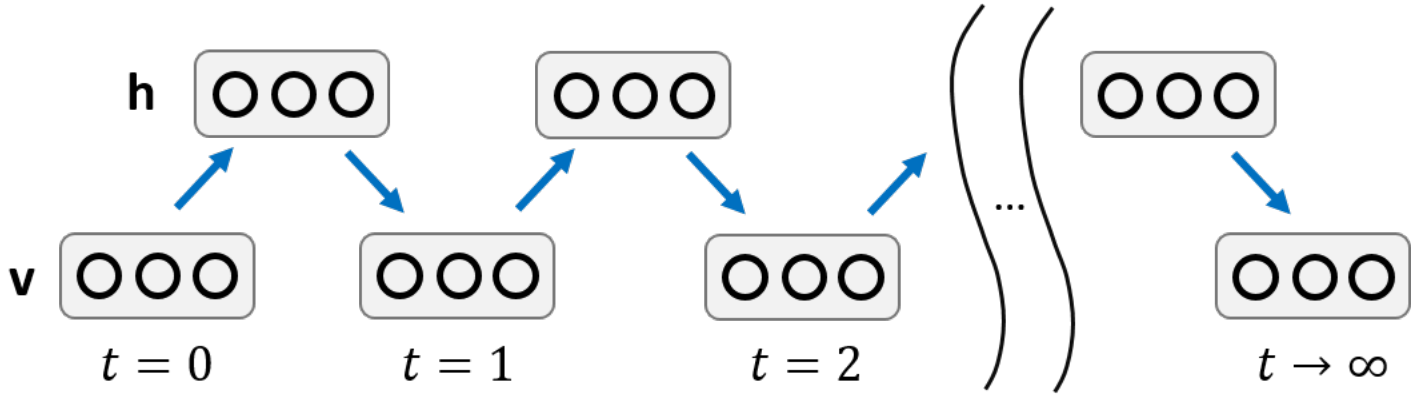
- Clamp data on **v**
- Sample $v_i h_j$ for all pairs of connected units
- Repeat for all elements of dataset

Dream

- Don't clamp units
- Let network reach equilibrium
- Sample $v_i h_j$ for all pairs of connected units
- Repeat many times to get a good estimate

Gibbs-Sampling RBM

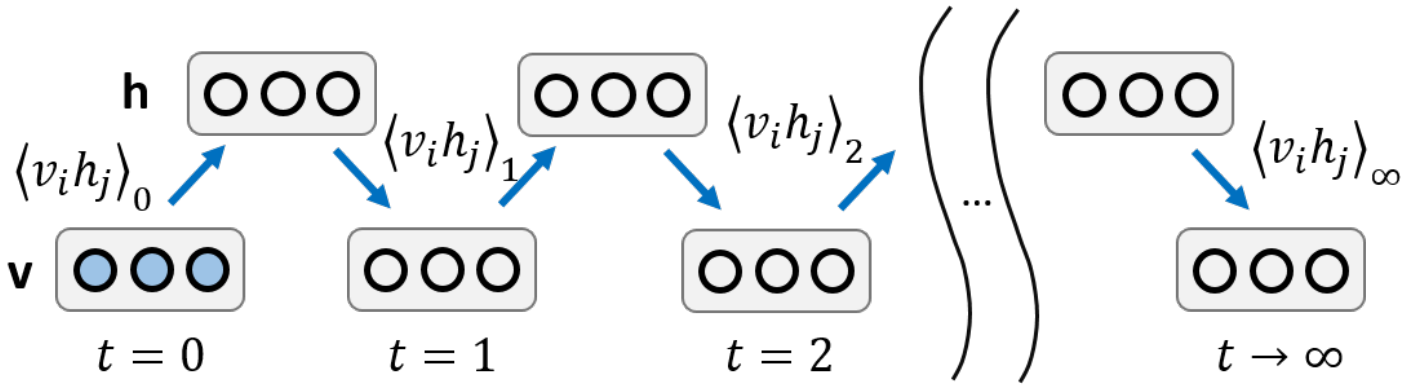
$$\frac{\partial \mathcal{L}}{\partial M_{ij}} = \underbrace{\langle v_i h_j \rangle_c}_{\text{data}} - \underbrace{\langle v_i h_j \rangle}_{\text{model}}$$



It is difficult to obtain an unbiased sample of the second term

Gibbs-Sampling RBM

Plugging-in Data

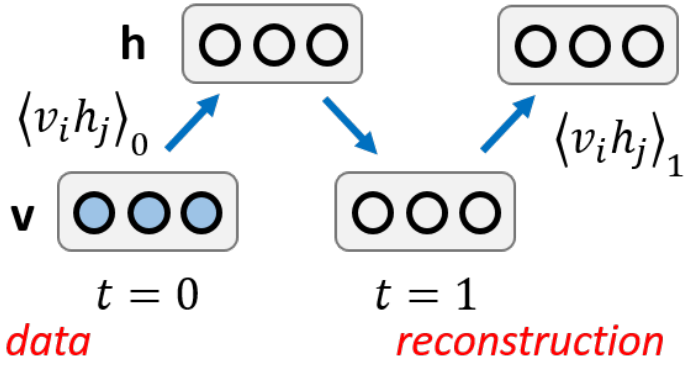


1. Start with a training vector on the visible units
2. Alternate between updating all the hidden units in parallel and updating all the visible units in parallel (iterate)

$$\frac{\partial \mathcal{L}}{\partial M_{ij}} = \underbrace{\langle v_i h_j \rangle_0}_{\text{data}} - \underbrace{\langle v_i h_j \rangle_\infty}_{\text{model}}$$

Contrastive-Divergence Learning

Gibbs sampling can be painfully slow to converge



1. Clamp a training vector $\mathbf{v}^l$ on visible units
2. Update all hidden units in parallel
3. Update the all visible units in parallel to get a *reconstruction*
4. Update the hidden units again

$$\underbrace{\langle v_i h_j \rangle_0}_{\text{data}} - \underbrace{\langle v_i h_j \rangle_1}_{\text{reconstruction}}$$

RBM-CD Algorithm

($N_e = 0$) Given input data $\mathbf{X} \in [0,1]^{D \times N_I}$ and random initial weights $\mathbf{M}$ in $[0,1]$

Repeat

1. ($N_e = N_e + 1$) Set $\Delta\mathbf{M} = 0$
2. **for** $n = 1$ **to** D
   1. Draw $\mathbf{v}_0 = \mathbf{X}(n,:) > randvec(N_I)$ and then compute $P(\mathbf{h}_0|\mathbf{v}_0)$
   2. Draw $\mathbf{h}_0 = P(\mathbf{h}_0|\mathbf{v}_0) > randvec(N_H)$
   3. Draw $\mathbf{v}_1 = P(\mathbf{v}_1|\mathbf{h}_0) > randvec(N_I)$
   4. Draw $\mathbf{h}_1 = P(\mathbf{h}_1|\mathbf{v}_1) > randvec(N_H)$
   5. $\Delta\mathbf{M} = \Delta\mathbf{M} + \langle \mathbf{v}_0^T \mathbf{h}_0 \rangle - \langle \mathbf{v}_1^T \mathbf{h}_1 \rangle$
3. Update weights $\mathbf{M} = \mathbf{M} + \epsilon\Delta\mathbf{M}$

Until $|E(N_e) - E(N_e - 1)| \approx 0$ **or** $N_e \geq maxEp$

What does Contrastive Divergence Learn?

- A very crude approximation of the gradient of the log-likelihood
  - It does not even follow the gradient closely
- More closely approximating the gradient of a objective function called the Contrastive Divergence
  - It ignores one tricky term in this objective function so it is not even following that gradient
- Sutskever and Tieleman (2010) have shown that it is not following the gradient of any function

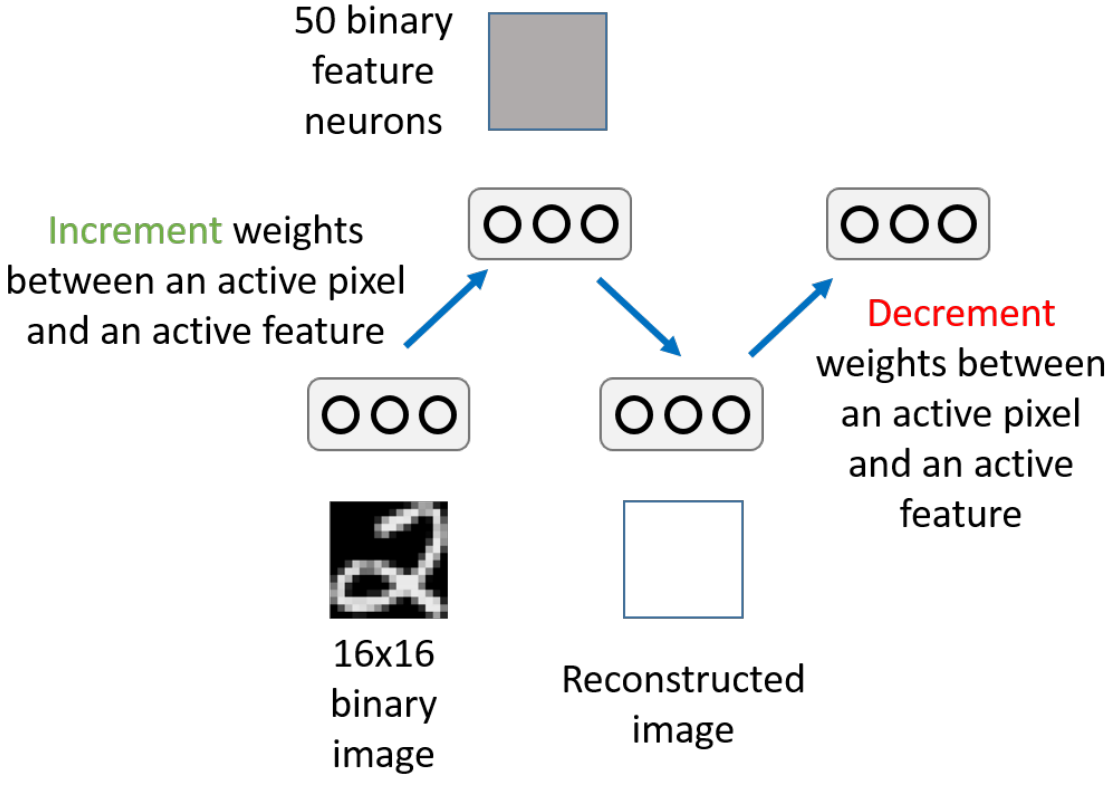
So Why Using it?

Because He says so!

It works well enough in many significant applications

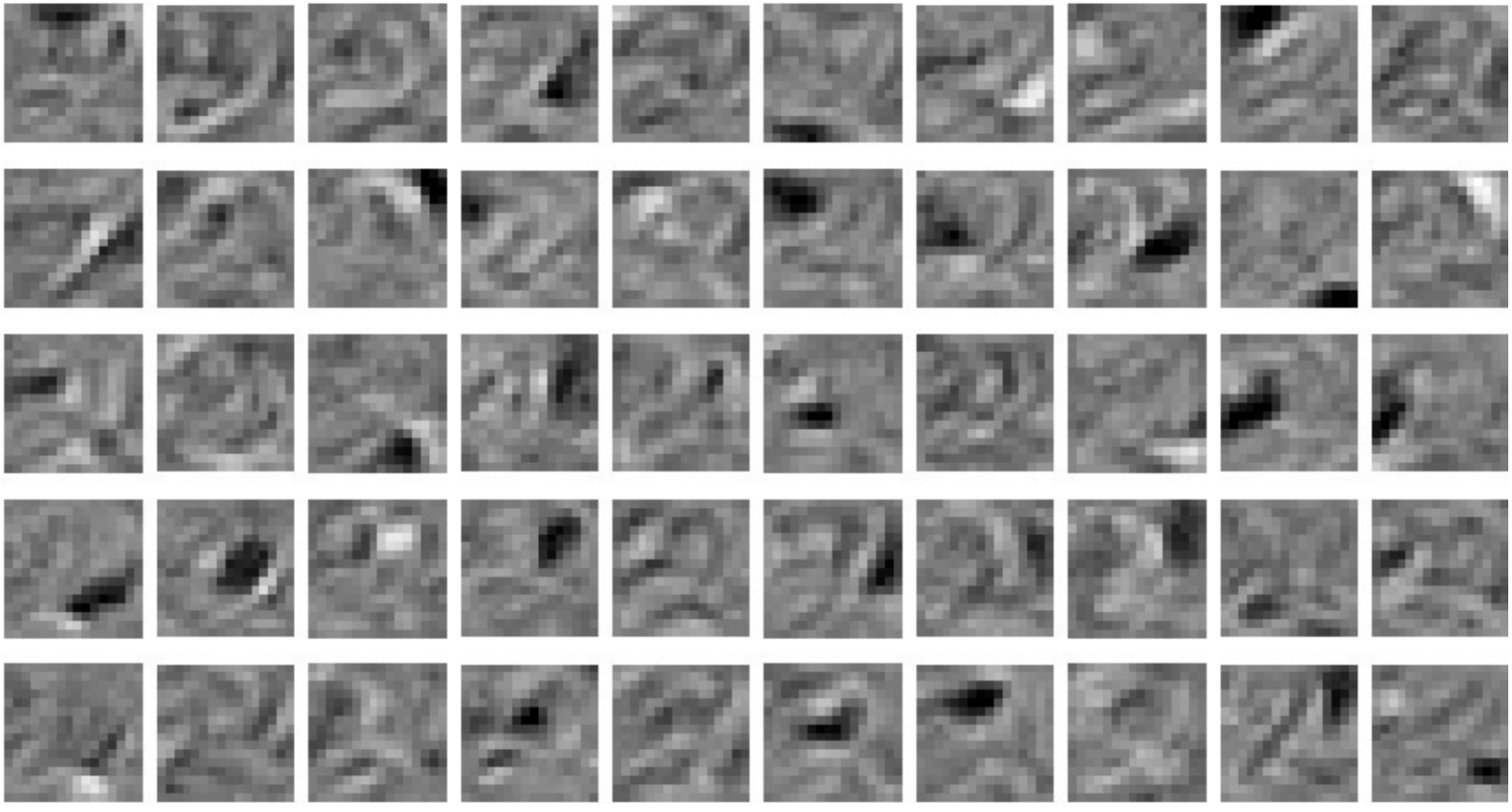
Character Recognition

Learning good features for reconstructing images of number 2 handwriting

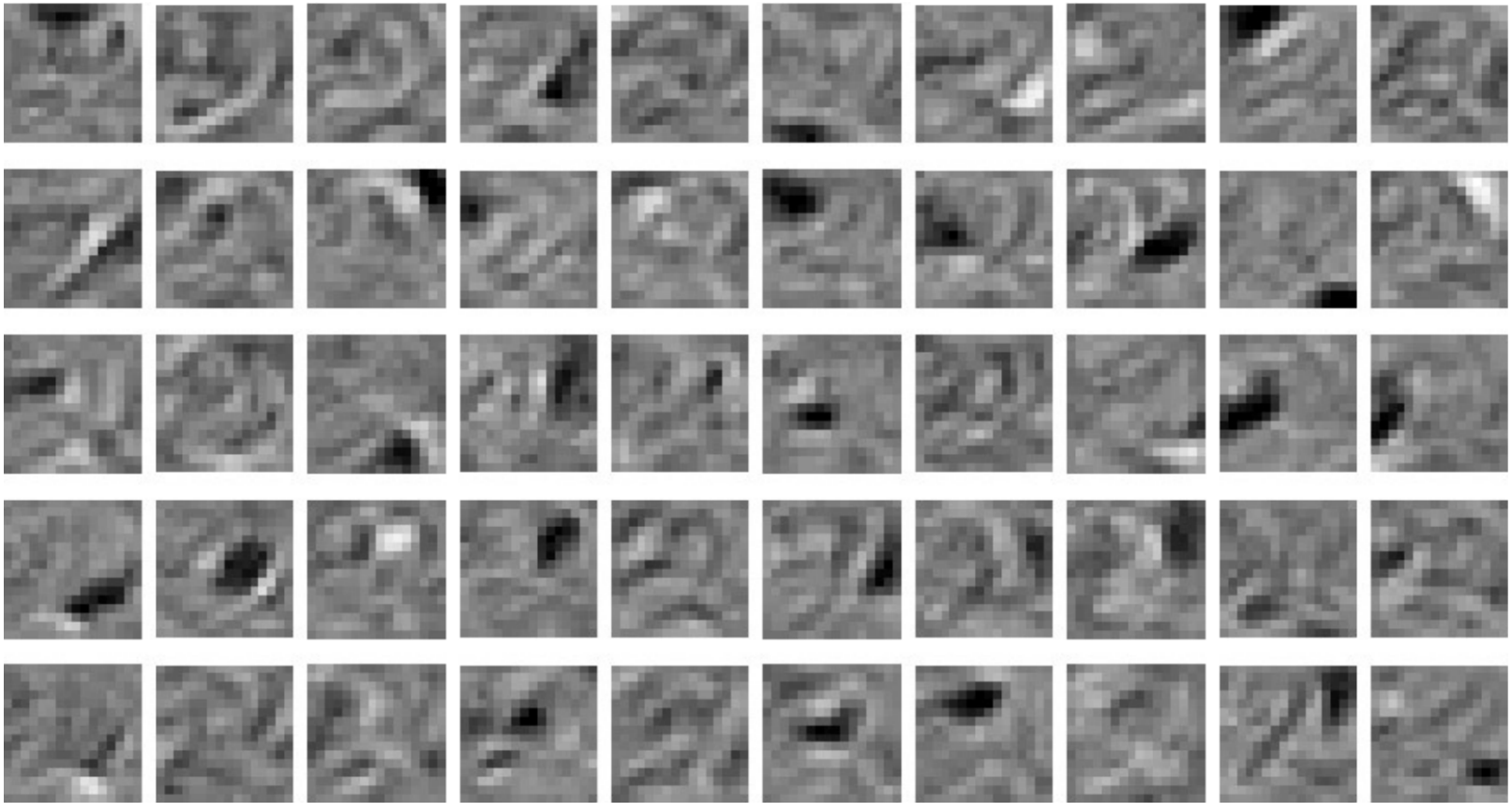


Slide credit goes to G. Hinton

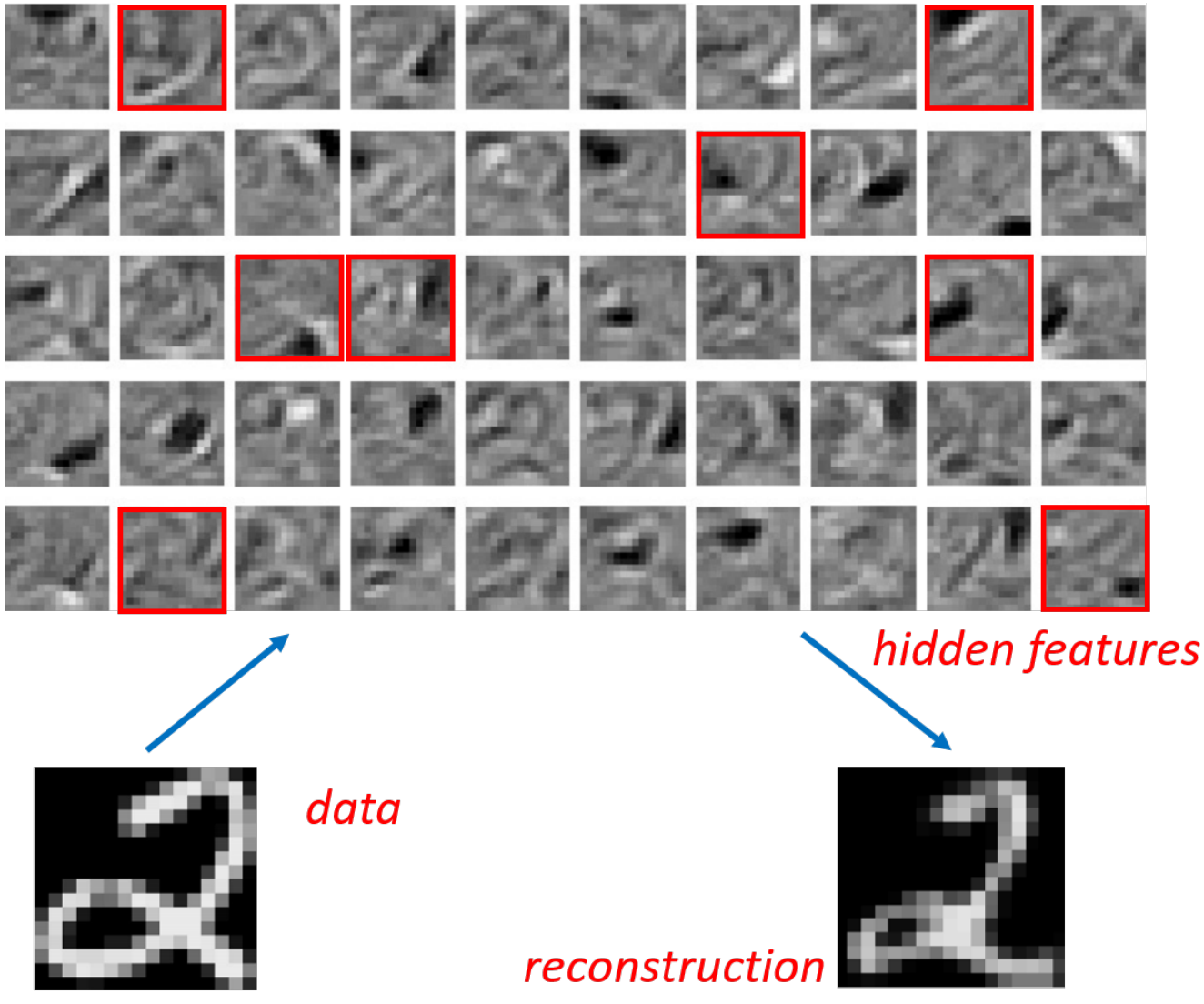
Weight Learning



Final Weights

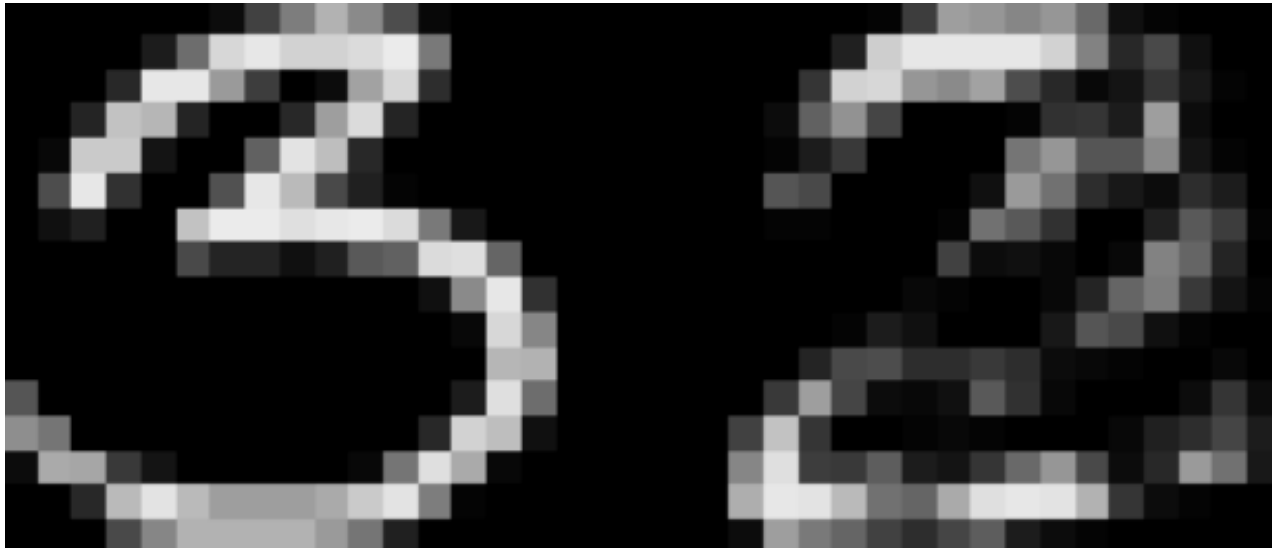


Digit Reconstruction



Digit Reconstruction (II)

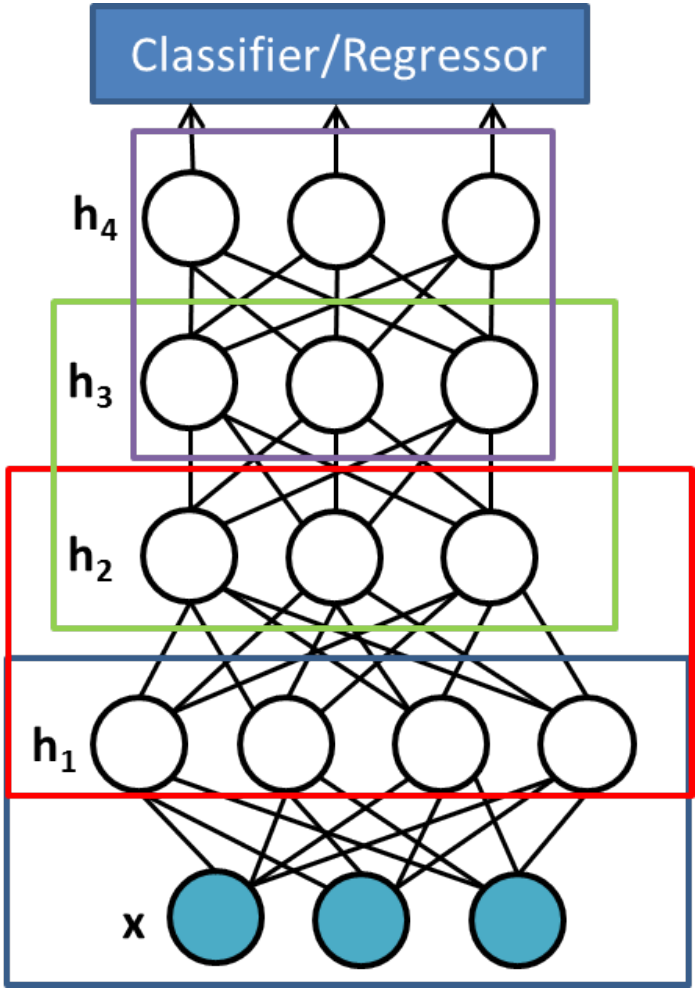
What would happen if we supply the RBM with a test digit that it is not a 2?



It will try anyway to see a 2 in whatever we supply!

One Last Final Reason for Introducing RBM

Deep Belief Network



The fundamental building block for one of the most popular deep learning architectures

A network of stacked RBM trained layer-wise by Contrastive Divergence plus a supervised read-out layer

Take Home Messages

- Stochastic networks as a paradigm that can explain neural variability and spontaneous activity in terms of distributions
- Boltzmann Machines
  - Hidden neurons required to explain high-order correlations
  - Training is a mix of Hebbian and anti-Hebbian
  - Multifaceted nature (recurrent network, undirected graphical model and energy-based network)
- Restricted Boltzmann Machines
  - Tractable model thanks to bipartite connectivity
  - Trained by a very short Gibbs sampling (contrastive divergence)
  - Can be very powerful if stacked (deep learning)

Next Lecture

Hands-on Lab

- Complete implementation of Hopfield Networks
- Try implementing Restricted Boltzmann Machines
  - I suggest you have a good look at reference [1] on the course wiki (pages $3 - 6$)
  - There will be time to finish the assignment on the lab of the 03rd of May