Autoencoders and Restricted Boltzmann Machines

Amir H. Payberah
payberah@kth.se
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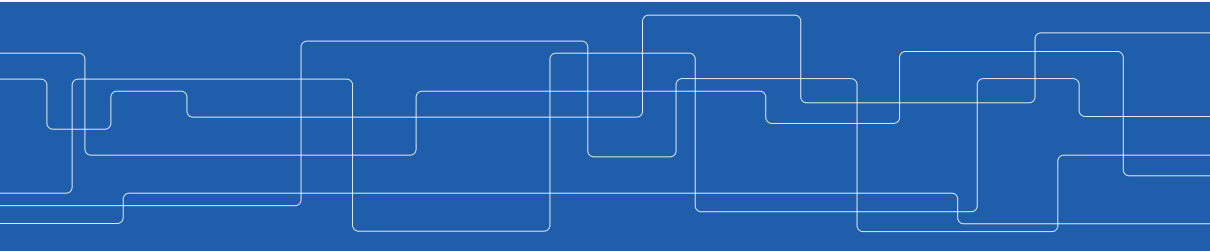
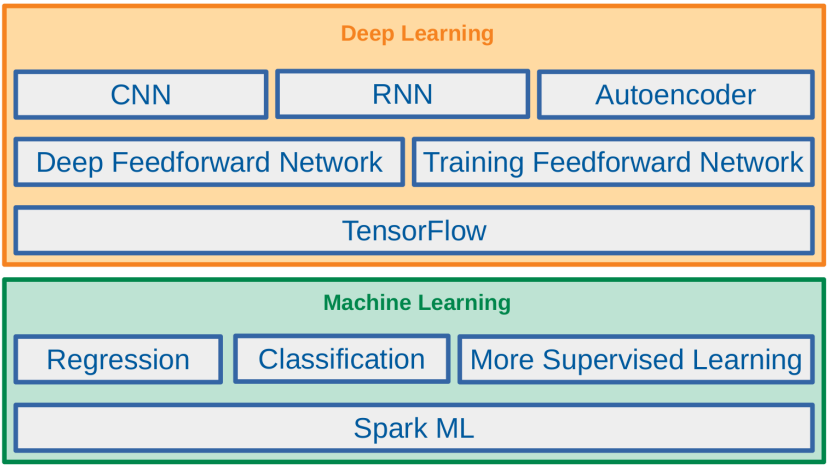


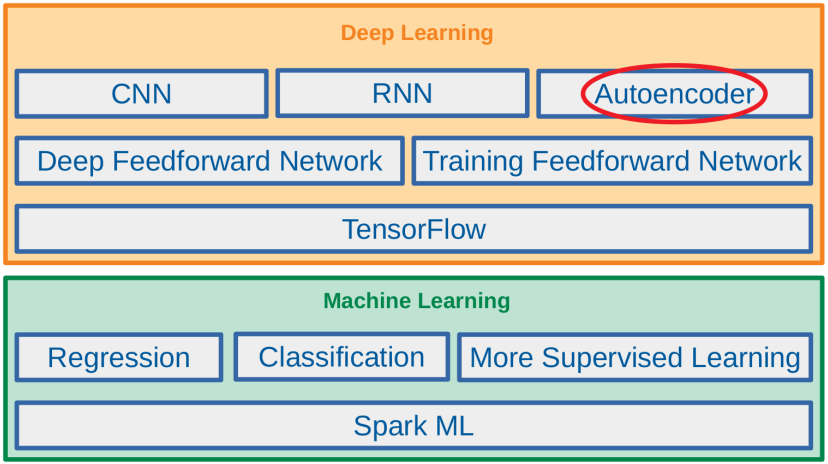
The Course Web Page

https://id2223kth.github.io

Where Are We?


Deep Learning
CNN
RNN
Autoencoder
Deep Feedforward Network
Training Feedforward Network
TensorFlow
Machine Learning
Regression
Classification
More Supervised Learning
Spark ML

Where Are We?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Let's Start With An Example

- Which of them is easier to memorize?
- Seq1: $40, 27, 25, 36, 81, 57, 10, 73, 19, 68$
- Seq2: $50, 25, 76, 38, 19, 58, 29, 88, 44, 22, 11, 34, 17, 52, 26, 13, 40, 20$

Seq1 : 40, 27, 25, 36, 81, 57, 10, 73, 19, 68

Seq2 : 50, 25, 76, 38, 19, 58, 29, 88, 44, 22, 11, 34, 17, 52, 26, 13, 40, 20

- Seq1 is shorter, so it should be easier.
- But, Seq2 follows two simple rules:
  - Even numbers are followed by their half.
  - Odd numbers are followed by their triple plus one.
- You don't need pattern if you could quickly and easily memorize very long sequences
- But, it is hard to memorize long sequences that makes it useful to recognize patterns.

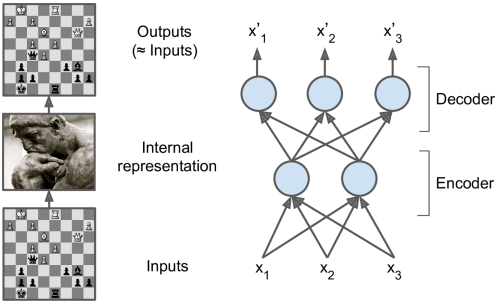
- 1970, W. Chase and H. Simon
- They observed that expert chess players were able to memorize the positions of all the pieces in a game by looking at the board for just 5 seconds.

- This was only the case when the pieces were placed in realistic positions, not when the pieces were placed randomly.
- Chess experts don't have a much better memory than you and I.
- They just see chess patterns more easily due to their experience with the game.
- Patterns helps them store information efficiently.

Autoencoders

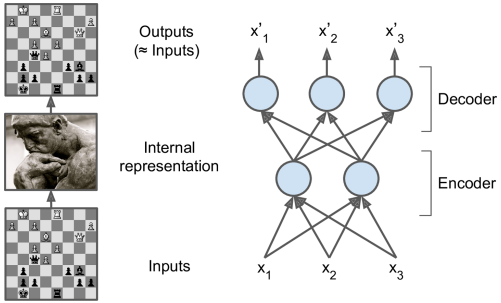
Autoencoders (1/5)

- Just like the chess players in this memory experiment.
- An autoencoder looks at the inputs, converts them to an efficient internal representation, and then spits out something that looks very close to the inputs.



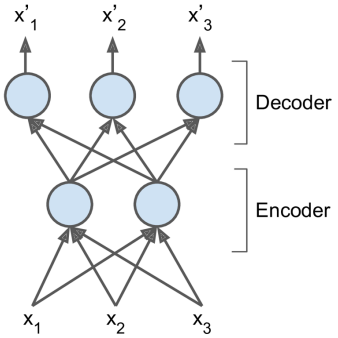
Autoencoders (2/5)

- The same architecture as a Multi-Layer Perceptron (MLP).
- Except that the number of neurons in the output layer must be equal to the number of inputs.



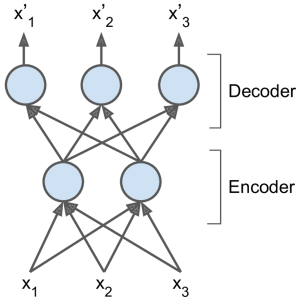
Autoencoders (3/5)

- An autoencoder is always composed of two parts.
- An encoder (recognition network), $\mathbf{h} = \mathtt{f}(\mathbf{x})$
  Converts the inputs to an internal representation.
- A decoder (generative network), $\mathbf{r} = \mathtt{g}(\mathbf{h})$
  Converts the internal representation to the outputs.
- If an autoencoder learns to set $\mathtt{g}(\mathtt{f}(\mathbf{x})) = \mathbf{x}$ everywhere, it is not especially useful, why?



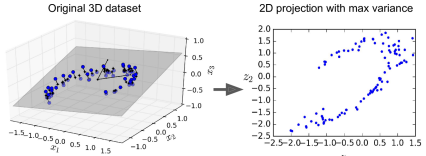
Autoencoders (4/5)

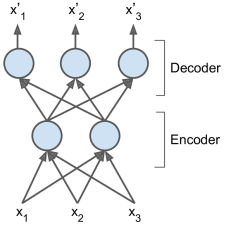
- Autoencoders are designed to be unable to learn to copy perfectly.
- The models are forced to prioritize which aspects of the input should be copied, they often learn useful properties of the data.



Autoencoders (5/5)

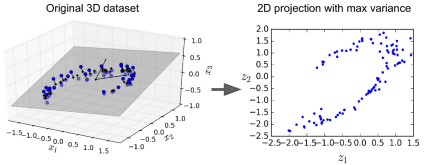
- Autoencoders are neural networks capable of learning efficient representations of the input data (called codings) without any supervision.
- Dimension reduction: these codings typically have a much lower dimensionality than the input data.

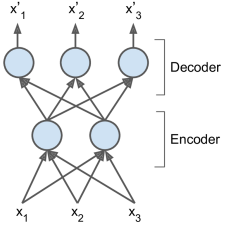




Dimension Reduction and PCA

- Principal Component Analysis (PCA) is the most popular dimensionality reduction algorithm.
- If the decoder is linear and the cost function is the Mean Squared Error (MSE), then it can be shown that it ends up performing PCA.
- Autoencoders with nonlinear encoder and decoder functions can thus learn a more powerful nonlinear generalization of PCA.





PCA with an Undercomplete Linear Autoencoder

- A linear autoencoder to perform PCA on a 3D dataset, projecting it to 2D.

```
n_inputs = 3  # 3D inputs
n_hidden = 2  # 2D codings
n_outputs = n_inputs
```

```
X = tf.placeholder(tf.float32, shape=[None, n_inputs])
hidden = tf.layers.dense(X, n_hidden) # the coding layer
outputs = tf.layers.dense(hidden, n_outputs)

cost = tf.reduce_mean(tf.square(outputs - X)) # MSE

optimizer = tf.train.AdamOptimizer(learning_rate=learning_rate)
training_op = optimizer.minimize(cost)

# the rest is as before
```

Different Types of Autoencoders

- Stacked autoencoders
- Denoising autoencoders
- Variational autoencoders

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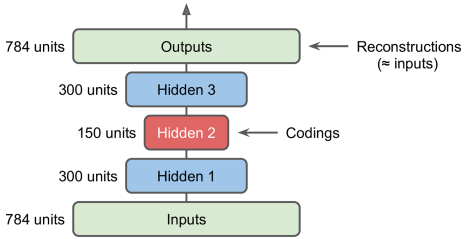
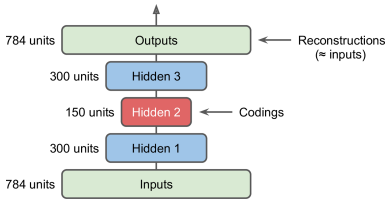
Stacked Autoencoders (1/3)

- Stacked autoencoder: autoencoders with multiple hidden layers.
- Adding more layers helps the autoencoder learn more complex codings.
- The architecture is typically symmetrical with regards to the central hidden layer.



Stacked Autoencoders (2/3)

- In a symmetric architecture, we can tie the weights of the decoder layers to the weights of the encoder layers.
- In a network with $\mathtt{N}$ layers, the decoder layer weights can be defined as $\mathtt{w}_{\mathtt{N}-\mathtt{l}+1} = \mathtt{w}_{\mathtt{l}}^{\mathtt{T}}$, with $\mathtt{l} = 1, 2, \cdots, \frac{\mathtt{N}}{2}$.
- This halves the number of weights in the model, speeding up training and limiting the risk of overfitting.



Stacked Autoencoders (3/3)

```
n_inputs = 28 * 28
n_hidden1 = 300
n_hidden2 = 150  # codings
n_hidden3 = n_hidden1
n_outputs = n_inputs

weights1 = tf.Variable(initializer([n_inputs, n_hidden1]), name="weights1")
weights2 = tf.Variable(initializer([n_hidden1, n_hidden2]), name="weights2")
weights3 = tf.transpose(weights2, name="weights3") # tied weights
weights4 = tf.transpose(weights1, name="weights4") # tied weights

hidden1 = tf.nn.elu(tf.matmul(X, weights1) + biases1)
hidden2 = tf.nn.elu(tf.matmul(hidden1, weights2) + biases2)
hidden3 = tf.nn.elu(tf.matmul(hidden2, weights3) + biases3)
outputs = tf.matmul(hidden3, weights4) + biases4
```

Different Types of Autoencoders

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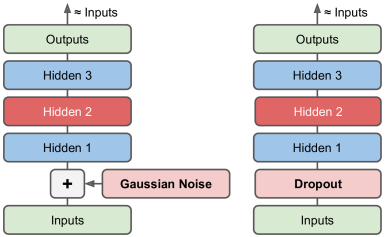
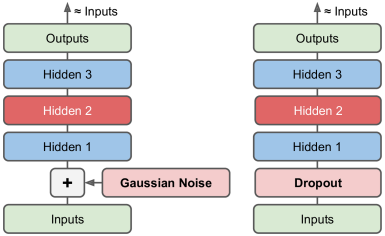
Denoising Autoencoders (1/3)

- One way to force the autoencoder to learn useful features is to add noise to its inputs, training it to recover the original noise-free inputs.
- This prevents the autoencoder from trivially copying its inputs to its outputs, so it ends up having to find patterns in the data.



Denoising Autoencoders (2/3)

- The noise can be pure Gaussian noise added to the inputs, or it can be randomly switched off inputs, just like in dropout.



Denoising Autoencoders (3/3)

```
n_inputs = 28 * 28
n_hidden1 = 300
n_hidden2 = 150  # codings
n_hidden3 = n_hidden1
n_outputs = n_inputs

X = tf.placeholder(tf.float32, shape=[None, n_inputs])
X_noisy = X + noise_level * tf.random_normal(tf.shape(X))

hidden1 = tf.layers.dense(X_noisy, n_hidden1, activation=tf.nn.relu, name="hidden1")
hidden2 = tf.layers.dense(hidden1, n_hidden2, activation=tf.nn.relu, name="hidden2")
hidden3 = tf.layers.dense(hidden2, n_hidden3, activation=tf.nn.relu, name="hidden3")
outputs = tf.layers.dense(hidden3, n_outputs, name="outputs")
```

Different Types of Autoencoders

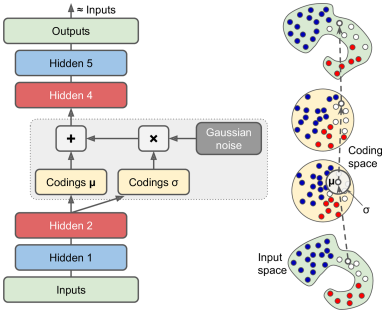
- Stacked autoencoders
- Denoising autoencoders
- Variational autoencoders

Variational Autoencoders (1/3)

- Variational autoencoders are probabilistic autoencoders.
- Their outputs are partly determined by chance, even after training.
  - As opposed to denoising autoencoders, which use randomness only during training.
- They are generative autoencoders, meaning that they can generate new instances that look like they were sampled from the training set.

Variational Autoencoders (2/3)

- Instead of directly producing a coding for a given input, the encoder produces a mean coding μ and a standard deviation σ.
- The actual coding is then sampled randomly from a Gaussian distribution with mean μ and standard deviation σ.
- After that the decoder just decodes the sampled coding normally.



Variational Autoencoders (3/3)

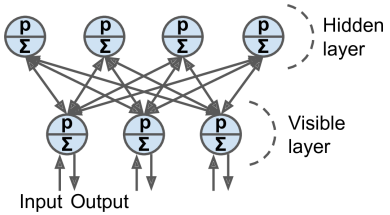
- The cost function is composed of two parts.
- 1. the usual reconstruction loss.
  - Pushes the autoencoder to reproduce its inputs.
  - Using cross-entropy.
- 2. the latent loss
  - Pushes the autoencoder to have codings that look as though they were sampled from a simple Gaussian distribution.
  - Using the KL divergence between the target distribution (the Gaussian distribution) and the actual distribution of the codings.
  - KL divergence measures the divergence between the two probabilities.


Original illustration: Sonia Jerrems

Restricted Boltzmann Machines

Restricted Boltzmann Machines

- A Restricted Boltzmann Machine (RBM) is a stochastic neural network.
- Stochastic meaning these activations have a probabilistic element, instead of deterministic functions, e.g., logistic or ReLU.
- The neurons form a bipartite graph:
  - One visible layer and one hidden layer.
  - A symmetric connection between the two layers.
  - There are no connections between neurons within a layer.



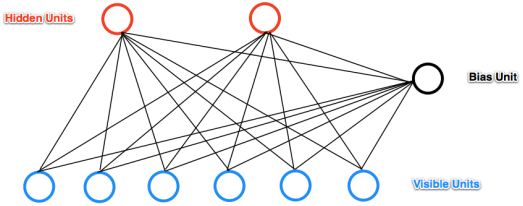
Let's Start With An Example

RBM Example (1/10)

- We have a set of six movies, and we ask users to tell us which ones they want to watch.
- We want to learn two latent units underlying movie preferences, e.g., SF/fantasy and Oscar winners

RBM Example (2/10)

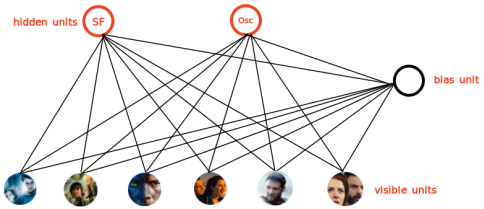
- Our RBM would look like the following.



RBM Example (3/10)

- Assume the given input x_i is the 0 or 1 for each visible neuron v_i.
  - 1: like a movie, and 0: dislike a movie
- Compute the activation energy at hidden neuron h_j:

$$a(h_j) = \sum_i w_{ij} v_i$$



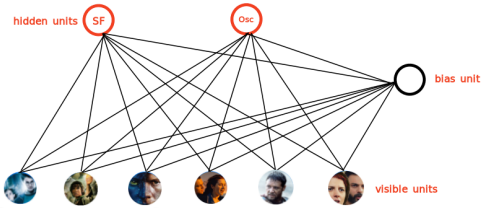
RBM Example (4/10)

- For each hidden neuron h_j, we compute the probability $p(h_j)$.

$$a(h_j) = \sum_i w_{ij} v_i$$

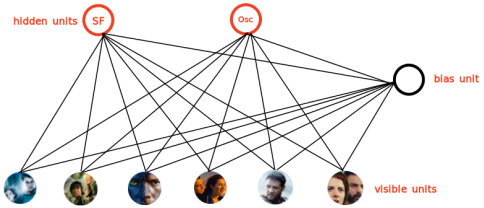
$$p(h_j) = \text{sigmoid}(a(h_j)) = \frac{1}{1 + e^{-a(h_j)}}$$

- We turn on the hidden neuron h_j with the probability $p(h_j)$, and turn it off with probability $1 - p(h_j)$.



RBM Example (5/10)

- Declaring that you like Harry Potter, Avatar, and LOTR, doesn't guarantee that the SF/fantasy hidden neuron will turn on.
- But it will turn on with a high probability.
  - In reality, if you want to watch all three of those movies makes us highly suspect you like SF/fantasy in general.
  - But there's a small chance you like them for other reasons.



RBM Example (6/10)

- Conversely, if we know that one person likes SF/fantasy (so that the SF/fantasy neuron is on)
- We can ask the RBM to generate a set of movie recommendations.
- The hidden neurons send messages to the visible (movie) neurons, telling them to update their states.

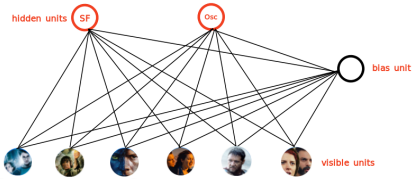
$$a(v_i) = \sum_j w_{ij} h_j$$

$$p(v_i) = \texttt{sigmoid}(a(v_i)) = \frac{1}{1 + e^{-a(v_i)}}$$

- Being on the SF/fantasy neuron doesn't guarantee that we'll always recommend all three of Harry Potter, Avatar, and LOTR.
  - For example not everyone who likes science fiction liked Avatar.

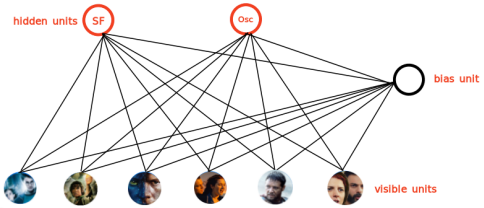
RBM Example (7/10)

- How do we learn the connection weights w_{ij} in our network?
- Assume, as an input we have a bunch of binary vectors $\mathbf{x}$ with six elements corresponding to a user's movie preferences.
- We do the following steps in each epoch:
- 1. Take a training instance $\mathbf{x}$ and set the states of the visible neurons to these preferences.



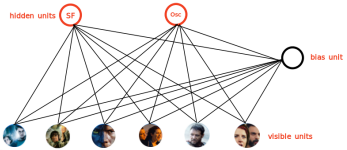
RBM Example (8/10)

- 2. Update the states of the hidden neurons.
  - Compute $a(h_j) = \sum_i w_{ij} v_i$ for each hidden neuron h_j.
  - Set h_j to 1 with probability $p(h_j) = \mathrm{sigmoid}(a(h_j)) = \frac{1}{1+e^{-a(h_j)}}$
- 3. For each edge e_{ij}, compute $\mathrm{positive}(e_{ij}) = v_i \times h_j$
  - I.e., for each pair of neurons, measure whether they are both on.



RBM Example (9/10)

- 4. Update the state of the visible neurons in a similar manner.
  - We denote the updated visible neurons with v'_i.
  - Compute $a(v'_i) = \sum_j w_{ij} h_j$ for each visible neuron v'_i.
  - Set v'_i to 1 with probability $p(v'_i) = \text{sigmoid}(a(v'_i)) = \frac{1}{1+e^{-a(v'_i)}}$
- 5. Update the hidden neurons again similar to step 2. We denote the updated hidden neurons with h'_j.
- 6. For each edge e_{ij}, compute $\text{negative}(e_{ij}) = v'_i \times h'_j$

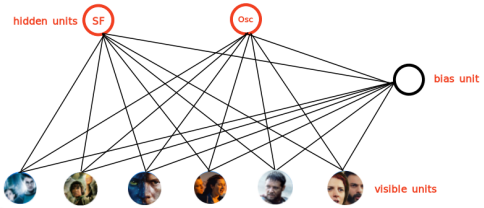


RBM Example (10/10)

- 7. Update the weight of each edge e_{ij}.

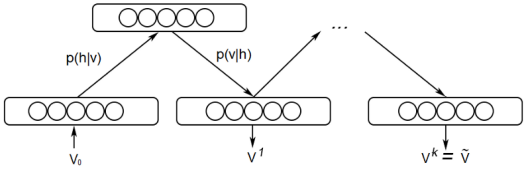
$$w_{ij} = w_{ij} + \eta(\text{positive}(e_{ij}) - \text{negative}(e_{ij}))$$

- 8. Repeat over all training examples.
- 9. Continue until the error between the training examples and their reconstructions falls below some threshold or we reach some maximum number of epochs.



RBM Training (1/2)

- Step 1, Gibbs sampling: what we have done in steps 1-6.
- Given an input vector $\mathbf{v}$, compute $p(\mathbf{h}|\mathbf{v})$.
- Knowing the hidden values $\mathbf{h}$, we use $p(\mathbf{v}|\mathbf{h})$ for prediction of new input values $\mathbf{v}$.
- This process is repeated k times.

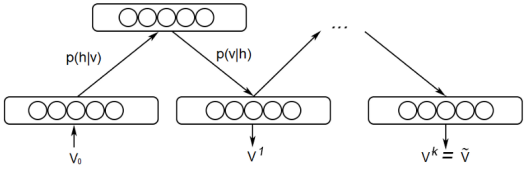


RBM Training (2/2)

- Step 2, contrastive divergence: what we have done in step 7.
  - Just a fancy name for approximate gradient descent.

$$\texttt{positive}(\mathbf{e}) = \mathbf{v}_0 \times \texttt{p}(\mathbf{h}_0|\mathbf{v}_0)$$
$$\texttt{negative}(\mathbf{e}) = \mathbf{v}_\texttt{k} \times \texttt{p}(\mathbf{h}_\texttt{k}|\mathbf{v}_\texttt{k})$$
$$\mathbf{w} = \mathbf{w} + \eta(\texttt{positive}(\mathbf{e}) - \texttt{negative}(\mathbf{e}))$$

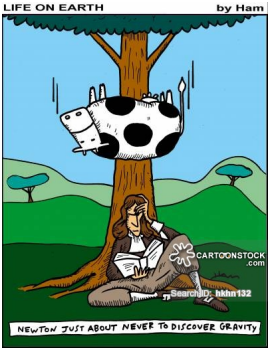
- $\mathbf{v}_0$ is the original input, and $\mathbf{v}_\texttt{k}$ is the input after $\texttt{k}$ iterations.



More Details about RBM

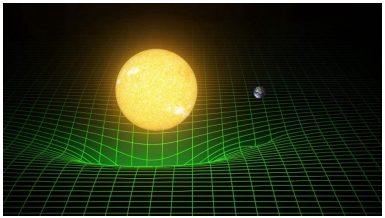
Energy-based Model (1/3)

- Energy a quantitative property of physics.
  - E.g., gravitational energy describes the potential energy a body with mass has in relation to another massive object due to gravity.



Energy-based Model (2/3)

- One purpose of deep learning models is to encode dependencies between variables.
- The capturing of dependencies happen through associating of a scalar energy to each state of the variables.
  - Serves as a measure of compatibility.
- A high energy means a bad compatibility.
- An energy based model tries always to minimize a predefined energy function.

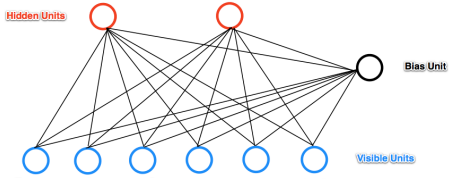


Energy-based Model (3/3)

- The energy function for the RBMs is defined as:

$$E(\mathbf{v}, \mathbf{h}) = -(\sum_{ij} w_{ij} v_i h_j + \sum_i b_i v_i + \sum_j c_j h_j)$$

- **v** and **h** represent the visible and hidden units, respectively.
- **w** represents the weights connecting visible and hidden units.
- **b** and **c** are the biases of the visible and hidden layers, respectively.



RBM is a Probabilistic Model

- At each point in time the RBM is in a certain state.
  - The state refers to the values of neurons in the visible and hidden layers $\mathbf{v}$ and $\mathbf{h}$.
- The probability of a certain state of $\mathbf{v}$ and $\mathbf{h}$:

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

- The probability that the network assigns to a visible vector $\mathbf{v}$, is given by summing over all possible hidden vectors $\mathbf{h}$.

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

Learning in Boltzmann Machines (1/2)

- RBMs try to learn a probability distribution from the data they are given.
- Given a training set of state vectors $\mathbf{v}$, learning consists of finding parameters $\mathbf{w}$ of $\mathrm{p}(\mathbf{v}, \mathbf{h})$, in a way that the training vectors have high probability $\mathrm{p}(\mathbf{v})$.

$$\mathrm{p}(\mathbf{v}|\mathbf{w}) = \frac{\sum_{\mathbf{h}} \mathrm{e}^{-\mathrm{E}(\mathbf{v},\mathbf{h})}}{\sum_{\mathbf{v},\mathbf{h}} \mathrm{e}^{-\mathrm{E}(\mathbf{v},\mathbf{h})}}$$

- Use the maximum-likelihood estimation.
- For a model of the form $\mathrm{p}(\mathbf{v})$ with parameters $\mathbf{w}$, the log-likelihood given a single training example $\mathbf{v}$ is:

$$\log \mathrm{p}(\mathbf{v}|\mathbf{w}) = \log \frac{\sum_{\mathbf{h}} \mathrm{e}^{-\mathrm{E}(\mathbf{v},\mathbf{h})}}{\sum_{\mathbf{v},\mathbf{h}} \mathrm{e}^{-\mathrm{E}(\mathbf{v},\mathbf{h})}} = \log \sum_{\mathbf{h}} \mathrm{e}^{-\mathrm{E}(\mathbf{v},\mathbf{h})} - \log \sum_{\mathbf{v},\mathbf{h}} \mathrm{e}^{-\mathrm{E}(\mathbf{v},\mathbf{h})}$$

Learning in Boltzmann Machines (1/2)

- The log-likelihood gradients for an RBM with binary units:

$$\frac{\partial \log p(\mathbf{v}|w_{ij})}{\partial w_{ij}} = \texttt{positive}(e_{ij}) - \texttt{negative}(e_{ij})$$

- Then, we can update the weight **w** as follows:

$$w_{ij}^{(\texttt{next})} = w_{ij} + \eta(\texttt{positive}(e_{ij}) - \texttt{negative}(e_{ij}))$$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Summary

Summary

- Autoencoders
  - Stacked autoencoders
  - Denoising autoencoders
  - Variational autoencoders
- Restricted Boltzmann Machine
  - Gibbs sampling
  - Contrastive divergence

Reference

- Ian Goodfellow et al., Deep Learning (Ch. 14, 20)
- Aurélien Géron, Hands-On Machine Learning (Ch. 15)

Questions?