Autoencoders and Restricted Boltzmann Machines

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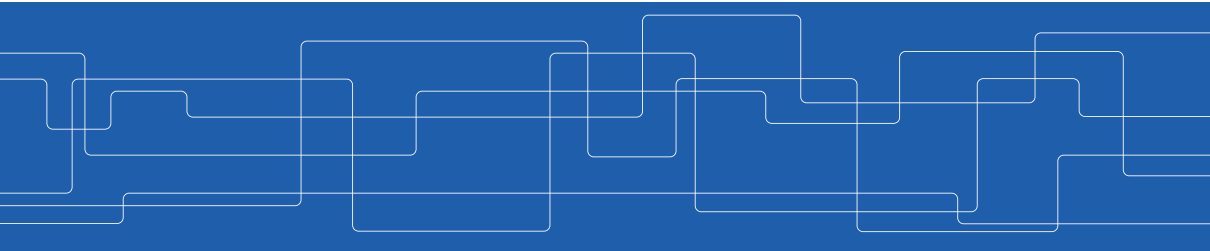
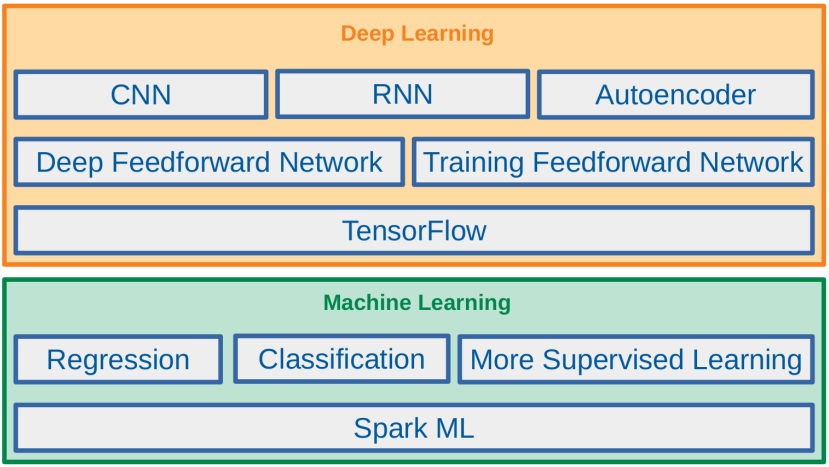
11/12/2018



The Course Web Page

https://id2223kth.github.io

Where Are We?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More Supervised Learning
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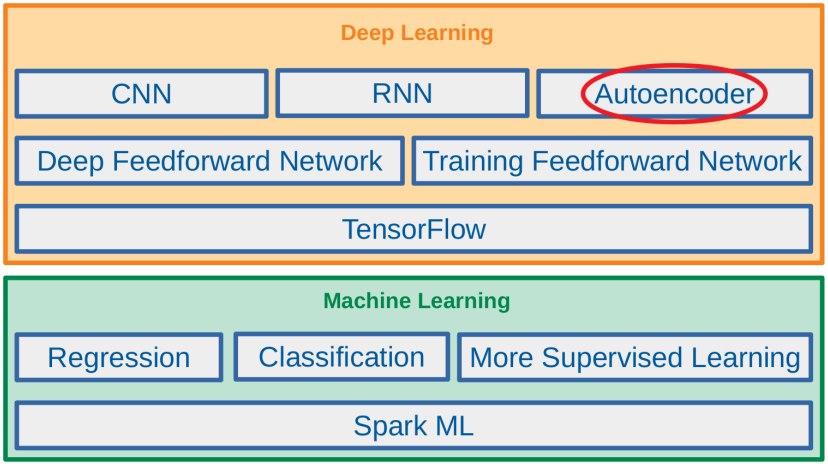
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Let's Start With An Example

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- Seq1: $40, 27, 25, 36, 81, 57, 10, 73, 19, 68$
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  - Even numbers are followed by their half.
  - Odd numbers are followed by their triple plus one.

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- 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.

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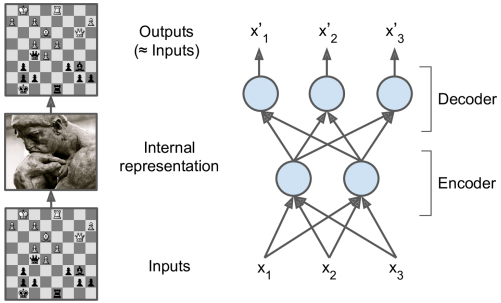
- Chess experts don't have a much better memory than you and I.
- They just see chess patterns more easily due to their experience with the game.
- Patterns helps them store information efficiently.

Autoencoders

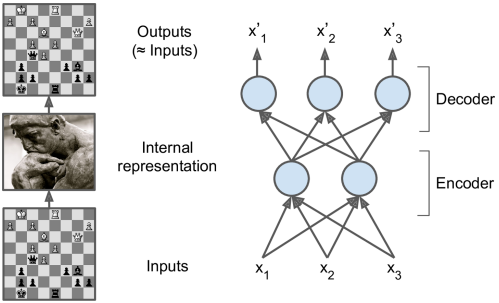
Autoencoders (1/5)

- Just like the chess players in this memory experiment.



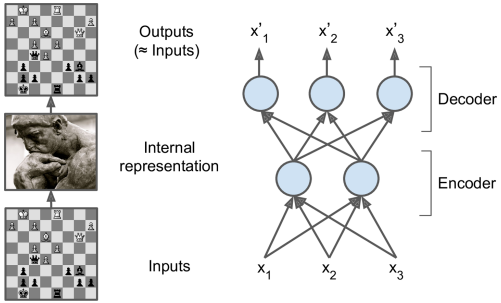
Autoencoders (1/5)

- 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.



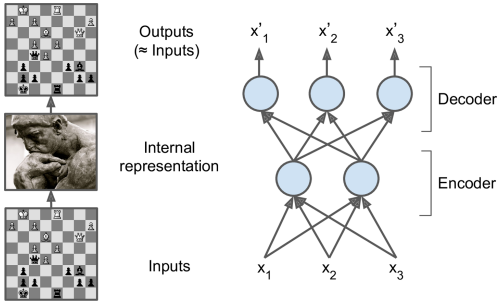
Autoencoders (2/5)

- The same architecture as a Multi-Layer Perceptron (MLP).



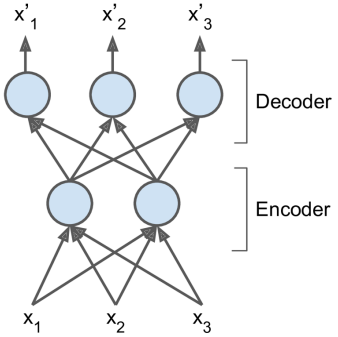
Autoencoders (2/5)

- 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.



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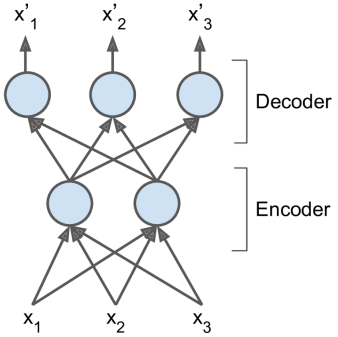
- An encoder (recognition network), $\mathbf{h} = f(\mathbf{x})$
  Converts the inputs to an internal representation.



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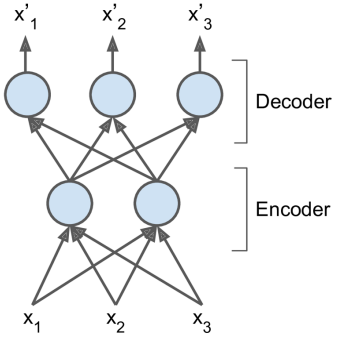
- A decoder (generative network), $\mathbf{r} = g(\mathbf{h})$
  Converts the internal representation to the outputs.



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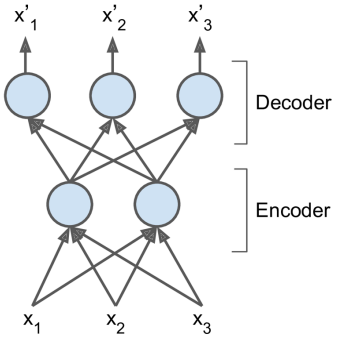
  Converts the internal representation to the outputs.
- If an autoencoder learns to set $\mathtt{g}(\mathtt{f}(\mathbf{x})) = \mathbf{x}$ everywhere, it is not especially useful, why?



Autoencoders (4/5)

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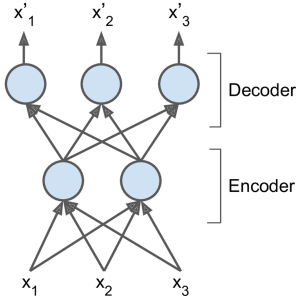
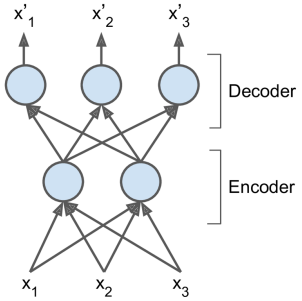


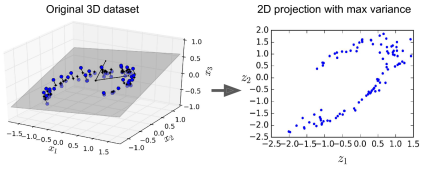
Autoencoders (4/5)

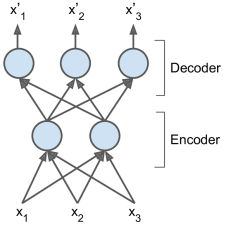
- Autoencoders are designed to be unable to learn to copy perfectly.
- The models are forced to prioritize which aspects of the input should be copied, they often learn useful properties of the data.



Autoencoders (5/5)

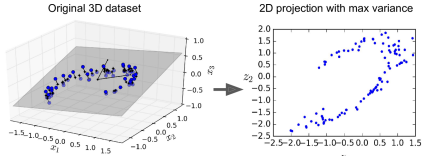
- Autoencoders are neural networks capable of learning efficient representations of the input data (called codings) without any supervision.

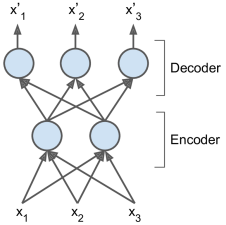




Autoencoders (5/5)

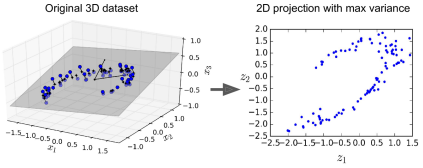
- Autoencoders are neural networks capable of learning efficient representations of the input data (called codings) without any supervision.
- Dimension reduction: these codings typically have a much lower dimensionality than the input data.

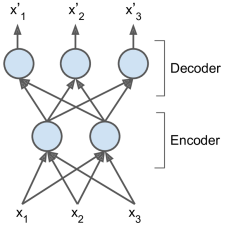




Dimension Reduction and PCA

- Principal Component Analysis (PCA) is the most popular dimensionality reduction algorithm.





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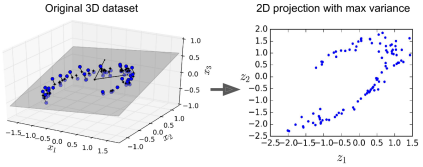
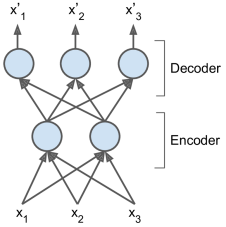
- If the decoder is linear and the cost function is the Mean Squared Error (MSE), then it can be shown that it ends up performing PCA.





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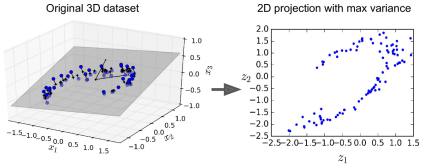
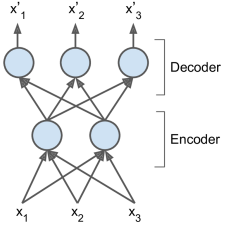
- Autoencoders with nonlinear encoder and decoder functions can thus learn a more powerful nonlinear generalization of PCA.





PCA with an Undercomplete Linear Autoencoder

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

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n_inputs = 3  # 3D inputs
n_hidden = 2  # 2D codings
n_outputs = n_inputs
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```
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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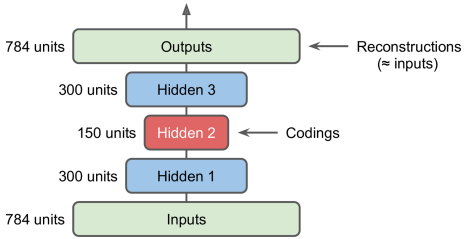
Stacked Autoencoders (1/3)

- Stacked autoencoder: autoencoders with multiple hidden layers.



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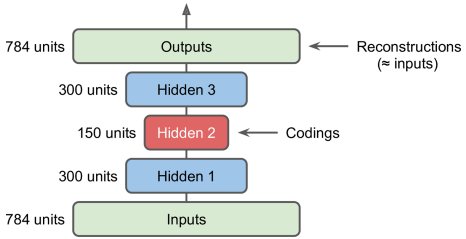
- Adding more layers helps the autoencoder learn more complex codings.



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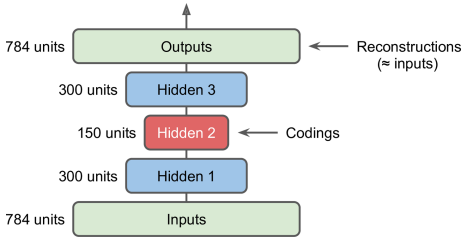
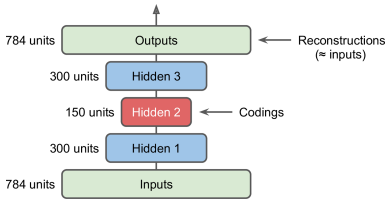
- Stacked autoencoder: autoencoders with multiple hidden layers.
- Adding more layers helps the autoencoder learn more complex codings.
- The architecture is typically symmetrical with regards to the central hidden layer.



Stacked Autoencoders (2/3)

- In a symmetric architecture, we can tie the weights of the decoder layers to the weights of the encoder layers.



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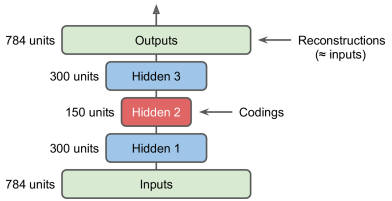
- In a network with $\mathtt{N}$ layers, the decoder layer weights can be defined as $\mathtt{w}_{\mathtt{N}-\mathtt{l}+1} = \mathtt{w}_{\mathtt{l}}^{\mathtt{T}}$, with $\mathtt{l} = 1, 2, \cdots, \frac{\mathtt{N}}{2}$.



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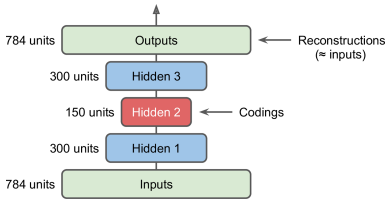
- This halves the number of weights in the model, speeding up training and limiting the risk of overfitting.



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
```

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- Denoising autoencoders
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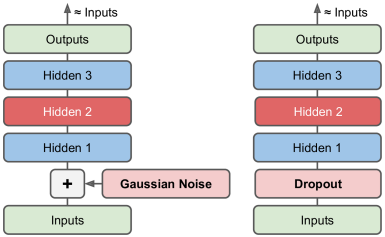
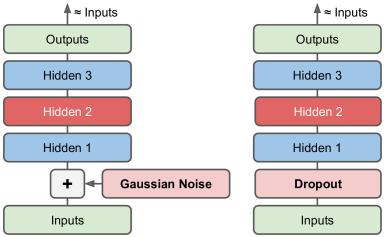
Denoising Autoencoders (1/3)

- 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.



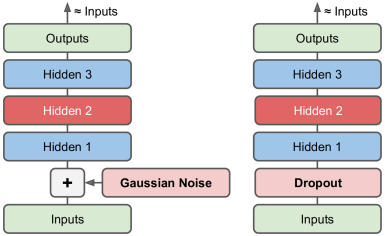
Denoising Autoencoders (1/3)

- 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.



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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")
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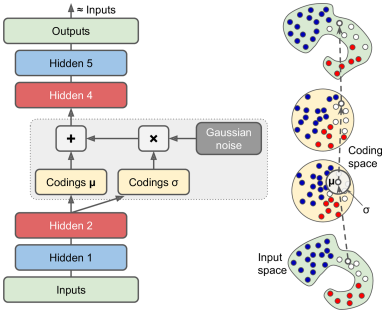
  - As opposed to denoising autoencoders, which use randomness only during training.
- They are generative autoencoders, meaning that they can generate new instances that look like they were sampled from the training set.

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.



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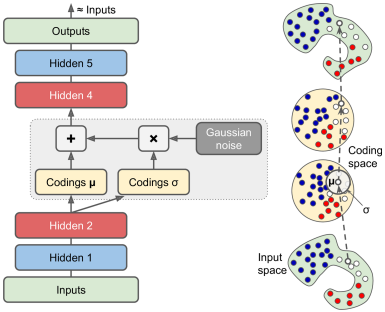

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- Instead of directly producing a coding for a given input, the encoder produces a mean coding μ and a standard deviation σ.
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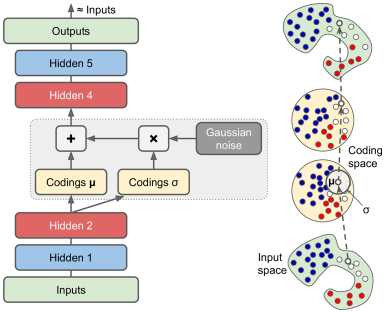
- After that the decoder just decodes the sampled coding normally.



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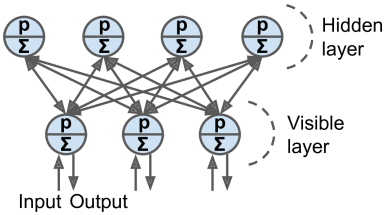
  - KL divergence measures the divergence between the two probabilities.


Original illustration: Sonia Jerrems

Restricted Boltzmann Machines

Restricted Boltzmann Machines

- A Restricted Boltzmann Machine (RBM) is a stochastic neural network.



Restricted Boltzmann Machines

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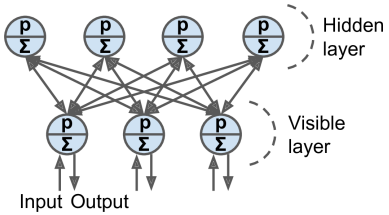
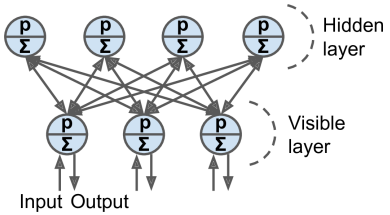
- Stochastic meaning these activations have a probabilistic element, instead of deterministic functions, e.g., logistic or ReLU.



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)

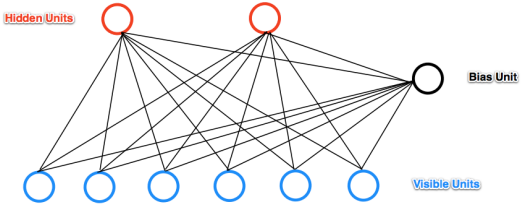
- We have a set of six movies, and we ask users to tell us which ones they want to watch.

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

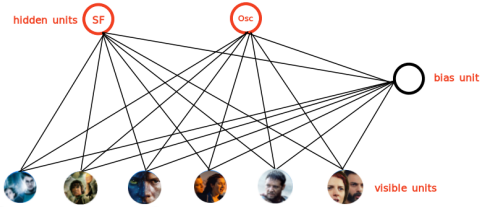
RBM Example (2/10)

- 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



RBM Example (3/10)

- Assume the given input x_i is the 0 or 1 for each visible neuron v_i.
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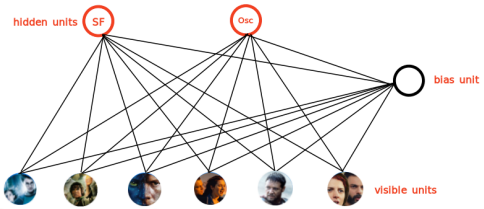

RBM Example (4/10)

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

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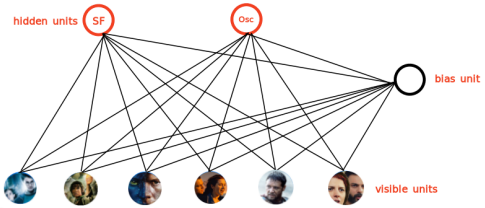

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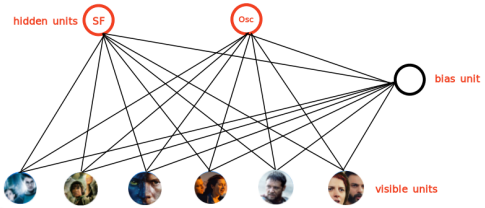
- We turn on the hidden neuron h_j with the probability $p(h_j)$, and turn it off with probability $1 - p(h_j)$.



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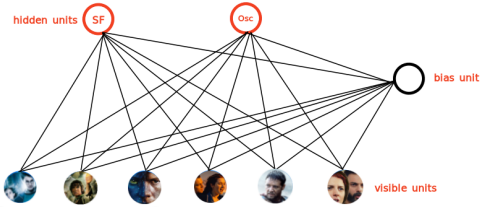

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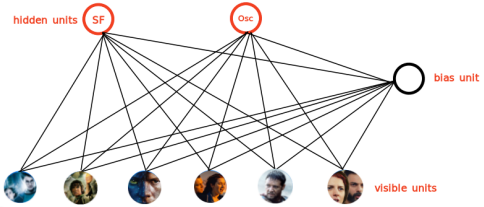

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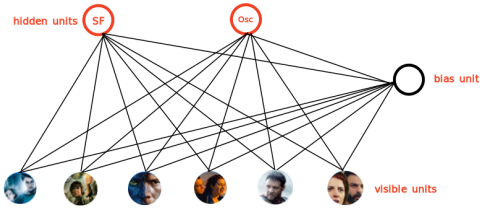
- But it will turn on with a high probability.
  - In reality, if you want to watch all three of those movies makes us highly suspect you like SF/fantasy in general.
  - But there's a small chance you like them for other reasons.



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- 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.

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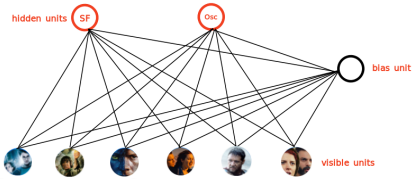
- How do we learn the connection weights w_{ij} in our network?



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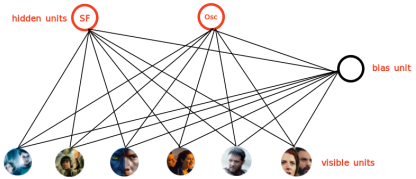

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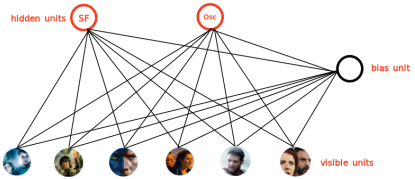

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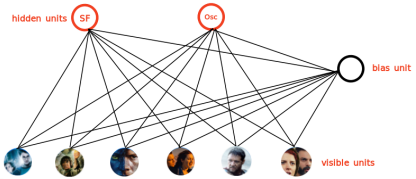

RBM Example (8/10)

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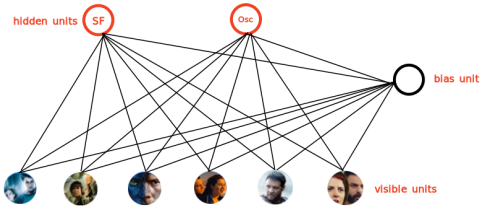

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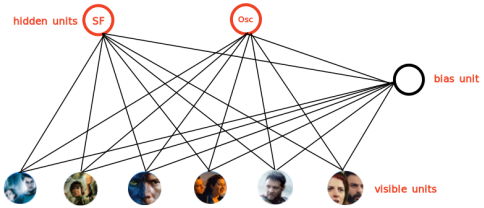

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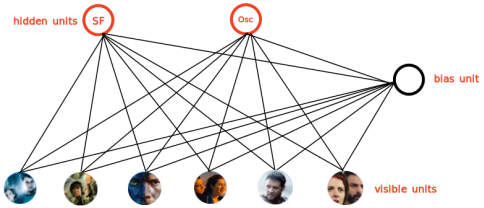

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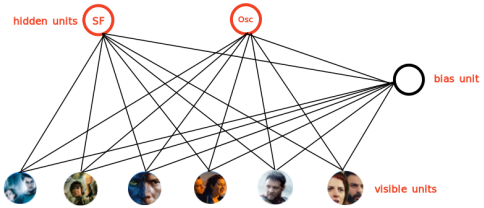
- 3. For each edge e_{ij}, compute $\mathrm{positive}(e_{ij}) = v_i \times h_j$
  - I.e., for each pair of neurons, measure whether they are both on.



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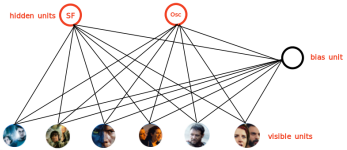

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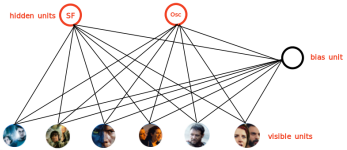

RBM Example (9/10)

- 4. Update the state of the visible neurons in a similar manner.
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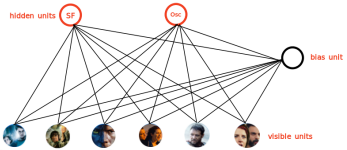
  - Set $\mathtt{v}'_\mathtt{i}$ to 1 with probability $\mathtt{p}(\mathtt{v}'_\mathtt{i}) = \mathtt{sigmoid}(\mathtt{a}(\mathtt{v}'_\mathtt{i})) = \frac{1}{1+\mathtt{e}^{-\mathtt{a}(\mathtt{v}'_\mathtt{i})}}$



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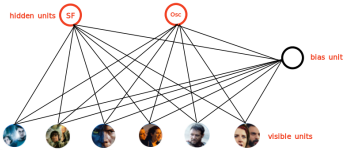
- 5. Update the hidden neurons again similar to step 2. We denote the updated hidden neurons with h'_j.



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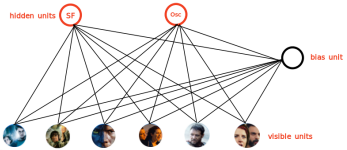
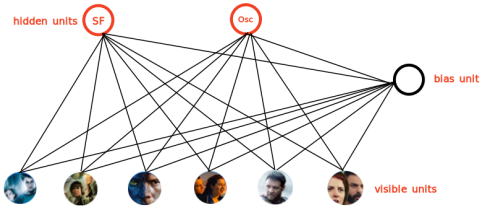
- 5. Update the hidden neurons again similar to step 2. We denote the updated hidden neurons with h'_j.
- 6. For each edge e_{ij}, compute $\text{negative}(e_{ij}) = v'_i \times h'_j$



RBM Example (10/10)

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

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



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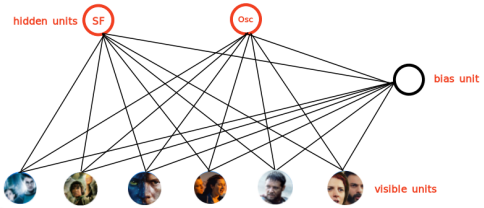

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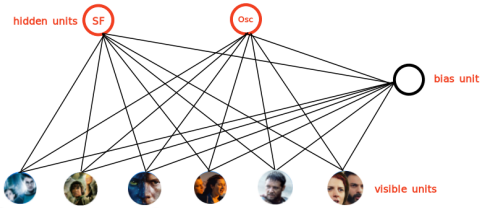
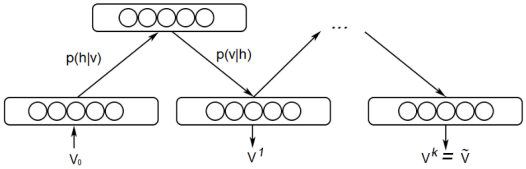
- 8. Repeat over all training examples.
- 9. Continue until the error between the training examples and their reconstructions falls below some threshold or we reach some maximum number of epochs.



RBM Training (1/2)

- Step 1, Gibbs sampling: what we have done in steps 1-6.



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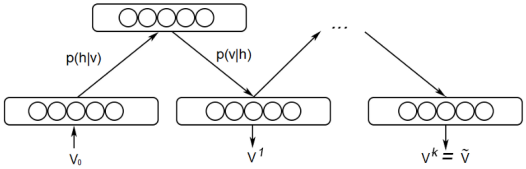

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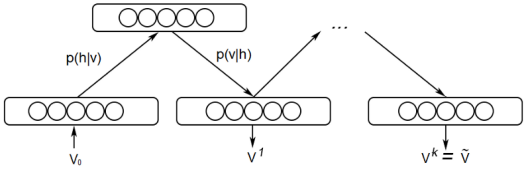

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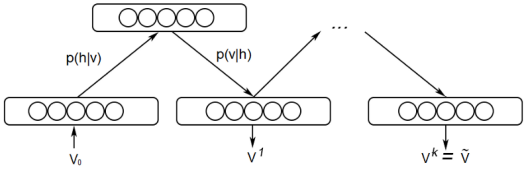

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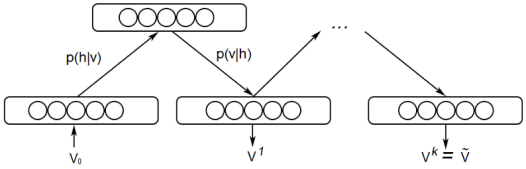

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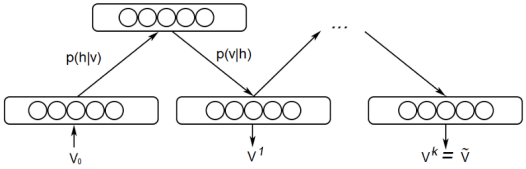
- $\mathbf{v}_0$ is the original input, and $\mathbf{v}_\texttt{k}$ is the input after $\texttt{k}$ iterations.



More Details about RBM

Energy-based Model (1/3)

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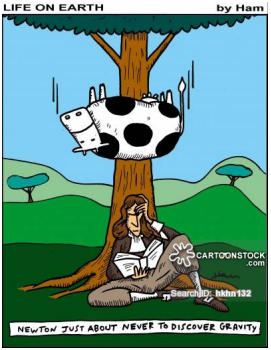

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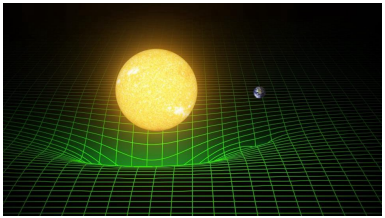

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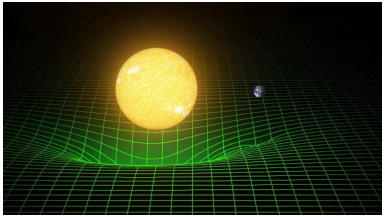

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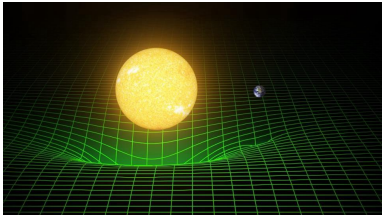

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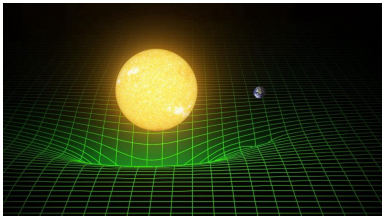
- An energy based model tries always to minimize a predefined energy function.



Energy-based Model (3/3)

- The energy function for the RBMs is defined as:

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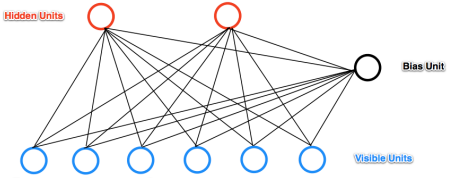

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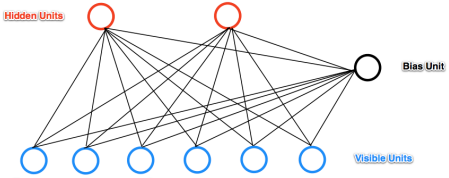

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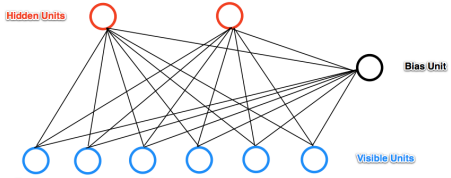

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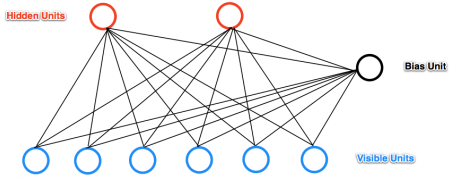

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- The probability that the network assigns to a visible vector $\mathbf{v}$, is given by summing over all possible hidden vectors $\mathbf{h}$.

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

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- 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:

$$\frac{\partial \log \mathrm{p}(\mathbf{v}|\mathtt{w}_{\mathtt{ij}})}{\partial \mathtt{w}_{\mathtt{ij}}} = \mathtt{positive}(\mathtt{e}_{\mathtt{ij}}) - \mathtt{negative}(\mathtt{e}_{\mathtt{ij}})$$

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

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


IT'S OVER
IT'S FINALLY OVER
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Summary

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- 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?