Autoencoders and Restricted Boltzmann Machines

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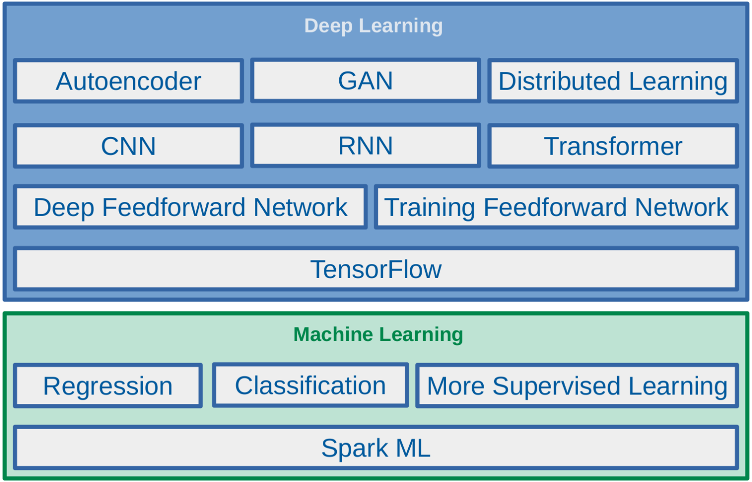
The Course Web Page

https://id2223kth.github.io

https://tinyurl.com/y6kcpmzy

Where Are We?



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

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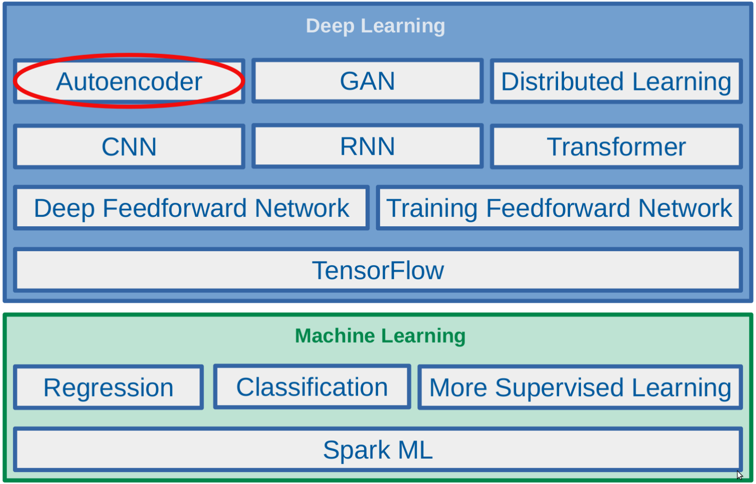
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Let's Start With An Example

- 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

$$\texttt{Seq1} : 40, 27, 25, 36, 81, 57, 10, 73, 19, 68$$

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

- 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.

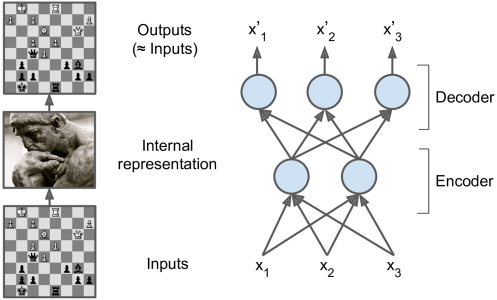
- 1970, W. Chase and H. Simon
- They observed that expert chess players were able to memorize the positions of all the pieces in a game by looking at the board for just 5 seconds.

- 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

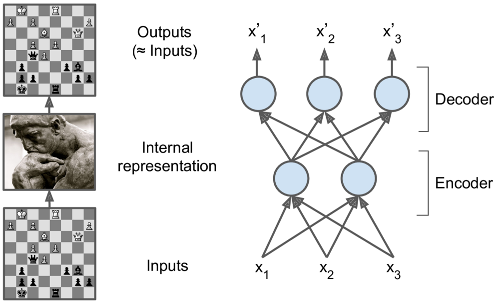
Autoencoders (1/5)

- 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.



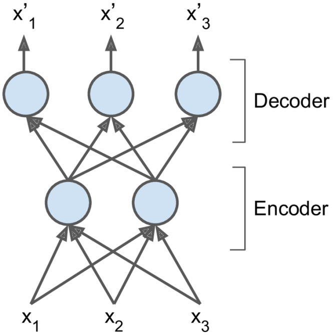
Autoencoders (2/5)

- 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.



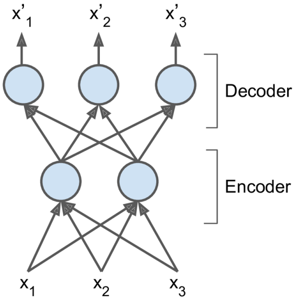
Autoencoders (3/5)

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



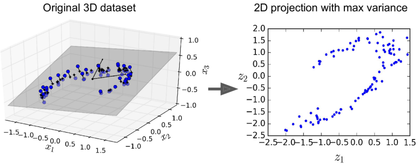
Autoencoders (4/5)

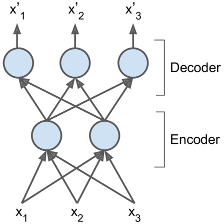
- Autoencoders are designed to be unable to learn to copy perfectly.
- The models are forced to prioritize which aspects of the input should be copied, they often learn useful properties of the data.



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.





Different Types of Autoencoders

- Stacked autoencoders
- Denoising autoencoders
- Sparse autoencoders
- Variational autoencoders

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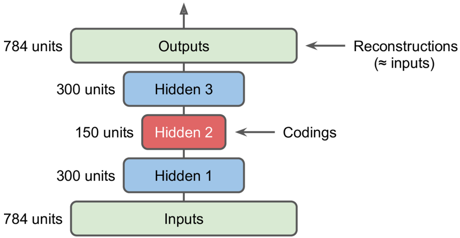
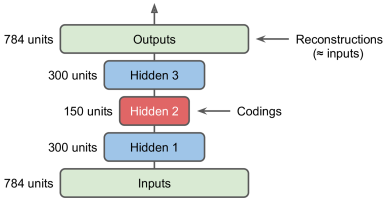
Stacked Autoencoders (1/3)

- 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)

```
stacked_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dense(100, activation="relu"),
    keras.layers.Dense(30, activation="relu"),
])
stacked_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="relu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])

model = keras.models.Sequential([stacked_encoder, stacked_decoder])
```

Different Types of Autoencoders

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- Denoising autoencoders
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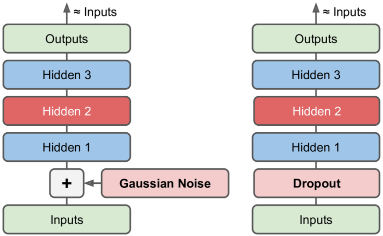
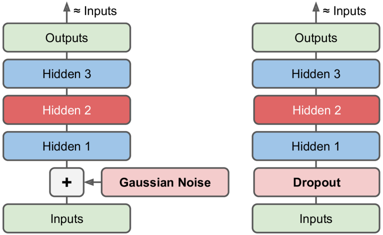
Denoising Autoencoders (1/4)

- 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 (2/4)

- 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 (3/4)

```
denoising_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dropout(0.5),
    keras.layers.Dense(100, activation="relu"),
    keras.layers.Dense(30, activation="relu")
])
denoising_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="relu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])

model = keras.models.Sequential([denoising_encoder, denoising_decoder])
```

Denoising Autoencoders (4/4)

```
denoising_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.GaussianNoise(0.2),
    keras.layers.Dense(100, activation="relu"),
    keras.layers.Dense(30, activation="relu")
])
denoising_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="relu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])

model = keras.models.Sequential([denoising_encoder, denoising_decoder])
```

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Sparse Autoencoders (1/2)

- Adding an appropriate term to the cost function to push the autoencoder to reducing the number of active neurons in the coding layer.
- This forces the autoencoder to represent each input as a combination of a small number of activations.
- As a result, each neuron in the coding layer typically ends up representing a useful feature.

Sparse Autoencoders (2/2)

```
sparse_l1_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dense(100, activation="selu"),
    keras.layers.Dense(300, activation="sigmoid", activity_regularizer=keras.regularizers.l1(1e-3))
])

sparse_l1_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="selu", input_shape=[300]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])

model = keras.models.Sequential([sparse_l1_encoder, sparse_l1_decoder])
```

Different Types of Autoencoders

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Variational Autoencoders (1/6)

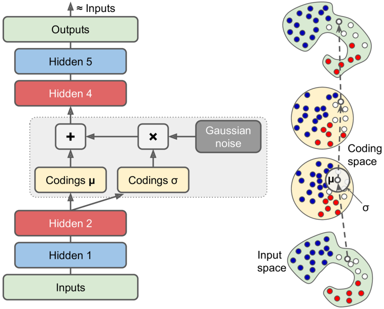
- Variational autoencoders are probabilistic autoencoders.
- Their outputs are partly determined by chance, even after training.
  - As opposed to denoising autoencoders, which use randomness only during training.
- They are generative autoencoders, meaning that they can generate new instances that look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

Variational Autoencoders (2/6)

- 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 (3/6)

- 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.
  - $latent\_loss = -\frac{1}{2}\sum_{1}^{K}(1 + log(\sigma_i^2) - \sigma_i^2 - \mu_i^2)$

Variational Autoencoders (4/6)

- Encoder part

```
inputs = keras.layers.Input(shape=[28, 28])
z = keras.layers.Flatten()(inputs)
z = keras.layers.Dense(150, activation="relu")(z)
z = keras.layers.Dense(100, activation="relu")(z)
codings_mean = keras.layers.Dense(10)(z)
codings_log_var = keras.layers.Dense(10)(z)
codings = Sampling()([codings_mean, codings_log_var]) # normal distribution
variational_encoder = keras.models.Model(inputs=[inputs], outputs=[codings])
```

Variational Autoencoders (5/6)

- Decoder part

```
decoder_inputs = keras.layers.Input(shape=[codings_size])
x = keras.layers.Dense(100, activation="relu")(decoder_inputs)
x = keras.layers.Dense(150, activation="relu")(x)
x = keras.layers.Dense(28 * 28, activation="sigmoid")(x)
outputs = keras.layers.Reshape([28, 28])(x)
variational_decoder = keras.models.Model(inputs=[decoder_inputs], outputs=[outputs])
```

Variational Autoencoders (6/6)

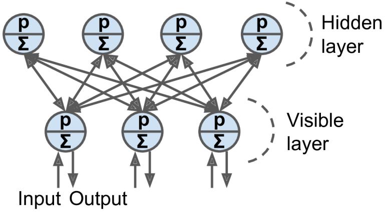
```
codings = variational_encoder(inputs)
reconstructions = variational_decoder(codings)
model = keras.models.Model(inputs=[inputs], outputs=[reconstructions])

latent_loss = -0.5 * K.sum(1 + codings_log_var - K.exp(codings_log_var)
                          - K.square(codings_mean), axis=-1)
model.add_loss(K.mean(latent_loss) / 784.)
```


S = k. log W
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.



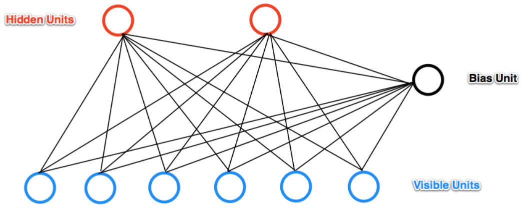
Let's Start With An Example

RBM Example (1/11)

- 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 neurons (hidden neurons) underlying movie preferences, e.g., SF/fantasy and Oscar winners

RBM Example (2/11)

- Our RBM would look like the following.



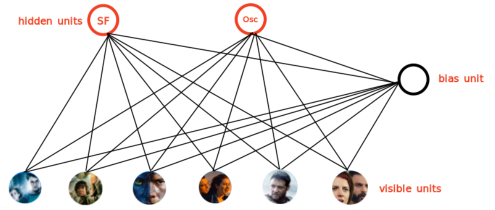
RBM Example (3/11)

- Alice: (HP=1, Avatar=1, LOTR=1, Glad=0, Titan=0, Sep=0), Big SF fan.
- Bob: (HP=1, Avatar=0, LOTR=1, Glad=0, Titan=0, Sep=0), SF fan, but not Avatar.
- Carol: (HP=1, Avat=1, LOTR=1, Glad=0, Titan=0, Sep=0), Big SF fan.
- David: (HP=0, Avat= 0, LOTR=1, Glad=1, Titan=1, Sep=1), Big Oscar winners fan.
- Eric: (HP=0, Avat=0, LOTR=1, Glad=1, Titan=0, Sep=1), Oscar winners fan, but not Titanic.
- Fred: (HP=0, Avat=0, LOTR=1, Glad=1, Titan=1, Sep=1), Big Oscar winners fan.

RBM Example (4/11)

- 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:

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



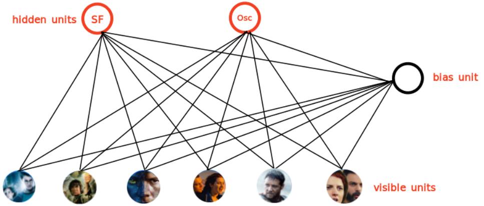
RBM Example (5/11)

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

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

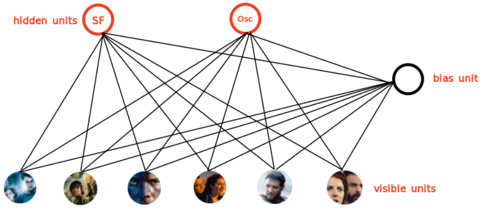
$$p(h_j) = \text{sigmoid}(a(h_j)) = \frac{1}{1 + e^{-a(h_j)}}$$

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



RBM Example (6/11)

- 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 (7/11)

- 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.

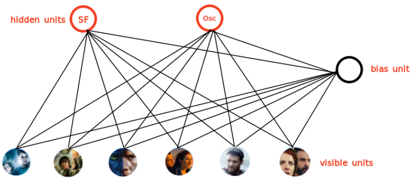
$$a(v_i) = \sum_j w_{ij} h_j$$

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

- 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.

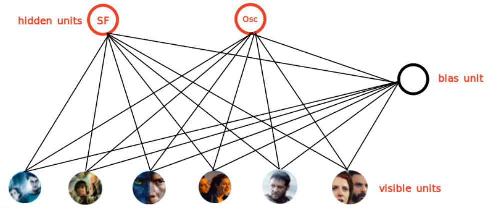
RBM Example (8/11)

- How do we learn the connection weights $\mathtt{w}_{\mathtt{ij}}$ 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.



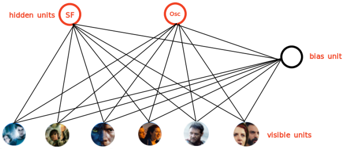
RBM Example (9/11)

- 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 (10/11)

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

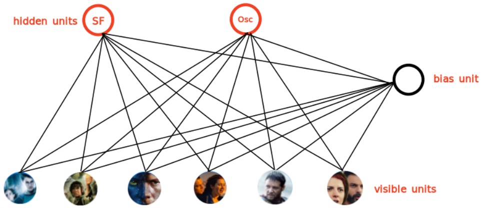


RBM Example (11/11)

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

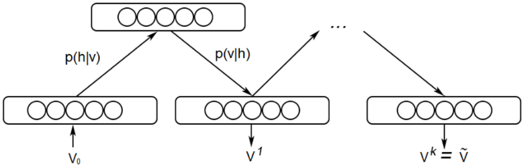
$$\mathtt{w_{ij}} = \mathtt{w_{ij}} + \eta(\mathtt{positive}(\mathtt{e_{ij}}) - \mathtt{negative}(\mathtt{e_{ij}}))$$

- 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 **v**, compute $p(\mathbf{h}|\mathbf{v})$.
- Knowing the hidden values **h**, we use $p(\mathbf{v}|\mathbf{h})$ for prediction of new input values **v**.
- This process is repeated k times.



RBM Training (2/2)

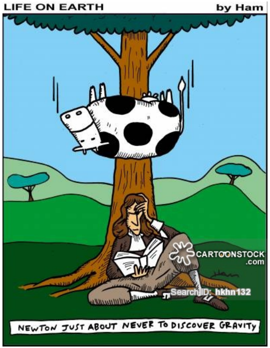
- Step 2, contrastive divergence: what we have done in step 7.
  - Just a fancy name for approximate gradient descent.

$$\mathbf{w} = \mathbf{w} + \eta(\texttt{positive}(\mathbf{e}) - \texttt{negative}(\mathbf{e}))$$

More Details about RBM

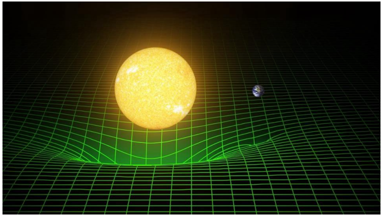
Energy-based Model (1/3)

- 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.

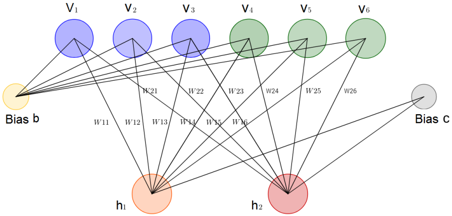


Energy-based Model (3/3)

- The energy function for the RBMs is defined as:

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

- $\mathbf{v}$ and $\mathbf{h}$ represent the visible and hidden units, respectively.
- $\mathbf{w}$ represents the weights connecting visible and hidden units.
- $\mathbf{b}$ and $\mathbf{c}$ are the biases of the visible and hidden layers, respectively.



RBM is a Probabilistic Model (1/2)

- The probability of a certain state of $\mathbf{v}$ and $\mathbf{h}$:

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

- In physics, the joint distribution $p(\mathbf{v}, \mathbf{h})$ is known as the Boltzmann Distribution or Gibbs Distribution.

- 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 $\mathbf{h}$.

RBM is a Probabilistic Model (2/2)

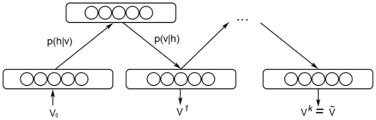
- It is difficult to calculate the joint probability due to the huge number of possible combination of **v** and **h**.

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

- Much easier is the calculation of the conditional probabilities of state **h** given the state **v** and vice versa (Gibbs sampling)

$p(\mathbf{h}|\mathbf{v}) = \Pi_i p(h_i|\mathbf{v})$

$p(\mathbf{v}|\mathbf{h}) = \Pi_j p(v_j|\mathbf{h})$



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 $p(\mathbf{v}, \mathbf{h})$, in a way that the training vectors have high probability $p(\mathbf{v})$.

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

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

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

Learning in Boltzmann Machines (2/2)

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

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

- Then, we can update the weight $\mathbf{w}$ as follows:

$$\mathtt{w}_{\mathtt{ij}}^{(\mathtt{next})} = \mathtt{w}_{\mathtt{ij}} + \eta(\mathtt{positive}(\mathtt{e}_{\mathtt{ij}}) - \mathtt{negative}(\mathtt{e}_{\mathtt{ij}}))$$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IT'S FINALLY OVER
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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. 17)

Questions?