

Week 6: Decision Trees and Variational Autoencoders

<http://mlvu.github.io>

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1 Decision trees

Imagine you do a newspaper round to help you get through these lean times. On your round, you encounter a number of dogs that either bark or (try to) bite. The dogs are described by the following binary features: *Heavy*, *Smelly*, *Big* and *Growling*. Consider the following set of instances:

Heavy	Smelly	Big	Growling	Bites
No	No	Yes	No	No
No	No	No	No	No
Yes	Yes	Yes	Yes	No
Yes	No	Yes	Yes	Yes
No	Yes	No	No	Yes
No	No	No	Yes	Yes
No	No	Yes	Yes	Yes
Yes	Yes	Yes	No	Yes

question 1: What is the entropy of the target value *Bites* in the data?

question 2: Which attribute would the ID3 algorithm choose to use for the root of the tree (without pruning)?

question 3: What is the information gain of the attribute you chose in the previous question?

question 4: Draw the full decision tree that would be learned for this data using ID3 without pruning.

question 5: Suppose three new dogs appear in your round as listed in the table below. Classify them using the tree from the previous question.

Dog	Heavy	Smelly	Big	Growling	Bites
Buster	Yes	Yes	Yes	Yes	?
Pluto	No	Yes	No	Yes	?
Zeus	Yes	Yes	No	No	?

question 6: Someone proposes a new scheme to prevent overfitting: she suggests to set a pre-defined maximum depth for the decision trees. When the standard algorithm reaches this depth, it terminates. Could this help to prevent overfitting? Why (not)?

question 7: In the maximum depth scheme introduced above, how would you determine a good value for the maximum depth for a given data set?

question 8: Why can't we apply L1-regularization to this decision tree learning problem?

2 Variational autoencoders

The maximum likelihood principle tells us to optimize the quantity $p(\mathbf{x} | \theta)$ as a function of θ (the model parameters). For complex models, this does not usually lead to a closed form solution. Instead, we will rewrite the maximum likelihood objective using the following decomposition.

$$\ln p(\mathbf{x} | \theta) = L(\mathbf{q}, \theta) + \text{KL}(\mathbf{q}, p)$$

with

$\mathbf{q}(z | \mathbf{x})$ any distribution on z

$\text{KL}(\mathbf{q}, p)$ the Kullback-Leibler divergence¹

between $\mathbf{q}(z | \mathbf{x})$ and $p(z | \mathbf{x}, \theta)$

$$L(\mathbf{q}, \theta) = \mathbb{E}_{\mathbf{q}} \ln \frac{p(\mathbf{x}, z | \theta)}{\mathbf{q}(z | \mathbf{x})}$$

¹The KL divergence can be defined using \log_2 or using \ln . The first leads to a value in *bits*, the second to a value in the slightly more abstract unit of *nats*. That is, the information distance between the two distributions is the same, but expressed in different units. In the context of the VAE, the natural logarithm \ln is preferred, mainly because it cancels out neatly against the exponent in the pdf of the normal distribution.

We will first prove that this equality holds. We start with the right hand side, fill in the components, and derive the left-hand side.

question 9: Fill in the blanks. We have written everything in terms of *expectations* \mathbb{E} to simplify the notation. The expectation is over the random variable \mathbf{z} , while \mathbf{x} has some definite value. Note that $\mathbb{E}f(\mathbf{z}) + \mathbb{E}g(\mathbf{z}) = \mathbb{E}[f(\mathbf{z}) + g(\mathbf{z})]$.

$$\begin{aligned}
 L(\mathbf{q}, \theta) + \text{KL}(\mathbf{q}, \mathbf{p}) &= \mathbb{E}_{\mathbf{q}} \ln \frac{p(\mathbf{x}, \mathbf{z} | \theta)}{q(\mathbf{z} | \mathbf{x})} - \mathbb{E}_{\mathbf{q}} \ln \frac{p(\mathbf{z} | \mathbf{x}, \theta)}{q(\mathbf{z} | \mathbf{x})} \\
 &= \dots \\
 &= \mathbb{E}_{\mathbf{q}} \ln p(\mathbf{x}, \mathbf{z} | \theta) - \mathbb{E}_{\mathbf{q}} \ln p(\mathbf{z} | \mathbf{x}, \theta) \\
 &= \mathbb{E}_{\mathbf{q}} \ln \frac{p(\mathbf{x}, \mathbf{z} | \theta)}{p(\mathbf{z} | \mathbf{x}, \theta)} = \dots \\
 &= \mathbb{E}_{\mathbf{q}} \ln p(\mathbf{x} | \theta) = \ln p(\mathbf{x} | \theta)
 \end{aligned}$$

In EM, we search by alternately (1) optimizing $L(\mathbf{q} | \theta)$ with respect to θ and (2) setting \mathbf{q} equal to \mathbf{p} (so that the KL term becomes zero).

question 10: For the variational autoencoder, we cannot (easily) perform this last step. Why not?

Instead, we *approximate* $p(\mathbf{z} | \mathbf{x}, \theta)$ with a neural network $q_{\mathbf{v}}(\mathbf{z} | \mathbf{x})$ that produces a distribution on \mathbf{z} given some \mathbf{x} . We call the neural network computing $p(\mathbf{x} | \mathbf{z}, \theta)$ $p_{\mathbf{w}}(\mathbf{x} | \mathbf{z})$, to make the notation a little more friendly. Here, \mathbf{w} , stands for all parameters of the \mathbf{p} network, and \mathbf{v} stands for all parameters of the \mathbf{q} network.²

This gives us an auto-encoder-like structure. An input is mapped to a distribution $q_{\mathbf{v}}(\mathbf{z} | \mathbf{x})$ by the **encoder**. We sample a single \mathbf{z} from this distribution and pass it through the **decoder** $p_{\mathbf{w}}(\mathbf{x} | \mathbf{z})$ to produce a distribution on \mathbf{x} (see the **slides** for diagrams).

To find a way to train such an architecture, we turn again to our decomposition of the likelihood. In our new notation:

$$\ln p_{\mathbf{w}}(\mathbf{x}) = L(\mathbf{v}, \mathbf{w}) + \text{KL}(\mathbf{q}, \mathbf{p}) .$$

²We've turned θ into \mathbf{w} and added parameters \mathbf{v} for our approximation \mathbf{q} on the conditional distribution on \mathbf{z} . We've also taken the parameters out of the conditional, because we will always talk about the function "given the parameter"; we will never talk about the probability on the parameters themselves.

The KL divergence term is difficult to compute: it's an expectation, and it contains the function $p_{\mathbf{w}}(\mathbf{z} | \mathbf{x})$ which requires us to invert the **decoder** neural network (that is, to reason about the inputs given the outputs).

However, because the KL divergence is always positive, we know that

$$\ln p_{\mathbf{w}}(\mathbf{x}) \geq L(\mathbf{v}, \mathbf{w})$$

for any $q_{\mathbf{v}}$ we choose. This is why L is called the variational *lower bound*.³ If we choose our parameters \mathbf{w}, \mathbf{v} to maximize L , we are also, indirectly, maximizing $\ln p_{\mathbf{w}}(\mathbf{x})$.⁴

To do so, we rewrite $L(\mathbf{v}, \mathbf{w})$ into two separate terms: a KL divergence and an expectation:

$$L(\mathbf{v}, \mathbf{w}) = -\text{KL}(q_{\mathbf{v}}(\mathbf{z} | \mathbf{x}), p_{\mathbf{v}}(\mathbf{z})) + \mathbb{E}_{q_{\mathbf{v}}} \ln p_{\mathbf{w}}(\mathbf{x} | \mathbf{z})$$

question 11: Show that this equation holds. That is, rewrite the left part into the right. We will assume that all expectations are over q .

$$\begin{aligned} L(\mathbf{v}, \mathbf{w}) &= \mathbb{E}_q \ln \frac{p_{\mathbf{w}}(\mathbf{x}, \mathbf{z})}{q_{\mathbf{v}}(\mathbf{z} | \mathbf{x})} \\ &= \dots \\ &= \dots \\ &= \dots \\ &= \mathbb{E} \ln p_{\mathbf{w}}(\mathbf{x} | \mathbf{z}) - [\mathbb{E} \ln q_{\mathbf{v}}(\mathbf{z} | \mathbf{x}) - \mathbb{E} \ln p_{\mathbf{w}}(\mathbf{z})] \\ &= \mathbb{E} \ln p_{\mathbf{w}}(\mathbf{x} | \mathbf{z}) - \text{KL}(q_{\mathbf{v}}(\mathbf{z} | \mathbf{x}), p_{\mathbf{w}}(\mathbf{z})) \end{aligned}$$

Thus, to optimize our variational autoencoder, we should maximize L . In other words, $-L$ is our loss function. The only problem left to solve is that the second term is an expectation (which we cannot compute explicitly).

question 12: How is this solved in practice?

³The word *variational* comes from the fact that one of its arguments, q , is a function (the calculus of functions is called *variational* calculus). For our purposes, this distinction doesn't matter much, since the function q is defined by a set of parameters \mathbf{v} , so ultimately we will take the derivative over those parameters, as we are used to.

⁴How close the lower bound L comes to the true value $\ln p_{\mathbf{w}}(\mathbf{x})$ depends on how well our encoder network $q_{\mathbf{v}}$ approximates the true conditional distribution on \mathbf{z} : $p_{\mathbf{w}}(\mathbf{z} | \mathbf{x})$. I.e. how small the KL term in the original decomposition is.