Bayesian Neural Networks and Probalistic Programming

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Water Center NN Meetings

Week 5: Oct. 17th, 2017

Disclaimer

Similiar to the week 1 presentation:

- None of this content is original; it is all adapted from Sections 1.6, 9.4 and 10.1 in Bishop 2006, as well as extensively from Edward's documentation at edwardlib.org (Tran et al. 2016), but any mistakes or typos are certainly my own.
- This is only intended for use within CWC, just because there is a lot of stuff I don't fully understand so there might be some errors that need to be ironed out. I think of it as a starting point that will hopefully inspire some future discussions which will help us learn this stuff together.

Differences between Bayesian Neural Nets (BNN) and the Neural Nets we've looked at?

- BNN are essentially the same, except any weights or parameters in the neural network will be random variables with a prior distribution.

Advantages/disadvantages of BNN

- Advantages
  - Model will represent uncertainty.
  - In some applications, BNN result in better models for data-sparse problems than other methods (including non-Bayesian neural nets, see Xiong, Barash, and Frey 2011 for example).
- Disadvantages
  - Numerical methods can be more complicated and some problems are intractable.
  - Sensitivity to prior?
    - Edward Box advocates critisizm of model (including choice of prior) which could overcome this (Box 1982).
  - Seems like BNN are a little less "plug and play." Hyperparameters, step sizes, etc. might need to be adjusted to get reasonable fits, and numerical methods for inference seem less universal (forum discourse.edward.org has some example issues users come across).

Pause

- We'll now look at a popular numerical method for inference in Bayesian problems, from the bigger picture fundamentals (taking an information theory perspective that was new to me) down to the numerical implementation.
- It's kind of dense so if it's more useful to skip to the practical exercises say the word!

Introduction - Information Theory (see section 1.6 in Bishop)

- Consider the amount of information gained/learned by an event or observation (we'll call x). We would receive more new information from a very surprising event than an event we expect (because we already know something about the expected event).
- So if we want to quantify this "amount of information" contained in an event we should use a function of the probability of the event ($p(x)$). The amount of information we'll call a function $h(\cdot)$, which will be a function of $p(x)$.

Guidance for the functional from of $h(\cdot)$

- If two events x and y are independent, then the amount of information gained by both events should be $h(x, y) = h(x) + h(y)$.
- We also know that the joint probability of x and y's occurrence would be: $p(x, y) = p(x)\ p(y)$.
- So the question is, what function $\hat{h}$ satisfies: $h(x, y) = \hat{h}(p(x)\ p(y)) = \hat{h}(p(x)) + \hat{h}(p(y))$?

Information Entropy

- $\hat{h}(\cdot) = \log(\cdot)$ satisfies
  $h(x, y) = \hat{h}(p(x)\, p(y)) = \hat{h}(p(x)) + \hat{h}(p(y))$, so
  $h(\cdot) = \log(p(\cdot))$.
- It's desirable for h to be positive, so because $0 \leq p \leq 1$, lets make it $h(\cdot) = -\log p(\cdot)$.
- Now say we have a bunch of random variables x for which we want to know the average amount of information (i.e. expectation of $h(x)$). This would be given by:

$$H[x] = -\sum_{x} p(x) \log p(x)$$

- This is known as the *entropy* of x.
- Extending this to continuous variables gives the *differential entropy*:

$$H[x] = -\int p(x)\, \log p(x)\, dx$$

[Bishop 2006, Shannon 1948]

So what does information entropy look like?

- From thermodynamics and statistical mechanics we have some idea of entropy as a measure of the disorder or randomness in a system. For information theory it is similar.[1]

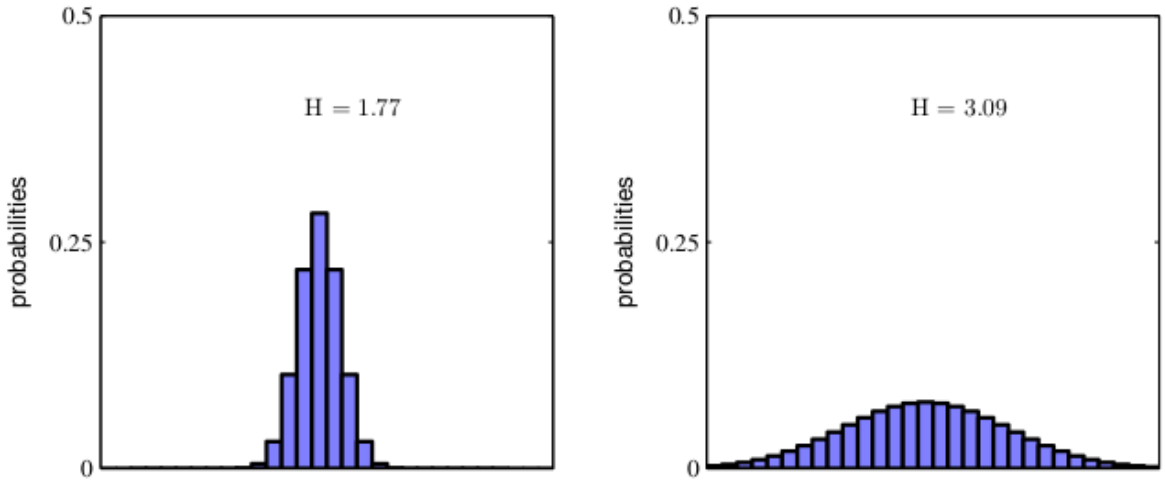

Figure 1: From Bishop 2006: Histograms of two probability distributions over thirty bins illustrating the higher value of entropy H for the broader distribution. The largest entropy would arise from a uniform distribution that would give $H = -\ln 1/30 = 3.40$

[1] von Neumann told Shannon he should also call it entropy because "nobody knows what entropy really is, so in any discussion you will always have an advantage."

Kullback-Leibler divergence

- Why should we even care about information theory or entropy?
  - Because we can use entropy ideas to approximate inference on a probalistic model (e.g. a Bayesian neural net), given data.
  - Say we have some phenomenon with a true probability distribution $p(x)$, which we are approximating with some [possibly parametric] distibution $q(x)$.
  - Then the additional necesary information required to communicate the value of x as consequence of using $q(x)$ would be:

$$\begin{aligned} KL(p\|q) &= -\int p(x) \ln q(x) dx - \left(-\int p(x) \ln p(x) dx\right) \\ &= -\int p(x) \ln \frac{q(x)}{p(x)} dx \end{aligned} \tag{1}$$

This is known as relative entropy or Kullback-Leibler (KL) divergence (Kullback and Leibler 1951).

Properties of Kullback-Leibler divergence

- Note that it is not a symmetrical quantity (e.g. $KL(p\|q) \neq KL(q\|p)$).
- Also, $KL(p\|q) \geq 0$,
- and $KL(p\|q) = 0$ only if p and q are identical (see Bishop 2006 for proof).
- So practically speaking KL diverpgence is very useful as a cost function quantifying the similarity between two probability distributions.

Equivalence of KL divergence and negative log liklihood

- Say we have N observations of data x_n from some unknown probaility distribution $p(x)$.
- We want to try to approximate $p(x)$ with a parametric disribution $q(x|\theta)$, by minimizing the KL diverence which can be approximated by:

$$KL(p\|q) \simeq \frac{1}{N}\sum_{n=1}^{N}[-\ln q(x_n|\theta) + In(p(x_n))] \tag{2}$$

- The second term is not a function of θ, and the first term is just the negative log liklihood. So for this example, minimizing KL-divergence is the same as minimizing the negative log liklihood, which we saw in Week 1!

KL divergence for Bayesian problems

- Say we have some group of latent variables z that define a hidden structure behind our data x. We can use Bayes' rule to define the distritbution of z given our observed data x (the *posterior*):

$$p(z \mid x) = \frac{p(x, z)}{\int p(x, z) dz} = \frac{p(x|z)p(z)}{p(x)}$$

- The main computational problem in calculating the posterior is that the normalizing constant is usually intractable. So instead of calcualting the posterior we will approximate the posterior.

Approximating the posterior

- We can approximate the posterior $p(z \mid x)$ with some probability distribution $q(z; \lambda)$, where q is a distribution of the latent varibles z parameterized by λ.
- Fortunately, we have already defined a tool (KL-divergence) that is a measure fo the difference between two probability distributions.
- So the problem then becomes:

$$\lambda^* = \text{argmin}_\lambda \text{divergence}(p(z|x), q(z; \lambda))$$

- Which we will frame as:

$$\lambda^* = \text{argmin}_\lambda \text{KL}(q(z; \lambda), p(z|x))$$

- But, we still have $p(z|x)$ so we need to get rid of that.

[Tran et al. 2016]

Minimizing KL-divergence

- To get rid of dependence of $p(z|x)$ we can use:

$$\log p(x) = KL(q(z;\lambda) \| p(z|x)) + \mathop{\mathbb{E}}_{q(z;\lambda)} [\log p(x,z) - \log q(z;\lambda)]$$

  - because $\log p(x)$ is invariant to λ, we can subtract this from $\mathrm{KL}(q(z;\lambda), p(z|x))$ without affecting λ^*.
  - in which case we are left with:

$$\lambda^* = \mathrm{argmin}_\lambda - \mathop{\mathbb{E}}_{q(z;\lambda)} [\log p(x,z) - \log q(z;\lambda)]$$

- So minimizing KL-divergence is the same as maximizing:

$$\mathrm{ELBO}(\lambda) = \mathop{\mathbb{E}}_{q(z;\lambda)} [\log p(x,z) - \log q(z;\lambda)]$$

  Where ELBO is an acronym standing for the "Evidence Lower Bound."

[Tran et al. 2016]

Maxmimizing ELBO using score function gradient

- Gradient descent/ascent is used to maximize ELBO. We are then interested in:

$$\nabla_\lambda ELBO(\lambda) = \nabla_\lambda \mathop{\mathbb{E}}_{q(z;\lambda)} [\log p(x,z) - \log q(z;\lambda)]$$

- This can be rewritten:

$$\nabla_\lambda ELBO = \mathop{\mathbb{E}}_{q(z;\lambda)} \nabla_\lambda \log q(z;\lambda) \left(\log p(x,z) - \log q(z;\lambda)\right) \tag{3}$$

- Where so long as we know the score function $\nabla_\lambda \log q(z;\lambda)$ we can use Monte Carlo integration to estimate both ELBO and its gradient:
  1. Draw S samples z_s from $q(z;\lambda)$.
  2. evaluate the terms in equation 3 using z_s.
  3. compute the empiracle mean across the samples of the evaluated terms from (2).

Gradient descent for ELBO

- From the previous slide: if we know the score function $\nabla_\lambda \log q(z;\lambda)$ we can use Monte Carlo integration to estimate both ELBO and its gradient:
  1. Draw S samples z_s from $q(z;\lambda)$.
  2. evaluate the terms in equation 3 using z_s.
  3. compute the empiracle mean across the samples of the evaluated terms from (2).
- Which gives the following estimate of the gradient:

$$\nabla_\lambda ELBO(\lambda) \approx \frac{1}{S}\sum_{s=1}^{S}\left[\left(\log p(x,z_s) - \log q(z_s;\lambda)\right)\nabla_\lambda \log q(z_s;\lambda)\right]$$

Psudocode for ELBO gradient descent

$$\nabla_\lambda ELBO(\lambda) \approx \frac{1}{S}\sum_{s=1}^{S}\left[\left(\log p(x, z_s) - \log q(z_s;\lambda)\right)\nabla_\lambda \log q(z_s;\lambda)\right]$$

Algorithm 1 Black Box Variational Inference

Input: data x, joint distribution p, mean field variational family q.
Initialize λ randomly, $t = 1$.
repeat
  // **Draw** S **samples from** q
  for $s = 1$ **to** S **do**
    $z[s] \sim q$
  end for
  $\rho = t$th value of a Robbins Monro sequence
  $\lambda = \lambda + \rho \frac{1}{S}\sum_{s=1}^{S} \nabla_\lambda \log q(z[s] \mid \lambda)(\log p(x, z[s]) - \log q(z[s] \mid \lambda))$
  $t = t + 1$
until change of λ is less than 0.01.

Figure 2: Reproduced from Ranganath, Gerrish, and Blei 2014.

References

See sections 1.6, 9.4, and 10.1 in Bishop, and edwardlib.org


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