Information Theory, Inference, and Learning Algorithms Chapter 28 Summary

CSCI-GA 3033 Bayesian Machine Learning
New York University
Yilun Kuang

Sep 29, 2022

28. 1 Occam's Razor

Model Comparison and Occam's Razor

Occam's Razor is a general principle that favors simpler hypotheses that explain the data. There are various aesthetic, epistemological, or empirical justifications for the usage of the Occam's Razor. However, this report will show that if we adopt the procedure of Bayesian inference, Occam's Razor automatically follows as a consequence of the probability theory [1]. Specifically, consider the Bayesian model selection problem

$$\frac{p(\mathcal{H}_1|D)}{p(\mathcal{H}_2|D)} = \frac{p(\mathcal{H}_1)}{p(\mathcal{H}_2)} \frac{p(D|\mathcal{H}_1)}{p(D|\mathcal{H}_2)},$$

where $p(\mathcal{H}_i)$ is the prior over the hypothesis $\mathcal{H}_i$ and the probability of the data D given model $\mathcal{H}_i$——$p(D|\mathcal{H}_i)$——is called *model evidence*, or *marginal likelihood*.

The aesthetic, empirical, and epistemological justifications of the Occam's Razor can be encoded in the ratio $\frac{p(\mathcal{H}_1)}{p(\mathcal{H}_2)}$ such that simpler hypotheses are a-priori preferred. However, even if we assume equal priors $p(\mathcal{H}_1) = p(\mathcal{H}_2)$, the marginal likelihood $p(D|\mathcal{H}_*)$ still points us towards simplier models. This is because for the simplier hypothesis $\mathcal{H}_1$, the support of possible data that can be explained by the $\mathcal{H}_1$ must be smaller than a more complicated model $\mathcal{H}_2$. Since $p(D|\mathcal{H}_*)$ is a normalized probability distribution, the density is more concentrated in a smaller area for $\mathcal{H}_1$. Thus if both $\mathcal{H}_1$ and $\mathcal{H}_2$ explain the data, it automatically follows that $p(D|\mathcal{H}_1)$ is higher than $p(D|\mathcal{H}_2)$ when evaluated at the currently observed data. The following figure provides an illustration.

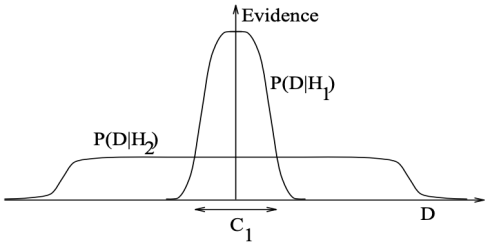


Figure 1: Model Evidence

[1] There are plethora of literatures in computational neuroscience and information theory that argues for the optimality of Bayesian inference as a model of perception and the necessity of efficient/sparse coding as a canonical neural mechanism for representation learning. In a way, the principle of parsimony embodied by the Occam's Razor has deep philosophical and scientific roots

Interlude: Marginal Likelihood for Deep Neural Networks

Let $\mathcal{H}_*$ be deep neural networks of various architectures. Generalization is determined by the 1) support and 2) inductive biases[2]. Support is the area where $p(D|\mathcal{H}_*)$ is non-zero. Inductive bias refers to the shape of the distribution, or the relative density in each location, over the support.

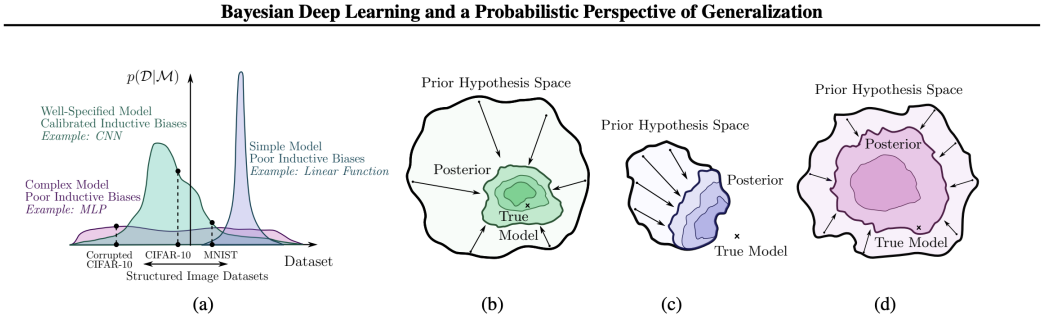


Figure 2. **A probabilistic perspective of generalization.** (a) Ideally, a model supports a wide range of datasets, but with inductive biases that provide high prior probability to a particular class of problems being considered. Here, the CNN is preferred over the linear model and the fully-connected MLP for CIFAR-10 (while we do not consider MLP models to in general have poor inductive biases, here we are considering a hypothetical example involving images and a very large MLP). (b) By representing a large hypothesis space, a model can contract around a true solution, which in the real-world is often very sophisticated. (c) With truncated support, a model will converge to an erroneous solution. (d) Even if the hypothesis space contains the truth, a model will not efficiently contract unless it also has reasonable inductive biases.

Figure 2: Model Evidence

A simple linear model has a small support as it can only represent a fixed set of functions. Linear model however has a particular inductive biases as the probability density is highly concentrated in one type of dataset. Thus if the data can be fully explained by a linear model, a MLP, and a CNN, by the Bayesian model selection we will prefer the linear model.

However, before observing any data, we should a-priori choose models with the largest support such that the data can be explained by the chosen model. The Occam's Razor comes only after the first inference step of model fitting. Thus we should choose CNN and MLP based on the marginal likelihood, which describes the probability of the observation under the prior model.

Notice that compared to MLP, CNN has a different inductive bias as it has higher density over datasets that obeys natural image statistics. Thus we can see that CNN is the best model here, as it both contains large support and also has good inductive biases for fast posterior contraction.

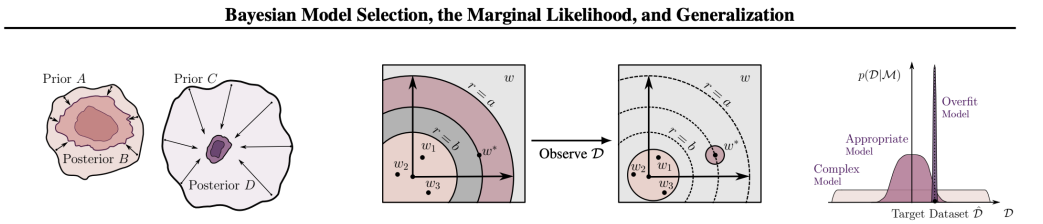
In practice, one should be cautious when doing model selection in deep learning with marginal likelihood. This is because marginal likelihood describes the probability of the observation given the prior model. In model selection, we usually compare trained neural networks, which roughly corresponds to a function draw from the posterior distribution. This is exemplified by the following figure[3], where the sharply contracted posterior D should be preferred over posterior B as it has a higher probability mass over the dataset. If we do marginal likelihood model selection based on the prior model, prior A is likely to be preferred even though its posterior B is worse than the posterior D induced by the prior C.

Interlude: Two Modes of Bayesian Inference

Bayesian Inference does not tell you how to invent models. Consider the problem settings where we would like to build an autonomous artificial agent capable of a variety of human and animal level tasks. The

[2]https://arxiv.org/pdf/2002.08791.pdf

[3]https://proceedings.mlr.press/v162/lotfi22a/lotfi22a.pdf



(a) Posterior contraction with a diffuse prior (b) Marginal likelihood underfitting (c) Marginal likelihood overfitting

Figure 1. **Pitfalls of marginal likelihood. (a)**: Prior B is vague, but contains easily identifiable solutions and quickly collapses to posterior D after observing a small number of datapoints. Prior A describes the data better than prior B, but posterior D describes the data better than posterior B. The marginal likelihood will prefer model A, but model C generalizes better. **(b)**: Example of misalignment between marginal likelihood and generalization. The marginal likelihood will pick prior scale b, and not include the best solution w^*, leading to suboptimal generalization performance. **(c)**: The complex model spreads its mass thinly on a broad support, while the appropriate model concentrates its mass on a particular class of problems. The overfit model is a δ-distribution on the target dataset $\hat{\mathcal{D}}$.

Figure 3: Model Evidence

most prominent route is self-supervised representation learning. Bayesian Inference, however, lets us 1) infer the optimal model parameters, or optimal functions and 2) infer what's the best model during the model selection phase.

The Mechanism of the Bayesian Razor: The Evidence and the Occam Factor

For frequentist, the maximum likelihood model choice prefer complex, over-parametrized models as it fits the data better but might generalizes poorly (take it with a grain of salt). Thus we need the Occam's Razor, which is embodied in the Bayesian inference as we'll show below.

There are two levels of inference in the Bayesian framework. The first level is the estimation of posterior measures on the parameters.

$$p(\mathbf{w}|D, \mathcal{H}_i) = \frac{p(D|\mathbf{w}, \mathcal{H}_i)p(\mathbf{w}|\mathcal{H}_i)}{p(D|\mathcal{H}_i)} \iff \text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

It's common to use gradient-based methods to find the maximum posterior $\mathbf{w}_{\text{MP}}$. We can then summarize the posterior distribution by the value of $\mathbf{w}_{\text{MP}}$, and error bars or confidence intervals on these best-fit parameters.

Error bars can be obtained from the curvature of the posterior by evaluating the Hessian at $\mathbf{w}_{\text{MP}}$, $\mathbf{A} = -\nabla\nabla \ln p(\mathbf{w}|D, \mathcal{H}_i)|_{\mathbf{w}_{\text{MP}}}$. We can then Taylor expand the log posterior probability with $\Delta\mathbf{w} = \mathbf{w} - \mathbf{w}_{\text{MP}}$.

$$p(\mathbf{w}|D, \mathcal{H}_i) \approx p(\mathbf{w}_{\text{MP}}|D, \mathcal{H}_i) \exp(-1/2\Delta\mathbf{w}^\top \mathbf{A}\Delta\mathbf{w})$$

i.e. the posterior can be locally approximated as a Gaussian with covariance matrix (equivalent to error bars) $\mathbf{A}^{-1}$.

The second level involves the inference process during model comparison.

$$p(\mathcal{H}_i|D) \propto p(D|\mathcal{H}_i)p(\mathcal{H}_i)$$

where

$$p(D|\mathcal{H}_i) = \int p(D|\mathbf{w}, \mathcal{H}_i)p(\mathbf{w}|\mathcal{H}_i)d\mathbf{w}$$

This integral can be approximated using the Laplace method by the peak of the integrand $p(D|\mathbf{w}, \mathcal{H}_i)p(\mathbf{w}|\mathcal{H}_i)$ times its width $\sigma_{\mathbf{w}|D}$:

$$\underbrace{p(D|\mathcal{H}_i)}_{\text{Evidence}} \approx \underbrace{p(D|\mathbf{w}_{\text{MP}}, \mathcal{H}_i)}_{\text{Best Fit Likelihood}} \times \underbrace{p(\mathbf{w}_{\text{MP}}|\mathcal{H}_i)\sigma_{\mathbf{w}|D}}_{\text{Occam Factor}}$$

Interpretation of the Occam Factor

Suppose $p(\mathbf{w}_{\text{MP}}|\mathcal{H}_i) = \frac{1}{\sigma_w}$, then the Occam Factor is given by

$$\text{Occam Factor} = \frac{\sigma_{w|D}}{\sigma_w}$$

which measures the factor by which the hypothesis space collapses when the data arrives. The Bayesian model comparison is an extension of the MLE model comparison as it's the likelihood itself multiplied by the Occam factor.

28. 2 Examples

Skipped

28. 3 Minimum Description Length (MDL)

The MDL framework can be viewed from a Bayesian perspective. One should prefer models that can communicate data in the smallest number of bits.

Remark: In fact, we can also connect this to the efficient / sparse coding ideas in neuroscience literatures (also Barlow-Twins). A criteria for learning representations is to have compact and efficient representations, i.e. the principle of parsimony and the maximal coding rate distortion idea. This is perhaps not as related to the model comparison itself but a reasonable desiderata in general.