Abstract

The predictive performance of any inferential model is critical to its practical success, but quantifying predictive performance is a subtle statistical problem. In this paper I show how the natural structure of any inferential problem defines a canonical measure of relative predictive performance and then demonstrate how approximations of this measure yield many of the model comparison techniques popular in statistics and machine learning.

Because any inferential method is built upon assumptions, one of the most important aspects of any statistical analysis is assessing the validity of the underlying assumptions. Although there are few model assessment approaches that claim to validate a model in isolation, there is a rich history of comparative techniques in the statistics literature, from visual residual analyses to scoring rules and predictive cross validation to the myriad of information criteria. The practical challenge in applying these methods, however, is in determining the ultimate accuracy of their assessments and hence which might be most appropriate to a given problem.

In this paper I demonstrate that any inferential system admits a canonical measure of comparative predictive performance, here termed a relative predictive performance score. Moreover, I show how many of the model comparison techniques in practice today arise as approximations to these canonical scores. This foundational perspective provides a common context for understanding the advantages and disadvantages of each technique both in theory and in practice.

After reviewing the basic assumptions common to most inferential techniques, in particular the assumptions of frequentist and Bayesian inference, I demonstrate first how relative predictive performance scores arise naturally from these assumptions and then how various approximations of these scores yield existing model comparison techniques. In the latter I emphasize how this foundational construction immediately identifies the practical consequences of each approximation.
1 Foundational Assumptions of Inference

The most fundamental assumption underlying any attempt at inference is the existence of some latent data generating process, \( \pi \), responsible for generating measurements. Formally we assume that measurements are drawn from some measurable space, \( (Y, \mathcal{Y}) \), and that the data generating process itself can be modeled mathematically by a single, time-invariant probability measure,

\[
\pi : \mathcal{Y} \to [0, 1].
\]

In order to make this construction as general as possible I impose no additional structure, such as a particular topology or metric, on \( Y \), nor make any philosophical interpretation of this latent data generating process, in particular its interpretation as an ontological truth or just an epistemological impression. Consequently the following results will hold regardless of any deeper meaning of the measurement process itself.

Inference is then a formal effort to learn the latent data generating process given a measurement, \( y \in Y \), by identifying \( \pi \) from the space of all probability measures, \( P \), on the measurement space. Unfortunately, exploring the entirety of \( P \) for any problem is far too unwieldy, and in order to construct practical inferential methods we first have to limit ourselves to a more manageable space of data generating processes.

An inferential model is the selection of a distinguished subset of data generating processes, \( X \subset P \); in the spirit of Dennis Lindley I refer to such subsets as small worlds \([1]\). As with the latent data generating process, I am careful not to assign any particular meaning to the small world – it can be a phenomenological model motivated by mathematical and practical convenience, a theoretical model motivated by a specific scientific hypothesis, or, as is most common in practice, a delicate combination of the two. In this paper I denote the measure corresponding to a given element of the small world, \( x \in X \), as

\[
\pi_x : \mathcal{Y} \to [0, 1].
\]

One assumption that I have explicitly not made is that the chosen small world need contain the latent data generating process (Figure \( 1 \)). In particular, assuming that the small world rarely, if ever, contains the latent data generation process formalizes the Boxian philosophy that “all models are wrong but some are useful” \([2]\). Although developments in computation and theory, such as statistical nonparametrics, have enabled the construction of increasingly complex models and less-small worlds, the intricacy of any realistic measurement should continue to inspire skepticism in the sufficiency of any small world.

From this perspective, the ultimate utility of any inferential procedure is not in whether it can find the latent data generating process exactly but rather in how well it can approximate the latent data generating process. In particular, the fidelity of a procedure is often judged based on its predictive performance. Exactly how we define predictive performance depends intimately on how inference is implemented, which itself depends on the fundamental interpretation of probability.
Figure 1: Inference requires the selection of a distinguished subset of data generating processes that (a) may or (b) may not contain the latent data generating process, $\pi$. The Boxian philosophy asserts that the former is impossible in practical problems but that we may still hope that some data generating process in $X$ will well-approximate $\pi$.

2 Inference in the Small World

We have already assumed that probability theory adequately describes the measurement process, but that does not have to be the only application of probability theory. While frequentist inference limits probabilities to the data, Bayesian inference also endows the small world with a probabilistic interpretation.

In the following sections I review the measure-theoretic construction of frequentist and Bayesian inference. The formality is a necessary evil in order to identify the canonical measures of predictive performance that do not rely on the additional structure of a particular measurement space.

2.1 Frequentist Inference

In frequentist inference probabilities are defined strictly as frequencies of repeatable events, namely measurements. Consequently probability theory applies to only the latent data generating process, $\pi$, and the data generating processes in the small world, $\{\pi_x\}$. Considered as a family of probability distribution functions on the measurement space, the small world,

$$\pi_x : X \times Y \rightarrow [0, 1],$$

is otherwise known as a likelihood function.

Given this rigid definition of probability, the only way we can construct a complete predictive distribution is by selecting a single element of the small world and utilizing the corresponding data generating process. One of the most prolific approaches to selecting such an element is with the use of estimators, functions of the data that identify some aspect of the latent data generating process. Formally, estimators are defined as maps from the measurement space to some auxiliary space, $\hat{e} : Y \rightarrow Z$. 

3
Given a set of estimators, $E$, we can quantify how well a given estimator identifies the latent data generating process with a loss function,

$$L : Y \times E \to \mathbb{R}.$$  

The corresponding risk of an estimator is defined as

$$R : X \times E \to \mathbb{R}$$

$$(x, \hat{e}) \mapsto \int_Y \pi_x(dy) L(y, \hat{e}),$$

and minimax estimators are defined by the optimality criterion,

$$\hat{e}_M = \arg\min_{\hat{e} \in E} \max_{x \in X} R(x, \hat{e}).$$

With a map $f : Z \to X$ we can then select a single element of the small world and define the subsequent predictive distribution for new data by

$$\tilde{\pi}_{Y|y} \equiv \pi_{f(\hat{e}_M(y))}.$$

For example, consider the circumstance where the small world contains the latent data generation process,

$$\pi = x_\pi \in X,$$

and take any map $g : X \to Z$ with a well-defined inverse, $g^{-1} : g(X) \to X$. If $Z$ is a metric space then a natural loss function is given by the distance function,

$$L(y, \hat{e}) = D(g(x_\pi), \hat{e}(y));$$

the resulting minimax estimator, $\hat{e}_M$, approximates the true value of the function, $g(x_\pi)$, which then identifies a unique element of the small world,

$$\hat{x} = g^{-1} \circ \hat{e}_M : Y \to X$$

$$y \mapsto g^{-1}(\hat{e}_M(y)).$$

Maximum likelihood estimators avoid the need for a loss function by using the likelihood itself. Given any reference measure, $\lambda$, with respect to which every element of the small world is absolutely continuous, the maximum likelihood estimator is defined as

$$\hat{x}_{\text{MLE}} : Y \to X$$

$$y \mapsto \arg\max_{x \in X} \frac{d\pi_x}{d\lambda}(y).$$
Provided that the maximum is unique, \( \hat{x}_{\text{MLE}} \) identifies a unique element of the small world and hence an unambiguous predictive distribution.

The practical utility of a frequentist estimator is a subtle issue. When the small world does not contain the latent data generating process, for example, any predictive distribution derived from an estimator will never be able to recover the latent data generating process exactly. Moreover, even if the small world does contain the true data generating process there is no guarantee that an estimator evaluated at a given measurement will identify it. A given estimator may be \emph{unidentified} and unable to select a single element of the small world at all, or it may simply be inaccurate or imprecise. In any case we must be skeptical of how well \( \pi_{Y|y} \) approximates the latent data generating process.

### 2.2 Bayesian Inference

Bayesian inference \[5,6\] considers a more general interpretation of probability that encompasses not just frequencies but any self-consistent system of uncertainty. Consequently we can assign probability distributions to not only the measurement space but also the small world itself given the choice of a \( \sigma \)-algebra, \( \mathcal{X} \), on \( X \).

From this perspective, the small world now defines a regular conditional probability distribution,

\[
\pi_{Y|x} : \mathcal{Y} \times X \to [0, 1],
\]

with respect to the canonical projection operator,

\[
\pi_x : Y \times X \to X,
\]

on the product space of measurements and the small world, \( Y \times X \). The difference between this regular conditional probability distribution and the frequentist likelihood function is largely one of interpretation and, following convention, I will refer to both objects as likelihoods.

Inference proceeds with the introduction of a \emph{prior distribution} over the small world,

\[
\pi_X : \mathcal{X} \to [0, 1],
\]

that encodes all information about the latent data generating process within the context of the small world before the current measurement is made. Together with the likelihood, the prior distribution defines a joint distribution on the product space of measurements and the small world, \( \pi_{Y \times X} \), and information about the small world given a measurement is encoded in the regular conditional probability distribution,

\[
\pi_{X|y} : \mathcal{X} \times Y \to [0, 1],
\]

defined with respect to the second canonical projection operator,

\[
\omega_Y : Y \times X \to Y.
\]
Conditioning $\pi_{X|y}$ on a given measurement, $y$, gives the posterior distribution over the small world,

$$
\pi_{X|y} = \left[ \frac{d\pi_{Y|x}}{d (\omega_Y)} \right] \pi_X.
$$

When $Y \sim X \sim \mathbb{R}^n$, the posterior density with respect to a reference Lebesgue measure is given by the celebrated Bayes’ Rule,

$$
\pi_{X|y}(x|y) = \frac{\pi_{Y|x}(y|x) \pi_X(x)}{\int_{\mathbb{R}^n} dx \pi_{Y|x}(y|x) \pi_X(x)}.
$$

Given the more general application of probability in Bayesian inference we can construct a predictive distribution not only by selecting a single element of the small world but also by averaging the elements of the small world with respect to a given probability distribution. The prior predictive distribution, for example, is given by weighting each element of the small world according to the prior distribution,

$$
\pi_{Y}^{\text{prior}}(d\tilde{y}) = \int_X \pi_X(dx) \pi_{Y|x}(d\tilde{y}, x).
$$

Similarly, the posterior predictive distribution is given by weighting each element of the small world according to the posterior distribution,

$$
\pi_{Y|y}^{\text{post}}(d\tilde{y}|y) = \int_X \pi_{X|y}(dx|y) \pi_{Y|X}(d\tilde{y}|x).
$$

Because it learns from the measured data, the posterior predictive distribution should be a better approximation of the latent data generating process provided that the modeling assumptions, such as the choice of the small world and the prior distribution, are compatible with the true data generating process.

As in frequentist inference, the performance of either predictive distribution depends critically on the assumptions in their construction. Some means of comparing the chosen predictive distribution to the latent data generating process is vital for validating the modeling assumptions and ensuring inferences that perform well in practice.

### 3 Validating Inference

Although the frequentist and Bayesian approaches have different means of inferring predictive distributions, they can both succumb to the same pathologies that jeopardize predictive performance.

The most obvious pathology is model misfit where the true data generating process is not contained within the small world, $\pi \notin X$, and any inferential method will be able to approximate the exact predictive distribution only so well (Figure 2). Even if the small
Figure 2: Because (a) frequentist estimators and (b) Bayesian prior and posterior distributions are limited to the small world, neither approach will be able to construct a predictive distribution capable of exactly modeling the latent data generating process, $\pi$, when it is not an element of the small world.

Figure 3: Even when the small world does contain the latent data generating process, $\pi$, inferences are not guaranteed to capture it. Here (a) a frequentist estimator evaluated at a given measurement strays from $\pi$ while (b) a Bayesian prior or posterior distribution concentrates away from $\pi$. In either case the predictive distributions will be biased away from the latent data generating process.

Consider, for example, the measurement space $Y = (\mathbb{R} \times \mathbb{R})^{N=12}$ with two data generating processes: a Gaussian distribution centered on a quartic polynomial

$$
y_{1,n} \sim U(-1, 1), \ y_{2,n} | y_{1,n} \sim \mathcal{N}\left(\sum_{k=0}^{4} c_k y_{1,n}^k \sigma^2\right), \ n = 1, \ldots, 12, \quad (1)
$$

and a Gaussian distribution centered on a constant,

$$
y_{1,n} \sim U(-1, 1), \ y_{2,n} \sim \mathcal{N}(c_0, \sigma^2), \ n = 1, \ldots, 12. \quad (2)
$$
Figure 4: Misfit occurs when an inferential model cannot capture the complexity of the latent data generating process, for example when models assuming the simple data generating process (2) are fit to (a) data generated according to the more complex process (1). Because the assumptions are too restrictive, the resulting (b) maximum likelihood predictive distribution and (c) posterior predictive distribution are poor approximations to the latent data generating process. Compare to Figure 2.

Misfit occurs when the measurement is generated from the more complex process (1) (Figure 4a) but the inferential models assume the simpler process (2); in this case the resulting predictive distributions (Figure 4b, c) will never be able to capture the latent data generating process. On the other hand, overfit occurs when the measurement is generating from the simpler process (Figure 5a) but the inferential models assume the more complex process. The resulting predictive distributions (Figure 5b, c) will overfit to the Gaussian noise, inducing a bias away from the latent data generating process. In both cases the Bayesian analysis uses the conjugate prior

$$\pi_X(c, \sigma) = \text{MultiNormalGamma}(\mu_0, \Lambda_0, \alpha_0, \beta_0)$$

with

$$\mu_0 = 0$$
$$\Lambda_0 = 0.001 \cdot I$$
$$\alpha_0 = 0.5$$
$$\beta_0 = 0.5.$$  

Reliable inferences consequently require some predictive validation to ensure that, even if the model misfits or overfits, the resulting predictive distribution approximates the latent data generating process sufficiently well. One immediate strategy is to test the model within a null hypothesis significance testing framework, rejecting if the measured data is sufficiently unlikely with respect to the inferred predictive distribution. By construction, however, we make no attempt to model anything outside of the small world, let alone its entire complement, which prevents us from constructing a valid alternative hypothesis.
Figure 5: Overfitting occurs when an inferential model has too much flexibility relative to the latent data generating process, for example when models assuming a complex data generating process (1) are fit to (a) data generating according to the simpler data generating process (2). Both the (b) maximum likelihood predictive distribution and (c) posterior predictive distribution recklessly fit to the Gaussian noise in the data, biasing predictions away from the latent data generating process. Compare to Figure 3.

needed to calibrate such tests. In order to quantify predictive performance without looking outside of the small world we need to compare the predictive distribution to the latent data generating process directly.

[7] considered many possible strategies for comparing predictive distributions to the latent data generating process, but almost all of them require endowing the small world with additional structure, such as a metric or a distinguished test function, that limits the ultimate scope of the validation. Only one of the approaches considered arises canonically from the general construction of inference – the Kullback-Leibler divergence [8]. In this section I discuss how the Kullback-Leibler divergence defines a measure of relative predictive performance, although one that cannot be computed in practice. I then consider a manipulation of the Kullback-Leibler divergence that defines scores of relative predictive performance that are amenable to approximations, and finally I show how various approximation strategies give rise to many of the model comparison techniques already popular in practice.

3.1 Relative Predictive Performance Measures

In order to construct a measure of predictive performance we have to compare some inferred predictive distribution, \( \tilde{\pi}_{Y|y} \), to the latent data generating process, \( \pi \). Without endowing the measurement space with any particular structure, the only canonical way of comparing two distributions, \( \mu \) and \( \nu \), on \( Y \) is with an \( f \)-divergence [9],

\[
D_f(\mu \parallel \nu) = \int_Y \nu(dy) f\left( \frac{d\mu}{d\nu}(y) \right),
\]

where
where \( f : \mathbb{R} \to \mathbb{R} \) is any convex function satisfying \( f(1) = 0 \). Moreover, the only \( f \)-divergence that respects any product structure of the measurement space and allows us to marginalize out irrelevant structure as necessary is the Kullback-Leibler divergence,

\[
\text{KL}(\mu || \nu) = -\int_Y \mu(dx) \log \frac{d\nu}{d\mu}(x).
\]

The Kullback-Leibler divergence vanishes only when the two measures are equal and monotonically increases as the two measures deviate, approaching infinity when \( \nu \) is not absolutely-continuous with respect to \( \mu \).

Because the Kullback-Leibler divergence is not symmetric there are two possible ways that we might use it to compare the latent data generating process and an inferred predictive distribution. Using the inferred predictive distribution as the base measure, \( \text{KL}(\tilde{\pi}_{Y|y} || \pi) \), considers the predictive performance only where \( \tilde{\pi}_{Y|y} \) concentrates and consequently does not penalize predictive distributions that completely ignore neighborhoods supported by \( \pi \). In an extreme limit, this divergence does not even penalize predictive distributions that are not absolutely continuous with respect to the latent data generating process. In order to truly assess the inferred predictive distribution we need to instead base the divergence on the latent data generating process itself,

\[
\text{KL}(\pi || \tilde{\pi}_{Y|y}) = -\int_Y \pi(dy) \log \frac{d\tilde{\pi}_{Y|y}}{d\pi}(\tilde{y}).
\]

Here we will use this form of the Kullback-Leibler divergence to quantify the validity of our modeling assumptions, but it can also be used to construct a more elaborate sensitivity analysis of those assumptions [10].

As with null hypothesis significance testing, the Kullback-Leibler divergence cannot be calibrated, in other words there is no canonical threshold below which we can declare our model assumptions valid. Unlike hypothesis testing, however, the difference between two divergences is meaningful, allowing us to quantify the relative performance of \( \tilde{\pi}_{Y|y} \) compared to some other predictive distribution. Although \( \text{KL}(\pi || \tilde{\pi}_{Y|y}) \) cannot be computed without assuming a priori knowledge of the true data generation process, we can manipulate the divergence into a more advantageous form without compromising its quantification of relative performance.

Let \( \lambda \) be any reference measure with respect to which both the true data generating process and the inferred predictive distribution are absolutely continuous. We can then define a relative predictive performance score as

\[
\delta(\pi || \tilde{\pi}_{Y|y}) = \text{KL}(\pi || \tilde{\pi}_{Y|y}) - \text{KL}(\pi || \lambda)
\]

\[
= -\int_Y \pi(dy) \log \frac{d\tilde{\pi}_{Y|y}}{d\lambda}(	ilde{y})
\]

\[
= -\mathbb{E}_\pi \left[ \log \frac{d\tilde{\pi}_{Y|y}}{d\lambda} \right].
\]
The difference between any relative predictive performance scores is the same as the difference of the equivalent Kullback-Leibler divergences and so they quantify the same relative performance, but because the densities \(d\tilde{\pi}_{Y|y}/d\lambda\) are independent of the latent data generating process these relative scores can be approximated using only sampled measurements from \(\pi\). Relative predictive performance scores also have the welcome interpretation as expected logarithmic score functions \([11, 5]\).

The ultimate utility of these relative predictive performance scores then depends on the accuracy and precision of the chosen approximation strategy.

### 3.2 Approximating Relative Predictive Performance Scores

Although relative predictive performance scores cannot be calculated exactly, their construction makes them amenable to a variety of approximations. For example, given an ensemble of \(N + 1\) measurements we could construct a Monte Carlo estimator,

\[
\hat{\delta}(\pi \mid \tilde{\pi}_{Y|y}) \approx -\frac{1}{N} \sum_{n=1}^{N} \log \frac{d\tilde{\pi}_{Y|y_{N+1}}}{d\lambda}(y_n),
\]

with vanishing bias and quantifiable variance. Unfortunately, in practice we rarely have an ensemble of measurements and instead have to consider approximations that utilize only a single measurement.

#### 3.2.1 Delta Estimators

An immediate approximation of relative predictive performance scores derives from making a delta approximation of the latent data generating process, \(\pi \approx \delta_y\), which gives

\[
\hat{\delta}_D(\pi \mid \tilde{\pi}_{Y|y}) \equiv -\log \frac{d\tilde{\pi}_{Y|y}}{d\lambda}(y).
\]

Using the same measurement to learn the model and then validate it introduces a bias that makes delta estimators susceptible to overfitting. Moreover, the underlying delta approximation typically induces a large variance in the estimator, making fine comparisons between models difficult if not impossible.

#### 3.2.2 Hold-out Estimators

More sophisticated estimates of relative predictive performance scores can be constructed by using the given measurement to simulate an ensemble of measurements.

Assuming that the measurement space has a product structure, \(Y = \prod_{n=1}^{N} Y_n\), any measurement can be partitioned in two subsets of size \(N_1\) and \(N_2\). Hold-out estimators use
one of these partitions, often denoted the training data, to infer a predictive distribution and the remaining partition, denoted the validation data, to construct a delta estimator,

\[ \hat{\delta}_H(\pi \parallel \tilde{\pi}_Y|y) \equiv - \log \left( \frac{d\tilde{\pi}_Y|y_1}{d\lambda}(y_2) \right)^{N/N_2} \]

\[ = - \frac{N}{N_2} \log \frac{d\tilde{\pi}_Y|y_1}{d\lambda}(y_2). \]

The simulated partitions in the validation data not only promise a more precise estimate but also admit the estimation of the estimator variance using the Monte Carlo standard error. This, however, comes with the assumption the naive scaling of the predictive density inferred from the training data is a reasonable approximation to the predictive density inferred from the full measurement. When data are sparse relative to the model complexity this assumption can severely bias the estimator; for example, predictive distributions inferred from small partitions are more susceptible to overfitting, artificially penalizing the predictive performance of model.

Moreover, the product structure of the measurement space necessary to construct hold-out estimators precludes many structured measurements, such as those arising from some hierarchical models, networks, and time series.

### 3.2.3 Jackknife Estimators

In order to compensate for some of the potential bias in hold-out estimators we can appeal to a jackknife estimator \cite{12} which averages over the possible assignments of training and validation data. Partitioning the measurement into \( K \) subsets of size \( M = N/K \), the jackknife estimator is given by

\[ \hat{\delta}_J(\pi \parallel \tilde{\pi}_Y|y) \equiv \frac{1}{K} \sum_{k=1}^{K} - \log \left( \frac{d\tilde{\pi}_Y|y\setminus y_k}{d\lambda}(y_k) \right)^{N/M} \]

\[ = \frac{1}{K} \sum_{k=1}^{K} - \log \left( \frac{d\tilde{\pi}_Y|y\setminus y_k}{d\lambda}(y_k) \right)^{K} \]

\[ = - \sum_{k=1}^{K} \log \frac{d\tilde{\pi}_Y|y\setminus y_k}{d\lambda}(y_k), \]

where \( y \setminus y_k \) are often denoted the \( k \)th training data and \( y_k \) the \( k \)th testing data. This approach can also be readily generalized to a bootstrap estimator \cite{13} which samples training and validation data with replacement.

The averaging over partitions typically reduces the bias of the relative predictive performance score estimation but the variance can still be quite large. Moreover, the \( K \) fits required to construct the jackknife estimator can be prohibitively expensive in practice.
3.3 Constructing Relative Predictive Performance Measures

When we apply these approximation strategies to the predictive distributions arising in frequentist and Bayesian inference we immediately recover many of the comparative methods that have arisen and proved empirically effective in statistical practice. In this section I detail many of these methods to emphasize the unifying nature of this foundational perspective.

3.3.1 Comparing Likelihoods

In frequentist methods the inferred predictive distribution is given by a single element in the small world or, equivalently, evaluating the likelihood at a single point.

Explicit use of delta estimators of likelihood-based relative predictive performance scores provide a formal justification of the visual residual analysis [14, 15] ubiquitous in not only statistics but also the physical sciences. Moreover, when augmented with an appropriate complexity penalty the reuse estimator reduces to the Akaike Information Criterion [16].

Hold-out and jackknife estimators of likelihood-based relative predictive performance scores immediately yields predictive log loss hold-out validation and cross validation, respectively, which have become almost fundamental principles in the practice of modern machine learning [17, 18].

The potential pathologies of these approximations manifest even in the simple misfit and overfit examples introduced above. I generate an ensemble of data from the latent data generating process and compare the exact likelihood predictive performance score based on a reference Lebesgue measure, $\delta$, to each estimate, $\hat{\delta}$ (Figures 6, 7). The partitions for the hold-out estimators consisted of six data each, the minimum required for finite maximum likelihood estimates, while the $K = 6$ jackknife partitions each consisting of $N - M = 10$ training data and $M = 2$ testing data.

In both cases the estimators are noisy with a substantial bias, with the hold-out estimator particularly sensitive to overfitting as expected. Although these errors may partially cancel when comparing models, any significant cancellation would be rather serendipitous.

3.3.2 Comparing Prior Predictive Distributions

Box [19, 20] was a strong proponent of the predictive validation of Bayesian methods, in particular the use of the prior predictive distribution.

One benefit of the prior predictive distribution is that, because it doesn’t depend on the measurement, the delta estimator is unbiased. In fact, the delta estimate

$$\delta_D\left(\pi \mid \pi^\text{prior}\right) \approx -\log \frac{d\pi^\text{prior}}{d\lambda}(y),$$
Figure 6: Even in the simple misfit model, approximations of likelihood-based relative predictive performance scores can leave much to be desired, as demonstrated by the 20%, 50%, and 80% quantiles of the estimator error over an ensemble of measurements from the latent data generating process.

Figure 7: The simple overfit model also exposes the weakness of approximations of likelihood-based relative predictive performance scores can leave much to be desired, as demonstrated by the 20%, 50%, and 80% quantiles of the estimator error over an ensemble of measurements from the latent data generating process. Hold-out estimators are particularly poor given how sensitive the hold-out fits are to overfitting.
Figure 8: Approximations of prior predictive-based relative predictive performance scores for the misfit are not terrible, as demonstrated by the 20%, 50%, and 80% quantiles of the estimator error over an ensemble of measurements from the latent data generating process, but nowhere near precise enough to compare models with similar predictive performance.

is exactly the logarithm of the marginal likelihood, or evidence, used in Bayesian model comparison [21, 5], and the difference of estimates between two models is exactly the log-odds ratio. Consequently classical Bayesian model comparison also has an interpretation in terms of predictive performance.

That said, the utility of this relative predictive performance score is limited both by the large variance of the estimator and a potential overfitting bias if the prior is modified during inference. In models where the prior is strongly constrained by previous measurements or theoretical conditions this bias may be less of an issue, but care should always be taken.

As in Section 3.3.1, the simple misfit and overfit examples demonstrate the limitations of each estimator (Figures 8, 9).

3.3.3 Comparing Posterior Predictive Distributions

Alternatively, we can construct relative predictive performance scores in the Bayesian paradigm by using the posterior predictive distribution.

Similar to the use of likelihoods, relative predictive performance scores constructed from reuse estimators provide motivation for many visual diagnostics such as Bayesian residual analyses [22] and, in particular, posterior-predictive checks [23, 24]. Likewise, the use of hold-out and jackknife estimators yields posterior predictive hold-out and cross validation, [25, 26, which continues to grow in popularity in the machine learning and statistics literature. Consideration of the example of Section 3.3.1 and 3.3.2 emphasizes the continued need to maintain vigilance in these applications (Figures 10, 11).

Posterior predictive cross validation also provides the basis for unifying many of the in-
Figure 9: The bootstrap estimator of prior predictive-based relative predictive performance scores is particularly sensitive to overfitting, as seen in the 20%, 50%, and 80% quantiles of the estimator error over an ensemble of measurements from the latent data generating process.

Figure 10: Approximations of posterior predictive-based relative predictive performance scores on the misfit example perform similarly to the approximations from other predictive distributions, once again demonstrated by the 20%, 50%, and 80% quantiles of the estimator error over an ensemble of measurements from the latent data generating process.
Figure 11: Approximations of posterior predictive-based relative predictive performance scores on the overfit example perform similarly to the approximations from other predictive distributions, once again demonstrated by the 20%, 50%, and 80% quantiles of the estimator error over an ensemble of measurements from the latent data generating process.

As with the reuse, hold-out, and jackknife estimators, the ultimate accuracy and precision of these information criteria relative to the true posterior predictive relative predictive performance score is paramount in any partial application.

4 Conclusion

In this paper I have shown how the Kullback-Leibler divergence between an inferred predictive distribution and the latent data generating process defines a canonical but incomputable measure of relative predictive performance. Moreover, I have demonstrated how it
can be simplified into relative predictive performance scores which quantify the same relative predictive performance while also being more amenable to practical approximations. Applying various approximation strategies to the relative predictive performance derived from predictive distributions in frequentist and Bayesian inference yields many of the model comparison techniques ubiquitous in practice, from predictive log loss cross validation to the Bayesian evidence and Bayesian information criteria.

The main benefit in unifying all of these existing methods into a single foundational perspective is that it provides a common framework for understanding the limitations of these methods and how they can be used responsibly. In particular, it emphasizes that these existing methods are all estimates, with uncertain variances and biases that make quantitative statements about relative predictive performance, and a hard selection of one model above all others under consideration, somewhat precarious.

This difficulty in making quantitative statements has motivated new approaches to model comparison that do not fit each model in isolation but rather fit them as components of a single, comprehensive model [30, 31]. Such an inclusive strategy offers unique computational benefits and an intriguing new interpretation of the small world, and it promises to be an exciting area of future research.

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