

# A relation between log-likelihood and cross-validation log-scores

## (with some remarks on models)

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*Note: Dear Reader & Peer, this manuscript is being peer-reviewed by you. Thank you.*

## 1 Introduction

The probability calculus unequivocally tells us how  $P(H_h | D I)$ , our degree of belief in a hypothesis  $H_h$  given data  $D$  and background information or assumptions  $I$ , is related to  $P(D | H_h I)$ , our degree of belief in observing those data when we entertain that hypothesis as true:

$$P(H_h | D I) = \frac{P(D | H_h I) P(H_h | I)}{P(D | I)} \quad (1a)$$

$$= \frac{P(D | H_h I) P(H_h | I)}{\sum_{h'} P(D | H_{h'} I) P(H_{h'} | I)}. \quad (1b)$$

$D, H_h, I$  denote propositions, which are usually about numeric quantities. I use the terms ‘degree of belief’, ‘belief’, and ‘probability’ as synonyms. By ‘hypothesis’ I mean either a scientific (physical, biological, etc.) hypothesis – a state or development of things capable of experimental verification, at least in a thought experiment; or more generally some proposition, often not precisely specified, which leads us to assign the particular degrees of belief  $P(\dots | H I)$ . In the latter case  $H$  is often called a ‘(probabilistic) model’.

The probability calculus, just like the truth calculus, proceeds purely syntactically rather than semantically. That is, if I tell you that  $H$  and  $H \Rightarrow D$  are true, you can conclude that  $D$  is true; similarly, if I tell you that  $P(H | I) = p$  and  $P(H \Rightarrow D | I) = q$ , you can conclude (try it as an exercise) that  $P(D | I) = p + q - 1$ . And in either case you don’t need to know what  $H$  and  $D$  are about – they could be about Donald Duck or parallel universes. Don’t we too often abuse of this syntactical property? We often say ‘under model  $H$  our belief about the value of quantity  $x$  is expressed by such and such distribution  $p(x | H) = f(x)$ ’,

without explaining what  $\theta$  really is and why it leads to  $f$ . Aren't terms such as 'model' and 'hypothesis', as often used in probability and statistics, convenient and respectable-looking carpets under which we can sweep the fact that we don't quite know what we're speaking about? The need to look under the carpet arises, though, the moment we have to specify our pre-data belief, the prior, about the mysterious  $H$ .

And yet again, semantics can very well be a by-product of syntax, or the distinction between the two be a chimera<sup>1</sup>. Such important matters are unfortunately rarely discussed in probability and statistics.

Expression (1b) assumes that we have a set  $\{H_h\}$  of mutually exclusive and exhaustive hypotheses under consideration, which is implicit in our knowledge  $I$  – in fact, the right side is only valid if

$$P(\bigvee_h H_h | I) = 1, \quad P(H_h \wedge H_{h'} | I) = 0 \quad \text{if } h \neq h'. \quad (2)$$

Only in extremely rare cases does the set of hypotheses  $\{H_h\}$  encompass and reflect the extremely complex and fuzzy hypotheses lying in the backs of our minds. The background knowledge  $I$  is therefore only a simplified picture of our actual knowledge. That's why  $I$  or the hypotheses  $\{H_h\}$  are often called *models*. 'A theory cannot duplicate nature, for if it did so in all respects, it would be isomorphic to nature itself and hence useless, a mere repetition of all the complexity which nature presents to us, that very complexity we frame theories to penetrate and set aside. If a theory were not simpler than the phenomena it was designed to model, it would serve no purpose. Like a portrait, it can represent only a part of the subject it pictures. This part it exaggerates, if only because it leaves out the rest. Its simplicity is its virtue, provided the aspect it portrays be that which we wish to study' (Truesdell<sup>2</sup>).

Expression (1a) is universally valid instead, but it's rarely possible to quantify its denominator  $P(D | I)$  unless we simplify our inferential problem by introducing a possibly unrealistic exhaustive set of hypotheses, thus falling back to (1b). We can bypass this problem if we are content with comparing our beliefs about any two hypotheses through their ratio, so that the term  $P(D | I)$  cancels out. See Jaynes's<sup>3</sup> insightful remarks about such binary comparisons, and also Good's<sup>4</sup>.

All terms in eq. (1) are always important in an inference problem, both at decision stages (for example, evaluating which hypotheses to

<sup>1</sup>Wittgenstein 1999, Girard 2001, 2003.

<sup>2</sup>Truesdell et al. 1980 Prologue p. xvi.

<sup>3</sup>Jaynes 2003 §§ 4.3–4.4.

<sup>4</sup>Good 1950 § 6.3–6.6.

include in our simplified set, or which hypothesis to finally choose – if we *have to* – discarding its competitors for future calculations; or if we must choose among possible medical treatment), and at exploratory stages (for example, examining whether a hypothesis leads to peculiar beliefs for peculiar kinds of data). But also other expressions are often used, either derived via the probability rules or constructed on more intuitive grounds.

My purpose is to show an exact relation between two specific quantities of either kind: the *log-likelihood* and the *leave-one-out cross-validation log-score*, although the relation can probably be extended to more general cross-validation log-scores.

## 2 Log-likelihood

The term  $P(D \mid H_h I)$  in eq. (1) is called the *likelihood* of the hypothesis given the data<sup>5</sup>. Its logarithm is surprisingly called log-likelihood:

$$\log P(D \mid H_h I), \quad (3)$$

where the logarithm can be taken in an arbitrary basis (Turing, Good<sup>6</sup>, Jaynes<sup>7</sup> recommend base  $10^{1/10}$ , leading to a measurement in decibels; see the cited works for the practical advantages of such choice).

The ratio of the likelihoods of two hypotheses, called *relative Bayes factor*, or its logarithm, the *relative weight of evidence*<sup>8</sup>, are often used to get an idea of how much the data favour our belief in one versus the other hypothesis (that is, assuming at least momentarily that they be exhaustive). ‘It is historically interesting that the expression “weight of evidence”, in its technical sense, anticipated the term “likelihood” by over forty years’<sup>9</sup>.

Recent literature<sup>10</sup> seems to exclusively deal with *relative Bayes factors*, so I’d like to mention that the non-relative Bayes factor for a hypothesis  $H_h$  provided by data  $D$  is actually defined as<sup>11</sup>

$$\frac{P(D \mid H_h I)}{P(D \mid \neg H_h I)} \equiv \frac{O(H_h \mid D I)}{O(H_h \mid I)} = \frac{P(D \mid H_h I) [1 - P(H_h \mid I)]}{\sum_{h' \neq h} P(D \mid H_{h'} I) P(H_{h'} \mid I)}, \quad (4)$$

<sup>5</sup>Good 1950 § 6.1 p. 62.

<sup>6</sup>e.g. Good 1985, 1950, 1969.

<sup>7</sup>Jaynes 2003 § 4.2.

<sup>8</sup>Good 1950 ch. 6, 1975, 1981, 1985, and many other works in Good 1983; Osteyee et al. 1974 § 1.4, MacKay 1992, Kass et al. 1995; see also Jeffreys 1983 chs V, VI, A.

<sup>9</sup>Osteyee et al. 1974 § 1.4.2 p. 12.

<sup>10</sup>for example Kass et al. 1995.

<sup>11</sup>Good 1981 § 2.

where the *odds*  $O$  is defined as  $O := P/(1 - P)$ . Looking at the expression on the right, which can be derived from the probability rules, it's clear that the Bayes factor for a hypothesis involves the likelihoods of *all* other hypotheses as well as their pre-data probabilities. This quantity and its logarithm, the (non-relative) weight of evidence, have important properties which *relative* Bayes factors don't enjoy. For example, the expected weight of evidence for a correct hypothesis is always positive, and for a wrong hypotheses always negative<sup>12</sup>. See Jaynes<sup>13</sup> for further discussion and a numeric example.

### 3 Cross-validation log-score

The literature in probability and statistics has also employed various ad-hoc measures to make exploratory analyses. Here I consider one in particular: the *leave-one-out cross-validation log-score* which I'll just call 'log-score' for brevity:

$$\frac{1}{d} \sum_{i=1}^d \log P(D_i \mid D_{-i} H_h I) \quad (5)$$

where every  $D_i$  is one datum in the data  $D \equiv \bigwedge_i D_i$ , and  $D_{-i}$  denotes the data with datum  $D_i$  excluded. The intuition behind this score, cursorily speaking, is this: 'let's see what my belief in one datum should be, on average, once I've observed the other data, if I consider  $H_h$  as true'. 'On average' means considering such belief for every single datum in turn, and then taking the geometric mean. Other variants of this score use more general partitions of the data into two disjoint subsets.

The literature presents some theoretical motivations and use of the log-score, as well as some debate<sup>14</sup>. The relation that I'm going to show in the next section might be of interest for such debate.

### 4 A relation between log-likelihood and log-score

I'd like to show an exact relation between the log-score (5) and the log-likelihood (3) which doesn't seem to appear in the literature. I find this relation very intriguing because it portrays the log-likelihood as a sort of full-scale use of the log-score.

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<sup>12</sup>Good 1950 § 6.7.

<sup>13</sup>Jaynes 2003 §§ 4.3–4.4.

<sup>14</sup>Bernardo et al. 1994 §§ 3.4, 6.1.6 gives the clearest motivation and explanation, see also Stone 1977, Geisser et al. 1979, Vehtari et al. 2012, 2002, Krnjajić et al. 2011, 2014, Gelman et al. 2014, Gronau et al. 2019, Chandramouli et al. 2019.

We can obviously write the likelihood as the  $d$ th root of its  $d$ th power:

$$P(D | HI) \equiv \left[ \underbrace{P(D | HI) \times \cdots \times P(D | HI)}_{d \text{ times}} \right]^{1/d} \quad (6)$$

where we have dropped the subscript  $h$  for simplicity. By the rules of probability we have

$$P(D | HI) = P(D_i | D_{-i} H_h I) \times P(D_{-i} | H_h I) \quad (7)$$

no matter which specific  $i \in \{1, \dots, d\}$  we choose (temporal ordering and similar matters are completely irrelevant in the formula above: it's a logical relation between propositions). So let's expand each of the  $d$  factors in the identity (6) using the product rule (7), using a different  $i$  for each of them. The result can be thus displayed:

$$\begin{aligned} P(D | HI) \equiv & \left[ P(D_1 | D_{-1} HI) \times P(D_{-1} | HI) \times \right. \\ & P(D_2 | D_{-2} HI) \times P(D_{-2} | HI) \times \\ & \quad \dots \times \\ & \left. P(D_d | D_{-d} HI) \times P(D_{-d} | HI) \right]^{1/d}. \end{aligned} \quad (8)$$

$\uparrow$   
 this column leads to the log-score

Upon taking the logarithm of this expression, the  $d$  factors vertically aligned on the left add up to the log-score (5), as indicated. But the mathematical reshaping we just did for  $P(D | HI)$  – that is, the root-product identity (6) and the expansion (8) – can be done for each of the remaining factors  $P(D_{-i} | HI)$  vertically aligned on the right in expression (8); and so on recursively. Here is an explicit example for

$d = 3$ :

$$P(D \mid HI) \equiv$$

$$\begin{aligned} & \left\{ P(D_1 \mid D_2 D_3 HI) \times [P(D_2 \mid D_3 HI) \times P(D_3 \mid HI) \times \right. \\ & \quad \left. P(D_3 \mid D_2 HI) \times P(D_2 \mid HI)]^{1/2} \times \right. \\ & P(D_2 \mid D_1 D_3 HI) \times [P(D_1 \mid D_3 HI) \times P(D_3 \mid HI) \times \\ & \quad \left. P(D_3 \mid D_1 HI) \times P(D_1 \mid HI)]^{1/2} \times \right. \\ & P(D_3 \mid D_1 D_2 HI) \times [P(D_1 \mid D_2 HI) \times P(D_2 \mid HI) \times \\ & \quad \left. P(D_2 \mid D_1 HI) \times P(D_1 \mid HI)]^{1/2} \right\}^{1/3}. \quad (9) \end{aligned}$$

In this example, the logarithm of the three vertically aligned factors in the left column is, as already noted, the log-score (5). The logarithm of the six vertically aligned factors in the central column is an average of the log-scores calculated for the three distinct subsets of pairs of data  $\{D_1 D_2\}$ ,  $\{D_1 D_3\}$ ,  $\{D_2 D_3\}$ . Likewise, the logarithm of the six factors vertically aligned on the right is the average of the log-scores for the three subsets of data singletons  $\{D_1\}$ ,  $\{D_2\}$ ,  $\{D_3\}$ .

In the general case with  $d$  data there are  $\binom{d}{k}$  subsets with  $k$  data points. We therefore obtain

$$\begin{aligned}
 \log P(D \mid H I) &\equiv \frac{1}{d} \sum_{i=1}^d \log P(D_i \mid D_{-i} H I) + \\
 &\quad \frac{1}{d} \sum_{i \in \{1, \dots, d\}} \frac{1}{d-1} \sum_{j \in \{1, \dots, d\}}^{j \neq i} \log P(D_{-i,j} \mid D_{-i,-j} H I) + \\
 &\quad \left( \binom{d}{d-2} \right)^{-1} \sum_{i,j \in \{1, \dots, d\}} \frac{1}{d-2} \sum_{k \in \{1, \dots, d\}}^{k \neq i,j} \log P(D_{-i,-j,k} \mid D_{-i,-j,-k} H I) + \\
 &\quad \dots + \\
 &\quad \left( \binom{d}{2} \right)^{-1} \sum_{i,j \in \{1, \dots, d\}} \frac{1}{2} [\log P(D_i \mid D_j H I) + \log P(D_j \mid D_i H I)] + \\
 &\quad \frac{1}{d} \sum_{i=1}^d \log P(D_i \mid H I), \quad (10)
 \end{aligned}$$

which can be compactly written

$$\log P(D \mid H I) \equiv \sum_{k=1}^d \binom{d}{k}^{-1} \sum_{\substack{\text{ordered} \\ k\text{-tuples}}} \frac{1}{k} \sum_{\substack{\text{cyclic} \\ \text{permutations}}} \log P(D_{i_1} \mid D_{i_2} \dots D_{i_k} H I). \quad (11)$$

That is, *the log-likelihood is the sum of all averaged log-scores that can be formed from all (non-empty) data subsets with  $k$  elements, the average for the  $k$ th-order log-scores being over the  $\binom{d}{k}$  subsets having the same cardinality  $k$ .*

There's also an equivalent form with a slightly different cross-validating interpretation: We take each datum  $D_j$  in turn and calculate our log-belief in it conditional on all possible subsets of remaining data, from the empty subset with no data (term  $k = 0$ ), to the only subset  $D_{-j}$  with all data except  $D_j$  (term  $k = d - 1$ ). These log-beliefs are averaged over the  $\binom{d-1}{k}$  subsets having the same cardinality  $k$ . The result can be

expressed as

$$\log P(D \mid HI) \equiv \frac{1}{d} \sum_{j=1}^d \sum_{k=0}^{d-1} \binom{d-1}{k}^{-1} \sum_{\substack{\text{ordered} \\ k\text{-tuples,} \\ j \text{ excluded}}} \log P(D_j \mid D_{i_1} \cdots D_{i_k} HI). \quad (12)$$

## 5 Discussion

The relation (11) just proven between the log-likelihood and the log-score brings forth several thoughts.

It's remarkable that the individual log-scores in expressions (11) and (12) above are computationally expensive, but their sum results in the log-likelihood, which is less expensive.

The relation (11) invites us to see the log-likelihood as a refinement and improvement of the log-score. The log-likelihood takes into account not only the log-score for the whole data, but also the log-scores for all possible subsets of data. Figuratively speaking it examines the relationship between data and hypothesis locally, globally, and on all intermediate scales.

To me this makes sense, because our interest is in how the hypothesis  $H$  relates to single data points as well as to any collection of them. A good portion of recent literature seems to focus on the relation between a hypothesis and *future* data rather than the collected data; but I think it's equally important to see how it relates to the data we already have. This tension between future and past data stems, in my opinion, from a misunderstanding about which model or hypothesis we're actually interested in. I hope to discuss this topic more at length in another work; but let me give a brief sketch of this misunderstanding.

As mentioned in the introduction,  $H$  sometimes denotes some unspecified knowledge that leads to a specific probabilistic model  $P(\dots \mid HI)$  (see the remark about syntax and semantics on p. 1). We must remember that the conjunction of  $H$  and some data  $D$  defines a new and *different* probabilistic model  $H' := DH$ . In the context of exchangeable models<sup>15</sup> there's an important distinction between two kinds of models:

<sup>15</sup>Bernardo et al. 2000 § 4.2, Dawid 2013, de Finetti 1937, Kingman 1978, Koch et al. 1982, see also Diaconis et al. 1980.



- (a) models that lead to the *same* belief about new data, independently of the data already observed:

$$P(D' | D H I) = P(D' | H I) \quad (\text{if } D \not\Rightarrow D'); \quad (13)$$

these are usually called ‘simple’ hypotheses or models<sup>16</sup>, but I prefer to call them *non-learning* models, because when we assume such a model, observed data become irrelevant for our beliefs about unobserved data (although observed data are of course relevant for our belief about the model);

- (b) models that lead to different beliefs about new data, depending on the data already observed:

$$P(D' | D H I) \neq P(D' | H I) \quad (\text{if } D \not\Rightarrow D'); \quad (14)$$

these are usually called ‘composite’ hypotheses or models<sup>16</sup>, but I prefer to call them *learning* models, for reasons analogous to the ones in the previous point.

Geometrically, learning models constitute a convex set, of which the non-learning models are the extreme points<sup>17</sup>.

Learning models have the important, factual property that *their conjunction with observed data tends to a non-learning model* as the number of observed data increases. Geometrically, as data accumulate, our model moves in the convex set mentioned above, approaching an extreme point.<sup>18</sup> I say ‘factual’ because this is not a mathematical theorem: we may imagine and do encounter sequences of data for which no convergence occurs<sup>19</sup>; but in practice this usually makes us replace our simplified set of hypotheses with a less simplified one and start anew. There’s a sort of Bayes theorem operating on a large hypothesis space which we keep on the back of our minds, of which the space represented on paper is just a necessarily simplified portrait or caricature (see Truesdell’s quote in § 1). Compare Jaynes’s<sup>20</sup> discussion about the ‘resurrection of dead hypotheses’.

the degrees of belief about data given some hypothesis only *after* some data have been collected, but I think it’s equally important to

<sup>16</sup>Bernardo et al. 2000 § 6.1.4.

<sup>17</sup>Lauritzen 1974a, 1988, 1984, Barndorff-Nielsen 2014, Dynkin 1978, Dawid 2013 gives a terse summary.

<sup>18</sup>compare Hjort in Barron et al. 1986, Hjort 1986 ch. 3.

<sup>19</sup>see e.g. Bruno 1964, Berk 1966, 1970, also Diaconis 1988 § 3.

<sup>20</sup>Jaynes 2003 § 4.4.1.

see how it relates to the data we already have. (compare for example<sup>21</sup>, although their motivation stems from o

If we see the symbol  $H$  as just a placeholder for a probabilistic model, rather than an empirical hypothesis (see the remark about syntax and semantics on p. 1), we must remember that the conjunction of  $H$  and some data  $D$  simply defines a new probabilistic model  $H' := H D$ .

The second point of view only holds for hypotheses  $\hat{H}$  which make any observed data irrelevant:

$$P(D \mid D' \hat{H} I) = P(D \mid \hat{H} I) \quad \text{if } D' \not\Rightarrow D, \quad (15)$$

or super-hypotheses  $H$  about such hypotheses, leading to exchangeable joint beliefs:

$$P(DD' \mid H I) = \sum_h P(D \mid \hat{H}_h H I) P(D' \mid \hat{H}_h H I) P(\hat{H}_h \mid H I) \quad \text{if } D' \not\Rightarrow D. \quad (16)$$

In either case the log-score can be seen as an approximation of the log-likelihood; more precisely of the log-likelihood per datum:

$$\frac{1}{d} \sum_{i=1}^d \log P(D_i \mid D_{-i} H I) \approx \frac{1}{d} \log P(D \mid H I). \quad (17)$$

This is in fact an exact equality if property (15) holds for  $H$ .

which lead to exchangeable beliefs about the data

Second, we can see This approximation is only valid

This approximation is reasonable if the amount of data is large with respect to the dimension of the space of a single datum, because \*\*\* (ref to geisser, stone, gelfandetal)

\*\*\* remark that  $D H$  is a *new* probability model: which of the two are we assessing? Connection with learning vs non-learning models which I hope to take up in another work.

\*\*\*<sup>22</sup> show the approximation only valid if number of data large enough – not very interesting situation in today's problems.

\*\*\* problems calculation with time-relevant hypotheses

'we cannot give a universal rule for them beyond the common-sense one, that if anybody does not know what his suggested value is, or whether there is one, he does not know what question he is asking and consequently does not know what his answer means'<sup>23</sup>.

<sup>21</sup>O'Hagan 1995, Berger et al. 1996, 1998.

<sup>22</sup>Bernardo et al. 1994 § 6.1.6.

<sup>23</sup>Jeffreys 1983 § 3.1 p. 124.

\*\*\* with similar procedure we can included all k-fold scores.

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