Bayesian Analysis Users Guide
Release 4.00, Manual Version 1

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Thermodynamic Integration

Thermodynamic Integration is a technique used in Bayesian probability theory to compute the posterior probability for a model. As a reminder, if a set of m models is designated as $M \in \{1, 2, \ldots, m\}$, then one can compute the posterior probability for the models by an application of Bayes' Theorem [1]

$$P(M|DI) \propto P(M|I)P(D|MI) \tag{C.1}$$

where we have dropped a normalization constant, $M = 1$ means we are computing the posterior probability for model 1, $M = 2$ the probability for model 2, etc. The three terms in this equation, going from left to right, are the posterior probability for the model indicator given the data and the prior information, $P(M|DI)$, the prior probability for the model given only the prior information, $P(M|I)$, and the marginal direct probability for the data given the model and the prior information, $P(D|MI)$.

The marginal direct probability for the data given a model can be computed from the joint posterior probability for the data and the model parameters, which we will call Ω, given the Model and the prior information

$$P(D|MI) = \int d\Omega P(\Omega|MI)P(D|\Omega MI). \tag{C.2}$$

Unfortunately, the integrals on the right-hand side of this equation can be very high dimensional. Consequently, although we know exactly what calculation must be done to compute the marginal direct probability, in most applications the integrals are not tractable.

The goal is to show how thermodynamic integration can be used to compute the desired posterior probability, taking the logarithm one obtains

$$\log P(M|DI) = \log P(M|I) + \log P(D|MI). \tag{C.3}$$

Note by taking the logarithm, we have essentially switched to a scale in which there is a arbitrary constant, the normalization constant, which we may or may not know. However, by comparing ratio's of of these logarithm of the logarithm of this normalization constant cancels and one can rank models by their logarithm of the odds ration.

Thermodynamic integration is a method of approximating these integrals. One derives this approximation, by introducing an annealing parameter β into the joint posterior probability for the parameters given the data and the model:

$$P(\Omega|M\beta DI) = \frac{P(\Omega|MI)P(D|\Omega MI)^{\beta}}{P(D|M\beta I)} \tag{C.4}$$

with

$$P(D|M\beta I) = \int d\Omega P(\Omega|MI)P(D|\Omega MI)^{\beta}. \tag{C.5}$$

Clearly, this expression is not the calculation we want to do, however it does have two interesting limits. First, when $\beta = 0$, the calculation is computing

$$P(D|M, \beta = 0, I) = \int P(\Omega|MI)d\Omega = 1 \tag{C.6}$$

which is just our normalization constant for the prior. Assuming a normalized prior then the above equality holds. Second, when $\beta = 1$, then

$$P(D|M, \beta = 1, I) = \int P(\Omega|MI)P(D|\Omega MI)d\Omega \tag{C.7}$$

is the exact calculation we wish to do.

If we take the derivative with respect to β of $\log P(D|M\beta I)$, one obtains

$$\frac{d}{d\beta}\log P(D|M\beta I) = \frac{1}{P(D|M\beta I)}\frac{d}{d\beta}P(D|M\beta I). \tag{C.8}$$

Substituting, Eq. (C.5), for $P(D|M\beta I)$, and rearranging the integral, one obtains

$$\frac{d}{d\beta}\log P(D|M\beta I) = \int \log P(D|M\Omega I)P(\Omega|MD\beta I)d\Omega \tag{C.9}$$

which is the expected value of the logarithm of the likelihood. Defining

$$\langle \log P(D|MI\rangle_{\beta} = \int \log P(D|M\Omega I)P(\Omega|MD\beta I)d\Omega \tag{C.10}$$

for this expectation, one obtains

$$\frac{d}{d\beta}\log P(D|M\beta I) = \langle \log P(D|MI\rangle_{\beta} \tag{C.11}$$

and integrating with respect to β, one obtains

$$\log P(D|MI) = \int_0^1 d\beta \langle \log P(D|MI\rangle_{\beta}. \tag{C.12}$$

So if we can calculate the integral on the right-side of this equation, it gives us an indirect method of computing the logarithm of the marginal direct probability for data given the model, Eq. (C.2). For more on thermodynamic integration and how to implement these types of calculations see [37, 45, 24, 25] and [46]

In an earlier versions of this Bayesian Analysis software, thermodynamic integration was implemented by varying β between zero and one in uniform steps and a simple sum was used to approximate the integral. As simple as it was, this procedure worked very well. More recently, implementing thermodynamic integration has become a bit more probabilistic because of the use of a nonuniform annealing schedule. Because the values of β are not evenly spaced, approximating the above integral is much harder. However, thermodynamic integration was never used to do model selection in the Bayesian calculations done in this software system. Rather the model selection programs implement model selection by directly sampling the discrete model indicators. Consequently, out model selection does not depend on how one anneals or performs the thermodynamic integration calculation. Thermodynamic integration was so that the user had a simple test to determine which of a selection of models was the most appropriate given the data and the prior information. To facilitate this, whenever an Ascii package runs it computes the expected logarithm of the likelihood and writes it into a file named "Bayes.prob.model" and this file can be viewed in the interface by activating the Text Report named "Probabilities".

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