A probabilistic diagnostic tool to assess Laplace approximations: proof of concept and non-asymptotic experimentation

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Abstract

In many statistical models, we need to integrate functions that may be high-dimensional. Such integrals may be impossible to compute exactly, or too expensive to compute numerically. Instead, we can use the *Laplace approximation* for the integral. This approximation is exact if the function is proportional to the density of a normal distribution; therefore, its effectiveness may depend intimately on the true shape of the function. To assess the quality of the approximation, we use *probabilistic numerics*: recasting the approximation problem in the framework of probability theory. In this probabilistic approach, uncertainty and variability don't come from a frequentist notion of randomness, but rather from the fact that the function may only be partially known. We use this framework to develop a diagnostic tool for the Laplace approximation, modelling the function and its integral as a Gaussian process and devising a "test" by conditioning on a finite number of function values.We will discuss approaches for designing and optimizing such a tool and demonstrate it on known sample functions, highlighting in particular the challenges one may face in high dimensions.

1 Introduction

Coming soon. Some combination of abstract (above) and framework (below). Specifically mention:

1. That we are building on the work of Zhou [1]

2. That this is non-asymptotic and not intended as a substitute for full-on MC integration or BQ - rather as a "middle-ground" amount of effort.

3. The goal is to "test" the assumptions underlying the Laplace approximation (e.g. "how Gaussian is this function?"). The Laplace approximation may still hold for a non-Gaussian shape, but such a function should be

rejected by our diagnostic ("sufficiently non-Gaussian things warrant further attention), at which point a more involved integration would show that the approximation was fine after all.

2 Framework and notation

Consider a positive function $f : \mathbb{R}^d \to \mathbb{R}_{>0}$. The object of interest for the diagnostic is the integral $F = \int_{\mathbb{R}^d} f(t)\mathrm{d}t$. In practical applications [citation needed], typically f and F are actually functions with an additional argument vector of structural parameters θ, with $t \in \mathbb{R}^d$ a vector of nuisance parameters to be marginalized. For instance, f may be a joint probability density for (θ, t), in which case F would be the marginal distribution of θ after integrating over t. To reflect this common setting, Zhou [1] called f and F the *full* and *target* functions, respectively. For the present discussion, non-marginalized arguments θ are not relevant, so any dependence on them is omitted and f and F are simply called the *true* function and integral, respectively.

Suppose now that f has all second-order partial derivatives[1], and a (local) maximum at some point $\hat{t} \in \mathbb{R}^d$. To reflect the use case where f is a density, $\hat{t}$ is called a *mode*. Let H be the Hessian of $\log f$ at $\hat{t}$, and suppose that it is negative-definite (i.e. that f is log-concave at the mode). The first step in arriving at the Laplace approximation [citation needed] for F is to take a second-order Taylor expansion of $\log f$ about $\hat{t}$. Noting that all first-order partial derivatives of $\log f$ are equal to zero at the mode, this approximation is

$$\log f(t) \approx \log f\left(\hat{t}\right) + \frac{1}{2}\left(t - \hat{t}\right)^{\top} H \left(t - \hat{t}\right). \tag{1}$$

Exponentiating the right side of (1) gives an approximation for f in the form of (up to normalizing constants) a Gaussian density centered at $\hat{t}$ with covariance matrix $-H^{-1}$. In turn, integrating this exponentiated function produces the *Laplace approximation*[2]

$$F \approx L\left(f\right) := f\left(\hat{t}\right) \int_{R^d} \exp\left[\frac{1}{2}\left(t - \hat{t}\right)^{\top} H \left(t - \hat{t}\right)\right]\mathrm{d}t$$

$$= f\left(\hat{t}\right) \sqrt{(2\pi)^d \det\left(-H^{-1}\right)}. \tag{2}$$

The Laplace approximation is exact (or "true") if f is itself proportional to a Gaussian density. There are other function shapes for which this may be the case, but such instances may be thought of as "coincidence". Certainly, the construction of the Laplace approximation via (1) is based on an assumption of approximately Gaussian shape, and this is assumption is our primary interest in developing a diagnostic.

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[1]TODO: check actual assumptions for Laplace. Are third derivatives necessary?

[2]TODO: get citation for this. In particular, there are a couple of variations I've seen in the form for "Laplace's method" in the Bayesian literature. For instance, sometimes $\log f$ is multiplied by a constant (usually sample size) before exponentiating.

References

[1] Haoxuan Zhou. Bayesian Integration for Assessing the Quality of the Laplace Approximation. Master's thesis, Simon Fraser University, nov 2017. URL `http://summit.sfu.ca/item/17765`.