The Laplace Approximation

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I. Introduction

In Bayesian statistics, available knowledge about parameters (θ) in a statistical model is updated with the information in observed data $(\mathcal{D})$ using Bayes' theorem :

$$\boxed{p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})} = \frac{p(\mathcal{D}|\theta)p(\theta)}{\int p(\mathcal{D}|\theta)p(\theta)d\theta}}.$$

However, then quantity $\int p(\mathcal{D}|\theta)p(\theta)d\theta$ is often **intractable**, except for simple special cases. To overcome this problem, one can use some methods like **Grid Approximation**, **Laplace Approximation**, **Variational Approximation**, **Markov Chain Monte Carlo (MCMC) Approximation**. So, here, we are focus on Laplace Approximation.

Main idea : $q(z) \approx p(z) = \mathcal{N}\left(z|z_0, A^{-1}\right)$

The **Laplace Approximation** is a simple and widely used framework which aims to find a **Gaussian approximation** to a probability density defined over a set of continuous variables. The mean equal to the **MAP** solution and precision equal to the observed **Fisher information**.

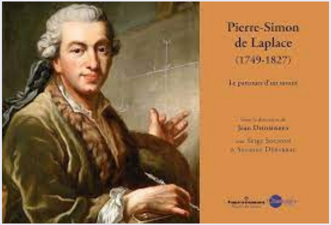


FIGURE: Pierre-Simon, Marquis de Laplace(23 March 1749–5 March 1827)

II. Development

II.1 Laplace approximation in 1d

Let's consider a **single continuous variable** z with distribution

$$p(z) = \frac{1}{Z} f(z) \text{ where } Z = \int f(z) dz$$

is the **normalisation coefficient** (**unknown**). The **goal** is to find a Gaussian approximation $q(z)$ which is centred on a mode of the distribution $p(z)$.

Steps

1. Find the mode of $p(z)$ (ie a point z_0 s.t. $p'(z_0) = 0$.)
2. Calculate the 2nd derivative (One may need Taylor expansion of $\log f(z)$ centred on z_0).
3. Write the Gaussian $q(z) \approx p(z) = \mathcal{N}\left(z|z_0, A^{-1}\right)$

Let's go

A Gaussian distribution has the property that its logarithm is a quadratic function of the variables. Let's consider now the Taylor expansion of $\ln f(z)$ centered on the mode z_0.

$$\ln f(z) \approx \ln f(z_0) + \frac{d}{dz}\left[\ln f(z_0)\right](z - z_0) + \frac{1}{2!}\frac{d^2}{dz^2}[\ln f(z_0)](z - z_0)^2$$

where

$$\frac{d}{dz}\left[\ln f(z_0)\right] = [\ln[f(z_0)]' = \ln'[f(z_0)]f'(z_0) = 0$$

Then,

$$\ln f(z) \approx \ln[f(z_0)] + 0 - \frac{1}{2}\left[-\frac{d^2}{dz^2}[\ln f(z_0)](z - z_0)^2\right]$$

$$\Rightarrow \ln f(z) \approx \ln[f(z_0)] - \frac{1}{2}A(z - z_0)^2 \text{ where } A = -\frac{d^2}{dz^2}[\ln f(z_0)]$$

$$\Rightarrow \exp\{\ln f(z)\} \approx \exp\left\{\ln[f(z_0)] - \frac{1}{2}A(z-z_0)^2\right\}$$

$$\Rightarrow f(z) \approx \exp\{\ln[f(z_0)]\} \cdot \exp\left\{-\frac{1}{2}A(z-z_0)^2\right\}$$

$$\Rightarrow f(z) \approx f(z_0)\exp\left\{-\frac{1}{2}A(z-z_0)^2\right\}$$

We obtain a normalized distribution $q(z)$ by making use of the standard result for the normalization of a gaussian. In fact,

$$
\begin{aligned}
Z &= \int f(z)dz \\
&= \int f(z_0) \exp\left\{-\frac{1}{2}A(z-z_0)^2\right\} dz \\
&= f(z_0) \int \exp\left\{-\frac{1}{2}A(z-z_0)^2\right\} dz \\
&= f(z_0) \int \exp\left\{-\frac{1}{2}(A^{-1})^{-1}(z-z_0)^2\right\} dz \\
&= f(z_0) \int \exp\left\{-\frac{1}{2}\frac{(z-z_0)^2}{A^{-1}}\right\} dz \\
&= f(z_0)\sqrt{2\pi A^{-1}}
\end{aligned}
$$

Then,

$$
\begin{aligned}
q(z) \approx p(z) &= \frac{1}{Z} f(z) \\
&= \frac{1}{f(z_0)\sqrt{2\pi A^{-1}}} f(z_0) \exp\left\{-\frac{1}{2} A (z-z_0)^2\right\} \\
&= \left(\frac{A}{\sqrt{2\pi}}\right)^{1/2} \exp\left\{-\frac{1}{2}\frac{(z-z_0)^2}{A^{-1}}\right\} \\
&= \frac{1}{\sqrt{2A^{-1}}} \exp\left\{-\frac{1}{2}\frac{(z-z_0)^2}{A^{-1}}\right\} \\
&= \mathcal{N}\left(z | z_0, A^{-1}\right)
\end{aligned}
$$

Example of Laplace approximation in 1d

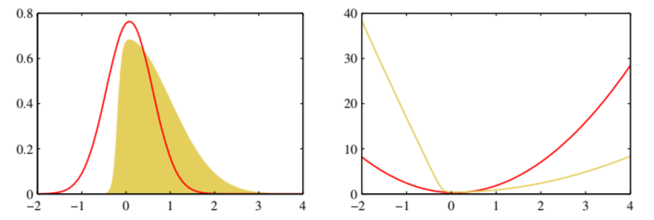


FIGURE: Illustration of the Laplace approximation applied to the distribution $p(z) \propto \exp(-z^2/2)\sigma(20z+4)$ where $\sigma(z)$ is the logistic sigmoid function defined by $\sigma(z) = \frac{1}{(1+e^{-z})}$. The left plot shows the normalized distribution $p(z)$ in yellow, together with the Laplace approximation centred on the mode z_0 of $p(z)$ in red. The right plot shows the negative logarithms of the corresponding curves. ([1, p.215])

Let's consider the same assumptions over $p(z)$, $f(z)$, Z_0 and $q(z)$ as before however, we are now in N-dimensional space. In fact, at the stationary point z_0, the gradient $\nabla f(x)$ will vanish. That's to say

$$\nabla_f(z_0) = 0.$$

By using Taylor expansion of $\ln f(z)$ at $z = z_0$, we have :

$$\ln f(z) \approx \ln f(z_0) + \nabla \ln f(z_0)(z - z_0) + \frac{1}{2!}(z - z_0)^T \nabla^2 \ln f(z_0)(z - z_0).$$

Then,

$$\ln f(z) \approx \ln f(z_0) + \frac{1}{2}(z - z_0)^T \nabla^2 \ln f(z_0)(z - z_0)$$

$$\Rightarrow \ln f(z) \approx \ln f(z_0) - \left[-\frac{1}{2}(z - z_0)^T \nabla^2 \ln f(z_0)(z - z_0)\right]$$

Let's say,

$$A = -\nabla^2 \ln f(z_0)$$

$$\Rightarrow \ln f(z) \approx \ln f(z_0) - \frac{1}{2}(z - z_0)^T A(z - z_0)$$

$$\Rightarrow \exp\{\ln f(z)\} \approx \exp\left\{\ln f(z_0) - \frac{1}{2}(z - z_0)^T A(z - z_0)\right\}$$

$$\Rightarrow f(z) \approx f(z_0) \exp\left\{-\frac{1}{2}(z - z_0)^T A(z - z_0)\right\}$$

As before, we obtain a normal distribution $q(z)$ by making use of the standard result for a normalized multivariate Gaussian :

$$\begin{aligned} Z &= \int f(z)dz \\ &= \int f(z_0) \exp\left\{-\frac{1}{2}(z - z_0)^T A(z - z_0)\right\} dz \\ &= f(z_0) \int \exp\left\{-\frac{1}{2}(z - z_0)^T A(z - z_0)\right\} dz \\ &= f(z_0) \int \exp\left\{-\frac{1}{2}(z - z_0)^T \left(A^{-1}\right)^{-1} (z - z_0)\right\} dz \\ &= f(z_0)\sqrt{|2\pi A^{-1}|} \end{aligned}$$

Then,

$$
\begin{aligned}
q(z) \approx p(z) &= \frac{1}{Z} f(z) \\
&= \frac{1}{f(z_0)\sqrt{(2\pi)^N |A^{-1}|}} f(z_0) \exp\left\{-\frac{1}{2}(z - z_0)^T A (z - z_0)\right\} \\
&= \left(\frac{A}{(2\pi)^N}\right)^{\frac{1}{2}} \exp\left\{-\frac{1}{2}(z - z_0)^T \left(A^{-1}\right)^{-1} (z - z_0)\right\} \\
&= \frac{1}{\sqrt{(2\pi)^N |A^{-1}|}} \exp\left\{-\frac{1}{2}(z - z_0)^T \left(A^{-1}\right)^{-1} (z - z_0)\right\}
\end{aligned}
$$

$$
q(z) \approx p(z) = \mathcal{N}\left(z | z_0, A^{-1}\right)
$$

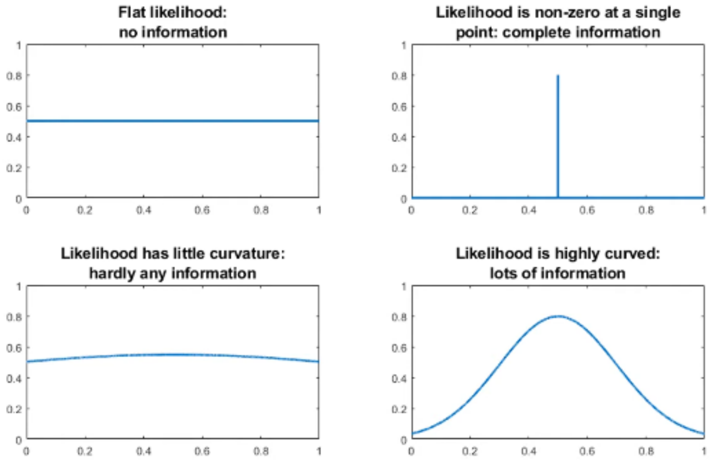
Where $|A|$ denotes the determinant of A. This gaussian distribution will be well defined provided its precision matrix, given by A, is positive definite.

II. 3 Fisher Information Matrix

- θ is parameter that models a distribution $p(X|\theta)$
- Fisher Information Matrix :

$$F(\theta) := \mathbb{E}_{p(X|\theta)}\left[\nabla \log p(X|\theta) \nabla \log p(X|\theta)^T\right]$$

- $F(\theta)$ measures the amount of information X carries about θ
- $F(\theta)$ measures the amount of curvature of the log-likelihood surface at its peak


Flat likelihood:
no information
Likelihood is non-zero at a single
point: complete information
Likelihood has little curvature:
hardly any information
Likelihood is highly curved:
lots of information
0
0.2
0.4
0.6
0.8
1

- $F(\theta)$ is the negative expected Hessian of the log likelihood [1] :

$$F(\theta) = -\mathbb{E}_{p(X|\theta)}\left[H_{\log p(X|\theta)}\right]$$

- In Laplace Approximation, $F(\hat{\theta})$ is the covariance of the fitted Gaussian

Implementation

See `Laplace_Apprximation_project.ipynb`

1. https ://agustinus.kristia.de/techblog/2018/03/11/fisher-information/

Laplace approximation framework

- Simple but widely used framework,
- Aims to find a Gaussian approximation to a probability density defined over a set of continuous variables, defined for both univariate and multivariate, directly applicable only to real variables.
- Method aims specifically at problems in which the distribution is unimodal, We can find the mode using a standard optimization method,
- Many distributions encountered in practice are multimodal :There will be different approximations according to which mode considered,

References : ([1][2][3])

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Acknowledgement

Thank you for your attention and participation !