

Bayesian Logistic Classification

3F8: Inference Coursework
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Abstract

Abstract goes here

1 Introduction

2 Laplace approximation for logistic regression

The Laplace approximation finds a Gaussian, $q(\mathbf{x})$, that provides a good approximation to a probability distribution $p(\mathbf{x})$ near a local maximum of $p(\mathbf{x})$. This is useful when the desired distribution $p(\mathbf{x})$ is intractable and difficult to manipulate.

In the previous report, the maximum-likelihood estimate for the model weights was used in classification¹. It is desirable instead to have a full posterior distribution of the weights:

$$p(\mathbf{w}|\mathbf{X}, \mathbf{y}) = \frac{p(\mathbf{X}|\mathbf{w}, \mathbf{y})p(\mathbf{w})}{p(\mathbf{X}|\mathbf{y})} \quad (1)$$

Calculating the normalising constant (also called the evidence) $p(\mathbf{X}|\mathbf{y})$ requires integrating a product of logistic functions, which is intractable. The Laplace approximation can be used to find an approximate posterior distribution and an approximate predictive distribution for the logistic classifier, while avoiding the difficult integral. The derivation of these results is found in Appendix A.

In this application, the prior on the model weights is chosen to be:

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; 0, \mathbf{I}\sigma_0^2) \quad (2)$$

This gives the posterior as:

$$p(\mathbf{w}|\mathbf{X}, \mathbf{y}) \approx \mathcal{N}(\mathbf{w}; \mathbf{w}_{\text{MAP}}, \mathbf{C}_N) \quad (3)$$

And the evidence as:

$$p(\mathbf{X}|\mathbf{y}) = \frac{(2\pi)^{\frac{N}{2}}}{\det \mathbf{C}_N^{-\frac{1}{2}}} p(\mathbf{X}|\mathbf{w} = \mathbf{w}_{\text{MAP}}, \mathbf{y}) p(\mathbf{w} = \mathbf{w}_{\text{MAP}}) \quad (4)$$

A Deriving Bayesian Logistic Classification using the Laplace Approximation

A.1 Laplace approximation

To define a probability distribution function (PDF) $p(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^N$ it is necessary to integrate a function to find the normalising constant K :

$$p(\mathbf{x}) := \frac{f(\mathbf{x})}{\int f(\mathbf{x}) d\mathbf{x}} = \frac{1}{K} f(\mathbf{x}) \quad (5)$$

¹For the model definition, and definitions of \mathbf{X} , \mathbf{y} , $\tilde{\mathbf{x}}$, etc, see the previous report.

In many cases, the integral $\int f(\mathbf{x})d\mathbf{x}$ is intractable or does not have a closed-form solution.

The Laplace approximation finds a Gaussian, $q(\mathbf{x})$, that provides a good approximation to $p(\mathbf{x})$ near a local maximum of $p(\mathbf{x})$. As $q(\mathbf{x})$ is Gaussian, its normalising constant is easy to find, so the problem of solving $\int f(\mathbf{x})d\mathbf{x}$ is avoided. To find $q(\mathbf{x})$, we start with the truncated Taylor expansion of $\ln f(\mathbf{x})$ around a local maximum \mathbf{x}_0 :

$$\ln f(\mathbf{x}) \approx \ln f(\mathbf{x}_0) + \nabla \ln f(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_0}(\mathbf{x} - \mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \nabla^2 \ln f(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_0}(\mathbf{x} - \mathbf{x}_0)$$

At a maximum of $f(\mathbf{x})$, $\nabla \ln f(\mathbf{x}) = 0$ as the logarithm is a monotonic function. Hence, close to \mathbf{x}_0 :

$$\begin{aligned} \ln f(\mathbf{x}) &\approx \ln f(\mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \nabla^2 \ln f(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_0}(\mathbf{x} - \mathbf{x}_0) \\ f(\mathbf{x}) &\approx f(\mathbf{x}_0) \exp\left(\frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \nabla^2 \ln f(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_0}(\mathbf{x} - \mathbf{x}_0)\right) \end{aligned} \quad (6)$$

Equation 6 is of the form of an un-normalised Gaussian. Let $\mathbf{P} = -\nabla^2 \ln f(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_0}$, and normalise Equation 6 to get an approximation for $p(\mathbf{x})$:

$$\begin{aligned} p(\mathbf{x}) &\approx \frac{1}{(2\pi)^{\frac{M}{2}} \det \mathbf{P}^{-\frac{1}{2}}} \exp\left(\frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \mathbf{P}(\mathbf{x} - \mathbf{x}_0)\right) \\ &= \mathcal{N}(\mathbf{x}; \mathbf{x}_0, \mathbf{P}^{-1}) \end{aligned} \quad (7)$$

For this to hold, \mathbf{P} must be positive definite, i.e. \mathbf{x}_0 must be a maximum.

This method can be used instead to find an approximate value of the normalising constant K. Substituting Equation 6 into the definition of K:

$$\begin{aligned} K = \int f(\mathbf{x})d\mathbf{x} &\approx f(\mathbf{x}_0) \int \exp\left(\frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \mathbf{P}(\mathbf{x} - \mathbf{x}_0)\right) d\mathbf{x} \\ &= \frac{(2\pi)^{\frac{N}{2}}}{\det \mathbf{P}^{\frac{1}{2}}} f(\mathbf{x}_0) \end{aligned} \quad (8)$$

A.2 Bayesian logistic regression

A.2.1 Posterior distribution

Given that the posterior Laplace approximation will be Gaussian, it is sensible to choose a Gaussian prior:

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \mathbf{m}_0, \mathbf{C}_0) \quad (9)$$

In order to apply the Laplace approximation, we need the location of a maximum in the posterior. Using the results for the likelihood of the logistic model in the previous report and the log of Equation 9, the log-posterior is:

$$\begin{aligned} \ln p(\mathbf{w}|\mathbf{X}, \mathbf{y}) &= \sum_{n=1}^N y_n \log \sigma(\mathbf{w}^T \tilde{\mathbf{x}}_n) + (1 - y_n) \log \sigma(-\mathbf{w}^T \tilde{\mathbf{x}}_n) \\ &\quad + \frac{1}{2}(\mathbf{w} - \mathbf{w}_0)^T \mathbf{C}_0^{-1}(\mathbf{w} - \mathbf{w}_0) \\ &\quad + \text{const} \end{aligned} \quad (10)$$

The value of \mathbf{w} at the maximum, \mathbf{w}_{MAP} , can be found by setting the derivative of Equation 10 to zero. As outlined in Section A.1 \mathbf{w}_{MAP} will be the mean of $q(\mathbf{w})$.

Using Equation 7, the covariance matrix of $q(\mathbf{w})$ can be found:

$$\begin{aligned} \mathbf{C}_N^{-1} &= -\nabla^2 \ln p(\mathbf{w}|\mathbf{X}, \mathbf{y})|_{\mathbf{w}=\mathbf{w}_{\text{MAP}}} \\ &= \mathbf{C}_0^{-1} + \sum_{n=1}^N \sigma(\mathbf{w}^T \tilde{\mathbf{x}}_n) \sigma(-\mathbf{w}^T \tilde{\mathbf{x}}_n) \tilde{\mathbf{x}}_n \tilde{\mathbf{x}}_n^T \end{aligned} \quad (11)$$

Defining $\boldsymbol{\sigma} = \sigma(\tilde{\mathbf{X}}^T \mathbf{w})$, this can be written in vector form as:

$$\mathbf{C}_N^{-1} = \mathbf{C}_0^{-1} + \tilde{\mathbf{X}} \tilde{\mathbf{X}}^T \boldsymbol{\sigma} (1 - \boldsymbol{\sigma}) \quad (12)$$

Hence, using Equation 7, the posterior distribution is:

$$p(\mathbf{w} | \mathbf{X}, \mathbf{y}) \approx \mathcal{N}(\mathbf{w}; \mathbf{w}_{\text{MAP}}, \mathbf{C}_N) \quad (13)$$

And using Equation 8, the normalizing constant is:

$$p(\mathbf{X} | \mathbf{y}) = \frac{(2\pi)^{\frac{N}{2}}}{\det \mathbf{C}_N^{-\frac{1}{2}}} p(\mathbf{X} | \mathbf{w} = \mathbf{w}_{\text{MAP}}, \mathbf{y}) p(\mathbf{w} = \mathbf{w}_{\text{MAP}}) \quad (14)$$

A.3 Predictive distribution

The predictive distribution can also be approximated using the Laplace method:

$$\begin{aligned} p(y^* = 1 | \mathbf{x}^*, \mathbf{y}, \mathbf{X}) &= \int p(y^* = 1 | \mathbf{x}^*, \mathbf{w}) p(\mathbf{w} | \mathbf{y}, \mathbf{X}) d\mathbf{w} \\ &\approx \int \sigma(\mathbf{w}^T \mathbf{x}^*) q(\mathbf{w}) d\mathbf{w} \end{aligned} \quad (15)$$

Using the sifting property of the delta function:

$$\sigma(\mathbf{w}^T \mathbf{x}) = \int \delta(a - \mathbf{w}^T \mathbf{x}) \sigma(a) da \quad (16)$$

Hence:

$$\begin{aligned} p(y^* = 1 | \mathbf{x}^*, \mathbf{y}, \mathbf{X}) &\approx \int \int \delta(a - \mathbf{w}^T \mathbf{x}^*) \sigma(a) q(\mathbf{w}) d\mathbf{w} da \\ &= \int \sigma(a) \int \delta(a - \mathbf{x}^{*T} \mathbf{w}) q(\mathbf{w}) d\mathbf{w} da \\ &= \int \sigma(a) \mathcal{N}(a; \mathbf{x}^{*T} \mathbf{w}_{\text{MAP}}, \mathbf{x}^{*T} \mathbf{C}_N \mathbf{x}^*) da \end{aligned} \quad (17)$$

In the final step, we have used the fact that the inner integral is applying a linear constraint to $q(\mathbf{w})$, as the argument of the delta function is 0 unless $a = \mathbf{x}^{*T} \mathbf{w}$