

Lecture 11

Laplace Approximation

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- Laplace approximation
- Bayesian logistic regression

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- Objective: construct a *Gaussian* distribution to approximate the target distribution
- Method: **second order Taylor expansion** at the posterior **mode** (i.e., MAP estimation)

- Given a joint probability $p(\boldsymbol{\theta}, \mathcal{D})$
- How to compute (approximate) $p(\boldsymbol{\theta}|\mathcal{D})$?

Let us do MAP estimation first

$$\boldsymbol{\theta}_0 = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \log p(\boldsymbol{\theta}, \mathcal{D}) = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \log p(\mathcal{D}|\boldsymbol{\theta})$$

- We then expand the log joint probability at the posterior mode

$$f(\boldsymbol{\theta}) \triangleq \log p(\boldsymbol{\theta}, \mathcal{D})$$

$$f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_0) + \nabla f(\boldsymbol{\theta}_0)^\top (\boldsymbol{\theta} - \boldsymbol{\theta}_0) \quad \nabla f(\boldsymbol{\theta}_0) = \mathbf{0}$$

$$+ \frac{1}{2} (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla \nabla f(\boldsymbol{\theta}_0) (\boldsymbol{\theta} - \boldsymbol{\theta}_0) \quad \nabla \nabla f(\boldsymbol{\theta}_0) \prec 0 \quad \text{Why?}$$

$$= f(\boldsymbol{\theta}_0) - \frac{1}{2} (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \mathbf{A} (\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

$$\mathbf{A} = -\nabla \nabla f(\boldsymbol{\theta}_0) \succ 0$$

$$\begin{aligned} f(\boldsymbol{\theta}) &\triangleq \log p(\boldsymbol{\theta}, \mathcal{D}) \\ &\approx f(\boldsymbol{\theta}_0) - \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \mathbf{A}(\boldsymbol{\theta} - \boldsymbol{\theta}_0) \end{aligned}$$

$$p(\boldsymbol{\theta}, \mathcal{D}) \approx p(\boldsymbol{\theta}_0, \mathcal{D}) \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \mathbf{A}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)\right)$$



Gaussian!

$$p(\boldsymbol{\theta}|\mathcal{D}) \approx \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\theta}_0, \mathbf{A}^{-1})$$

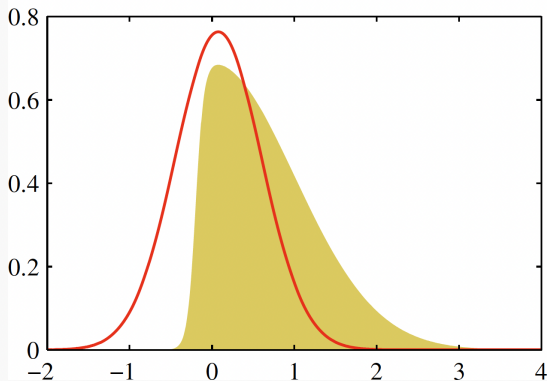
$$\boldsymbol{\theta}_0 = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \log p(\boldsymbol{\theta}, \mathcal{D})$$

$$\mathbf{A} = -\nabla\nabla \log p(\boldsymbol{\theta}, \mathcal{D})|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0}$$

$$p(z) \propto \exp(-z^2/2)\sigma(20z + 4)$$

Yellow: true

Red: Laplace approx.



- Laplace approximation
- Bayesian logistic regression

- Given a dataset $\{\phi_n, t_n\}$, where $t_n \in \{0, 1\}$, $\phi_n = \phi(\mathbf{x}_n)$ and $n = 1, \dots, N$, the likelihood function is given by

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} | \mathbf{m}_0, \mathbf{S}_0)$$

$$p(\mathbf{t} | \mathbf{w}) = \prod_{n=1}^N y_n^{t_n} \{1 - y_n\}^{1-t_n}$$

$$\mathbf{t} = (t_1, \dots, t_N)^T$$

$$y_n = p(\mathcal{C}_1 | \phi_n) = \sigma(\mathbf{w}^T \phi_n)$$



$$p(\mathbf{w} | \mathbf{t}) \propto p(\mathbf{w}) p(\mathbf{t} | \mathbf{w})$$

$$\log p(\mathbf{w}, \mathbf{t}) = -\frac{1}{2}(\mathbf{w} - \mathbf{m}_0)^T \mathbf{S}_0^{-1}(\mathbf{w} - \mathbf{m}_0) + \sum_{n=1}^N \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\} + \text{const}$$



$$\frac{d\sigma}{da} = \sigma(1 - \sigma).$$

$$\mathbf{S}_N = -\nabla \nabla \ln p(\mathbf{w} | \mathbf{t}) = \mathbf{S}_0^{-1} + \sum_{n=1}^N y_n(1 - y_n) \phi_n \phi_n^T$$



$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w} | \mathbf{w}_{\text{MAP}}, \mathbf{S}_N^{-1})$$

- Predictive distribution: given a new input ϕ

$$\begin{array}{ccc} a = \phi^\top \mathbf{w} & & q(\mathbf{w}) = \mathcal{N}(\mathbf{w} | \mathbf{w}_{\text{MAP}}, \mathbf{S}_N^{-1}) \\ \swarrow & & \searrow \\ q(a) = \mathcal{N}(a | \mathbf{w}_{\text{MAP}}^\top \phi, \phi^\top \mathbf{S}_N^{-1} \phi) & & \\ \downarrow & & \\ p(\mathcal{C}_1 | \mathbf{t}) = \int \sigma(a) q(a) da & & \text{Numerical quadrature} \end{array}$$

- The general idea of Laplace's Approximation
- Being able to implement it