

Lecture 3. Variational Bayes

Introduction to Bayesian Statistical learning

18.03.2024-22.03.2024 Instructors: Alina Bazarova, Oleg Filatov. Technical issues: Alexandre Strube

Analytic Variational Bayes (slightly heavier on the math)

Formula for posterior distribution (reminder)

$$p(\theta | X) = \frac{p(\theta)p(X | \theta)}{\int_{\mathbb{R}} p(\theta)p(X | \theta)d\theta} = \frac{p(X, \theta)}{\int_{\mathbb{R}} p(\theta)p(X | \theta)d\theta}$$

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Assume there is a distribution density function $q(\theta)$ which is in turn parametrised by a series of hyper-parameters.

Free energy and Kullback-Leibler divergence

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Note, that KL divergence is always ≥ 0 and hence $\log p(X) \geq \int q(\theta) \log \frac{p(X, \theta)}{q(\theta)} d\theta$

Moreover, $\int q(\theta) \log \frac{q(\theta)}{p(\theta | X)} d\theta = \int q(\theta) \log q(\theta) d\theta - \int q(\theta) \log p(\theta | X) d\theta$ **measure of how close $q(\theta)$ and $p(\theta | X)$ are**

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Hence **maximising free energy** is equivalent to **minimising KL divergence**

Mean-field approximation

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The key property of q_{θ_i} :

$$\log q(\theta_i) \propto \int q_{\theta_{-i}}(\theta_{-i}) p(X, \theta) d\theta_{-i} \quad q_{\theta_{-i}}(\theta_{-i}) = \prod_{j \neq i} q_{\theta_j}(\theta_j)$$

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The proof of the above stems from the calculus of variations.

Sketch of the proof

We need to maximise free energy $F = \int q(\theta) \log \frac{p(X, \theta)}{q(\theta)} d\theta$ with respect to each factorised $q_{\theta_i}(\theta_i)$

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From variational calculus this is equivalent to solving: $\frac{\partial}{\partial q_{\theta_i}(\theta_i)} \int q(\theta) \log \frac{p(X, \theta)}{q(\theta)} d\theta_{-i} = 0$

Sketch of the proof

$$\frac{\partial}{\partial q_{\theta_i}(\theta_i)} \int q(\theta) \log \frac{p(X, \theta)}{q(\theta)} d\theta_{-i} = 0, \text{ recall } q(\theta) = \prod_i q(\theta_i)$$

use differentiation by parts

$$\int q_{\theta_{-i}}(\theta_{-i}) \log p(X, \theta) d\theta_{-i} - \int q_{\theta_{-i}}(\theta_{-i}) \log q(\theta_{-i}) d\theta_{-i} - \int q_{\theta_{-i}}(\theta_{-i}) \log q(\theta_i) d\theta_{-i} + \text{const} = 0$$

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$$\log q(\theta_i) \propto \int q_{\theta_{-i}} \log p(X, \theta) d\theta_{-i} \blacksquare$$

Algorithm (Mean field variational Bayes for 2 parameters θ_1, θ_2)

1. Initialise $q(\theta_1)$

2. Given $q(\theta_1)$ update $q(\theta_2)$ using $\log q(\theta_2) \propto \int \log p(X, \theta) q(\theta_1) d\theta_1$

3. Given $q(\theta_2)$ update $q(\theta_1)$ using $\log q(\theta_1) \propto \int \log p(X, \theta) q(\theta_2) d\theta_2$

4. Iterate until stopping condition is met.

Example: a single Gaussian

Assume we draw measurements $y = (y_1, \dots, y_n)$ from a Gaussian distribution with

mean μ and precision β :
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$$\text{Recall } q(\mu) \sim N(m, \nu) \text{ and hence } m = \frac{m_0 + \nu_0bcs_1}{1 + N\nu_0bc} \text{ and } \nu = \frac{\nu_0}{1 + N\nu_0bc} \text{ where } s_1 = \sum_n y_n$$

Update on β

We apply a similar procedure to derive an update on β .

$$\log q(\beta) = \int Lq(\mu)d\mu = \int LN(\mu, m, \nu)d\mu = \left(\frac{N}{2} + c_0 - 1\right) \log \beta + \frac{\beta}{b_0} - \frac{\beta}{2} \int \sum_n (y_n - \mu)^2 N(\mu, m, \nu) d\mu + \text{const}\{\beta\}$$

$$\log q(\beta) = \left(\frac{N}{2} + c_0 - 1\right) \log \beta - \left(\frac{1}{b_0} + \frac{X}{2}\right) \beta, \text{ where } X \text{ is the integral above:}$$

$$X = \frac{1}{2} \int (s_2 - 2\mu s_1 + \mu^2) N(\mu, m, \nu) d\mu = \frac{1}{2} s_2 - 2s_1 m + N(m + \nu^2), \text{ where } s_2 = \sum_n y_n^2$$

$$\text{Hence, } \frac{1}{b} = \frac{1}{b_0} + \frac{X}{2} \text{ and } c = \frac{N}{2} + c_0.$$

We can now proceed in an iterative procedure (fix β , update μ and the other way round until necessary)!

Jupyter notebook avb_gaussian

Non-linear models and convergence issues

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Convergence.

- Convergence of VB is guaranteed since it is a generalisation of Expectation Maximisation algorithm
- As soon as we use Taylor approximation, the theory breaks down, and convergence becomes more empirical: e.g. monitoring free energy F , stop when it reaches maximum

Stochastic Variational Bayes

Recall that the problem we discussed previously is maximising free energy

$$F = \int q(\theta) \log \frac{p(X, \theta)}{q(\theta)} d\theta.$$

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$$F \approx \frac{1}{L} \sum_l \log p(X, \theta^l) - \log \frac{q(\theta^l)}{p(\theta^l)}, \text{ where } \theta^l \text{ are drawn from } q(\theta)$$

$$\text{Moreover, } \nabla_{\phi} F \approx \frac{1}{L} \sum_l \nabla_{\phi} \left(\log p(X, \theta^l) - \log \frac{q(\theta^l)}{p(\theta^l)} \right)$$

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Can be even simpler: $q(\theta) \sim N(\theta; \mu, \sigma)$. Generate $\varepsilon \sim N(0,1)$, then $\theta = \mu + \sigma\varepsilon$

How to choose L ?

In practice even $L = 1$ can be sufficient, however we need to choose **gradient descent algorithm** which deals with **stochastic optimisation**, e.g. **Adam**

To improve computational efficiency use **mini-batches**: divide data into subsets and performing optimisation on each batch in turn.

Very common technique in the machine learning!

Example: fitting a Gaussian distribution

Assume we draw measurements $y = (y_1, \dots, y_n)$ from a Gaussian distribution with mean μ and precision β : $P(y \mid \mu, \beta) = \left(\frac{\beta}{2\pi}\right)^{\frac{n}{2}} e^{-\frac{\beta}{2} \sum (y_i - \mu)^2}$.

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Recall $MVN(m, C)$ has a pdf function

$$p(x, m, C) = (2\pi)^{-n/2} |C|^{-1/2} \exp \left((x - m)^T C^{-1} (x - m) \right)$$

Free energy

$$\int q(\theta) \log \frac{p(\theta)p(y|\theta)}{q(\theta)} d\theta \approx - \int q(\theta) \log \frac{q(\theta)}{p(\theta)} d\theta + \frac{1}{L} \sum_l \log p(y|\theta^l)$$

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Jupyter notebooks `svb_gaussian_tf2`, `svb_biexp_tf2`