Basics of Bayesian inferences and Bayesian deep learning

-Summary-

• Difference between frequentist and Bayesian approaches for statistical inference:

Frequentist versus Bayesian Methods

- In frequentist inference, probabilities are interpreted as long run frequencies. The goal is to create procedures with long run frequency guarantees.
- In Bayesian inference, probabilities are interpreted as subjective degrees of belief. The goal is to state and analyze your beliefs.

- Bayesian inference procedure:
 - 1. Choose prior distribution for $p(\theta)$: express our beliefs about a parameter θ before we see any data.
 - 2. Choose statistical model $p(x|\theta)$: reflects our beliefs about x given θ .
 - 3. After observing data $\mathcal{D}_n = \{X_1, ... X_n\}$, we update our beliefs and calculate the posterior distributions $p(\theta | \mathcal{D}_n)$.

- Our goal is to find posterior distribution $p(\theta|\mathcal{D}_n)$ and estimate $E[g(\theta)|\mathcal{D}_n]$ by $\sum_{i=1}^n g(\theta^{(s)})$
 - When $p(\theta|\mathcal{D}_n)$ can be computed explicitly -> Use Monte Carlo (MC) method:

<MC algorithm>:

for
$$j = 1$$
 to s :

1. Sample $\theta^{(j)} \sim p(\theta | \mathcal{D}_n)$

This algorithm gives independent Samples $\{ \boldsymbol{\theta}^{(1)}, ... \, \boldsymbol{\theta}^{(s)} \}$

For example : $x_i | \mu, \tau \sim N(\mu, \frac{1}{\tau}), \mu | \tau, x \sim N(\mu_0, \frac{1}{\tau}), \tau \sim \text{Gamma}(\alpha, \beta)$:

$$p(\mu|x_1, \dots x_n) \propto \left(2\beta + (\mu - \mu_0)^2 + \sum_{i=1}^n (x_i - \mu)^2\right)^{-\alpha - \frac{(n+1)}{2}}$$

$$p(\tau|x_1, \dots x_n) = dGamma\left(\alpha + \frac{n}{2}, \beta + \frac{1}{2} \sum_{i=1}^n (x_i - \bar{x})^2 + \frac{n}{2(n+1)} (\bar{x} - \mu_0)^2\right)$$

• When the posterior distribution $p(\theta|\mathcal{D}_n)$ is intractable (or cannot given by implicit form):

(Let's denote
$$\theta = (\theta_1, \dots \theta_k), \theta_{-i} = (\theta_1, \dots \theta_{i-1}, \theta_{i+1}, \dots, \theta_k)$$
)

If the full conditional distribution $p(\theta_i | \theta_{-i}, \mathcal{D}_n)$ is **known** -> Use Gibbs sampling:

<Gibbs sampling algorithm> :

Given the current state $\theta^{(s)} = \left(\theta_1^{(s)}, \dots \theta_k^{(s)}\right)$

(# $\theta^{(0)}$ can be chosen by appropriate estimator of θ)

1. Sample
$$\theta_1^{(s+1)} \sim p\left(\theta \middle| \theta_{-1}^{(s)}, x_1, ... x_n\right)$$

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K. Sample
$$\theta_k^{(s+1)} \sim p\left(\theta \middle| \theta_{-k}^{(s)}, x_1, \dots x_n\right)$$

K+1. Set
$$\theta^{(s+1)} = (\theta_1^{(s+1)}, \dots \theta_k^{(s+1)})$$

This algorithm gives dependent Samples $\{\theta^{(1)}, ... \theta^{(s)}\}$

• When the posterior distribution $p(\theta|\mathcal{D}_n)$ is intractable (or cannot given by implicit form): If the full conditional distribution $p(\theta_i|\theta_{-i},\mathcal{D}_n)$ is unknown: -> Use Metropolis Algorithm

<Metropolis algorithm> :

Given the current state $\theta^{(s)} = (\theta_1^{(s)}, \dots \theta_k^{(s)})$

This algorithm gives dependent Samples $\{\theta^{(1)}, ... \theta^{(s)}\}$

- 1. Sample $\theta^* \sim J(\theta | \theta^{(s)})$
- 2. Compute the acceptance ratio:

$$r = \frac{p(\theta^*|x_1, ..., x_n)}{p(\theta^{(s)}|x_1, ..., x_n)} = \frac{p(x_1, ... x_n | \theta^*) p(\theta^*)}{p(x_1, ... x_n | \theta^{(s)}) p(\theta^{(s)})}$$

3. Set
$$\theta^{(s+1)} = \begin{cases} \theta^* & \text{with probability} & \min(r,1) \\ \theta^{(s)} & \text{with probability} & 1 - \min(r,1) \end{cases}$$

Note: $J(\theta | \theta^{(s)})$ is a symmetric proposal distribution

(ex:
$$J(\theta|\theta^{(s)}) = \text{uniform}(\theta^{(s)} - \delta, \theta^{(s)} + \delta) \text{ or } N(\theta^{(s)}, \delta^2)$$
, where δ is given)

• Can we **generalize** the Gibbs sampling and Metropolis algorithm? -> Metropolis-Hasting

<Metropolis-Hasting algorithm> :

Given the current state $\theta^{(s)} = (\theta_1^{(s)}, \dots \theta_k^{(s)})$:

for i = 1 to k:

1. Update θ_i :

- a. Sample $\theta_i^* \sim J_i(\theta_i | \theta^{(s)})$
- b. Compute the acceptance ratio:

Note:

1. This terms becomes 1 when J_i is symmetric.

(the algorithm regresses to Metropolis algorithm)

2. Acceptance ratio r=1 when J_i is full conditional distribution of θ_i .

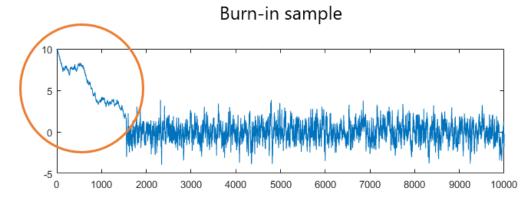
(the algorithm regresses to Gibbs Sampling)

$$r = \frac{p(\theta_{i}^{*}, \theta_{-i}^{(s)})}{p(\theta_{i}^{(s)}, \theta_{-i}^{(s)})} \times \frac{J_{i}(\theta_{i}^{(s)} | \theta_{i}^{*}, \theta_{-i}^{(s)})}{J_{i}(\theta_{i}^{*} | \theta_{i}^{(s)}, \theta_{-i}^{(s)})}$$

c. Set
$$\theta_i^{(s+1)} = \begin{cases} \theta_i^* & \text{with probability} & \min(r, 1) \\ \theta_i^{(s)} & \text{with probability} & 1 - \min(r, 1) \end{cases}$$

• Here, $J_i(\theta_i|\theta^{(s)})$ does not need to be symmetric (i.e : $J_i(\theta_a|\theta_b) \neq J_i(\theta_b|\theta_a)$)

- Recall that the Gibbs sampling / Metropolis (-Hasting) algorithms give 'dependent' samples.
 - In other words, the samples will be autocorrelated within a Markov chain, and we want independent samples. (How to obtain nearly independent samples among them??)
 - Q: Given s samples by MCMC, how many independent samples can be induced (or considered) from these samples? -> Check **Effective Sample Size** (ESS)
 - Q: Under the MCMC process, Are all the samples important as samples? -> No (Use **burn-in**, for example: drop 1500 samples at the initial MCMC process)



- Recall that the Gibbs sampling / Metropolis (-Hasting) algorithms give 'dependent' samples.
 - How to select samples to make nearly independent sample set? -> Use thinning:
 - Check autocorrelation of MCMC chain
 - 2. Pick lag number so that ACF is reasonably low. (here, lag = 40).
 - Among attained s samples by MCMC, pick every 40th samples to make a nearly independent sample set.

