Variational Inference

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Introduction

Bayesian ML: Recap

- We assume a prior distribution over the parameters of the model given as $P(\theta)$
- We assume a likelihood function $P(D|\theta)$
- We use Bayes' rule to find the posterior distribution of the parameters given the data: $P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$
- Typically, we can not compute the posterior distribution analytically as the denominator is intractable

Bayesian ML: Methods

Laplace Approximation

Approximates the posterior with a Gaussian distribution parameterized by $\Psi = (\mu, \Sigma)$.

$$q_\Psi(\theta) = \mathcal{N}(\mu, \Sigma)$$

where μ is the mode of the posterior and Σ is the negative inverse Hessian of the log joint distribution evaluated at θ_{MAP}.

MCMC (Markov Chain Monte Carlo)

Generates samples from the posterior distribution by constructing a Markov chain.

$$P(\theta|D) \propto P(D|\theta)P(\theta)$$

Variational Inference

Poses posterior inference as an optimization problem. The approximating distribution is parameterized by Ψ.

$$\Psi^* = \arg\min_{\Psi} \mathrm{KL}(q_\Psi(\theta)||P(\theta|D))$$

KL Divergence

- KL divergence is a measure of dissimilarity between two distributions.
- It is defined as: $\mathrm{KL}(q||p) = \int q(\theta) \log \frac{q(\theta)}{p(\theta)} d\theta$
- Or, can be written in terms of expectations as: $\mathrm{KL}(q||p) = \mathbb{E}_{q(\theta)} \left[\log \frac{q(\theta)}{p(\theta)} \right]$

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Compute the KL divergence between two Gaussian distributions $q(\theta) = \mathcal{N}(\mu_q, \sigma_q^2)$ and $p(\theta) = \mathcal{N}(\mu_p, \sigma_p^2)$.

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- $\mathrm{KL}(q||p) = \mathbb{E}_{q(\theta)}\left[\log \frac{q(\theta)}{p(\theta)}\right]$
- Expanding $q(\theta) = \mathcal{N}(\mu_q, \sigma_q^2) = \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp\left(-\frac{(\theta-\mu_q)^2}{2\sigma_q^2}\right)$

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- $\mathrm{KL}(q||p) = \mathbb{E}_{q(\theta)}\left[\log \frac{q(\theta)}{p(\theta)}\right] =$
  $\mathbb{E}_{q(\theta)}\left[\log \frac{\frac{1}{\sqrt{2\pi\sigma_q^2}} \exp\left(-\frac{(\theta-\mu_q)^2}{2\sigma_q^2}\right)}{\frac{1}{\sqrt{2\pi\sigma_p^2}} \exp\left(-\frac{(\theta-\mu_p)^2}{2\sigma_p^2}\right)}\right]$

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The answer is: $\frac{1}{2}\left(\log \frac{\sigma_2^2}{\sigma_1^2} + \frac{\sigma_1^2+(\mu_1-\mu_2)^2}{\sigma_2^2} - 1\right)$

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- Now using linearity of expectation, we get:

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Aside:

$\theta \sim q(\theta) = \mathcal{N}(\mu_q, \sigma_q^2)$

$\mathbb{E}_{q(\theta)}\left[\theta\right] = \mu_q$

$\mathbb{E}_{q(\theta)}\left[\theta^2\right] = \sigma_q^2 + \mu_q^2$

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- Using the aside, we expand the expectation:

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- $\mathrm{KL}(q||p)$ = Term 1 + Term 2 + Term 3 + Term 4 + Term 5 + Term 6 + Term 7

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- Using the aside, we expand the expectation:
- $\text{KL}(q||p) =$ Term 1 + Term 2 + Term 3 + Term 4 + Term 5 + Term 6 + Term 7
- Term 1 $= \log \frac{\sigma_p}{\sigma_q}$

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- $\text{KL}(q||p) = \text{Term 1} + \text{Term 2} + \text{Term 3} + \text{Term 4} + \text{Term 5} + \text{Term 6} + \text{Term 7}$
- $\text{Term 1} = \log \frac{\sigma_p}{\sigma_q}$
- Term 2: $\mathbb{E}_{q(\theta)}\left(-\frac{\theta^2}{2\sigma_q^2}\right) = -\frac{1}{2}\mathbb{E}_{q(\theta)}\left(\frac{\theta^2}{\sigma_q^2}\right) = -\frac{1}{2}\left(\frac{\sigma_q^2+\mu_q^2}{\sigma_q^2}\right)$

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- Term 3: $\mathbb{E}_{q(\theta)}\left(\frac{2\theta\mu_q}{2\sigma_q^2}\right) = \frac{2\mu_q}{2\sigma_q^2}\mathbb{E}_{q(\theta)}(\theta) = \frac{2\mu_q^2}{2\sigma_q^2}$

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- Term 7: $\mathbb{E}_{q(\theta)}\left(\frac{\mu_p^2}{2\sigma_p^2}\right) = \frac{\mu_p^2}{2\sigma_p^2}$
- Overall after simplification, we get:
  $\mathrm{KL}(q||p) = \frac{1}{2}[\log\frac{\sigma_p^2}{\sigma_q^2} - 1 + \frac{(\mu_p-\mu_q)^2}{\sigma_p^2} + \frac{\sigma_q^2}{\sigma_p^2}]$

Notebook demo

Optimizing

Notebook demo

Monte Carlo Sampling

Notebook demo

Repameterization Trick

Notebook demo

ELBO

Worked out example: Coin Toss

Worked out example: Linear Regression

Worked out example: Neural Networks