Statistical Models & Computing Methods

Lecture 15: Advanced VI – I



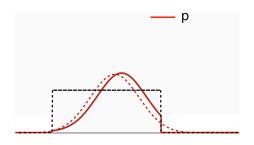
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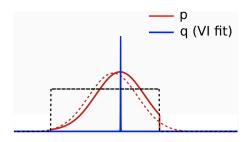
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Introduction

- ➤ So far, we have only used the KL divergence as a distance measure in VI.
- ▶ Other than the KL divergence, there are many alternative statistical distance measures between distributions that admit a variety of statistical properties.
- ▶ In this lecture, we will introduce several alternative divergence measures to KL, and discuss their statistical properties, with applications in VI.



- ▶ VI does not work well for non-smooth potentials
- ► This is largely due to the zero-avoiding behaviour
 - The area where $p(\theta)$ is close to zero has very negative $\log p$, so does the variational distribution q when trained to minimize the KL.
- ► In this truncated normal example, VI will fit a delta function!



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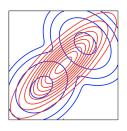


 \triangleright Recall that the KL divergence from q to p is

$$D_{\mathrm{KL}}(q||p) = \mathbb{E}_q \log \frac{q(x)}{p(x)} = \int q(x) \log \frac{q(x)}{p(x)} dx$$

► An alternative: the reverse KL divergence

$$D_{\mathrm{KL}}^{\mathrm{Rev}}(p||q) = \mathbb{E}_p \log \frac{p(x)}{q(x)} = \int p(x) \log \frac{p(x)}{q(x)} \ dx$$









KL



ightharpoonup The f-divergence from q to p is defined as

$$D_f(q||p) = \int p(x)f\left(\frac{q(x)}{p(x)}\right) dx$$

where f is a convex function such that f(1) = 0.

ightharpoonup The f-divergence defines a family of valid divergences

$$D_f(q||p) = \int p(x)f\left(\frac{q(x)}{p(x)}\right) dx$$

$$\geq f\left(\int p(x)\frac{q(x)}{p(x)} dx\right) = f(1) = 0$$

and

$$D_f(q||p) = 0 \Rightarrow q(x) = p(x)$$
 a.s.



Many common divergences are special cases of f-divergence, with different choices of f.

- ightharpoonup KL divergence. $f(t) = t \log t$
- ightharpoonup reverse KL divergence. $f(t) = -\log t$
- ► Hellinger distance. $f(t) = \frac{1}{2}(\sqrt{t} 1)^2$

$$H^{2}(p,q) = \frac{1}{2} \int (\sqrt{q(x)} - \sqrt{p(x)})^{2} dx = \frac{1}{2} \int p(x) \left(\sqrt{\frac{q(x)}{p(x)}} - 1 \right)^{2} dx$$

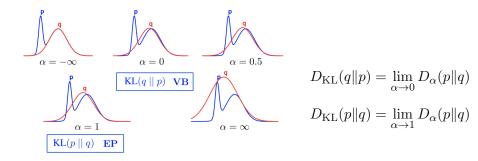
▶ Total variation distance. $f(t) = \frac{1}{2}|t-1|$

$$d_{\text{TV}}(p,q) = \frac{1}{2} \int |p(x) - q(x)| dx = \frac{1}{2} \int p(x) \left| \frac{q(x)}{p(x)} - 1 \right| dx$$



When $f(t) = \frac{t^{\alpha} - t}{\alpha(\alpha - 1)}$, we have the Amari's α -divergence (Amari, 1985; Zhu and Rohwer, 1995)

$$D_{\alpha}(p||q) = \frac{1}{\alpha(1-\alpha)} \left(1 - \int p(\theta)^{\alpha} q(\theta)^{1-\alpha} d\theta \right)$$



Adapted from Hernández-Lobato et al.



$$D_{\alpha}(q||p) = \frac{1}{\alpha - 1} \log \int q(\theta)^{\alpha} p(\theta)^{1 - \alpha} d\theta$$

- ightharpoonup Some special cases of Rényi's α -divergence
 - $D_1(q||p) := \lim_{\alpha \to 1} D_{\alpha}(q||p) = D_{\mathrm{KL}}(q||p)$
 - $D_0(q||p) = -\log \int_{q(\theta)>0} p(\theta) d\theta = 0 \text{ iff } supp(p) \subset supp(q).$
 - $D_{+\infty}(q||p) = \log \max_{\theta} \frac{q(\theta)}{p(\theta)}$
 - $D_{\frac{1}{2}}(q||p) = -2\log(1 \text{Hel}^2(q||p))$
- ► Importance properties
 - ightharpoonup Rényi divergence is non-decreasing in α

$$D_{\alpha_1}(q||p) \ge D_{\alpha_2}(q||p), \quad \text{if } \alpha_1 \ge \alpha_2$$

• Skew symmetry: $D_{1-\alpha}(q||p) = \frac{1-\alpha}{\alpha}D_{\alpha}(p||q)$



- ► Consider approximating the exact posterior $p(\theta|x)$ by minimizing Rényi's α -divergence $D_{\alpha}(q(\theta)||p(\theta|x))$ for some selected $\alpha > 0$
- ▶ Using $p(\theta|x) = p(\theta, x)/p(x)$, we have

$$D_{\alpha}(q(\theta)||p(\theta|x)) = \frac{1}{\alpha - 1} \log \int q(\theta)^{\alpha} p(\theta|x)^{1 - \alpha} d\theta$$
$$= \log p(x) - \frac{1}{1 - \alpha} \log \int q(\theta)^{\alpha} p(\theta, x)^{1 - \alpha} d\theta$$
$$= \log p(x) - \frac{1}{1 - \alpha} \log \mathbb{E}_q \left(\frac{p(\theta, x)}{q(\theta)}\right)^{1 - \alpha}$$

► The Rényi lower bound (Li and Turner, 2016)

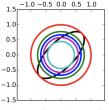
$$L_{\alpha}(q) \triangleq \frac{1}{1-\alpha} \log \mathbb{E}_q \left(\frac{p(\theta, x)}{q(\theta)} \right)^{1-\alpha}$$



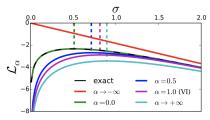
▶ Theorem(Li and Turner 2016). The Rényi lower bound is continuous and non-increasing on $\alpha \in [0,1] \cup \{|L_{\alpha}| < +\infty\}$. Especially for all $0 < \alpha < 1$

$$L_{\text{VI}}(q) = \lim_{\alpha \to 1} L_{\alpha}(q) \le L_{\alpha}(q) \le L_{0}(q)$$

 $L_0(q) = \log p(x) \text{ iff } supp(p(\theta|x)) \subset supp(q(\theta)).$



(a) Approximated posterior.



(b) Hyper-parameter optimisation.



► Monte Carlo estimation of the Rényi lower bound

$$\hat{L}_{\alpha,K}(q) = \frac{1}{1-\alpha} \log \frac{1}{K} \sum_{i=1}^{K} \left(\frac{p(\theta_i, x)}{q(\theta_i)} \right)^{1-\alpha}, \quad \theta_i \sim q(\theta)$$

- ▶ Unlike traditional VI, here the Monte Carlo estimate is **biased**. Fortunately, the bias can be characterized by the following theorem
- ▶ **Theorem**(Li and Turner, 2016). $\mathbb{E}_{\{\theta_i\}_{i=1}^K}(\hat{L}_{\alpha,K}(q))$ as a function of α and K is
 - ▶ non-decreasing in K for fixed $\alpha \leq 1$, and converges to $L_{\alpha}(q)$ as $K \to +\infty$ if $supp(p(\theta|x)) \subset supp(q(\theta))$.
 - continuous and non-increasing in α on $[0,1] \cup \{|L_{\alpha}| < +\infty\}$



▶ When $\alpha = 0$, the Monte Carlo estimate reduces to the multiple sample lower bound (Burda et al., 2015)

$$\hat{L}_K(q) = \log \left(\frac{1}{K} \sum_{i=1}^K \frac{p(x, \theta_i)}{q(\theta_i)} \right), \quad \theta_i \sim q(\theta)$$

- ▶ This recovers the standard ELBO when K = 1.
- ▶ Using more samples improves the tightness of the bound (Burda et al., 2015)

$$\log p(x) \ge \mathbb{E}(\hat{L}_{K+1}(q)) \ge \mathbb{E}(\hat{L}_K(q))$$

Moreover, if $p(x,\theta)/q(\theta)$ is bounded, then

$$\mathbb{E}(\hat{L}_K(q)) \to \log p(x)$$
, as $K \to +\infty$



Using the reparameterization trick

$$\theta \sim q_{\phi}(\theta) \Leftrightarrow \theta = g_{\phi}(\epsilon), \ \epsilon \sim q_{\epsilon}(\epsilon)$$

$$\nabla_{\phi} \hat{L}_{\alpha,K}(q_{\phi}) = \sum_{i=1}^{K} \left(\hat{w}_{\alpha,i} \nabla_{\phi} \log \frac{p(g_{\phi}(\epsilon_i), x)}{q_{\phi}(g_{\phi}(\epsilon_i))} \right), \quad \epsilon_i \sim q_{\epsilon}(\epsilon)$$

where

$$\hat{w}_{\alpha,i} \propto \left(\frac{p(g_{\phi}(\epsilon_i), x)}{q_{\phi}(g_{\phi}(\epsilon_i))}\right)^{1-\alpha},$$

the normalized importance weight with finite samples. This is a biased estimate of $\nabla_{\phi} L_{\alpha}(q_{\phi})$ (except $\alpha = 1$).

- $ightharpoonup \alpha = 1$: Standard VI with the reparamterization trick
- $ightharpoonup \alpha = 0$: Importance weighted VI (Burda et al., 2015)



- ► Full batch training for maximizing the Rényi lower bound could be very inefficient for large datasets
- ► Stochastic optimization is non-trivial since the Rényi lower bound can not be represented as an expectation on a datapoint-wise loss, except for $\alpha = 1$.
- ► Two possible methods:
 - ▶ derive the fixed point iteration on the whole dataset, then use the minibatch data to approximately compute it (Li et al., 2015)
 - ▶ approximate the bound using the minibatch data, then derive the gradient on this approximate objective (Hernández-Lobato et al., 2016)

Remark: the two methods are equivalent when $\alpha = 1$ (standard VI).



► Suppose the true likelihood is

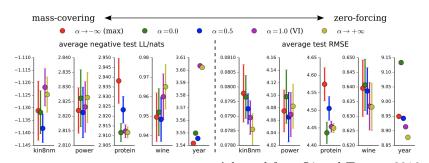
$$p(x|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

► Approximate the likelihood as

$$p(x|\theta) \approx \left(\prod_{n \in \mathcal{S}} p(x_n|\theta)\right)^{\frac{N}{|\mathcal{S}|}} \triangleq \bar{f}_{\mathcal{S}}(\theta)^N$$

▶ Use this approximation for the energy function

$$\tilde{L}_{\alpha}(q, \mathcal{S}) = \frac{1}{1 - \alpha} \log \mathbb{E}_{q} \left(\frac{p_{0}(\theta) \bar{f}_{\mathcal{S}}(\theta)^{N}}{q(\theta)} \right)^{1 - \alpha}$$



Adapted from Li and Turner, 2016

- ▶ The optimal α may vary for different data sets.
- Large α improves the predictive error, while small α provides better test log-likelihood.
- $\sim \alpha = 0.5$ seems to produce overall good results for both test LL and RMSE.

▶ In standard VI, we often minimize $D_{KL}(q||p)$. Sometimes, we can also minimize $D_{KL}(p||q)$ (can be viewed as MLE).

$$q^* = \underset{q}{\operatorname{arg\,min}} D_{\mathrm{KL}}(p||q) = \underset{q}{\operatorname{arg\,max}} \mathbb{E}_p \log q(\theta)$$

ightharpoonup Assume q is from the exponential family

$$q(\theta|\eta) = h(\theta) \exp\left(\eta^{\top} T(\theta) - A(\eta)\right)$$

▶ The optimal η^* satisfies

$$\eta^* = \underset{\eta}{\arg \max} \mathbb{E}_p \log q(\theta|\eta)$$
$$= \underset{\eta}{\arg \max} \left(\eta^\top \mathbb{E}_p \left(T(\theta) \right) - A(\eta) \right) + \text{Const}$$

ightharpoonup Differentiate with respect to η

$$\mathbb{E}_p\left(T(\theta)\right) = \nabla_{\eta} A(\eta^*)$$

▶ Note that $q(\theta|\eta)$ is a valid distribution $\forall \eta$

$$0 = \nabla_{\eta} \int h(\theta) \exp\left(\eta^{\top} T(\theta) - A(\eta)\right) d\theta$$
$$= \int q(\theta|\eta) \left(T(\theta) - \nabla_{\eta} A(\eta)\right) d\theta$$
$$= \mathbb{E}_{q} \left(T(\theta)\right) - \nabla_{\eta} A(\eta)$$

► The KL divergence is minimized if the expected sufficient statistics are the same

$$\mathbb{E}_{q}\left(T(\theta)\right) = \mathbb{E}_{p}\left(T(\theta)\right)$$



- ► An approximate inference method proposed by Minka 2001.
- ► Suitable for approximating product forms. For example, with iid observations, the posterior takes the following form

$$p(\theta|x) \propto p(\theta) \prod_{i=1}^{n} p(x_i|\theta) = \prod_{i=0}^{n} f_i(\theta)$$

► We use an approximation

$$q(\theta) \propto \prod_{i=0}^{n} \tilde{f}_i(\theta)$$

One common choice for \tilde{f}_i is the exponential family

$$\tilde{f}_i(\theta) = h(\theta) \exp\left(\eta_i^{\top} T(\theta) - A(\eta_i)\right)$$

▶ Iteratively refinement of the terms $\tilde{f}_i(\theta)$



ightharpoonup Take out term approximation i

$$q^{\setminus i}(\theta) \propto \prod_{j \neq i} \tilde{f}_j(\theta)$$

 \triangleright Put back in term i

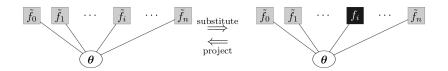
$$\hat{p}(\theta) \propto f_i(\theta) \prod_{j \neq i} \tilde{f}_j(\theta)$$

 \blacktriangleright Match moments. Find q such that

$$\mathbb{E}_q(T(\theta)) = \mathbb{E}_{\hat{p}}(T(\theta))$$

▶ Update the new term approximation

$$\tilde{f}_i^{\text{new}}(\theta) \propto \frac{q(\theta)}{q^{\setminus i}(\theta)}$$



▶ Minimize the KL divergence from \hat{p} to q

$$D_{\mathrm{KL}}(\hat{p}||q) = \mathbb{E}_{\hat{p}} \log \left(\frac{\hat{p}(\theta)}{q(\theta)} \right)$$

ightharpoonup Equivalent to moment matching when q is in the exponential family.

- ▶ The approximating distributions that we discussed so far are assumed to have a parametric form, that is $q_{\theta}(x)$ with parameter θ .
- ► This parametric form often limits the power of the approximating distributions.
- ► In what follows, we will introduce a particle based VI introduced by Liu et al. that uses non-parameteric approximating distributions.



- ► A general theoretical tool for bounding differences between distributions, introduced by Charles Stein.
- ▶ The key idea is to characterize a distribution p with a Stein operator A_p , such that

$$p = q \iff \mathbb{E}_{x \sim q}[\mathcal{A}_p f(x)] = 0, \quad \forall f \in \mathcal{F}$$

For continuous distributions with smooth density p(x),

$$\mathcal{A}_p f(x) := s_p(x)^T f(x) + \nabla_x \cdot f(x)$$

where $s_p(x) = \nabla_x \log p(x)$ is the score function.

Note that $s_p(x)$ does not dependent on the normalizing constant of p(x), so p(x) can be unnormalized.



▶ When p = q, we have Stein's Identity

$$\mathbb{E}_{x \sim p} \left[s_p(x)^T f(x) + \nabla_x \cdot f(x) \right] = 0$$

- ightharpoonup Stein's identity defines an infinite number of identities indexed by test function f, widely applied in learning probabilistic models, variance reduction, optimization and many more.
- ▶ When $p \neq q$, we have (also by Stein's Identity)

$$\mathbb{E}_{x \sim q}[\mathcal{A}_p f(x)] = \mathbb{E}_{x \sim q}[(s_p(x) - s_q(x))^T f(x)] \tag{1}$$

Easy to find test function f(x) such that (1) is non-zero. For example:

$$f(x) = s_p(x) - s_q(x)$$



 \blacktriangleright We therefore, define Stein Discrepancy between p and q as follows

$$D(q||p) := \max_{f \in \mathcal{F}} \mathbb{E}_{x \sim q}[\mathcal{A}_p f(x)]$$
 (2)

where \mathcal{F} is a rich enough set of functions.

- ightharpoonup Traditionally, Stein's method takes \mathcal{F} to be sets of functions with bounded Lipschitz norm, which is computationally difficult for practical use.
- ▶ We can use a kernel trick to construct a reproducing kernel Hilbert space (RKHS) where there is a closed form solution to (2).



Let k(x, x') be a positive definite kernel, that is

$$\int_{\mathcal{X}} g(x)k(x, x')g(x') \ dxdx' > 0, \quad \forall \ 0 < \|g\|_{2}^{2} < \infty.$$

By Mercer's theorem,

$$k(x, x') = \sum_{i} \lambda_i e_i(x) e_i(x')$$

 \blacktriangleright We can define a RKHS $\mathcal H$ that contains linear combinations of these eigenfunctions

$$f(x) = \sum_{i} f_{i} e_{i}(x), \quad \langle f, g \rangle_{\mathcal{H}} = \sum_{i} \frac{f_{i} g_{i}}{\lambda_{i}}$$
 with $||f||_{\mathcal{H}}^{2} = \langle f, f \rangle_{\mathcal{H}} = \sum_{i} f_{i}^{2} / \lambda_{i}$.

► Reproducing Property

$$f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}}, \quad k(x, x') = \langle k(\cdot, x), k(\cdot, x') \rangle_{\mathcal{H}}.$$



▶ Given a positive definite kernel k(x, x'), Liu et al. define a **kernelized Stein discrepancy** (KSD) D(q||p) as follows

$$D(q||p) = \sqrt{\mathbb{E}_{x,x' \sim q}[\delta_{p,q}(x)^T k(x,x') \delta_{p,q}(x')]}$$

where $\delta_{p,q}(x) = s_p(x) - s_q(x)$. Obviously,

$$D(q||p) \ge 0$$
, $D(q||p) = 0 \Leftrightarrow q = p$.

▶ With the spectral decomposition, we can rewrite KSD as

$$D(q||p) = \sqrt{\sum_{i} \lambda_{i} ||\mathbb{E}_{x \sim q}[\mathcal{A}_{p}e_{i}(x)]||_{2}^{2}}$$

- ▶ It turns out that KSD can be viewed as standard Stein discrepancy over a specific family of functions \mathcal{F} , i.e, the unit ball of $\mathcal{H}^d = \mathcal{H} \times \cdots \times \mathcal{H}$.
- ▶ Denote $\beta(x') = \mathbb{E}_{x \sim q}[A_p k_{x'}(x)]$, then

$$D(q||p) = ||\beta||_{\mathcal{H}^d}$$

► Moreover, we have

$$\langle \beta, f \rangle_{\mathcal{H}^d} = \mathbb{E}_{x \sim q}[\mathcal{A}_p f(x)], \quad \forall f \in \mathcal{H}^d$$

► Therefore,

$$D(q||p) = \max_{f \in \mathcal{F}} \mathbb{E}_{x \sim q}[\mathcal{A}_p f(x)]$$

where $\mathcal{F} = \{ f \in \mathcal{H}^d : ||f||_{\mathcal{H}^d} \leq 1 \}$. The maximum is achieved at $f^* = \beta/||\beta||_{\mathcal{H}^d}$.



Proposed by Liu and Wang, 2016.

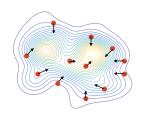
Idea: represent the distribution using a collection of particles $\{x_i\}_{i=1}^n$ and iteratively move these particles toward the target p by updates of form

$$x_i \leftarrow T(x_i), \quad T(x) = x + \epsilon \phi(x)$$

where ϕ is a perturbation direction chosen to maximumly decrease the KL divergence.

$$\phi = \operatorname*{arg\,max}_{\phi \in \mathcal{F}} \left\{ \left. - \frac{\partial}{\partial \epsilon} D_{\mathrm{KL}}(q_T \| p) \right|_{\epsilon = 0} \right\}$$

where q_T is the density of x' = T(x) when the current density of x is q(x).



▶ Perturbation direction is closely related to Stein operator

$$-\frac{\partial}{\partial \epsilon} D_{\mathrm{KL}}(q_T || p) \bigg|_{\epsilon=0} = \mathbb{E}_{x \sim q} [\mathcal{A}_p \phi(x)]$$

▶ This gives another interpretation of Stein discrepancy

$$D(q||p) = \max_{\phi \in \mathcal{F}} \left\{ -\frac{\partial}{\partial \epsilon} D_{\mathrm{KL}}(q_T ||p) \Big|_{\epsilon=0} \right\}$$

▶ Most importantly, the optimum direction has a closed form when \mathcal{F} is the unit ball of RKHS \mathcal{H}^d :

$$\phi^*(\cdot) = \mathbb{E}_{x \sim q}[\mathcal{A}_p k(x, \cdot)]$$

= $\mathbb{E}_{x \sim q}[\nabla_x \log p(x) k(x, \cdot) + \nabla_x k(x, \cdot)]$

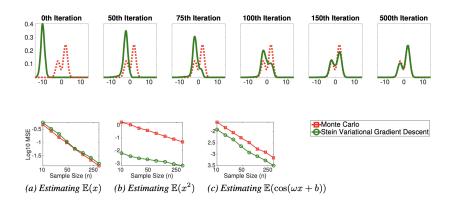


We can approximate the expectation $E_{x\sim q}$ with the empirical average over current particles

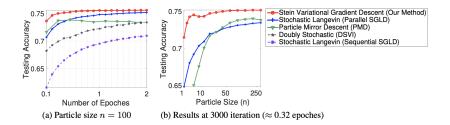
$$x_i \leftarrow x_i + \epsilon \frac{1}{n} \sum_{j=1}^n \left[\nabla_x \log p(x_j) k(x_j, x_i) + \nabla_{x_j} k(x_j, x_i) \right], \ 1 \le i \le n$$

- ▶ Deterministically transport probability mass from initial q_0 to target p.
- ▶ Reduces to standard gradient ascent for MAP when using a single particle (n = 1).
- $\nabla_x \log p(x_j)$: the gradient term moves the particles towards high probability domains of p(x).
- ▶ $\nabla_x k(x_j, x_i)$: the repulsive force term enforces diversity in the particles and prevents them from collapsing to the modes of p(x).









Liu et al., 2016



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