MATHÉMATIQUES
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Stein Variational Gradient Descent: Main ideas

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1 Goal

Given a smooth density π supported on $\mathcal{X} \subseteq \mathbb{R}^d$, find μ on $\mathcal{X}$ as close as possible to π.

2 Stein framework

Stein identity: Let $\mathcal{A}_\pi$ a Stein operator s.t.

$$\mathcal{A}_\pi \phi = \nabla \log \pi(\cdot)^\top \phi(\cdot) + \nabla \cdot \phi(\cdot)$$

with $\phi(x) = [\phi_1(x), ..., \phi_d(x)]^\top$. Then, if ϕ is in the Stein class of π i.e. $\phi(x)\pi(x) = 0$ for all $x \in \partial\mathcal{X}$ if $\mathcal{X}$ is compact or $\lim_{||x|| \to \infty} \phi(x)\pi(x) = 0$ if $\mathcal{X} = \mathbb{R}^d$, we have:

$$\mathbb{E}_{x\sim\pi}[\mathcal{A}_\pi \phi(x)] = 0 \tag{1}$$

Proof.

$$\begin{aligned}
\mathbb{E}_{x\sim\pi}[\mathcal{A}_\pi \phi(x)] &= \int_{\mathcal{X}} \left(\nabla \log \pi(\cdot)^\top \phi(\cdot) + \nabla \cdot \phi(\cdot)\right)\pi(x)dx \\
&= \int_{\mathcal{X}} \nabla \log \pi(\cdot)^\top \phi(\cdot)\pi(x)dx + \int_{\mathcal{X}} \nabla \cdot \phi(\cdot)\pi(x)dx \\
&= \int_{\mathcal{X}} \nabla \log \pi(\cdot)^\top \phi(\cdot)\pi(x)dx + \int_{\mathcal{X}} \sum_{k=1}^d \frac{\partial \phi_k}{\partial x_k}\pi(x)dx \\
&= \int_{\mathcal{X}} \nabla \log \pi(\cdot)^\top \phi(\cdot)\pi(x)dx + \sum_{k=1}^d \left([\pi(x)\phi_k(x)]_{\mathcal{X}} - \int_{\mathcal{X}} \frac{\partial \pi(x)}{\partial x_k}\phi_k(x)dx \right) \\
&= \int_{\mathcal{X}} \nabla \log \pi(\cdot)^\top \phi(\cdot)\pi(x)dx - \int_{\mathcal{X}} \sum_{k=1}^d \frac{\partial \pi(x)}{\partial x_k}\phi_k(x)dx \\
&= \int_{\mathcal{X}} \pi(x) \sum_{k=1}^d \frac{\partial \log \pi(x)}{\partial x_k}\phi_k(x) - \pi(x) \sum_{k=1}^d \frac{\partial \log \pi(x)}{\partial x_k}\phi_k(x)dx \quad \text{(log trick)} \\
&= 0
\end{aligned}$$

■

Now, let μ a smooth density supported on $\mathcal{X}$ different from π. Now, Eq. 1 do not hold anymore with $x \sim \mu$. However, we can use $\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)]$ as a discrepancy measure between μ and π, as its magnitude relates to how different μ and π are (see Liu and Wang [2016] & Liu [2017]). Indeed, if we assume ϕ to be in the Stein class of μ as well (this is mild condition as π and μ are two densities on $\mathcal{X}$, one can choose ϕ to be in the Stein class of all distribution on $\mathcal{X}$. E.g. if $\mathcal{X} = \mathbb{R}^d$, one can pick

$\phi(x) = \exp\big[-\|x-y\|^2\big]$), we have:

$$\begin{aligned}
\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)] &= \int_{\mathcal{X}} \big(\nabla \log \pi(x)^\top \phi(x) + \nabla\cdot\phi(x)\big)\mu(x)dx \\
&= \int_{\mathcal{X}} \nabla \log \pi(x)^\top \phi(x)\mu(x)dx + \sum_{k=1}^{d}\left([\mu(x)\phi_k(x)]_{\mathcal{X}} - \int_{\mathcal{X}} \frac{\partial \mu(x)}{\partial x_k}\phi_k(x)dx\right) \\
&= \int_{\mathcal{X}} \mu(x)\sum_{k=1}^{d}\frac{\partial \log \pi(x)}{\partial x_k}\phi_k(x) - \mu(x)\sum_{k=1}^{d}\frac{\partial \log \mu(x)}{\partial x_k}\phi_k(x)dx \ \ \text{(log trick)} \\
&= \int_{\mathcal{X}} \mu(x)\left[\sum_{k=1}^{d}\phi_k(x)\left(\frac{\partial \log \pi(x)}{\partial x_k} - \frac{\partial \log \mu(x)}{\partial x_k}\right)\right]dx \\
&= \int_{\mathcal{X}} \mu(x)\left[\sum_{k=1}^{d}\phi_k(x)\left(\frac{\partial \log \frac{\pi(x)}{\mu(x)}}{\partial x_k}\right)\right]dx.
\end{aligned} \tag{2}$$

As expected, the scale of $\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)]$ increases w.r.t. the difference between μ and π.

Therefore, one can define an objective to find a density μ^* close to π:

$$\mu^* = \arg\min_{\mu} \ \mathbb{S}(\mu,\pi) = \arg\min_{\mu} \ \max_{\phi\in\mathcal{H}}\{\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)]\}, \tag{3}$$

as $\mathbb{S}(\mu,\pi) = 0$ iff $\mu = \pi$ and $\mathbb{S}(\mu,\pi) > 0$ otherwise with $\mathcal{H}$ sufficiently large. The choice of $\mathcal{H}$ is therefore crucial. One way to ensure it is both rich enough and computationally tractable is to let $\mathcal{H}$ be a RKHS.

2.1 Kernelized Stein Discrepancy

Let $\mathcal{H}_0$ be a RKHS with a kernel $k(x,x')$ in the Stein class of π and μ. Let $\mathcal{H} = (\mathcal{H}_0^{(1)},\dots,\mathcal{H}_0^{(d)})$. The KSD maximizes ϕ in the unit ball of $\mathcal{H}$. The objective in (3) is then:

$$\mathbb{S}(\mu,\pi) = \max_{\phi\in\mathcal{H}}\{\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)], \ s.t. \ \|\phi\|_{\mathcal{H}} \le 1\}. \tag{4}$$

Within this framework, one can show that the optimal solution of (4) is given by:

$$\phi(x) = \frac{\phi^*(x)}{\|\phi^*\|_{\mathcal{H}}} \text{ , where } \phi^*(.) = \mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \otimes k(x,\cdot)] = \int_{\mathcal{X}} k(x,\cdot)\nabla\log\pi(x) + \nabla k(x,\cdot)d\mu(x), \tag{5}$$

where $\mathcal{A}_\pi \otimes f(x) = f(x)\nabla\log\pi(x) + \nabla f(x)$, is a variant of Stein operator. Moreover, $\mathbb{S}(\mu,\pi) = \|\phi^*\|_{\mathcal{H}}$.

Proof. We first need to prove that

$$\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi f(x)] = \langle f, \phi^*\rangle_{\mathcal{H}}, \ \forall f \in \mathcal{H} :$$

$$\begin{aligned}
\langle f, \phi^*\rangle_{\mathcal{H}} &= \sum_{l=1}^{d}\Big\langle f^{(l)}, \mathbb{E}_{x\sim\mu}\Big[k(x,\cdot)\nabla\log\pi(x)^{(l)} + \nabla k(x,\cdot)^{(l)}\Big]\Big\rangle_{\mathcal{H}^0} \\
&= \mathbb{E}_{x\sim\mu}\left[\sum_{l=1}^{d}\Big\langle f^{(l)}, k(x,\cdot)\nabla\log\pi(x)^{(l)} + \nabla k(x,\cdot)^{(l)}\Big\rangle_{\mathcal{H}^0}\right] \\
&= \mathbb{E}_{x\sim\mu}\left[\sum_{l=1}^{d}\nabla\log\pi(x)^{(l)}\Big\langle f^{(l)}, k(x,\cdot)\Big\rangle_{\mathcal{H}^0} + \Big\langle f^{(l)}, \nabla k(x,\cdot)^{(l)}\Big\rangle_{\mathcal{H}^0}\right] \\
&= \mathbb{E}_{x\sim\mu}\left[\sum_{l=1}^{d}\nabla\log\pi(x)^{(l)} f^{(l)}(x) + \nabla_{x_l} f(x)^{(l)}\right] \ \text{(see Zhou [2008])} \\
&= \mathbb{E}_{x\sim\mu}\big[\nabla\log\pi(x)^\top f(x) + \nabla\cdot f(x)\big] \\
&= \mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi f(x)].
\end{aligned} \tag{6}$$

Moreover, $\langle f, \phi* \rangle_{\mathcal{H}} \leq \|f\|_{\mathcal{H}} \|\phi^*\|_{\mathcal{H}}$. Thus,

$$\mathbb{S}(\mu, \pi) = \max_{f \in \mathcal{H}} \{\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi f(x)] = \langle f, \phi^* \rangle_{\mathcal{H}},\ s.t.\ \|f\|_{\mathcal{H}} \leq 1\} \leq \|\phi^*\|_{\mathcal{H}}.$$

Let $f = \frac{\phi^*}{\|\phi^*\|_{\mathcal{H}}}$, then $\|f\|_{\mathcal{H}} = 1$ and

$$\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)] = \langle f, \phi^* \rangle_{\mathcal{H}} = \|\phi^*\|_{\mathcal{H}},$$

ending the proof. ■

3 Link with Kullback-Leibler Divergence

Let $T : \mathcal{X} \to \mathcal{X}$, $x \mapsto (I + \gamma\phi)(x)$. One can show that (see Liu and Wang [2016] Theorem 3.1):

$$\nabla_\gamma KL(T_\# \mu || \pi) = -\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)]. \tag{7}$$

Therefore, assuming $\phi \in \mathcal{H}$ with $\mathcal{H}$ as defined as in Section 2.1, using (5), we know that:

$$\phi^*(.) = \int_{\mathcal{X}} k(x, \cdot)\nabla \log \pi(x) + \nabla k(x, \cdot) d\mu(x) \tag{8}$$

minimizes $\nabla_\gamma KL(T_\# \mu || \pi)$. Furthermore, one can show that:

$$\begin{aligned}
P_\mu \nabla \log \frac{\mu}{\pi}(\cdot) &= \int_{\mathcal{X}} k(x, \cdot)\nabla \log \mu(x) d\mu(x) - \int_{\mathcal{X}} k(x, \cdot)\nabla \log \pi(x) d\mu(x) \\
&= \int_{\mathcal{X}} k(x, \cdot)\nabla \mu(x) dx - \int_{\mathcal{X}} k(x, \cdot)\nabla \log \pi(x) d\mu(x) \\
&= -\int_{\mathcal{X}} \nabla k(x, \cdot) d\mu(x) - \int_{\mathcal{X}} k(x, \cdot)\nabla \log \pi(x) d\mu(x) \\
&= -\int_{\mathcal{X}} k(x, \cdot)\nabla \log \pi(x) + \nabla k(x, \cdot) d\mu(x) \\
&= -\phi^*(\cdot)
\end{aligned} \tag{9}$$

The Stein Variational Gradient Descent (SVGD) algorithm consists in an iterative procedure where one apply successive transformations to an initial density μ_0 towards the "direction" ϕ^* that minimizes the gradient of the Kullback-Leibler divergence:

$$\mu_{n+1} = (I + \gamma\phi^*)_\# \mu_n = \left(I - \gamma P_\mu \nabla \log \frac{\mu}{\pi}\right)_\# \mu_n. \tag{10}$$

4 Not understood yet

- $k(x, \cdot)$ in the Stein class of π and μ?
- Link with Wasserstein distance?
- Why did they defined so much about their RKHS?

Bibliography

Qiang Liu. Stein variational gradient descent as gradient flow, 2017. URL `https://arxiv.org/abs/1704.07520`.

Qiang Liu and Dilin Wang. Stein variational gradient descent: A general purpose bayesian inference algorithm, 2016. URL `https://arxiv.org/abs/1608.04471`.

Ding-Xuan Zhou. Derivative reproducing properties for kernel methods in learning theory. *Journal of Computational and Applied Mathematics*, 220(1-2):456–463, October 2008. doi: 10.1016/j.cam.2007.08.023. URL `https://doi.org/10.1016/j.cam.2007.08.023`.

A Lemmas

Lemma 1. *Let two distributions μ and π on $\mathcal{X} \subseteq \mathbb{R}^d$. Let $\phi : \mathcal{X} \to \mathbb{R}^d$ be in the Stein class of μ and $\mathcal{A}_\pi \phi(x) = \nabla \log \pi(x)^\top \phi(x) + \nabla \cdot \phi(x)$ Then,*

$$\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)] = \mathbb{E}_{x\sim\mu}\Big[(\nabla \log \pi(x) - \nabla \log \mu(x))^\top \phi(x)\Big]$$

Proof.

$$\begin{aligned}
\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)] &= \mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x) - \mathcal{A}_\mu \phi(x)] \\
&= \mathbb{E}_{x\sim\mu}\big[\nabla \log \pi(x)^\top \phi(x) - \nabla \cdot \phi(x) - \nabla \log \mu(x)^\top \phi(x) + \nabla \cdot \phi(x)\big] \\
&= \mathbb{E}_{x\sim\mu}\Big[(\nabla \log \pi(x) - \nabla \log \mu(x))^\top \phi(x)\Big]
\end{aligned}$$

■

Lemma 2. *Let two distributions μ and π on $\mathcal{X} \subseteq \mathbb{R}^d$. Let $\phi : \mathcal{X} \to \mathbb{R}$ be in the Stein class of μ and $\mathcal{A}_\pi \otimes \phi(x) = \phi(x)\nabla \log \pi(x) + \nabla \phi(x)$ Then,*

$$\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \otimes \phi(x)] = \mathbb{E}_{x\sim\mu}[(\nabla \log \pi(x) - \nabla \log \mu(x))\phi(x)]$$

Proof. Same proof as Lemma 1. ■