

On Nonconvex SVGD

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1 Setup

$$F = \frac{1}{n} \sum_{i=1}^n f_i, \quad \pi \sim e^{-F}$$

$$f_n = \frac{1}{n_0} \sum_{i \in I} f_i, \quad \#I = n_0, \quad \sigma_n \sim e^{-f_n}$$

$$\phi_t(x) = \left(I - tP_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) \right) (x), \quad \mu_t = (\phi_t)_\# \mu_n$$

$$\varphi(t) = \int \log \left(\frac{\mu_t}{\pi} \right) d\mu_t$$

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We define the update rule as:

$$S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\sigma_{n+1}} \right) = \begin{cases} S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\pi} \right) & p, \\ S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) + S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\sigma_{I'}} \right) - S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_{I'}} \right) & 1-p \end{cases},$$

where $\sigma_{I'} \sim \exp^{-f_{I'}}$, $f_{I'} = \frac{1}{b'} \sum_{i \in I'} f_i$.

3 Main Proof

$$\phi(\gamma) \leq \phi(0) + \gamma \left\langle S_{\mu_n} \nabla \log \frac{\mu_n}{\pi}, S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) \right\rangle_H + \frac{C \cdot \gamma^2}{2} \left\langle S_{\mu_n} \nabla \log \frac{\mu_n}{\sigma_n}, S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) \right\rangle_H$$

then by similar calculation as in PAGE, we have,

$$\begin{aligned} \varphi(\gamma) &\leq \varphi(0) - \frac{\gamma}{2} \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \right\|_H^2 - \left(\frac{1}{2\gamma} - \frac{c}{2} \right) \cdot \gamma^2 \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) \right\|_H^2 \\ &\quad + \frac{\gamma}{2} \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) - S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) \right\|_H^2 \end{aligned}$$

Then a direct calculation now reveals that,

$$\mathbf{E} \left[\left\| S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\pi} \right) - S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\sigma_{n+1}} \right) \right\|_H^2 \right]$$

$$\begin{aligned}
&= p \cdot 0 + (1-p) \cdot \mathbb{E} \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) + S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\sigma_{I'}} \right) - S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_{I'}} \right) - S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\pi} \right) \right\|_H^2 \\
&= (1-p) \cdot \mathbb{E} \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) + S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\sigma_{I'}} \right) - S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_{I'}} \right) - \right. \\
&\quad \left. S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\pi} \right) + S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \right\|_H^2 + (1-p) \cdot \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) - S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_I} \right) \right\|_H^2
\end{aligned}$$

4 Inequality

we need to estimate

$$\left\| S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\pi} \right) - S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \right\|_H^2$$

and

$$\left\| S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\sigma_{I'}} \right) - S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_{I'}} \right) \right\|_H^2$$

$$\begin{aligned}
&S_{\mu_{n+1}} \nabla \log \left(\frac{\mu_{n+1}}{\pi} \right) - S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \\
&= \int k(y, \cdot) \nabla \log(\mu_{n+1}(y)) \mu_{n+1}(y) dy - \int k(\phi_\gamma(x), \cdot) \nabla \log(\mu_n(x)) \mu_n(x) dx \\
&\quad + \int k(\phi_\gamma(x), \cdot) \nabla \log(\pi(x)) \mu_n(x) dx - \int k(y, \cdot) \nabla \log(\pi(y)) \mu_{n+1}(y) dy + \int k(\phi_\gamma(x), \cdot) \nabla \log \left(\frac{\mu_n(x)}{\pi(x)} \right) \mu_n(x) dx - \\
&\quad \int k(x, \cdot) \nabla \log \left(\frac{\mu_n(x)}{\pi(x)} \right) \mu_n(x) dx = I + II + III
\end{aligned}$$

$$\|II\|_H^2 = \int \int k(\phi_\gamma(x), \phi_\gamma(x')) (\nabla \log(x) - \nabla \log(\pi(\phi_\gamma(x)))) (\nabla \log(x') - \nabla \log(\pi(\phi_\gamma(x')))) \mu(x) \mu(x') dx dx'$$

since F is L-smooth, so

$$|\nabla \log(x') - \nabla \log(\pi(\phi_\gamma(x')))| \leq L \cdot |x - \phi_\gamma(x)| = L \cdot \gamma \cdot |P_{\mu_\gamma} \nabla \log \left(\frac{\mu_n(x)}{\sigma_n(x)} \right)| \leq C \cdot \gamma \cdot \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) \right\|_H$$

then by Cauchy-Schwartz inequality and μ_n is weekly compact(will see this in the end), we derive

$$\|II\|_H^2 \leq C \cdot \gamma^2 \cdot \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) \right\|_H^2$$

$$\begin{aligned}
\|I\|_H^2 &= \left\| \int k(y, \cdot) \nabla \log(\mu_{n+1}(y)) \mu_{n+1}(y) dy - \int k(\phi_\gamma(x), \cdot) \nabla \log(\mu_n(x)) \mu_n(x) dx \right\|_H^2 \\
&= \int \int k(y, y') \nabla \log(\mu_{n+1}(y)) \nabla \log(\mu_{n+1}(y')) \mu_{n+1}(y) \mu_{n+1}(y') dy dy' \\
&\quad - \int \int k(y, \phi_\gamma(x)) \nabla \log(\mu_{n+1}(y)) \nabla \log(\mu_n(x')) \mu_{n+1}(y) \mu_n(x') dy dx' \\
&\quad - \int \int k(\phi_\gamma(x), y') \nabla \log(\mu_{n+1}(y')) \nabla \log(\mu_n(x)) \mu_{n+1}(y') \mu_n(x) dy' dx \\
&\quad + \int \int k(\phi_\gamma(x), \phi_\gamma(x')) \nabla \log(\mu_n(x)) \nabla \log(\mu_n(x')) \mu_n(x) \mu_n(x') dx dx' \\
&= \int \int tr \nabla_{1,2}^2 k(y, y') \mu_{n+1}(y) \mu_{n+1}(y') dy dy' \\
&\quad - \int \int tr(\nabla_{1,2}^2 k(y, \phi_\gamma(x')) J \phi_\gamma(x')) \mu_{n+1}(y) \mu_n(x') dy dx' \\
&\quad - \int \int tr(\nabla_{1,2}^2 k(\phi_\gamma(x), y') J \phi_\gamma(x)) \mu_n(x) \mu_{n+1}(y') dx dy' \\
&\quad + \int \int tr(\nabla_{1,2}^2 K(\phi_\gamma(x), \phi_\gamma(x')) J \phi_\gamma(x) J \phi_\gamma(x')) \mu_n(x) \mu_n(x') dx dx' \\
&= \int \int tr(\nabla_{1,2}^2 K(\phi_\gamma(x), \phi_\gamma(x')) (I - J \phi_\gamma(x)) (I - J \phi_\gamma(x'))) \mu_n(x) \mu_n(x') dx dx'
\end{aligned}$$

$$\text{assume } |\nabla_{1,2}^2 K(\cdot, \cdot)| \leq C, \text{ then } tr(\nabla_{1,2}^2 K(\phi_\gamma(x), \phi_\gamma(x')) (I - J \phi_\gamma(x)) (I - J \phi_\gamma(x'))) \leq C \cdot \gamma^2 \cdot \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) \right\|_H^2$$

$$\text{so } \|I\|_H^2 \leq C \cdot \gamma^2 \cdot \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\sigma_n} \right) \right\|_H^2$$

$$\|III\|_H^2 = \int \int (k(\phi_\gamma(x), \phi_\gamma(x')) - k(\phi_\gamma(x), x') - k(x, \phi_\gamma(x')) + k(x, x')) \nabla \log \left(\frac{\mu_n(x)}{\pi(x)} \right) \nabla \log \left(\frac{\mu_n(x')}{\pi(x')} \right) \mu_n(x) \mu_n(x') dx dx'.$$

$$\text{denote } F(x, x') := k(\phi_\gamma(x), \phi_\gamma(x')) - k(\phi_\gamma(x), x') - k(x, \phi_\gamma(x')) + k(x, x')$$

then by integration by part, we have

$$\|III\|_H^2 = \int \int (tr(\nabla_{1,2}^2 F(x, x')) + \nabla_2 F(x, x') \nabla \log(\pi(x)) + \nabla_1 F(x, x') \nabla \log(\pi(x')) + F(x, x') \nabla \log(\pi(x)) \nabla \log(\pi(x')))) \mu_n(x) \mu_n(x')$$

We need to know the order of $F(x, x')$, $\nabla_1 F(x, x')$, $\nabla_2 F(x, x')$, $\nabla_{1,2}^2 F(x, x')$

in the following we assume supremum norm the second, third and fourth order derivatives of k are finite, and we miss $O(|\phi_\gamma(x) - x|^2)$ and $O(|\phi_\gamma(x') - x'|^2)$ in the derivation.

$$\begin{aligned}
|F(x, x')| &= | \langle \phi_\gamma(x' - x'), \nabla_2 k(\phi_\gamma(x), x') \rangle + \langle x' - \phi_\gamma(x'), \nabla_2 k(x, x') \rangle | \\
&\leq |\nabla_{1,2}^2 k(x, x')(\phi_\gamma(x) - x)(\phi_\gamma(x') - x')| \leq C \cdot \gamma^2 \cdot \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right) \right\|_H^2 \\
|\nabla_1 F(x, x')| &= |\nabla_1 k(\phi_\gamma(x), \phi_\gamma(x')) J \phi_\gamma(x) - \nabla_1 k(\phi_\gamma(x), x') J \phi_\gamma(x) - \nabla_1 k(x, \phi_\gamma(x')) + \nabla_1 k(x, x')| \\
&= |\nabla_{1,2}^2 k(\phi_\gamma(x), x')(\phi_\gamma(x') - x') J \phi_\gamma(x) - \nabla_{1,2}^2 k(x, x')(\phi_\gamma(x') - x')| \\
&= |\nabla_{11,2}^3 k(x, x')(\phi_\gamma(x') - x')(\phi_\gamma(x) - x) + \nabla_{1,2}^2 k(\phi_\gamma(x), x)(\phi_\gamma(x') - x')(J \phi_\gamma(x) - I)| \leq C \cdot \gamma^2 \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right) \right\|_H^2 \\
&\text{similarly } |\nabla_2 F(x, x')| \leq C \cdot \gamma^2 \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right) \right\|_H^2 \\
tr \nabla_{1,2}^2 F(x, x') &= tr(J \phi_\gamma(x) \nabla_{1,2}^2 k(\phi_\gamma(x), \phi_\gamma(x')) J \phi_\gamma(x') - J \phi_\gamma(x) \nabla_{1,2}^2 k(\phi_\gamma(x), x') - \nabla_{1,2}^2 k(x, \phi_\gamma(x')) J \phi_\gamma(x') + \\
&\nabla_{1,2}^2 k(x, x')), \\
&\text{denote } J \phi_\gamma(x') = I - \gamma J P_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right)(x') = I - \gamma P', J \phi_\gamma(x) = I - \gamma J P_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right)(x) = I - \gamma P \\
&\text{then} \\
tr \nabla_{1,2}^2 F(x, x') &= tr((I - \gamma P) \nabla_{1,22}^3 k(\phi_\gamma(x), x')(\phi_\gamma(x') - x') - (I - \gamma P) \nabla_{1,2}^2 k(\phi_\gamma(x), \phi_\gamma(x'))(\gamma P') \\
&- \nabla_{1,22}^3 k(x, x')(\phi_\gamma(x') - x') + (\gamma P') \nabla_{1,2}^2 k(x, \phi_\gamma(x')))) \\
&= tr(\nabla_{11,22}^4 k(x, x')(\phi_\gamma(x) - x)(\phi_\gamma(x') - x') - (\gamma P') \nabla_{11,2}^3 k(x, \phi_\gamma(x'))(\phi_\gamma(x) - x) - (\gamma P) \nabla_{1,22}^3 k(\phi_\gamma(x), x')(\phi_\gamma(x') - \\
&x') + (\gamma P) \nabla_{1,2}^2 k(x, x')(\gamma P'))
\end{aligned}$$

$$|tr \nabla_{1,2}^2 F(x, x')| \leq C \cdot \gamma^2 \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right) \right\|_H^2$$

then by weak compactness, we know,

$$\|III\|_H^2 \leq C \cdot \gamma^2 \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right) \right\|_H^2$$

similarly, since the set of $\{\sigma_{I'}\}$ is finite and have similar property with π , so

$$\left\| S_{\mu_{n+1}} \nabla \log\left(\frac{\mu_{n+1}}{\sigma_{I'}}\right) - S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_{I'}}\right) \right\|_H^2 \leq C \cdot \gamma^2 \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right) \right\|_H^2$$

Finally,

$$\mathbf{E} \left\| S_{\mu_{n+1}} \nabla \log\left(\frac{\mu_{n+1}}{\pi}\right) - S_{\mu_{n+1}} \nabla \log\left(\frac{\mu_{n+1}}{\sigma_{n+1}}\right) \right\|_H^2 \leq (1-p) \cdot \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\pi}\right) - S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right) \right\|_H^2 + C \cdot \gamma^2 \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right) \right\|_H^2$$

So if γ is small enough (depend on constant C), then

$$\mathbf{E}(\Phi_{n+1}) \leq \mathbf{E}(\Phi_n) - \frac{\gamma}{2} \mathbf{E} \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\pi}\right) \right\|_H^2,$$

where

$$\Phi_n := KL(\mu_n | \pi) + \frac{\gamma}{2p} \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\pi}\right) - S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\sigma_n}\right) \right\|_H^2$$

(you see Φ_n is decreasing, so $KL(\mu_n | \pi) \leq C$, so $\{\mu_n\}$ is weakly compact)

Problem: is $\int |x|^2 \mu_n(x) dx$ weakly continuous?

If we cannot prove this, then we need more assumption on π , that is : there exists a constant $a > 0$ and a point x_0 such that $\int e^{ad(x_0, x)^2} \pi(dx) < +\infty$, then by a theorem from Vilani's book "optimal transport

old and new" page 592. we have T_1 inequality $W_p(\mu, \nu) \leq \sqrt{\frac{2H_\nu(\mu)}{\lambda}}$, $p = 1, \lambda$ is some constant. So we have $W_1(\mu_n, \pi) \leq C$, by L-smoothness of F we have $\int |\nabla \log(\pi(x))| \mu_n(x) dx \leq C \cdot \int |x| \mu_n(x) dx \leq C$