Regularized Stein Variational Gradient Descent -Talk in BIRS Stein's method workshop

Ye He, University of California Davis

joint work with Krishnakumar Balasubramanian, Bharath K Sriperumbudur and Jianfeng Lu

Apr.12, 2022

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LMC (---> SVGD

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The talk includes discussion of 4 parts:

- Prelimilary on RKHS
- A regularized formulation of SVGD
- Some analysis on the regularized SVGD
- Future work



Prelimilary on RKHS Introduction to the Reproducing kernel Hilbert Space(RKHS)

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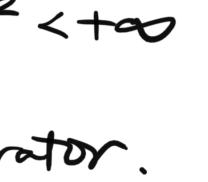
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Prelimilary on RKHS The integral operator and its adjoint





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x) < g, k(·,x) > mdx)



Prelimilary on RKHS Properties of the operators

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Prelimilary on RKHS Interpolation spaces between RKHS and L^2

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Here Leips bit then is an inclusion.
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Here Leips bit then is an inclusion.
Isophie Leips $\rightarrow L_{2}(\mu)$
 $T_{Here} = \overline{\Sigma}_{i=1}^{\infty} \lambda_{i} \langle P_{i} \overline{P}_{2} \mu_{i} \rangle^{e_{i}}$ with $\lambda_{i} \ge 2\lambda_{i} \ge$$$

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Stein variational formulation

Goal: to generate samples following
$$\pi \propto e^{-V}$$

• optimization formulation:
 $\chi \longrightarrow \chi + \varepsilon \phi(\chi) := T(\chi)$, $\chi \varepsilon R^{d}$, $\chi \rightarrow$
- to find the optimal ϕ^* sit. $KL(T \# p | \pi)$ def
In [Q.Lin et al 2016],
 $\phi^* = \operatorname{outgmax}_{\phi t \#} \{ E_{x \approx p} [S_{\pi} | \phi(x)] \}$, constrain
Where $S_{\pi} \phi(\chi) := -\nabla V(\chi) \cdot \phi(\chi) + \nabla \cdot \phi(\chi)$
 $\sum Stein operator.$

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x~p, \$:12d→12d derays fastest.

traints on p_{J}^{2}

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Stein variational formulation -Langevin dynamics

Choose
$$\mathcal{F} = L_{2}^{d}(p)$$
, constraint: $|| \neq |$
We get
 $\psi^{*} \propto - \nabla V_{1\times 3} - \frac{\nabla \rho_{1\times 3}}{\rho_{1\times 3}} = - \nabla \cdot$
and
 $\chi \longrightarrow T_{1\times 3} = \chi - \varepsilon \nabla \log \frac{1}{K}$
Let $\varepsilon \Rightarrow 0^{+}$,
 $\partial_{\varepsilon} p = \nabla \cdot \left(p \nabla \log \frac{1}{K} \right)$
 $\stackrel{1}{\longrightarrow}$ Forker Planck equation to

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 $I_{2}d_{p} \leq 1$







Stein variational formulation -SVGD

Choose $f = H_R^d$, constraint: $\| \cdot \phi \|_{H_R^d} \leq 1$ In [Q. Lin et 2016], \$ × - ikp vlog£ and $\chi \longrightarrow T(\chi) = \chi - \varepsilon i \kappa \rho \nabla \log f(\chi)$ Lot E->ot, in [Lustal 2018], $\partial_{\tau} \rho = \nabla \cdot \left(\rho \dot{k} \rho \nabla log + \right)$

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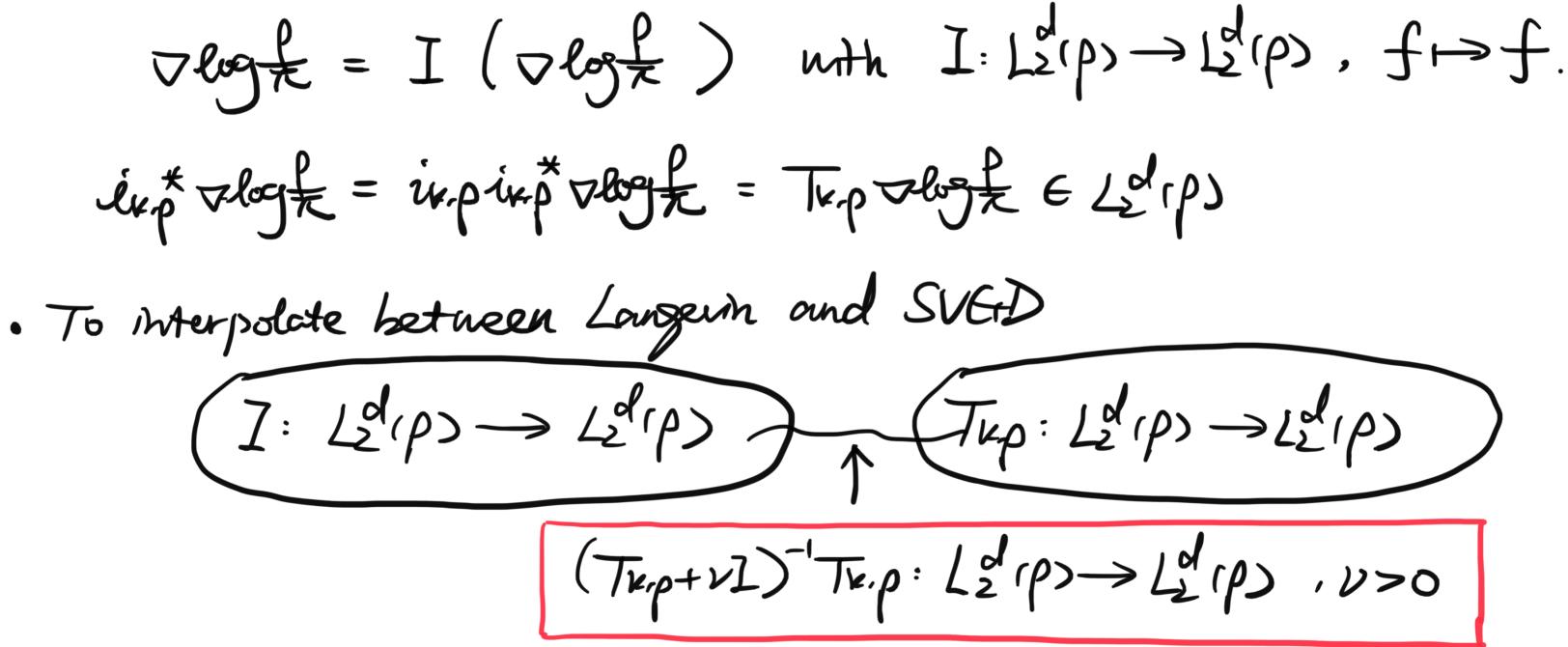






Stein variational formulation Comparison between Langevin and SVGD

- Langern: $\partial_t \rho = \nabla \cdot (\rho \nabla \log f)$ SVGD: $\partial t \rho = \nabla \cdot (\rho \dot{u} \rho \nabla log f)$
- · Obsense that,



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Stein variational formulation -regularized SVGD

[Krishnakumar et al 2017] Choose $f = H_R^d$, constraint: $\mathcal{V} \| \phi \|_{\mathcal{M}}^2 + \| \phi \|_{\mathcal{M}} \leq 1$ • $\mathcal{V}_{II} = \langle \phi, (i_k p^{*} i_k p + \nu Z_k) \hat{\mathcal{V}}_{k} \phi \mathcal{V}_{k} d$ · Exp[Stopros] = < \$, inp* vlog & > He We get \$\$ ~ (inp inp+rip) Timp tologh & Hpd C L2(p) \$\$ ~ imp(inp*inp+v2n) inp* thogh ELdip) likep (ikep*ikep+vIp) jie.p* = (ikeprikep*+vI) ikepikep* Clam: D +* ~ (Tr.p+VI) Tr.p vlogt.



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Stein variational formulation -regularized SVGD

Population limit:

$$\rho^{n+1} = (I_d - h_{n+1}(\iota_{k,\rho^n}\iota_{k,\rho^n}^* + \nu I_d)^{-1}\iota_{k,\rho^n})^{-1}$$

Mean-field PDE:

$$\begin{cases} \partial_t \rho = \nabla \cdot \left(\rho \left(\iota_{k,\rho} \iota_{k,\rho}^* + \nu I_d \right)^{-1} \iota_{k,\rho} \iota_{k,\rho} \right) \\ \rho(0,\cdot) = \rho_0(\cdot). \end{cases}$$

• Finite particle system: $(X_n^i)_{i=1}^N$ are the N-particles at step n. $\bar{X}_n := [X_n^1, \cdots, X_n^N]^T$. For all $f : \mathbb{R}^d \to \mathbb{R}^d$, $L_n f := [f(X_n^1), \cdots, f(X_n^N)]^T$.

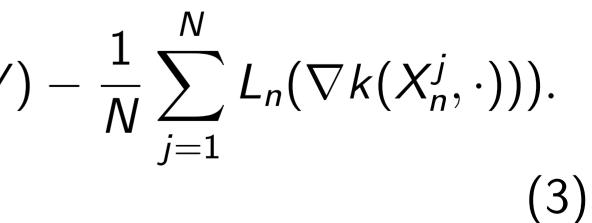
$$\bar{X}_{n+1} = \bar{X}_n - h_{n+1} (\frac{1}{N} K_n + \nu I_N)^{-1} (\frac{1}{N} K_n L_n (\nabla V)^{-1} (\frac{1}{N} K_n (\nabla$$

where $K_n \in \mathbb{R}^{N \times N}$ is the Gram matrix with $(K_n)_{i,i} = k(X_n^i, X_N^j)$.

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 $\sum_{k,\rho^n} \iota_{k,\rho^n}^* \nabla \log \frac{\rho^n}{\pi})_{\#\rho^n}.$ (1)

 $\iota_{k,\rho}^*(\nabla\log\frac{\rho}{\pi})),$ (2)



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Analysis on the regularized SVGD the mean-field PDE

- . Existence and uniqueness of neak solution
- . Stability in Wp
- · KL-divergence decour / Fisher information convergence

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Analysis on the regularized SVGD the mean-field PDE

Existence and uniqueness of heak solution
• neak solution,
$$p \in C(E_{0},\infty), P_{V})$$
 sit for a
 $\int_{0}^{+\infty} \int_{\mathbb{R}^{d}} \frac{\partial e}{\partial t} \frac{\partial t}{\partial t} \frac{\partial$

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for ∀ Po ∈ PV, ([0,00), Pu) to

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Analysis on the regularized SVGD the mean-field PDE

(1) Characteristic gradient flow holded by (1):

$$\begin{cases}
\frac{d}{dt} \stackrel{\text{d}}{=} (t_{1} \times \rho_{0}) = -(T_{u} \rho_{t} + \nu I)^{-1} T_{u} \rho_{t} \nabla \log \frac{f_{t}}{\pi} (t_{1} + \rho_{0}) + \rho_{0} \\
\frac{f_{t}}{f_{t}} = (\frac{g}{f_{t}} + \rho_{0}) + \rho_{0} \\
\frac{g}{f_{t}} = (\frac{g}{f_{t}} + \rho_{0}) + \rho_{0} \\
\frac{g}{f_{t}} = \frac{g}{f_{t}} + \rho_{0} + \rho_{0} \\
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(2)

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Some reasonable Banach space



Analysis on the regularized SVGD the mean-field PDE

. Theorem. Under assumptions on k and V, let p.p. ER be the hitsol conditions to PDE (1) S.t. // Pillp:=/ipa/xippildx) <+co, i=12, pE(1,+00). Let putits and pritits be the two corresponding neak solutions, ne have

$$\sup_{t \in t_{0}, T_{J}} W_{P}(\rho, u_{t}, \gamma, \rho_{2}(t_{r})) \leq C$$

$$1$$

$$depending$$

Wp(PI.P2)

on R. V. P. P. T. U



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Analysis on the regularized SVGD the mean-field PDE

KL-divergence Deceuy Let Prixs be the neak solution to PDE (1). · dt KL(A+1x) = - < inp vloge, (inpitup +vla) inp vloge Jud $:= I_{V,Stein}(\rho_t|\pi) \leq O$ · Properties of Iristein (M/T) (1) $I_{V.Spein}(\mu|\pi) = \sum_{i=1}^{\infty} \frac{\lambda_i}{\lambda_i + \nu} |\langle \nabla \log \mathcal{A}, e_i \rangle_{L_{2}(\mu)}|^2$ where 入」を… き入;ま… >0 feigin ONis of Lim).



Analysis on the regularized SVGD the mean-field PDE

Properties of
$$\overline{J}_{\nu}$$
 sign($\nu | \pi$):
(2) Approximation to the Fisher information.
- $\overline{I}(\mu | \pi)$: = $\int_{|P^{d}|} |\nabla \log \frac{\mu}{\pi} \sin^{2} \mu dx$)
= $\overline{I}_{|P^{d}|} |\nabla \log \frac{\mu}{\pi} \sin^{2} \mu dx$)
- $\overline{I}(\mu | \pi)$: = \overline{J}_{ν} stein $(\mu | \pi) + \overline{\Sigma}_{|1-1} \frac{\nu}{\Delta_{1}+\nu} | k$
Recall: $\nabla \log \frac{\mu}{\pi} \in L_{2}(\mu)$, $\exists \gamma \in (0, \frac{1}{2}]$ so. $\nabla \log \frac{\mu}{\pi}$
 $\Rightarrow I(\mu | \pi) = I_{\nu}$ stein $(\mu | \pi) + \overline{\Sigma}_{|1-1} \frac{\nu}{\Delta_{1}+\nu} | k$
 $\in I_{\nu}$ stein $(\mu | \pi) + \nu^{2\gamma} || k ||_{L_{2}(\mu)}^{2}$
 $\Rightarrow I(\mu | \pi) - \nu^{2\gamma} || k ||_{L_{2}(\mu)}^{2} \in \overline{I}_{\nu}$ stein $(\mu | \pi) + \varepsilon$

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 $tem(\mu | \pi)$ $k = T_{\mu,\mu} \cdot h, h \in L_{\mu}$

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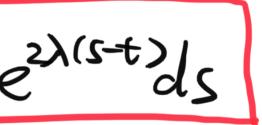
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Analysis on the regularized SVGD the mean-field PDE

Decay of KL-divergence
Assume
$$\pi \sim LSI(\lambda)$$
, i.e. $KL(\mu|\pi) \in \frac{1}{2\lambda} Z_{\mu}$
 $\frac{d}{dt} KL(\mu|\pi) \leq -I(\mu|\pi) + \nu^{2\lambda t} R_{\mu} \lambda^{2}$
 $\leq -2\lambda KL(\mu|\pi) + \nu^{2\lambda t} R_{\mu} \lambda^{2}$
 $\neq KL(\mu|\pi) \leq e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} KL(\mu|\pi) + \int_{0}^{t} \nu^{2\lambda t} R_{\mu} \lambda^{2} e^{-2\lambda t} R_{\mu} \lambda^{2}$

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 $(\mu|\pi)$, we have $R(t) = \| T_{upt} - Y_t \|_{L_1(p_t)} < +\infty$



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Analysis on the regularized SVGD Comparison to Langevin dynamics

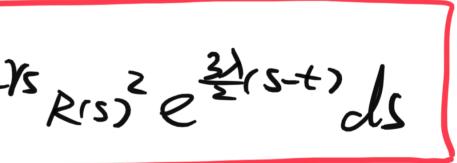
Let
$$\mu_{\text{H}}(x)$$
 be the solution to the FPE to Langer
with initial andrition $\mu_{\text{O}}(x)$.
Assume $\pi \sim \text{LSI(\lambda)}$ and we choose μ_{O} st. μ_{H}
then we get
 $\frac{d}{dt} \text{KL}(\mu_{\text{O}}) \leq -\frac{3\lambda}{2} \text{KL}(\mu_{\text{H}}) + \nu^{2\lambda_{\text{H}}} R$
 \Rightarrow
 $\text{KL}(\mu_{\text{H}}) \leq e^{-\frac{3\lambda_{\text{H}}}{2}} \text{KL}(\mu_{\text{O}}) + \int_{0}^{t} \nu^{2\lambda_{\text{H}}} R$

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in dynamics

~LSI(X) for Ut=0,

(H)²





Analysis on the regularized SVGD Decay of KL-divergence along the population

Recall:

$$\rho^{n+1} = (I_d - h_{n+1}(\iota_{k,\rho} n \iota_{k,\rho}^* n + \nu_{n+1} I_d)^{-1} \iota_{k,\rho} n \iota_{k,\rho}^* n$$

Assumption A1

- There exists B > 0 such that for all $x \in \mathbb{R}^d$: $\|\nabla k(x, \cdot)\|_{\mathcal{H}^d_L} \leq B$. (1)
- The potential function $V : \mathbb{R}^d \to \mathbb{R}$ is twice continuous differentiable and gradient Lipschitz with parameter L. (2)
- Along the population limit, $I(\rho^n | \pi) < \infty$ for all fixed $n \ge 0$. (3)



$$abla \log rac{
ho^n}{\pi})_{\#
ho^n}.$$



Analysis on the regularized SVGD Decay of KL-divergence along the population

Theorem 1

Assume that π satisfies the log-Sobolev inequality with parameter λ . Under the A1, Let (ρ^n) be the population limit of regularized SVGD described in (1) with initial condition $\rho^0 = \rho_0$ such that $KL(\rho_0|\pi) \leq R$. By choosing ν_{n+1} and the step-size h_{n+1} such that for all $n \ge 0$:

$$\begin{split} \nu_{n+1} &\leq \left(\frac{l(\rho^{n}|\pi)}{2 \left\| (\iota_{k,\rho^{n}} \iota_{k,\rho^{n}}^{*})^{-\gamma_{n}} \nabla \log \frac{\rho^{n}}{\pi} \right\|_{L_{2}^{d}(\rho^{n})}^{2}} \right)^{\frac{1}{2\gamma_{n}}}, \\ h_{n+1} &< \min \left\{ L^{-1}, \sqrt{2}B^{-1}(\alpha-1)\alpha^{-1}\nu_{n+1}^{\gamma_{n}}l(\rho^{n}|\pi)^{-\frac{1}{2}} \left(\sup_{i} \frac{\lambda_{i}^{(n)^{1+2\gamma_{n}}}}{(\lambda_{i}^{(n)}+\nu_{n+1})^{2}} \right)^{-\frac{1}{2}} \\ & \frac{1}{2}B^{-2}\alpha^{2}\nu_{n+1}^{2\gamma_{n}}(\sup_{i} \frac{\lambda_{i}^{(n)^{1+2\gamma_{n}}}}{(\lambda_{i}^{(n)}+\nu_{n+1})^{2}})^{-1}, 4\lambda^{-1} \right\}. \end{split}$$

where for each n, $\gamma_n \in (0, \frac{1}{2}]$ and $(\iota_{k,\rho} n \iota_{k,\rho}^* n)^{-\gamma_n} \nabla \log \frac{\rho^n}{\pi} \in L_2^d(\rho^n)$. $\{\lambda_i^{(n)}\}$ is the sequence of positive eigenvalues of the operator $\iota_{k,\rho} n \iota_{k,\rho} n *$ in the order of decreasing values. α is some constant and $\alpha \in (1,2)$. Then for all $n \geq 1$,

$$KL(\rho^{n}|\pi) \leq \prod_{i=1}^{n} (1 - \frac{1}{4}\lambda h_{i})R$$

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(4)





Analysis on the regularized SVGD Convergence of Fisher information along the population

Theorem 2

Under the A1, Let (ρ^n) be the population limit of regularized SVGD described in (1) with initial condition $\rho^0 = \rho_0$ such that $KL(\rho_0|\pi) \leq R$. By choosing ν_{n+1} and the step-size h_{n+1} such that for all $n \geq 0$:

$$h_{n+1} < \min\left\{L^{-1}, \sqrt{2}B^{-1}(\alpha-1)\alpha^{-1}\nu_{n+1}^{\gamma_n}I(\rho^n|\pi)^{-\frac{1}{2}} \left(\sup_{i}\frac{\lambda_i^{(n)}+2\gamma_n}{(\lambda_i^{(n)}+\nu_{n+1})^2}\right)^{-\frac{1}{2}}\right\}.$$

where for each n, $\gamma_n \in (0, \frac{1}{2}]$, $(\iota_{k,\rho} n \iota_{k,\rho}^* n)^{-\gamma_n} \nabla \log \frac{\rho^n}{\pi} \in L_2^d(\rho^n)$ and $R_n := \left\| (\iota_{k,\rho} n \iota_{k,\rho}^* n \iota_{k,\rho})^{-\gamma_n} \nabla \log \frac{\rho^n}{\pi} \right\|$

 $\{\lambda_i^{(n)}\}\$ is the sequence of positive eigenvalues of the operator $\iota_{k,\rho} n \iota_{k,\rho} n * in$ the ord constant and $\alpha \in (1,2)$. Then for all $n \geq 1$,

$$\sum_{n=0}^{\infty} \frac{h_{n+1}}{2} I(\rho^n | \pi) \le \sum_{n=0}^{\infty} \nu_{n+1}^{2\gamma_n} h_{n+1} \left(1 + \frac{1}{2} \nu_{n+1}^{-\frac{1}{2}} \alpha^2 B^2 h_{n+1} \right) R_n^2 + R.$$

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$$(\mathcal{L}_{k,\rho}^{n} \iota_{k,\rho}^{*})^{-\gamma_{n}} \nabla \log \frac{\rho^{n}}{\pi} \Big\|_{L_{2}^{d}(\rho^{n})}$$

der of decreasing values. α is some

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• To analyze on the finite particle system

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