Variational Wasserstein Gradient Flow

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Amirhossein Taghvaei

Joint work with J. Fan, Y. Chen

Department of Aeronautics & Astronautics
University of Washington, Seattle

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Outline

- Overview of the problem and related questions
- Variational approach for implementing WGF

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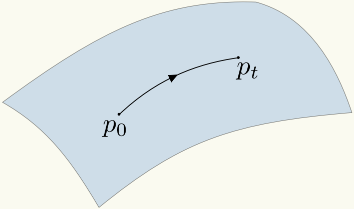
Problem overview



Question: How to numerically implement a flow on the space of probability distributions?

Examples:

- $\{p_t\}_{t\geq 0}$ is the solution to the Fokker-Plank eq.: $\partial_t p = \mathcal{L}p$
- $\{p_t\}_{t\geq 0}$ is the posterior in a nonlinear filtering problem: $\mathrm{d}p = \mathcal{L}p\mathrm{d}t + p(h - \hat{h}_t)\mathrm{d}I_t$

Two approaches:

- pde-based (does not scale with the dimension)
- probabilistic (approximate with an empirical distribution of particles)

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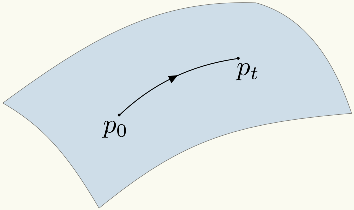

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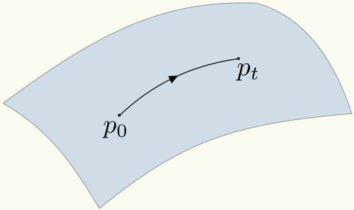

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Objective: numerically implement a given flow $\{p_t\}_{t\geq 0}$:

- Step 1: Construct a stochastic process $\{\bar{X}_t\}_{t\geq 0}$ s.t.

$$\text{Law}(\bar{X}_t) = p_t \quad \forall t \geq 0$$

- Step 2: Realize $\bar{X}_t$ with a system of (interacting) particles $\{X_t^1, \ldots, X_t^N\}$

$$\frac{1}{N}\sum_{i=1}^{N} \delta_{X_t^i} \approx \text{Law}(\bar{X}_t)$$

Questions:

(I) How to construct $\bar{X}_t$? $\Rightarrow$ uniqueness issue

(II) How to realize $\bar{X}_t$ with system of interacting particles?

(III) Error analysis for particle approximation (propagation of chaos)

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  where $I(x, p_t^{(N)})$ is approximation of $\nabla \log \bar{p}_t(x)$

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Gaussian approximation

In order to approximate $\nabla \log(\bar{p}_t)$ in terms of particles $\{X_t^1, \dots, X_t^N\}$:

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Question (III): Error analysis
comparison between stochastic and deterministic method

- Assume the target distribution is $N(\bar{x}, Q)$, i.e. $V = (x-\bar{x})^T Q^{-1}(x-\bar{x})$
- Compare the error in estimating mean or variance:

$$\text{error} = \mathbb{E}[\|m_t^{(N)} - \bar{x}\|^2]$$

- deterministic:

$$\text{error} \le e^{-\lambda t}\mathbb{E}[\|m_0^{(N)} - \bar{x}\|^2]$$

- stochastic:

$$\text{error} \le e^{-\lambda t}\mathbb{E}[\|m_0^{(N)} - \bar{x}\|^2] + \frac{C}{N}$$

- same result for covariance, but not other moments

Observation:

Gaussian approx. $\Rightarrow$ more accurate estimation of mean and variance

Question: does the observation generalize?

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- Assume the target distribution is $N(\bar{x}, Q)$, i.e. $V = (x - \bar{x})^T Q^{-1} (x - \bar{x})$
- Compare the error in estimating mean or variance:

$$\text{error} = \mathbb{E}[\|m_t^{(N)} - \bar{x}\|^2]$$

- deterministic:

$$\text{error} \leq e^{-\lambda t} \mathbb{E}[\|m_0^{(N)} - \bar{x}\|^2]$$

- stochastic:

$$\text{error} \leq e^{-\lambda t} \mathbb{E}[\|m_0^{(N)} - \bar{x}\|^2] + \frac{C}{N}$$

- same result for covariance, but not other moments

Observation:

Gaussian approx. $\Rightarrow$ more accurate estimation of mean and variance

Question: does the observation generalize?

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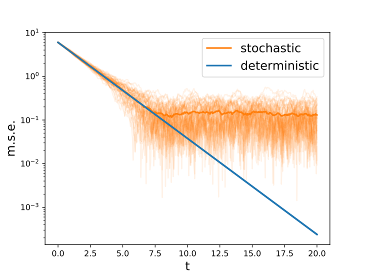

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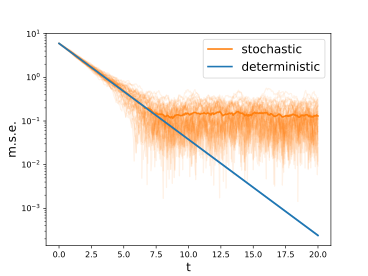

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Outline

- Overview of the problem and related questions
- Variational approach for implementing WGF

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Wasserstein gradient flow

- Optimization problem:

$$\min_{p \in \mathcal{P}_2(\mathbb{R}^n)} F(p)$$

- Wasserstein gradient flow:

$$\frac{\partial p}{\partial t} = \nabla \cdot (p \nabla \frac{\delta F}{\delta p})$$

where $\frac{\delta F}{\delta p}$ is the L_2-derivative.

- Example: $F(p) = D(p \| e^{-V})$ (KL divergence)

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Related works

- pde-based approach (Peyre, 2015; Benamou et al., 2016; Carlier et al., 2017; Li et al., 2020; Carrillo et al., 2021)
- JKO scheme + ICNN (Mokrov et al., 2021; Alvarez-Melis et al., 2021; Yang et al., 2020; Bunne et al., 2021; Bonet et al., 2021)
- Kernel Stein Discrepancy Descent (Korba et. al. 2021)
- SVGD (Liu & Wang, 2016; Chewi, et. al., 2020)
- MMD (Mroueh et al., 2019; Arbel et al., 2019)
- Wasserstein Proximal Gradient. (Salim, et. al., 2020)
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Proposed approach:

- Modify the objective function so that is well defined on empirical distributions
- Directly apply gradient flow on particles
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Variational f-divergences

- Consider f-divergence objective functionals

$$F(p) = D_f(p\|q) := \int f(\frac{p(x)}{q(x)})q(x)\mathrm{d}x$$

where $f : [0, \infty] \to \mathbb{R}$ is convex and $f(1) = 0$ (e.g. $f(x) = x\log(x) \to$ KL)

- It admits variational representation

$$D_f(p\|q) = \sup_{h\in\mathcal{C}} \left\{ \int h(x)p(x)\mathrm{d}x - \int f^*(h(x))q(x)\mathrm{d}x \right\}$$

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Properties of the approximate f divergence

- upper-bound:

$$D_f^{\mathcal{H}}(p\|q) \leq D_f(p\|q) \quad \text{with equality if} \quad f'(\frac{p}{q}) \in \mathcal{H}$$

- positivity: If $\mathcal{H}$ contains all constant functions, then

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where h_t is the maximizer for $p = p_t$

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Computational algorithms

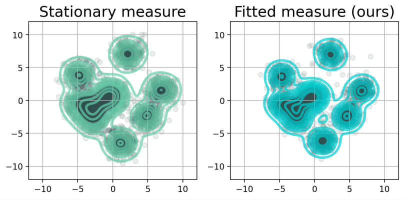
- time discretization with JKO scheme

$$\bar{X}_{k+1} = \nabla\phi_k(\bar{X}_k),$$
$$\phi_k = \arg\min_{\phi\in\mathsf{ICNN}} \max_{h\in\mathcal{H}} \{\frac{1}{2\Delta t} W_2^2(\bar{p}_k, \nabla\phi\#\bar{p}_k) + \mathcal{V}(h, \nabla\phi\#\bar{p}_k)\}$$

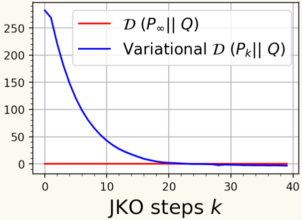
- results in min-max optimization at each time-step
- solve using stochastic optimization algorithms
- represent ϕ with input convex neural networks (ICNN) (Amos et al., 2017)
- represent h with feed-forward neural networks

Setup:

- objective function is $D(p\|q)$
- target is Gaussian mixture with 10 components

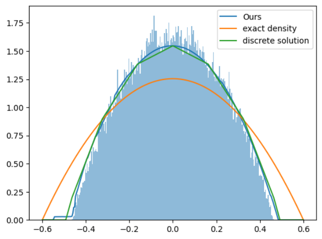


dimension $= 128$

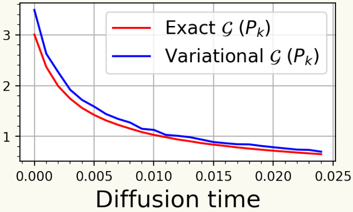


Setup:

- objective function is generalized entropy $\mathcal{G}(p) = \dfrac{1}{m-1}\displaystyle\int p^m(x)\,\mathrm{d}x$
- gradient flow is $\dfrac{\partial p}{\partial t} = \Delta p^m$



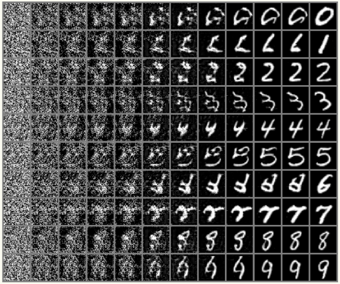
comparison with exact solution



convergence of the objective function

Setup:

- objective function is JS distance $\mathrm{JSD}(p\|q) = D(p\|\frac{p+q}{2}) + D(q\|\frac{p+q}{2})$
- assuming access to samples from q (GAN setup)



MNIST dataset

CIFAR dataset

Concluding remarks

Summary:

- Variational approach to construct gradient flows

$$\min_p F(p) \quad \rightarrow \quad \min_p \max_{h\in\mathcal{H}} \mathcal{V}(p,h)$$

- established elementary results about the variational divergence
- numerical results illustrating scalability with dimension

Open questions:

- Does the gradient flow converge

$$D_f^{\mathcal{H}}(p_t\|q) \rightarrow 0, \quad \text{as} \quad t\rightarrow\infty$$

- Under what conditions we have log-Sobolev type inequality

$$\frac{\mathrm{d}}{\mathrm{d}t} D_f^{\mathcal{H}}(p_t\|q) \leq -\lambda D_f^{\mathcal{H}}(p_t\|q)$$

- For sampling, what is the benefit compared to simulating Langevin eq.?

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