Design of Gradient Flows for Sampling

Energy Functionals, Invariance and Gaussian Approximation

Yifan Chen

Courant Institute, New York University

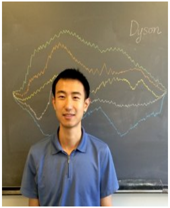
SCIML seminar, Oct 2023

The Paper

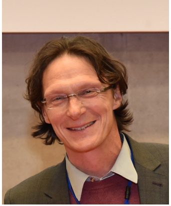
[Chen, Huang, Huang, Reich, Stuart 2023]

Sampling via Gradient Flows in the Space of Probability Measures

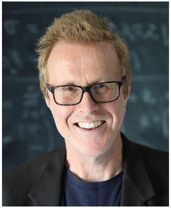
Daniel Huang
Peking University



Jiaoyang Huang
University of Pennsylvania



Sebastian Reich
University of Potsdam



Andrew Stuart
Caltech

Link: `https://arxiv.org/abs/2310.03597`.

Context

The sampling problem

Goal: draw (approximate) samples from

$$\rho^\star(\theta) \propto \exp(-V(\theta))$$

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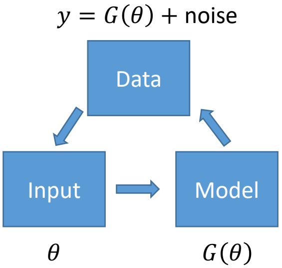
Many applications in

- Uncertainty quantification
- Bayes inverse problems
- Filtering
- Active learning
- ...



Methodology

Dynamics for sampling

Idea: construct a **dynamics of ρ_t** that gradually converges to

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  - Sequential Monte Carlo, e.g., $\rho_t \propto \exp(-tV(\theta))$, ...

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  - Sequential Monte Carlo, e.g., $\rho_t \propto \exp(-tV(\theta))$, ...
- **Infinite time dynamics** $\rho_\infty = \rho^\star$, from arbitrary ρ_0
  - MCMC, Langevin's dynamics, ...

Dynamics through Gradient Flows (GFs)

Gradient flow dynamics for sampling

Idea: construct a **gradient flow** **dynamics of** ρ_t that converges to

$$\rho^\star(\theta) \propto \exp(-V(\theta))$$

Namely, dynamics comes from gradient based optimization methods

- Langevin's dynamics and Wasserstein GFs
  [Jordan, Kinderlehrer, Otto 1998], ...
- Stein variational GD and Stein variational GFs
  [Liu, Wang 2016], [Liu 2017], ...
- Interaction between optimization and sampling
  [Wibisono 2018], ...
- A recent review paper
  [Trillos, Hosseini, Sanz-Alonso 2023]
- ...

Gradient Flows

Ingredients in gradient flows

Formally: ($\mathcal{P}$ is the space of probability densities)

- **An energy functional** to minimize

$$\mathcal{E} : \mathcal{P} \to \mathbb{R}$$

- **A metric** for descent direction

$$g_\rho : T_\rho\mathcal{P} \times T_\rho\mathcal{P} \to \mathbb{R}, \quad g_\rho(\sigma_1, \sigma_2) = \langle M(\rho)\sigma_1, \sigma_2 \rangle_{L^2}$$

$$\Longrightarrow \text{ Flow: } \quad \frac{\partial \rho_t}{\partial t} = -\nabla_g \mathcal{E}(\rho_t) = -M(\rho_t)^{-1} \frac{\delta \mathcal{E}}{\delta \rho}|_{\rho=\rho_t}$$

- $T_\rho\mathcal{P}$ (tangent space) is the space of measures integrated to 0
- $\frac{\delta \mathcal{E}}{\delta \rho}$ is the first variation of $\mathcal{E}$ at ρ
- $M(\rho_t)^{-1}$ can be understood as a **preconditioner**

Sampling through Numerical Approximation of GFs

Gradient flow equation

$$\frac{\partial \rho_t}{\partial t} = -M(\rho_t)^{-1}\frac{\delta \mathcal{E}}{\delta \rho}|_{\rho=\rho_t}$$

Numerical approximations of GFs then lead to sampling methods

- Particle methods such as mean field SDEs

$$\mathrm{d}\theta_t = f(\theta_t;\rho_t,\rho^\star)\mathrm{d}t + h(\theta_t;\rho_t,\rho^\star)\mathrm{d}W_t$$

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Example: Langevin's dynamics

- $\mathcal{E}(\rho) = \mathrm{KL}[\rho \| \rho^\star]$ and $M(\rho)^{-1} = -\nabla \cdot (\rho \nabla \cdot)$
- The PDE: $\frac{\partial \rho_t}{\partial t} + \nabla \cdot (\rho_t \nabla_\theta \log \rho^\star) = \Delta \rho_t$
- The SDE: $\mathrm{d}\theta_t = \nabla_\theta \log \rho^\star(\theta_t)\mathrm{d}t + \sqrt{2}\mathrm{d}W_t$

The Focus of this Talk

The question:

Any guiding principles for designing $\mathcal{E}$ and $M(\rho)$?

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Some desired properties of gradient flows for sampling:

- **Numerical approximation is tractable**
  - e.g. Langevin dynamics $\mathrm{d}\theta_t = \nabla_\theta \log \rho^\star(\theta_t)\mathrm{d}t + \sqrt{2}\mathrm{d}W_t$ does not need the normalization constants of $\rho^\star$
- **Fast convergence of the flow**
  - e.g. Langevin dynamics converges fast for well conditioned, single mode distributions, but may struggle for others

Design of Gradient Flows for Sampling

1. On Choosing Energy Functionals: KL is Special
2. On Choosing Metrics: Fisher-Rao is Special
3. On Numerical Approximations by Gaussians and Mixtures

On Choosing the Energy Functionals

Recap: Gradient flow equation

$$\frac{\partial \rho_t}{\partial t} = -M(\rho_t)^{-1} \frac{\delta \mathcal{E}}{\delta \rho}|_{\rho=\rho_t}$$

- Most popular choice of $\mathcal{E}(\rho)$: Kullback–Leibler divergence

$$\mathcal{E}(\rho; \rho^\star) = \mathrm{KL}[\rho \| \rho^\star] = \int \rho \log\left(\frac{\rho}{\rho^\star}\right) \mathrm{d}\theta$$

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- Property: $\mathcal{E}(\rho; c\rho^\star) = \mathcal{E}(\rho; \rho^\star) - \log c$ for any $c \in \mathbb{R}_+$

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  $\Rightarrow$ the gradient flow equation is independent of c

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  $\Rightarrow$ the gradient flow equation is independent of c

Implication: no need to worry about **normalization consts** of $\rho^\star$

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The answer is **NO** among a large class of $\mathcal{E}$

KL Divergence is Special

Theorem [Chen, Huang, Huang, Reich, Stuart 2023]

Among all f-**divergence** with continuously differentiable f, KL divergence is the only one, up to scaling, whose first variation is **invariant to the normalization consts of $\rho^\star$**

- f-divergence: for $f(0) = 1$ and f convex

$$D_f[\rho \| \rho^\star] = \int \rho^\star f\Big(\frac{\rho}{\rho^\star}\Big) \mathrm{d}\theta$$

  - Kullback–Leibler divergence: $f(x) = x \log x$
  - χ^2 divergence: $f(x) = (x-1)^2$
  - Hellinger distance: $f(x) = (\sqrt{x} - 1)^2$
  - ...

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Use KL divergence from now on

Design of Gradient Flows for Sampling

Two Metrics

Wasserstein metric [Jordan, Kinderlehrer, Otto 1998]

Metric: $M(\rho)^{-1}\psi = -\nabla \cdot (\rho \nabla \psi)$

Flow: $\frac{\partial \rho_t}{\partial t} = -\nabla_\theta \cdot (\rho_t \nabla_\theta \log \rho^\star) + \nabla \cdot (\nabla \rho_t)$

SDEs: $\mathrm{d}\theta_t = \nabla_\theta \log \rho^\star \mathrm{d}t + \sqrt{2}\mathrm{d}W_t$

- Optimal transport [Villani 2003, 2008]

Fisher-Rao metric [Rao 1945]

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Flow: $\frac{\partial \rho_t}{\partial t} = \rho_t(\log \rho^\star - \log \rho_t) - \rho_t \mathbb{E}_{\rho_t}[\log \rho^\star - \log \rho_t]$

- Information geometry [Amari 2016], [Ay, Jost, Lê, Schwachhöfer, 2017]

Convergence Property of Wasserstein Gradient Flow

Theorem [Markowich, Villani 2000]

Assume $\exists \lambda > 0$ such that

$$-D^2 \log \rho^\star(\cdot) \succeq \lambda I$$

Then, for all $t \geq 0$,

$$\mathrm{KL}[\rho_t \| \rho^\star] \leq \mathrm{KL}[\rho_0 \| \rho^\star] e^{-2\lambda t}$$

Rate of exponential convergence depends on $\rho^\star$

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A Closer Look at Fisher-Rao

Fisher-Rao gradient flow

$$\frac{\partial \rho_t}{\partial t} = \rho_t\big(\log \rho^\star - \log \rho_t\big) - \rho_t \mathbb{E}_{\rho_t}[\log \rho^\star - \log \rho_t]$$

Apply transformation of any **diffeomorphism** $\varphi : \mathbb{R}^{d_\theta} \to \mathbb{R}^{d_\theta}$

- $\tilde{\rho}_t = \varphi \# \rho_t$ is the transformed distribution at time t
- $\tilde{\rho}^\star = \varphi \# \rho^\star$ is the transformed target distribution

Then, the form of the flow equation remains **invariant**

$$\frac{\partial \tilde{\rho}_t}{\partial t} = \tilde{\rho}_t\big(\log \tilde{\rho}^\star - \log \tilde{\rho}_t\big) - \tilde{\rho}_t \mathbb{E}_{\tilde{\rho}_t}[\log \tilde{\rho}^\star - \log \tilde{\rho}_t]$$

Why Care About Invariance?

Implication of invariance

Convergence rates of the gradient flow are **the same** for general $\rho^\star$ and **Gaussian** $\rho^\star$

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- Assume there exists a diffeomorphism φ such that

$$\tilde{\rho}^\star = \varphi\#\rho^\star = \text{Gaussian}$$

- Recall the property of the KL divergence

$$\mathrm{KL}[\rho_t \| \rho^\star] = \mathrm{KL}[\varphi\#\rho_t \| \varphi\#\rho^\star] = \mathrm{KL}[\tilde{\rho}_t \| \tilde{\rho}^\star]$$

Thus, a general $\rho^\star$ problem $\sim$ a simpler **Gaussian** $\rho^\star$ problem

Convergence of Fisher-Rao gradient flows

[Chen, Huang, Huang, Reich, Stuart 2023]

Let ρ_t satisfy the Fisher-Rao gradient flow. Assume

- there exist constants $K, B > 0$ such that ρ_0 satisfies

$$e^{-K(1+|\theta|^2)} \leq \rho_0(\theta)/\rho^\star(\theta) \leq e^{K(1+|\theta|^2)}$$

- the second moments of $\rho_0, \rho^\star$ are both bounded by B

Then, for any $t \geq \log\big((1+B)K\big)$,

$$\mathrm{KL}[\rho_t \| \rho^\star] \leq (2 + B + eB)Ke^{-t}$$

See also: **[Lu, Slepčev, Wang 2022], [Domingo-Enrich, Pooladian 2023]**

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“Unconditional” uniform exponential convergence

- In sharp contrast to Wasserstein gradient flows whose convergence rates depend on $\rho^\star$

Does This Mean Fisher-Rao is All You Need?

Numerical approximations of Fisher-Rao GFs can be tricky

Particle methods (i.e. Diracs ansatz)

- Birth-death dynamics [Lu, Lu, Nolen 2019], [Lu, Slepčev, Wang 2022]
- Ensemble MCMC [Lindsey, Weare, Zhang 2021]

Need ways to move the support of the particles to explore the space and choices of smoothing kernels

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The question:

Any other choices of metric having such invariance property?

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The answer is again, **NO**

Fisher-Rao Metric is Special

Unique property of Fisher-Rao metric

[Cencov 2000], [Ay, Jost, Lê, Schwachhöfer 2015], [Bauer, Bruveris, Michor 2016]

The Fisher-Rao metric is the **only Riemannian metric on smooth positive densities** (up to scaling) that is invariant under any diffeomorphism of the parameter space.

No other alternatives if we ask for **diffeomorphism invariance***!*

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But can ask for a relaxed **affine invariance**

- Affine invariant MCMC [Goodman, Weare 2010]
- Preconditioned Langevin and Kalman-Wasserstein GFs [Reich Cotter 2015], [Leimkuhler, Matthews, Weare 2018], [Garbuno-Inigo, Hoffmann, Li, Stuart 2020]
- Other affine invariant gradient flow examples in the paper
  - e.g., affine invariant Stein gradient flow

Design of Gradient Flows for Sampling

Numerical Approximation of the Fisher-Rao Gradient Flow

Particle methods (i.e. Diracs ansatz)

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Need ways to move the support of the particles to explore the space and choices of smoothing kernels

Our focus: **parametric approximation** (full support ansatz)

- Gaussian approximations
- Gaussian mixtures for multimodal problems

Gaussian Approximation by Moment Closures

The general procedures:

- Consider any dynamics in the **density space**

$$\frac{\partial \rho_t(\theta)}{\partial t} = \sigma_t(\theta, \rho_t)$$

- Write down the dynamics of the **mean and covariance**

$$\frac{\mathrm{d}m_t}{\mathrm{d}t} = \int \sigma_t(\theta, \rho_t)\theta \mathrm{d}\theta$$
$$\frac{\mathrm{d}C_t}{\mathrm{d}t} = \int \sigma_t(\theta, \rho_t)(\theta - m_t)(\theta - m_t)^T \mathrm{d}\theta$$

- Closure: replace ρ_t in the above RHS by $\rho_{a_t} = \mathcal{N}(m_t, C_t)$
  Notation: $a_t = (m_t, C_t)$

References: Moment closure in variational Kalman filtering [Särkkä, 2007], and in Wasserstein gradient flow [Lambert, Chewi, Bach, Bonnabel, Rigollet 2022]

Gaussian Approximation by Moment Closures

Gaussian approximate Fisher-Rao gradient flow

$$\frac{\mathrm{d}m_t}{\mathrm{d}t} = C_t \mathbb{E}_{\rho_{a_t}}[\nabla_\theta \log \rho^\star],$$
$$\frac{\mathrm{d}C_t}{\mathrm{d}t} = C_t + C_t \mathbb{E}_{\rho_{a_t}}[\nabla_\theta \nabla_\theta \log \rho^\star] C_t$$

- Derived using Stein's lemma
- Equivalent to **natural gradient** flow [Amari 1998] for

Gaussian variational inference: $\min_{m,C} \mathrm{KL}[\mathcal{N}(m, C) \| \rho^\star]$

Key: Fisher information matrix is used for preconditioning

$$\frac{\mathrm{d}}{\mathrm{d}t}(m_t, C_t) = -\mathrm{FI}(m_t, C_t)^{-1} \nabla_{m_t, C_t} \mathrm{KL}$$

Convergence Guarantee

Gaussian target

If $\rho^\star = \mathcal{N}(m_\star, C_\star)$, and $C_0 = \lambda_0 I, \lambda_0 > 0$, then

$$\|m_t - m_\star\|_2 = \mathcal{O}(e^{-t}), \quad \|C_t - C_\star\|_2 = \mathcal{O}(e^{-t})$$

- Same story, due to invariance property

Convergence Guarantee

Logconcave target [Chen, Huang, Huang, Reich, Stuart 2023]

Assume

- $\alpha I \preceq -\nabla_\theta \nabla_\theta \log \rho^\star \preceq \beta I$
- $\lambda_{0,\min} I \preceq C_0 \preceq \lambda_{0,\max} I$

Then

$$\mathrm{KL}[\rho_{a_t} \| \rho^\star] - \mathrm{KL}[\rho_{a_\star} \| \rho^\star] \leq e^{-Kt}(\mathrm{KL}[\rho_{a_0} \| \rho^\star] - \mathrm{KL}[\rho_{a_\star} \| \rho^\star])$$

where

- $a_t = (m_t, C_t), \rho_{a_t} = \mathcal{N}(m_t, C_t)$
- $a_\star = \mathrm{argmin}_a \ \mathrm{KL}[\rho_a \| \rho^\star]$
- $K = \alpha \min\{1/\beta, \lambda_{0,\min}\}$

- Inspired by the proof for the Wasserstein gradient flow in Gaussian variational inference for logconcave target

  [Lambert, Chewi, Bach, Bonnabel, Rigollet 2022]

Local Convergence Rates: Linearized Analysis

Theorem [Chen, Huang, Huang, Reich, Stuart 2023]

Assume $\alpha I \preceq -\nabla_\theta \nabla_\theta \log \rho^\star \preceq \beta I$. For $N_\theta = 1$, let $\lambda_{\star,\max} < 0$ denote the largest eigenvalue of the linearized Jacobian matrix of the flow around $a_\star$. Then we have

$$-\lambda_{\star,\max} \geq \frac{1}{(7 + \frac{4}{\sqrt{\pi}})\big(1 + \log\big(\frac{\beta}{\alpha}\big)\big)}$$

Moreover, the bound is sharp: it is possible to construct a sequence of triplets $\rho_n^\star$, α_n and β_n, where $\lim_{n\to\infty} \frac{\beta_n}{\alpha_n} = \infty$, such that, if we let $\lambda_{\star,\max,n}$ denote the corresponding largest eigenvalues of the linearized Jacobian matrix for the n-th triple, then, it holds that

$$-\lambda_{\star,\max,n} = \mathcal{O}\left(1/\log\frac{\beta_n}{\alpha_n}\right)$$

Convergence rates only depend on $\log($condition number$)$

Numerical Examples

- **2D Convex Potential**: $\theta = (\theta^{(1)}, \theta^{(2)})$

$$V(\theta) = \frac{(\sqrt{\lambda}\theta^{(1)} - \theta^{(2)})^2}{20} + \frac{(\theta^{(2)})^4}{20} \quad \text{with} \quad \lambda = 0.01,\ 0.1,\ 1$$

- **Method**: Gaussian approximation of Fisher-Rao GF, Wasserstein GF and vallina GF
- **Configuration**: we initialize the Gaussian at

$$\mathcal{N}\Big(\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}4 & 0\\0 & 4\end{bmatrix}\Big)$$

We integrate the mean and covariance dynamics to $t = 15$

Numerical Examples

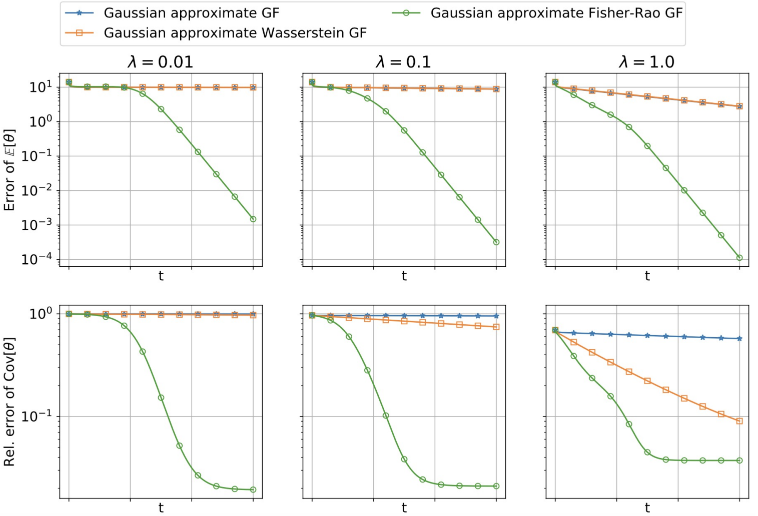

Figure: x axis is from $t = 0$ to 15. Convergence rate of Gaussian approximate Fisher-Rao gradient flows not influenced by values of λ

Ongoing Work: Gaussian Mixtures + Kalman Methods

Consider the 2d Darcy flow problem ($\theta \in \mathbb{R}^{128}$)

$$-\nabla \cdot (a(x,\theta)\nabla p(x)) = f(x) = 1000 \sin\big(4\pi x_{(2)}\big) \qquad x \in D$$
$$p(x) = 0 \qquad x \in \partial D$$

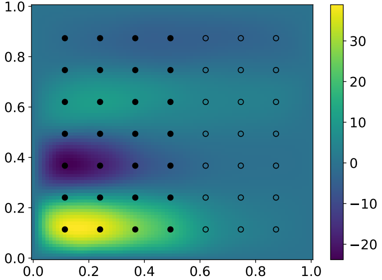

Figure: The reference pressure field p and observations $\frac{p([x_{(1)},x_{(2)}]^T)+p([1-x_{(1)},x_{(2)}]^T)}{2}$ at 28 equidistant points (solid black dots) and their mirroring points (empty black dots).

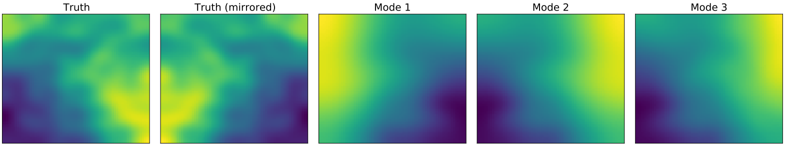

Figure: The truth log permeability field $a(x;\theta_{ref})$, and log permeability fields obtained by 3-mode GMKI (Gaussian Mixture Kalman Inversion)

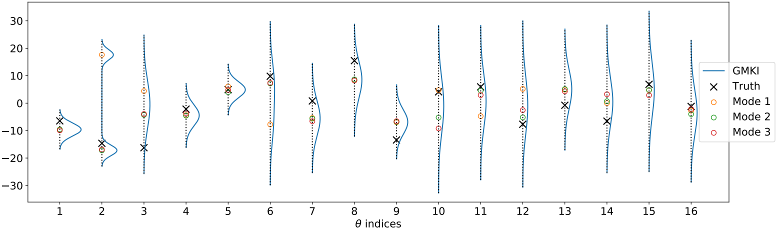

Figure: The truth expansion parameters $\theta_{(i)}$ (black crosses), and mean estimations of $\theta_{(i)}$ for each modes (circles) and the associated marginal distributions obtained GMKI at the 30-th iteration.

Summary

Gradient flows for sampling

- **Energy functional**: KL divergence is special
  - Invariance to normalization consts
- **Metric**: Fisher-Rao metric is special
  - Invariance to any diffeomorphism of the parameter space $\Rightarrow$ unconditional uniform exponential convergence
  - Relaxed to affine invariance and many constructions
- **Gaussian approximation**
  - Moment closures = natural gradient in Gaussian VI
  - Convergence guarantee for Gaussian and logconcave targets
- **Further directions**
  - Gaussian mixture approximations for multimodal targets
  - Derivative free approximations via Kalman's methodology
  - Other approximations to sample curved distributions

Thank You!

[Chen, Huang, Huang, Reich, Stuart 2023]

Sampling via Gradient Flows in the Space of Probability Measures

Link: `https://arxiv.org/abs/2310.03597`.