# Gradient Flows for Sampling

## Energy Functionals, Invariance and Gaussian Approximation

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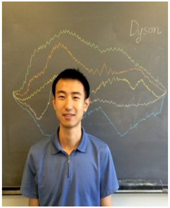
*University of South Carolina, July 2023*

# The Paper

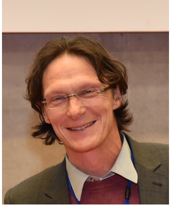
**[Chen, Huang, Huang, Reich, Stuart 2023]**

Gradient flows for sampling:
Mean-field models, Gaussian approximations and affine invariance

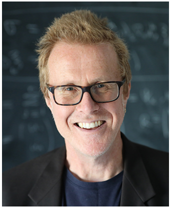
Daniel Huang
Caltech



Jiaoyang Huang
University of Pennsylvania



Sebastian Reich
University of Potsdam



Andrew Stuart
Caltech

Link: `https://arxiv.org/abs/2302.11024`.

# Outline

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**The sampling problem**

Goal: draw (approximate) samples from

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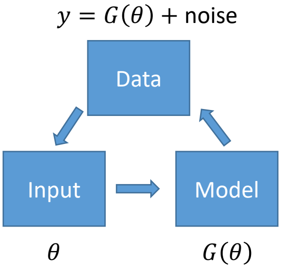
Many applications in

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



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**Dynamics for sampling**

Idea: construct a **dynamics of $\rho_t$** that gradually converges to

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  - Sequential Monte Carlo, ...

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The focus of this talk: **Infinite time dynamics**

# Dynamics through Gradient Flows (GFs)

**Gradient flow dynamics for sampling**

Idea: construct a **gradient flow** **dynamics of** $\rho_t$ that converges to

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*Namely, dynamics comes from gradient based optimization methods*

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

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

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

# Sampling through Numerical Approximation of GFs

**Gradient flow equation**

$$\frac{\partial \rho_t}{\partial t} = - \underbrace{M(\rho_t)^{-1}}_{\text{preconditioner}} \underbrace{\frac{\delta \mathcal{E}}{\delta \rho}\Big|_{\rho=\rho_t}}_{\text{first variation}}$$

**Numerical approximations** of GFs lead to sampling methods

- Particle methods such as SDEs

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

  e.g., Langevin's dynamics $\mathrm{d}\theta_t = \nabla_\theta \log \rho^\star(\theta_t)\mathrm{d}t + \sqrt{2}\mathrm{d}W_t$

- Parametric approximations such as Gaussian approximation
  e.g., Gaussian variational inference, Kalman filters

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

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

We approach the question through the **perspective of invariance**

- In energy functionals: invariance to normalization consts
- In metrics: invariance to transformation of the space

We then discuss numerical approximations of the resulting flow

# Outline

# On Choosing the Energy Functionals

**Recap: Gradient flow equation**

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

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

- 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 $\rho^\star$**

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

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Use KL divergence from now on

# Outline

# Two Metrics

**Wasserstein metric [Jordan, Kinderlehrer, Otto 1998]**

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

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

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

**Fisher-Rao metric [Rao 1945]**

$$\text{Metric: } M(\rho)^{-1}\psi = \rho(\psi - \mathbb{E}_\rho[\psi])$$

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

- Optimal transport [Villani 2003, 2008]
- 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

$$D^2 V(\cdot) \succeq \lambda I$$

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 problem**

# A Closer Look at Fisher-Rao

**Fisher-Rao gradient flow**

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**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

Recall the definition of the push-forward operator

$$\tilde{\rho}_t(\theta) = \rho_t(\varphi^{-1}(\theta)) |\det \nabla \varphi^{-1}|$$
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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** $\rho^\star$

- Assume there exists a diffeomorphism $\varphi$ such that

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

- 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

# Theoretical Results of Fisher-Rao

### Convergence of Fisher-Rao gradient flows

**[Lu, Slepčev, Wang 2022], [Chen, Huang, Huang, Reich, Stuart 2023]**

Let $\rho_t$ satisfy the Fisher-Rao gradient flow. Assume

- there exist constants $K, B > 0$ such that $\rho_0$ satisfies

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

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

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

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

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**Unconditional uniform exponential convergence**

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

# Numeric Approximation and Further Thoughts

**Simulating the Fisher-Rao gradient flow is not easy**

- Birth-death dynamics, Wasserstein-Fisher-Rao gradient flow
  [Lu, Lu, Nolen 2019], [Lu, Slepčev, Wang 2022]
- Gaussian approximation **[Chen, Huang, Huang, Reich, Stuart 2023]**
  Derivative-free Kalman method [Huang, Huang, Reich, Stuart 2022]

We will talk about it later ...

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**The question:**

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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.

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No other alternatives if we ask for diffeomorphism invariance!

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  - Kalman-Wasserstein gradient flows
    [Garbuno-Inigo, Hoffmann, Li, Stuart 2020]

$$\frac{\partial \rho_t}{\partial t} = -\nabla_\theta \cdot (\rho_t C(\rho_t) \nabla_\theta \log \rho^\star) + \nabla \cdot (C(\rho_t) \nabla \rho_t)$$
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$\Rightarrow$ Uniform exponential convergence for any **Gaussian** $\rho^\star$

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- Other affine invariant gradient flow examples in our paper
  - e.g., affine invariant Stein gradient flow

# Outline

# Numerical Approximation of the Fisher-Rao Gradient Flow

- Birth-death dynamics, Wasserstein-Fisher-Rao gradient flow
  [Lu, Lu, Nolen 2019], [Lu, Slepčev, Wang 2022]
- **Gaussian approximation** **[Chen, Huang, Huang, Reich, Stuart 2023]**
  Derivative-free Kalman method [Huang, Huang, Reich, Stuart 2022]

The focus of this talk: **Gaussian approximation**

# 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 $\rho_t$ 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**

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

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- It is equivalent to the Fisher-Rao gradient flow constrained to Gaussians geometrically **[Chen, Huang, Huang, Reich, Stuart 2023]**
- 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

# Convergence Guarantee **[Chen, Huang, Huang, Reich, Stuart 2023]**

**Gaussian target**

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

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

# Convergence Guarantee **[Chen, Huang, Huang, Reich, Stuart 2023]**

**Logconcave target**

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

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

- See also the case of Wasserstein gradient flow in Gaussian variational inference for logconcave target

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

# Local Convergence Rates

**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

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

Moreover, the bound is sharp: it is possible to construct a sequence of triplets $\rho_n^\star$, $\alpha_n$ and $\beta_n$, 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

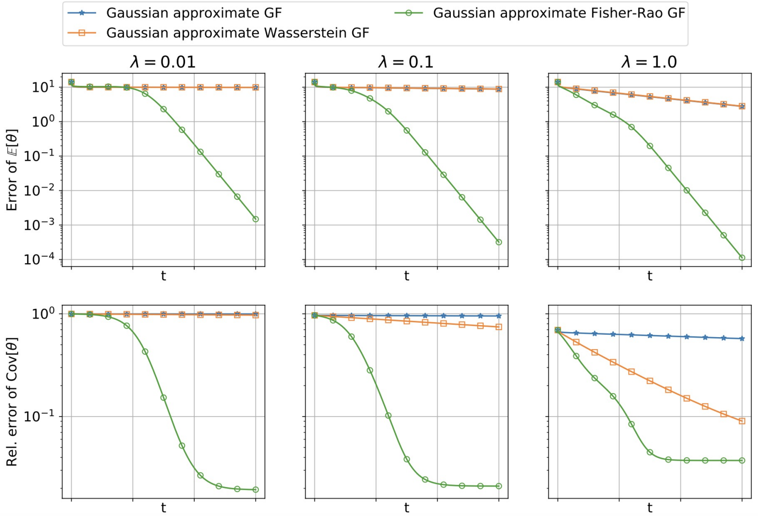


Figure: $x$ axis is from $t = 0$ to $15$. Convergence rate of Gaussian approximate Fisher-Rao gradient flows not influenced by values of $\lambda$

# Outline

# Summary

Gradient flows for sampling **[Chen, Huang, Huang, Reich, Stuart 2023]**

- **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 via moment closures**
  - equivalent to Gaussian variational inference
  - convergence guarantee for Gaussian and logconcave targets
- **Further directions**
  - optimal convergence rates in variational inference
  - Gaussian mixture approximations
  - derivative free approximations via Kalman's methodology

# Thank You

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

Gradient flows for sampling:
Mean-field models, Gaussian approximations and affine invariance

Link: `https://arxiv.org/abs/2302.11024`.