What are ... generative probability flows for sampling?

Viktor Stein, Technical University of Berlin

"What is ... ?" Seminar

07.11.2025

1. Two types of generative modelling

2. Gradient flows - from Euclidean to metric

3. Optimal transport and the Wasserstein metric

4. Wasserstein gradient flow

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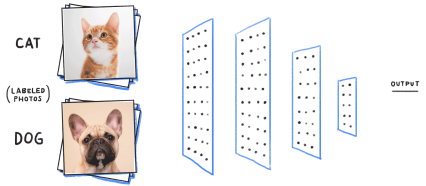

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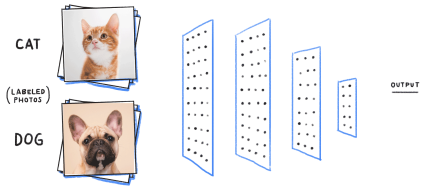

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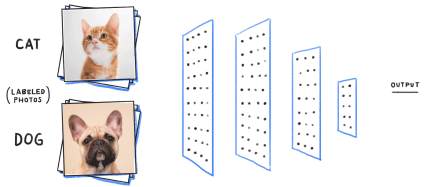

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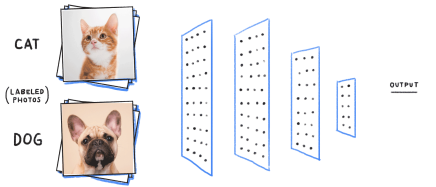

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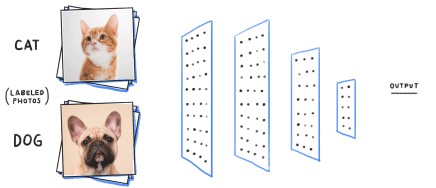

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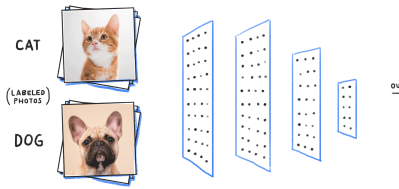

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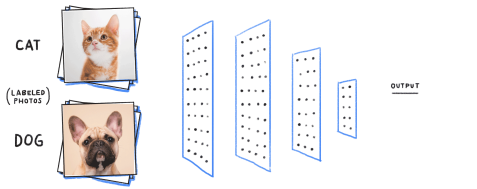

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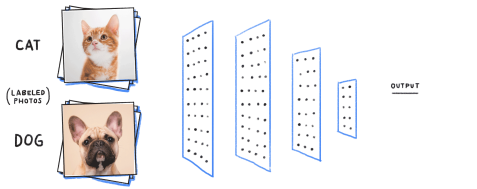

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Another example. π represents hand-written digits (784-dimensional)

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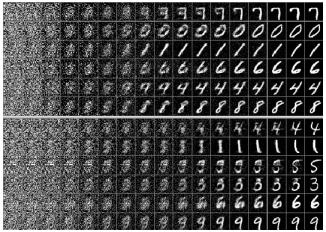

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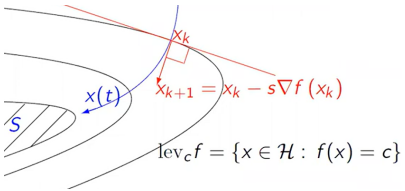

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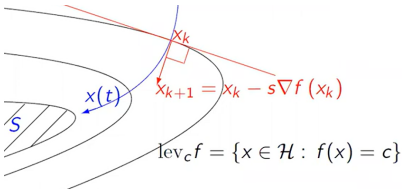

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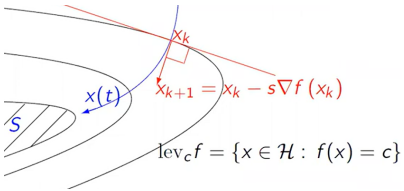

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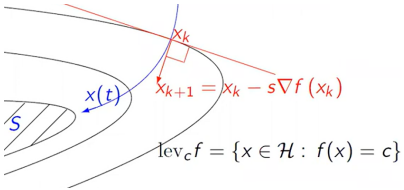

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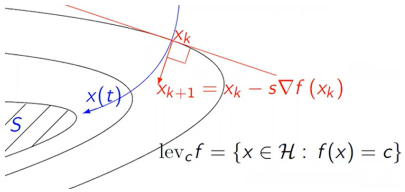

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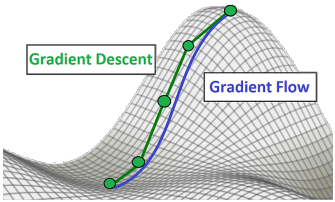
ii) Both $\|u'(t)\|_2 = \|\nabla\Phi(u(t))\|_2$ *and* $\frac{\mathrm{d}}{\mathrm{d}t}\Phi(u(t)) = -\|\nabla\Phi(u(t))\|_2\|u'(t)\|_2$ *hold for* $t > 0$.

iii) $\frac{\mathrm{d}}{\mathrm{d}t}\Phi(u(t)) \le -\frac{1}{2}\big\|\nabla\Phi\big(u(t)\big)\big\|_2^2 - \frac{1}{2}\|u'(t)\|_2^2$ *for* $t > 0$.

The **scalar** quantities $\|u'(t)\|_2,\ \|\nabla\Phi(u(t))\|_2$

can be given sense when replacing $\mathbb{R}^d$ by a metric space.

$\rightsquigarrow$ new scalar formulation of gradient flow



Let (X, d) be a complete metric space.

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Definition (Absolute continuity)

A curve $u\colon (0,\infty) \to X$ is p-locally absolutely continuous for $p \in [1,\infty]$ and we write $u \in \mathrm{AC}^p_{\mathrm{loc}}\big((0,\infty); X\big)$ if there exists a $m \in L^p_{\mathrm{loc}}(0,\infty)$ with (if $p = 1$, we omit exponent)

$$d\big(u(t), u(s)\big) \leq \int_s^t m(r)\,\mathrm{d}r \qquad \forall 0 < s \leq t < \infty.$$

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Definition (Metric derivative)

The *metric derivative* of a curve $u \in \mathrm{AC}_{\mathrm{loc}}\big((0,\infty); X\big)$ at $t \in (0,\infty)$ is

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The gradient norm $\|\nabla\Phi\|_2$ is replaced by an *upper gradient*, a function g such that

$$\big|\Phi(u(t)) - \Phi(u(s))\big| \leq \int_s^t g(u(s))|u'|(s)\,\mathrm{d}s \qquad \forall u \in \mathrm{AC}_{\mathrm{loc}}\big((0,\infty); X\big),\ 0 < s \leq t < \infty.$$

The **Wasserstein-2 space** is

$$\mathcal{P}_2(\mathbb{R}^d) := \left\{ \mu \in \mathcal{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} \|x\|_2^2 \, \mathrm{d}\mu(x) < \infty \right\}$$

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$$W_2(\mu, \nu)^2 = \min_{\pi \in \Gamma(\mu,\nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|_2^2 \, \mathrm{d}\pi(x, y), \;\; \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d),$$

the transport polytope is $\Gamma(\mu, \nu) \coloneqq \{\pi \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) : (P_1)_{\#}\pi = \mu, (P_2)_{\#}\pi = \nu\}$, and $f_{\#}\mu \coloneqq \mu \circ f^{-1}$.

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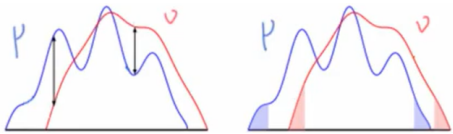

Vertical (L^2) vs. horizontal (W_2) mass displacement.

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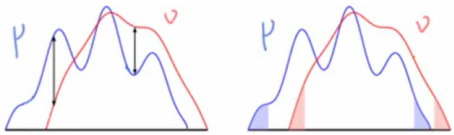

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Theorem (Brenier (early 90s))

If $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ has a density (and $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ is arbitrary), then there exists a transport map $T\colon \mathbb{R}^d \to \mathbb{R}^d$ with $T_{\#}\mu = \nu$ (and $T = \nabla\varphi$ for some convex function $\varphi\colon \mathbb{R}^d \to \mathbb{R}$) solving the Monge problem

$$\inf_{\substack{T\colon \mathbb{R}^d \to \mathbb{R}^d, \\ T_{\#}\mu = \nu}} \int_{\mathbb{R}^d} \|T(x) - x\|_2^2 \, \mathrm{d}\mu(x) = W_2(\mu,\nu)^2, \qquad \pi = (\mathrm{id}, T).$$

Density perspective: A curve $\mu\colon (0,\infty) \to \mathcal{P}_2(\mathbb{R}^d)$ is *absolutely continuous* if $\exists$ L^2-Borel velocity field $v\colon \mathbb{R}^d \times (0,\infty) \to \mathbb{R}^d$ s.t.

$$\partial_t \mu_t + \nabla \cdot (v_t \mu_t) = 0, \qquad (t,x) \in (0,\infty) \times \mathbb{R}^d, \text{ weakly.} \tag{Continuity Eq.}$$

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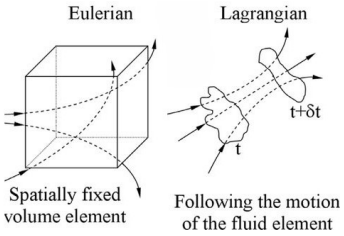

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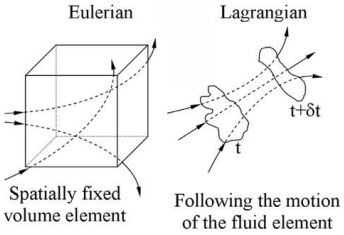
Particle perspective: Under regularity assumptions on $(v_t)_t$, there exists a solution ("flow map")

$$\partial_t \varphi(t,x) = v_t(\varphi(t,x)), \qquad \varphi(0,x) = x$$

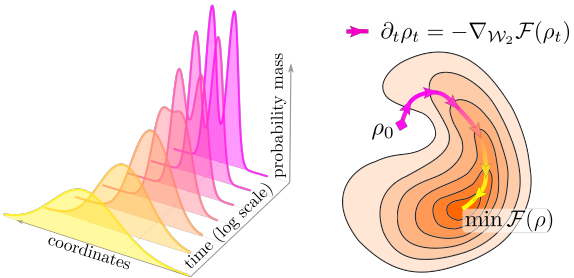
with $\mu_t = \varphi(t,\cdot)_{\#}\mu_0$.



Definition (Wasserstein gradient flow)

A locally absolutely continuous curve $\mu\colon (0,\infty) \to \mathcal{P}_2(\mathbb{R}^d)$ with velocity field $v_t \in \mathrm{T}_{\mu_t}\,\mathcal{P}_2(\mathbb{R}^d)$ is a *Wasserstein gradient flow with respect to* $\mathcal{F}\colon \mathcal{P}_2(\mathbb{R}^d) \to (-\infty,\infty]$ (assumed sufficiently regular) if

$$v_t \in -\partial_{W_2}\mathcal{F}(\mu_t), \quad \text{for a.e. } t > 0.$$



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(Altekrüger, Hertrich, et al. 2023)

Thank you for your attention!

I am happy to take any questions

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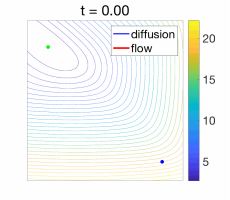
Definition (Fréchet subdifferential in Wasserstein space)

The (reduced) **Fréchet subdifferential** of $\mathcal{F}\colon \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, \infty]$ at $\mu \in \operatorname{dom}(\mathcal{F})$ is

$$\partial \mathcal{F}(\mu) \coloneqq \left\{ \xi \in L^2(\mathbb{R}^d; \mu) : \mathcal{F}(\nu) - \mathcal{F}(\mu) \geq \inf_{\pi \in \Gamma^{\mathrm{opt}}(\mu,\nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi(x_1), x_2 - x_1 \rangle \, \mathrm{d}\pi(x, y) + o(W_2(\mu, \nu)) \right\}$$

Gradient flows in $\mathbb{R}^d$



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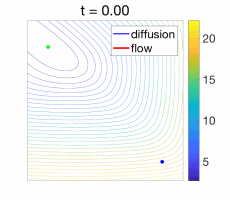

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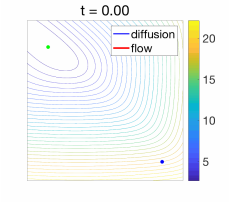

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relevant AG papers (Altekrüger, P. Hagemann, et al. 2023; Chemseddine, P. Hagemann, et al. 2025; Chemseddine, Wald, et al. 2024; Wald and Steidl 2025; P. Hagemann, Schütte, et al. 2025; P. Hagemann, Hertrich, et al. 2024; Hertrich, Gräf, et al. 2024; Duong et al. 2025; Altekrüger, Hertrich, et al. 2023; Chemseddine, Kornhardt, et al. 2025; P. L. Hagemann et al. 2023)