Mirror and Preconditioned Gradient Descent in Wasserstein Space

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CSD Seminar
20/02/2025

Motivations

Let $\mathcal{P}_2(\mathbb{R}^d) = \{\mu \in \mathcal{P}(\mathbb{R}^d),\ \int \|x\|_2^2\ \mathrm{d}\mu(x) < \infty\}$, $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$.

Goal:

$$\min_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \mathcal{F}(\mu)$$

Applications:

- Sampling from $\nu \propto e^{-V}$ (Wibisono, 2018)
- Generative modeling
- Learning neural networks (Mei et al., 2018; Chizat and Bach, 2018)
- Modeling dynamic of populations of cells (Schiebinger et al., 2019)

Example of functionals

- Free energies: $\mathcal{F}(\mu) = \int V \mathrm{d}\mu + \iint W(x,y)\ \mathrm{d}\mu(x)\mathrm{d}\mu(y) + \mathcal{H}(\mu)$ where $\mathcal{H}(\mu) = \int \log\big(\mu(x)\big)\ \mathrm{d}\mu(x)$ for $\mu \ll \mathrm{Leb}$
- $\mathcal{F}(\mu) = \mathrm{KL}(\mu||\nu) = \int V \mathrm{d}\mu + \mathcal{H}(\mu)\ (+C)$ for sampling from $\nu \propto e^{-V(x)}$
- $\mathcal{F}(\mu) = D(\mu, \nu)$ for sampling from ν

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Gradient Descent on $\mathbb{R}^d$

Let $f : \mathbb{R}^d \to \mathbb{R}$.

Goal: $\min_{x \in \mathbb{R}^d} \; f(x)$ via gradient flow

$$\frac{\mathrm{d}x_t}{\mathrm{d}t} = -\nabla f(x_t), \quad x_0 = x_0$$

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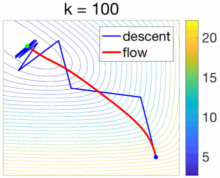
Main algorithm: **Gradient Descent** (GD)



From (Bach, 2020)

$$\forall k \geq 0, \; x_{k+1} = x_k - \tau \nabla f(x_k)$$
$$= \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \; \frac{1}{2}\|x - x_k\|_2^2 + \tau \langle \nabla f(x_k), x - x_k \rangle$$

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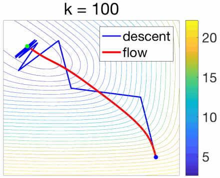

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$$\begin{aligned}\forall k \geq 0,\; x_{k+1} &= x_k - \tau \nabla f(x_k) \\ &= \operatorname*{argmin}_{x \in \mathbb{R}^d} \; \frac{1}{2}\|x - x_k\|_2^2 + \tau \langle \nabla f(x_k), x - x_k \rangle\end{aligned}$$

Convergence Analysis

- f β-smooth $\implies$ $f(x_{k+1}) \leq f(x_k) - \frac{1}{2\beta}\|\nabla f(x_k)\|_2^2 = f(x_k) - \frac{\beta}{2}\|x_{k+1} - x_k\|_2^2$
- f β-smooth and α-convex $\implies$ $f(x_k) - f(x^*) \leq \frac{\beta - \alpha}{2k}\|x_0 - x^*\|_2^2$

Reminder:

- f β-smooth $\iff$ $\forall x, y \in \mathbb{R}^d,\; f(x) - f(y) - \langle \nabla f(y), x - y \rangle \leq \frac{\beta}{2}\|x - y\|_2^2$
- f α-convex $\iff$ $f - \alpha\frac{\|\cdot\|_2^2}{2}$ convex

Mirror Descent on $\mathbb{R}^d$ (Beck and Teboulle, 2003)

If f not β-smooth: no guarantees for GD $\rightarrow$ change geometry

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Definition (Bregman Divergence)

Let $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ be strictly convex, then the Bregman divergence is defined as

$$\forall x, y \in \mathbb{R}^d,\ \mathrm{d}_\phi(x, y) = \phi(x) - \phi(y) - \langle \nabla \phi(y), x - y \rangle.$$

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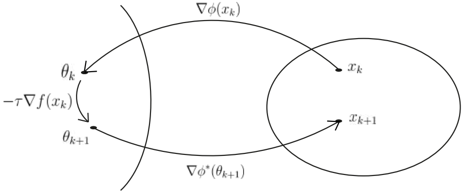
Mirror Descent algorithm:

$$\begin{aligned}\forall k \geq 0,\ x_{k+1} &= \underset{x\in\mathbb{R}^d}{\operatorname{argmin}}\ \mathrm{d}_\phi(x, x_k) + \tau\langle\nabla f(x_k), x - x_k\rangle \\ &= \nabla\phi^*\big(\nabla\phi(x_k) - \tau\nabla f(x_k)\big).\end{aligned}$$

Remark: For $\phi(x) = \frac{1}{2}\|x\|_2^2$, MD = GD and $\mathrm{d}_\phi(x,y) = \frac{1}{2}\|x-y\|_2^2$



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Convergence analysis (Lu et al., 2018)

- f β-smooth relative to ϕ, *i.e.* $\mathrm{d}_f(x, y) \leq \beta\mathrm{d}_\phi(x, y)$ (equivalently $\beta\phi - f$ convex) $\implies f(x_{k+1}) \leq f(x_k) - \beta\mathrm{d}_\phi(x_k, x_{k+1})$
- f β-smooth and α-convex relative to ϕ, *i.e.* $\alpha\mathrm{d}_\phi(x, y) \leq \mathrm{d}_f(x, y)$ (equivalently $f - \alpha\phi$ convex) $\implies f(x_k) - f(x^*) \leq \frac{\beta-\alpha}{k}\mathrm{d}_\phi(x^*, x_0)$

Proof of convergence

Lemma (Three-Point Inequality)

Let $g : \mathbb{R}^d \to \mathbb{R}$ be a convex function, $\phi : \mathbb{R}^d \to \mathbb{R}$ strictly convex. Let $z_0 \in \mathbb{R}^d$ and $z^* = \operatorname{argmin}_z \ \mathrm{d}_\phi(z, z_0) + g(z)$. Then, for all $z \in \mathbb{R}^d$,

$$g(z) + \mathrm{d}_\phi(z, z_0) \geq g(z^*) + \mathrm{d}_\phi(z^*, z_0) + \mathrm{d}_\phi(z, z^*).$$

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Using smoothness, Three-point inequality on $g(x) = \frac{1}{\beta}\langle \nabla f(x_k), x - x_k \rangle$ and strong convexity we get for all $x \in \mathbb{R}^d$,

$$\begin{aligned} f(x_{k+1}) &\leq f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \beta \mathrm{d}_\phi(x_{k+1}, x_k) \\ &\leq f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \beta \mathrm{d}_\phi(x, x_k) - \beta \mathrm{d}_\phi(x, x_{k+1}) \\ &\leq f(x) + (\beta - \alpha)\mathrm{d}_\phi(x, x_k) - \beta \mathrm{d}_\phi(x, x_{k+1}). \end{aligned}$$

By induction and using the monotonicity of f, and taking $x = x^*$, we get the desired rates: $f(x_k) - f(x) \leq \frac{\alpha \mathrm{d}_\phi(x, x_0)}{\left(1 + \frac{\alpha}{\beta - \alpha}\right)^k - 1} \leq \frac{\beta - \alpha}{k} \mathrm{d}_\phi(x, x_0)$.

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Remarks: (1) the proof works replacing β with $1/\tau$ if $\tau \leq 1/\beta$, (2) we need smoothness and convexity in specific directions.

Preconditioned Gradient Descent (Maddison et al., 2021)

Let $h : \mathbb{R}^d \to \mathbb{R}$ strictly convex, $g : \mathbb{R}^d \to \mathbb{R}$.

Preconditioned Gradient Descent scheme:

$$\begin{aligned} \forall k \geq 0,\ y_{k+1} &= y_k - \tau \nabla h^*\big(\nabla g(y_k)\big) \\ &= \operatorname*{argmin}_{y \in \mathbb{R}^d}\ h\left(\frac{y_k - y}{\tau}\right)\tau + \langle \nabla g(y_k), y - y_k \rangle \end{aligned}$$

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Closely related to MD (Kim et al., 2023) as for $g = \phi^*$, $h^* = f$, $y = \nabla\phi(x)$,

$$\nabla\phi(x_{k+1}) = \nabla\phi(x_k) - \tau\nabla f(x_k) \iff x_{k+1} = \nabla\phi^*\big(\nabla\phi(x_k) - \tau\nabla f(x_k)\big).$$

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Convergence analysis (Maddison et al., 2021)

- h^* β-smooth relative to g^* $\implies h^*\big(\nabla g(y_{k+1})\big) \leq h^*\big(\nabla g(y_k)\big) - \beta \mathrm{d}_g(y_{k+1}, y_k)$
- h^* β-smooth and α-convex relative to g^*
  $\implies \forall k \geq 1,\ h^*\big(\nabla g(y_k)\big) - h^*(0) \leq \frac{\alpha-\beta}{k}\big(g(y_0) - g(y^*)\big)$
  $\implies \forall k \geq 0,\ g(y_k) - g(y^*) \leq (1 - \alpha/\beta)^k\big(g(y_0) - g(y^*)\big)$

Relation between MD and Preconditoned GD

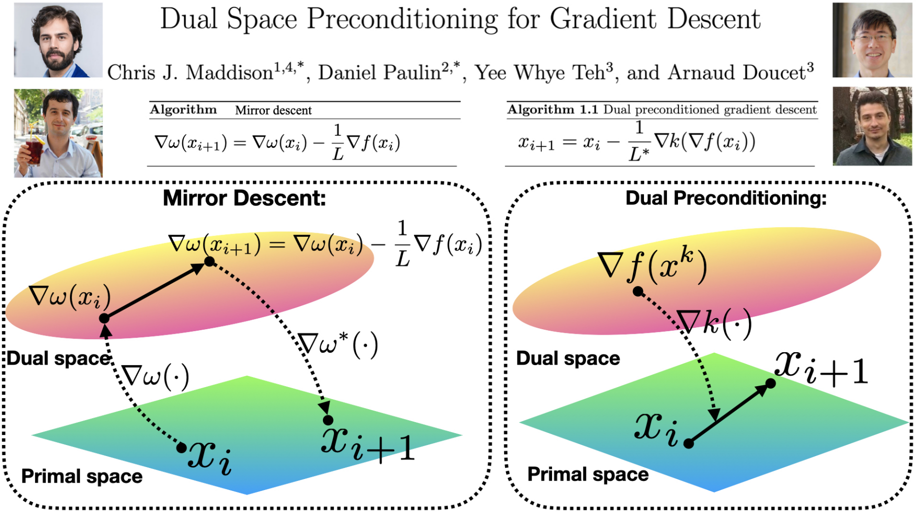

Figure: Taken from a tweet of Konstantin Mishchenko [1]

[1] https://mobile.x.com/konstmish/status/1431983100561592323/photo/1

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Wasserstein Geometry

Definition (Wasserstein distance)

Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ and denote by $\Pi(\mu,\nu)$ the set of coupling between μ, ν. Then, the Wasserstein distance is

$$\mathrm{W}_2^2(\mu,\nu) = \inf_{\gamma\in\Pi(\mu,\nu)} \int \|x-y\|_2^2 \ \mathrm{d}\gamma(x,y).$$

Properties:

- W_2 distance, $(\mathcal{P}_2(\mathbb{R}^d), \mathrm{W}_2)$: Wasserstein space
- **Brenier's theorem**: If $\mu \ll \mathrm{Leb}$, then there exists a unique T_μ^ν such that

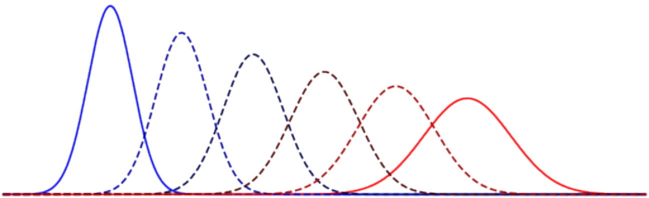
1. $(\mathrm{T}_\mu^\nu)_\#\mu = \nu$ $\big(\mathrm{T}_\#\mu(A) = \mu\big(\mathrm{T}^{-1}(A)\big)$ for all $A \subset \mathbb{R}^d\big)$
2. $\mathrm{W}_2^2(\mu,\nu) = \int \|x - \mathrm{T}_\mu^\nu(x)\|_2^2 \ \mathrm{d}\mu(x) = \|\mathrm{Id} - \mathrm{T}_\mu^\nu\|_{L^2(\mu)}^2$

- **Riemannian structure**

Riemannian Structure of the Wasserstein Space

- Geodesics between $\mu \ll \mathrm{Leb}$ and $\nu \in \mathcal{P}_2(\mathbb{R}^d)$:

$$\forall t \in [0,1],\ \mu_t = \big((1-t)\mathrm{Id} + t\mathrm{T}_\mu^\nu\big)_\#\mu$$



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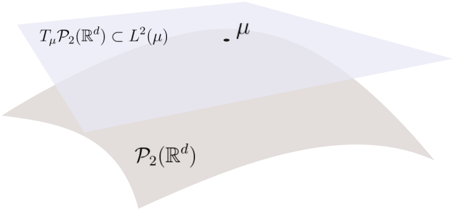
- Tangent space at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ (Ambrosio et al., 2005):

$$\mathcal{T}_\mu \mathcal{P}_2(\mathbb{R}^d) = \overline{\{\nabla\psi,\ \psi \in C_c^\infty(\mathbb{R}^d)\}} \subset L^2(\mu),$$

where $L^2(\mu) = \{f \in \mathbb{R}^d \to \mathbb{R}^d,\ \int \|f(x)\|_2^2\, \mathrm{d}\mu(x) < \infty\}$.



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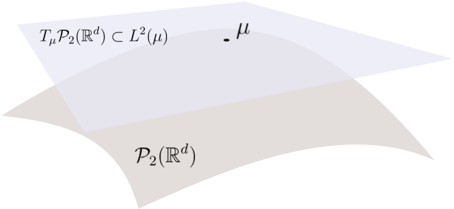

- $\mathcal{F}$ is α-geodesically convex if $t \mapsto \mathcal{F}(\mu_t)$ is α-convex, *i.e.* for all $t \in [0,1]$,

$$\mathcal{F}(\mu_t) \le (1-t)\mathcal{F}(\mu_0) + t\mathcal{F}(\mu_1) - \frac{\alpha t(1-t)}{2}\mathrm{W}_2^2(\mu_0,\mu_1).$$

Wasserstein Gradient

Definition (Wasserstein gradient (Bonnet, 2019))

Let $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. $\nabla_{\mathrm{W}_2}\mathcal{F}(\mu) \in L^2(\mu)$ is a Wasserstein gradient of $\mathcal{F}$ at μ if for any $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ and any optimal coupling $\gamma \in \Pi_o(\mu,\nu)$,

$$\mathcal{F}(\nu) = \mathcal{F}(\mu) + \int \langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu)(x), y - x\rangle \,\mathrm{d}\gamma(x,y) + o\big(\mathrm{W}_2(\mu,\nu)\big).$$

If such a gradient exists, then we say that $\mathcal{F}$ is W_2-differentiable at μ.

Properties:

- There is a unique gradient in $\mathcal{T}_\mu\mathcal{P}_2(\mathbb{R}^d)$ (Lanzetti et al., 2022, Proposition 2.5)
- Differential are strong (Lanzetti et al., 2022, Proposition 2.6), *i.e.* for any $\gamma \in \Pi(\mu,\nu)$,

$$\mathcal{F}(\nu) = \mathcal{F}(\mu) + \int \langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu)(x), y - x\rangle \,\mathrm{d}\gamma(x,y) + o\left(\sqrt{\int \|x-y\|_2^2 \,\mathrm{d}\gamma(x,y)}\right)$$

  In particular, for $\gamma = (\mathrm{Id},\mathrm{T})_\#\mu$,

$$\mathcal{F}(\mathrm{T}_\#\mu) = \mathcal{F}(\mu) + \langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu), \mathrm{T}-\mathrm{Id}\rangle_{L^2(\mu)} + o(\|\mathrm{T}-\mathrm{Id}\|_{L^2(\mu)})$$

Wasserstein Gradient

Example of functionals

- Potential energies $\mathcal{V}(\mu) = \int V \mathrm{d}\mu$: For V differentiable and smooth,

$$\nabla_{\mathrm{W}_2}\mathcal{V}(\mu) = \nabla V$$

- Interaction energies $\mathcal{W}(\mu) = \iint W(x-y)\ \mathrm{d}\mu(x)\mathrm{d}\mu(y)$: For W even, differentiable and smooth,

$$\nabla_{\mathrm{W}_2}\mathcal{W}(\mu) = \nabla W \star \mu$$

Negative entropy

$\mathcal{H}(\mu) = \int \log\big(\mu(x)\big)\ \mathrm{d}\mu(x)$ not W_2-differentiable but can consider subgradients under regularity assumptions:

$$\forall x \in \mathbb{R}^d,\ \nabla_{\mathrm{W}_2}\mathcal{H}(\mu)(x) = \nabla \log \mu(x)$$

Wasserstein Gradient Flows (Ambrosio et al., 2005)

Wasserstein gradient flow of $\mathcal{F}$: curve $t \mapsto \mu_t$ satisfying (weakly)

$$\partial_t \mu_t = \mathrm{div}\big(\mu_t \nabla_{\mathrm{W}_2} \mathcal{F}(\mu_t)\big).$$

Particles: $x_t \sim \mu_t \iff \frac{\mathrm{d}x_t}{\mathrm{d}t} = -\nabla_{\mathrm{W}_2} \mathcal{F}(\mu_t)(x_t)$.

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Time discretization of the flow:

- Implicit/Backward (JKO) scheme (Jordan et al., 1998):

$$\mu_{k+1} = \operatorname*{argmin}_{\mu\in\mathcal{P}_2(\mathbb{R}^d)} \ \frac{1}{2}\mathrm{W}_2^2(\mu,\mu_k) + \tau\mathcal{F}(\mu)$$

  If $\mu_k \ll \mathrm{Leb}$, $\mu_{k+1} = \mathrm{T}_\#\mu_k$ with

$$\mathrm{T} = \operatorname*{argmin}_{\mathrm{T}\in L^2(\mu_k)} \ \frac{1}{2}\|\mathrm{T}-\mathrm{Id}\|^2_{L^2(\mu_k)} + \tau\mathcal{F}(\mathrm{T}_\#\mu_k)$$

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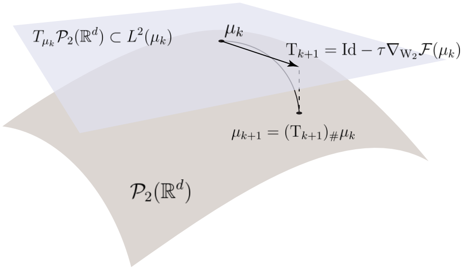
$$\mathrm{T} = \operatorname*{argmin}_{\mathrm{T} \in L^2(\mu_k)} \frac{1}{2} \|\mathrm{T} - \mathrm{Id}\|_{L^2(\mu_k)}^2 + \tau \mathcal{F}(\mathrm{T}_\# \mu_k)$$

- Explicit/Forward scheme

$$\begin{cases} \mathrm{T}_{k+1} = \mathrm{argmin}_{\mathrm{T} \in L^2(\mu_k)} \ \frac{1}{2} \|\mathrm{T} - \mathrm{Id}\|_{L^2(\mu_k)}^2 + \tau \langle \nabla_{\mathrm{W}_2} \mathcal{F}(\mu_k), \mathrm{T} - \mathrm{Id} \rangle_{L^2(\mu_k)} \\ \mu_{k+1} = (\mathrm{T}_{k+1})_\# \mu_k \end{cases}$$

Taking the FOC: $\mathrm{T}_{k+1} = \mathrm{Id} - \tau \nabla_{\mathrm{W}_2} \mathcal{F}(\mu_k)$

Wasserstein Gradient Descent



Wasserstein Gradient Descent:

$$\begin{cases} \mathrm{T}_{k+1} = \mathrm{argmin}_{\mathrm{T}\in L^2(\mu_k)} \ \frac{1}{2}\|\mathrm{T}-\mathrm{Id}\|^2_{L^2(\mu_k)} + \tau\langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k), \mathrm{T}-\mathrm{Id}\rangle_{L^2(\mu_k)} \\ \mu_{k+1} = (\mathrm{T}_{k+1})_\#\mu_k \end{cases}$$

Taking the FOC: $\mathrm{T}_{k+1} = \mathrm{Id} - \tau\nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k)$

Particle approximation: $\hat{\mu}_k^n = \frac{1}{n}\sum_{i=1}^n \delta_{x_i^k}$, $x_i^{k+1} = \mathrm{T}_{k+1}(x_i^k)$ for all $i \in \{1,\dots,n\}$.

Contributions

Study schemes of the form

$$\begin{cases} \mathrm{T}_{k+1} = \mathrm{argmin}_{\mathrm{T}\in L^2(\mu_k)}\ \mathrm{d}(\mathrm{T},\mathrm{Id}) + \tau\langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k), \mathrm{T}-\mathrm{Id}\rangle_{L^2(\mu_k)} \\ \mu_{k+1} = (\mathrm{T}_{k+1})_{\#}\mu_k, \end{cases}$$

and provide **convergence conditions**.

Considered divergences:

- For $\mathrm{d}(\mathrm{T},\mathrm{Id}) = \frac{1}{2}\|\mathrm{T}-\mathrm{Id}\|^2_{L^2(\mu)}$: **Wasserstein gradient descent**
- For $\mathrm{d}_{\phi_\mu}(\mathrm{T},\mathrm{Id}) = \phi_\mu(\mathrm{T}) - \phi_\mu(\mathrm{Id}) - \langle \nabla\phi_\mu(\mathrm{Id}), \mathrm{T}-\mathrm{Id}\rangle_{L^2(\mu)}$ (**Bregman divergence** on $L^2(\mu)$): extends **Mirror Descent** (Beck and Teboulle, 2003) to $\mathcal{P}_2(\mathbb{R}^d)$.
- For $\mathrm{d}(\mathrm{T},\mathrm{Id}) = \int h\big(\mathrm{T}(x)-x\big)\ \mathrm{d}\mu(x)$: extends **Preconditioned Gradient Descent** (Maddison et al., 2021) to $\mathcal{P}_2(\mathbb{R}^d)$.

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Background on $L^2(\mu)$

Definition (Bregman Divergence (Frigyik et al., 2008))

Let $\phi_\mu : L^2(\mu) \to \mathbb{R}$ be convex. The Bregman divergence is defined for all $\mathrm{T}, \mathrm{S} \in L^2(\mu)$ as

$$\mathrm{d}_{\phi_\mu}(\mathrm{T}, \mathrm{S}) = \phi_\mu(\mathrm{T}) - \phi_\mu(\mathrm{S}) - \langle \nabla \phi_\mu(\mathrm{S}), \mathrm{T} - \mathrm{S} \rangle_{L^2(\mu)}.$$

- If $\phi_\mu(\mathrm{T}) = \frac{1}{2}\|\mathrm{T}\|^2_{L^2(\mu)}$, $\mathrm{d}_{\phi_\mu}(\mathrm{T}, \mathrm{S}) = \frac{1}{2}\|\mathrm{T} - \mathrm{S}\|^2_{L^2(\mu)}$
- We call ϕ_μ pushforward compatible if there exists $\phi : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ such that

$$\forall \mu \in \mathcal{P}_2(\mathbb{R}^d),\ \forall \mathrm{T} \in L^2(\mu),\ \phi_\mu(\mathrm{T}) = \phi(\mathrm{T}_\# \mu).$$

  In this case, if ϕ is W_2-differentiable, then ϕ_μ is Fréchet differentiable and $\nabla \phi_\mu(\mathrm{T}) = \nabla_{\mathrm{W}_2} \phi(\mathrm{T}_\# \mu) \circ \mathrm{T}$.
- Let $\phi_\mu, \psi_\mu : L^2(\mu) \to \mathbb{R}$ convex.
  - ϕ_μ is β-smooth relative to ψ_μ if for all $\mathrm{T}, \mathrm{S} \in L^2(\mu)$, $\mathrm{d}_{\phi_\mu}(\mathrm{T}, \mathrm{S}) \leq \beta \mathrm{d}_{\psi_\mu}(\mathrm{T}, \mathrm{S})$.
  - ϕ_μ is α-convex relative to ψ_μ if for all $\mathrm{T}, \mathrm{S} \in L^2(\mu)$, $\mathrm{d}_{\phi_\mu}(\mathrm{T}, \mathrm{S}) \geq \alpha \mathrm{d}_{\psi_\mu}(\mathrm{T}, \mathrm{S})$.

Convexity on $\mathcal{P}_2(\mathbb{R}^d)$

Let $\mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, $\mu_0 \ll \mathrm{Leb}$, and $\mu_t = \big((1-t)\mathrm{Id} + t\mathrm{T}_{\mu_0}^{\mu_1}\big)_\#\mu_0$.

- $\mathcal{F}$ is α-geodesically convex if $t \mapsto \mathcal{F}(\mu_t)$ is α-convex, *i.e.* for all $t \in [0,1]$,

$$\mathcal{F}(\mu_t) \leq (1-t)\mathcal{F}(\mu_0) + t\mathcal{F}(\mu_1) - \frac{\alpha t(1-t)}{2}\mathrm{W}_2^2(\mu_0, \mu_1),$$

or equivalently

$$\begin{aligned} \frac{\alpha}{2}\mathrm{W}_2^2(\mu_0,\mu_1) = \frac{\alpha}{2}\|\mathrm{T}_{\mu_0}^{\mu_1} - \mathrm{Id}\|_{L^2(\mu_0)}^2 &\leq \mathcal{F}(\mu_1) - \mathcal{F}(\mu_0) - \langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_0), \mathrm{T}_{\mu_0}^{\mu_1} - \mathrm{Id}\rangle_{L^2(\mu_0)} \\ &= \mathrm{d}_{\tilde{\mathcal{F}}_{\mu_0}}(\mathrm{T}_{\mu_0}^{\mu_1}, \mathrm{Id}) \end{aligned}$$

with $\tilde{\mathcal{F}}_\mu(\mathrm{T}) = \mathcal{F}(\mathrm{T}_\#\mu)$.

Convexity on $\mathcal{P}_2(\mathbb{R}^d)$

Let $\mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, $\mu_0 \ll \mathrm{Leb}$, and $\mu_t = \big((1-t)\mathrm{Id} + t\mathrm{T}_{\mu_0}^{\mu_1}\big)_\# \mu_0$.

- $\mathcal{F}$ is α-geodesically convex if $t \mapsto \mathcal{F}(\mu_t)$ is α-convex, *i.e.* for all $t \in [0,1]$,

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  or equivalently

$$\begin{aligned}\frac{\alpha}{2}\mathrm{W}_2^2(\mu_0,\mu_1) = \frac{\alpha}{2}\|\mathrm{T}_{\mu_0}^{\mu_1} - \mathrm{Id}\|_{L^2(\mu_0)}^2 &\leq \mathcal{F}(\mu_1) - \mathcal{F}(\mu_0) - \langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_0), \mathrm{T}_{\mu_0}^{\mu_1} - \mathrm{Id}\rangle_{L^2(\mu_0)} \\ &= \mathrm{d}_{\tilde{\mathcal{F}}_{\mu_0}}(\mathrm{T}_{\mu_0}^{\mu_1}, \mathrm{Id})\end{aligned}$$

  with $\tilde{\mathcal{F}}_\mu(\mathrm{T}) = \mathcal{F}(\mathrm{T}_\#\mu)$.

Definition

Let $\mathcal{F}, \mathcal{G} : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$, $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, $\mathrm{T}, \mathrm{S} \in L^2(\mu)$, $\mu_t = (\mathrm{T}_t)_\#\mu$ with $\mathrm{T}_t = (1-t)\mathrm{S} + t\mathrm{T}$ for all $t \in [0,1]$.

- $\mathcal{F}$ β-smooth relative to $\mathcal{G}$ along $t \mapsto \mu_t$ if $\forall s,t \in [0,1]$, $\mathrm{d}_{\tilde{\mathcal{F}}_\mu}(\mathrm{T}_s, \mathrm{T}_t) \leq \beta \mathrm{d}_{\tilde{\mathcal{G}}_\mu}(\mathrm{T}_s, \mathrm{T}_t)$.
- $\mathcal{F}$ α-convex relative to $\mathcal{G}$ along $t \mapsto \mu_t$ if $\forall s,t \in [0,1]$, $\mathrm{d}_{\tilde{\mathcal{F}}_\mu}(\mathrm{T}_s, \mathrm{T}_t) \geq \alpha \mathrm{d}_{\tilde{\mathcal{G}}_\mu}(\mathrm{T}_s, \mathrm{T}_t)$.

Mirror Descent on the Wasserstein Space

Let $\phi_\mu : L^2(\mu) \to \mathbb{R}$ be strictly convex, proper and differentiable.

Mirror Descent scheme:

$$\begin{cases} \mathrm{T}_{k+1} = \mathrm{argmin}_{\mathrm{T}\in L^2(\mu_k)}\ \mathrm{d}_{\phi_{\mu_k}}(\mathrm{T}, \mathrm{Id}) + \tau\langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k), \mathrm{T} - \mathrm{Id}\rangle_{L^2(\mu_k)} \\ \mu_{k+1} = (\mathrm{T}_{k+1})_\#\mu_k. \end{cases}$$

By FOC: $\nabla\phi_{\mu_k}(\mathrm{T}_{k+1}) = \nabla\phi_{\mu_k}(\mathrm{Id}) - \tau\nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k)$

Computing the scheme:

- For $\phi_\mu(\mathrm{T}) = \int V \circ \mathrm{T}\ \mathrm{d}\mu$, $\mathrm{T}_{k+1} = \nabla V^* \circ \big(\nabla V - \tau\nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k)\big)$
- For ϕ_μ pushforward compatible:

$$\nabla_{\mathrm{W}_2}\phi(\mu_{k+1}) \circ \mathrm{T}_{k+1} = \nabla_{\mathrm{W}_2}\phi(\mu_k) - \tau\nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k)$$

  In general: implicit in $\mathrm{T}_{k+1} \to$ Newton method
- Other particular cases with closed-forms, *e.g.* $\phi_\mu(\mathrm{T}) = \frac{1}{2}\|P_\mu \mathrm{T}\|^2_{L^2(\mu)}$ recovers SVGD (Liu and Wang, 2016) or EKS (Garbuno-Inigo et al., 2020).

Descent Lemma

Let $\phi_\mu : L^2(\mu) \to \mathbb{R}$ be strictly convex, proper and differentiable.

Mirror Descent scheme:

$$\begin{cases} \mathrm{T}_{k+1} = \mathrm{argmin}_{\mathrm{T}\in L^2(\mu_k)} \ \mathrm{d}_{\phi_{\mu_k}}(\mathrm{T}, \mathrm{Id}) + \tau \langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k), \mathrm{T} - \mathrm{Id}\rangle_{L^2(\mu_k)} \\ \mu_{k+1} = (\mathrm{T}_{k+1})_\# \mu_k. \end{cases}$$

Proposition (Descent Lemma)

Assumptions:

- *For all $k \geq 0$, $\mathcal{F}$ is β-smooth relative to ϕ along $t \mapsto \big((1-t)\mathrm{Id} + t\mathrm{T}_{k+1}\big)_\# \mu_k$*

Then, for all $k \geq 0$,

$$\mathcal{F}(\mu_{k+1}) \leq \mathcal{F}(\mu_k) - \beta \mathrm{d}_{\phi_{\mu_k}}(\mathrm{Id}, \mathrm{T}_{k+1}).$$

Remark: β-smoothness implies $\beta \mathrm{d}_{\phi_{\mu_k}}(\mathrm{T}_{k+1}, \mathrm{Id}) \geq \mathrm{d}_{\tilde{\mathcal{F}}_{\mu_k}}(\mathrm{T}_{k+1}, \mathrm{Id})$

Sketch of the proof:

1. Apply β-smoothness
2. Apply 3-point inequality

Convergence

Proposition

Assumptions: Let $\beta > 0, \alpha \geq 0$ *and* $\mathrm{T}_{\phi_{\mu_k}}^{\mu_k,\mu^*} = \mathrm{argmin}_{\mathrm{T}_\#\mu_k=\mu^*}\ \mathrm{d}_{\phi_{\mu_k}}(\mathrm{T}, \mathrm{Id})$.

- $\mathcal{F}$ *β-smooth relative to ϕ along* $t \mapsto \big((1-t)\mathrm{Id} + t\mathrm{T}_{k+1}\big)_\#\mu_k$
- $\mathcal{F}$ *α-convex relative to ϕ along* $t \mapsto \big((1-t)\mathrm{Id} + t\mathrm{T}_{\phi_{\mu_k}}^{\mu_k,\mu^*}\big)_\#\mu_k$
- *Assume* $\mathrm{d}_{\phi_{\mu_k}}(\mathrm{T}_{\phi_{\mu_k}}^{\mu_k,\mu^*}, \mathrm{T}_{k+1}) \geq \mathrm{d}_{\phi_{\mu_{k+1}}}(\mathrm{T}_{\phi_{\mu_{k+1}}}^{\mu_{k+1},\mu^*}, \mathrm{Id})$

Then, for all $k \geq 1$, $\mathcal{F}(\mu_k) - \mathcal{F}(\mu^*) \leq \frac{\beta-\alpha}{k}\mathrm{d}_{\phi_{\mu_0}}(\mathrm{T}_{\phi_{\mu_0}}^{\mu_0,\mu^*}, \mathrm{Id})$.

If $\alpha > 0$, *for all* $k \geq 0$, $\mathrm{d}_{\phi_{\mu_k}}(\mathrm{T}_{\phi_{\mu_k}}^{\mu_k,\mu^*}, \mathrm{Id}) \leq \left(1 - \frac{\alpha}{\beta}\right)^k \mathrm{d}_{\phi_{\mu_0}}(\mathrm{T}_{\phi_{\mu_0}}^{\mu_0,\mu^*}, \mathrm{Id})$.

Let ϕ_μ be pushforward compatible. Define the OT problem:

$$\begin{aligned}\mathrm{W}_\phi(\nu,\mu) &= \inf_{\gamma\in\Pi(\nu,\mu)}\ \phi(\nu) - \phi(\mu) - \int \langle \nabla_{\mathrm{W}_2}\phi(\mu)(y), x-y\rangle\ \mathrm{d}\gamma(x,y) \\ &\leq \mathrm{d}_{\phi_\eta}(\mathrm{T},\mathrm{S}) \quad \text{for} \quad (\mathrm{T},\mathrm{S})_\#\eta \in \Pi(\nu,\mu)\end{aligned}$$

Property: If $\mu \ll \mathrm{Leb}$ and $\nabla_{\mathrm{W}_2}\phi(\mu)$ is invertible, then $\gamma^* = (\mathrm{T}_{\phi_\mu}^{\mu,\nu}, \mathrm{Id})_\#\mu$, and $\mathrm{W}_\phi(\nu,\mu) = \mathrm{d}_{\phi_\mu}(\mathrm{T}_{\phi_\mu}^{\mu,\nu}, \mathrm{Id})$.

Continuous Formulation

Informally, for ϕ_μ pushforward compatible:

$$\begin{cases} \varphi(\mu_k) = \nabla_{\mathrm{W}_2}\phi(\mu_k) \\ \varphi(\mu_{k+1}) \circ \mathrm{T}_{k+1} = \varphi(\mu_k) - \tau \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k) \end{cases} \xrightarrow[\tau \to 0]{} \begin{cases} \varphi(\mu_t) = \nabla_{\mathrm{W}_2}\phi(\mu_t) \\ \frac{\mathrm{d}}{\mathrm{d}t}\varphi(\mu_t) = -\nabla_{\mathrm{W}_2}\mathcal{F}(\mu_t). \end{cases}$$

Continuous Formulation

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$$\frac{\mathrm{d}}{\mathrm{d}t}\varphi(\mu_t) = \frac{\mathrm{d}}{\mathrm{d}t}\nabla_{\mathrm{W}_2}\phi(\mu_t) = \mathrm{H}\phi_{\mu_t}(v_t),$$

with $\mathrm{H}\phi_{\mu_t} : L^2(\mu_t) \to L^2(\mu_t)$ Hessian operator defined such that

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\phi(\mu_t) = \langle \mathrm{H}\phi_{\mu_t}(v_t), v_t \rangle_{L^2(\mu_t)} \quad \text{with} \quad \partial_t \mu_t + \mathrm{div}(\mu_t v_t) = 0.$$

Mirror flow:

$$\partial_t \mu_t - \mathrm{div}\left(\mu_t (\mathrm{H}\phi_{\mu_t})^{-1} \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_t)\right) = 0.$$

Related works:

- For $\phi(\mu) = \int V \mathrm{d}\mu$, $\mathcal{F}(\mu) = \mathrm{KL}(\mu||\mu^*)$, coincides with continuous formulation of Mirror Langevin (Ahn and Chewi, 2021)
- For $\phi = \mathcal{F}$, coincides with Information Newton's flows (Wang and Li, 2020)
- For $\phi(\mu) = \frac{1}{2}\mathrm{W}_2^2(\mu, \nu)$, $\mathcal{F}(\mu) = \mathrm{KL}(\mu||\mu^*)$, coincides with Sinkhorn flows (Deb et al., 2023)

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Preconditioned GD

Let $h : \mathbb{R}^d \to \mathbb{R}$ strictly convex, proper and differentiable.

Preconditioned Gradient Descent scheme: Let $\phi_\mu^h(\mathrm{T}) = \int h \circ \mathrm{T} \, \mathrm{d}\mu$,

$$\begin{cases} \mathrm{T}_{k+1} = \mathrm{argmin}_{\mathrm{T} \in L^2(\mu_k)} \ \phi_{\mu_k}^h\left(\frac{\mathrm{Id}-\mathrm{T}}{\tau}\right)\tau + \langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k), \mathrm{T} - \mathrm{Id}\rangle_{L^2(\mu_k)} \\ \mu_{k+1} = (\mathrm{T}_{k+1})_\# \mu_k \end{cases}$$

By FOC: $\mathrm{T}_{k+1} = \mathrm{Id} - \tau \nabla h^* \circ \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k)$

Preconditioned GD

Let $h : \mathbb{R}^d \to \mathbb{R}$ strictly convex, proper and differentiable.

Preconditioned Gradient Descent scheme: Let $\phi_\mu^h(\mathrm{T}) = \int h \circ \mathrm{T}\, \mathrm{d}\mu$,

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By FOC: $\mathrm{T}_{k+1} = \mathrm{Id} - \tau \nabla h^* \circ \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k)$

Proposition (Descent Lemma)

Assumptions: For all $k \geq 0$,

- *$\mathcal{F}$ convex along $t \mapsto \big((1-t)\mathrm{T}_{k+1} + t\mathrm{Id}\big)_\# \mu_k$*
- *ϕ^{h^*} β-smooth relative to $\mathcal{F}^*$ along a suitable curve*

Then, for all $k \geq 0$,

$$\phi_{\mu_{k+1}}^{h^*}\big(\nabla_{\mathrm{W}_2}\mathcal{F}(\mu_{k+1})\big) \leq \phi_{\mu_k}^{h^*}\big(\nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k)\big) - \beta \mathrm{d}_{\tilde{\mathcal{F}}_{\mu_k}}(\mathrm{T}_{k+1}, \mathrm{Id}).$$

Preconditioned GD

Let $h : \mathbb{R}^d \to \mathbb{R}$ strictly convex, proper and differentiable.

Preconditioned Gradient Descent scheme: Let $\phi_\mu^h(\mathrm{T}) = \int h \circ \mathrm{T} \,\mathrm{d}\mu$,

$$\begin{cases} \mathrm{T}_{k+1} = \mathrm{argmin}_{\mathrm{T} \in L^2(\mu_k)} \ \phi_{\mu_k}^h\left(\frac{\mathrm{Id}-\mathrm{T}}{\tau}\right)\tau + \langle \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k), \mathrm{T} - \mathrm{Id}\rangle_{L^2(\mu_k)} \\ \mu_{k+1} = (\mathrm{T}_{k+1})_\# \mu_k \end{cases}$$

By FOC: $\mathrm{T}_{k+1} = \mathrm{Id} - \tau \nabla h^* \circ \nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k)$

Proposition

Assumptions: For all $k \geq 0$, *denoting* $\bar{\mathrm{T}} = \mathrm{argmin}_{\mathrm{T}, \mathrm{T}_\#\mu_k = \mu^*} \ \mathrm{d}_{\tilde{\mathcal{F}}_{\mu_k}}(\mathrm{Id}, \mathrm{T})$,

- $\mathcal{F}$ *convex along* $t \mapsto \big((1-t)\mathrm{T}_{k+1} + t\mathrm{Id}\big)_\# \mu_k$
- ϕ^{h^*} β*-smooth relative to* $\mathcal{F}^*$ *along a suitable curve*
- ϕ^{h^*} α*-convex relative to* $\mathcal{F}^*$ *along a suitable curve*

Then, for all $k \geq 1$, $\phi_{\mu_k}^{h^*}\big(\nabla_{\mathrm{W}_2}\mathcal{F}(\mu_k)\big) - h^*(0) \leq \frac{\beta-\alpha}{k}\big(\mathcal{F}(\mu_0) - \mathcal{F}(\mu^*)\big)$.
Moreover, assuming that h^* *attains its minimum at* 0 *and* $\alpha > 0$, *for all* $k \geq 0$, $\mathcal{F}(\mu_k) - \mathcal{F}(\mu^*) \leq (1-\tau\alpha)^k \big(\mathcal{F}(\mu_0) - \mathcal{F}(\mu^*)\big)$.

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Showing Relative Smoothness and Convexity

Relative smoothness of $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ relative to $\phi : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$?

- Let $\mathcal{F}(\mu) = \int V \mathrm{d}\mu$ and $\phi(\mu) = \int U \mathrm{d}\mu$:

$$V \ \beta\text{-smooth relative to } U \implies \mathcal{F} \ \beta\text{-smooth relative to } \phi$$
$$V \ \alpha\text{-convex relative to } U \implies \mathcal{F} \ \alpha\text{-convex relative to } \phi$$

- Let $\mathcal{F}(\mu) = \iint W(x-y) \ \mathrm{d}\mu(x)\mathrm{d}\mu(y)$ and $\phi(\mu) = \iint K(x-y) \ \mathrm{d}\mu(x)\mathrm{d}\mu(y)$:

$$W \ \beta\text{-smooth relative to } K \implies \mathcal{F} \ \beta\text{-smooth relative to } \phi$$
$$W \ \alpha\text{-convex relative to } K \implies \mathcal{F} \ \alpha\text{-convex relative to } \phi$$

- For $\mathcal{F} = \mathcal{G} + \mathcal{H}$, $\mathrm{d}_{\tilde{\mathcal{F}}_\mu} = \mathrm{d}_{\tilde{\mathcal{G}}_\mu} + \mathrm{d}_{\tilde{\mathcal{H}}_\mu}$ and $\mathcal{F}$ 1-convex relative to $\mathcal{G}$ and $\mathcal{H}$
- In general: look at the Hessian

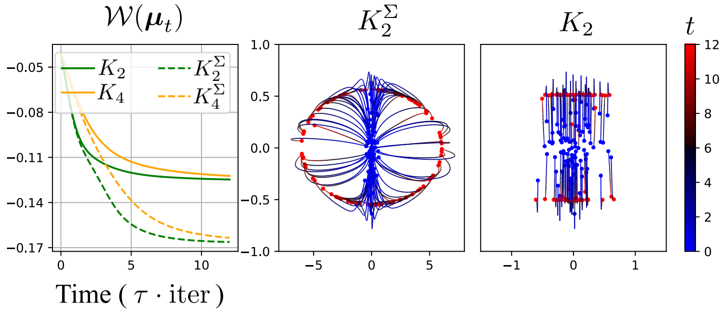
Mirror Descent on Interaction Energy

Goal: Let $\Sigma \in S_d^{++}(\mathbb{R})$ possibly ill-conditioned,

$$\min_{\mu} \ \mathcal{W}(\mu) = \iint W(x-y)\ \mathrm{d}\mu(x)\mathrm{d}\mu(y) \quad \text{with} \quad W(z) = \frac{1}{4}\|z\|_{\Sigma^{-1}}^4 - \frac{1}{2}\|z\|_{\Sigma^{-1}}^2$$

Bregman potential: $\phi_\mu(\mathrm{T}) = \iint K\big(\mathrm{T}(x) - \mathrm{T}(y)\big)\ \mathrm{d}\mu(x)\mathrm{d}\mu(y)$ with

$$K_2(z) = \frac{1}{2}\|z\|_2^2, \quad K_2^\Sigma(z) = \frac{1}{2}\|z\|_{\Sigma^{-1}}^2,$$
$$K_4(z) = \frac{1}{4}\|z\|_2^4 + \frac{1}{2}\|z\|_2^2, \quad K_4^\Sigma(z) = \frac{1}{4}\|z\|_{\Sigma^{-1}}^4 + \frac{1}{2}\|z\|_{\Sigma^{-1}}^2.$$



Mirror Descent on Gaussian

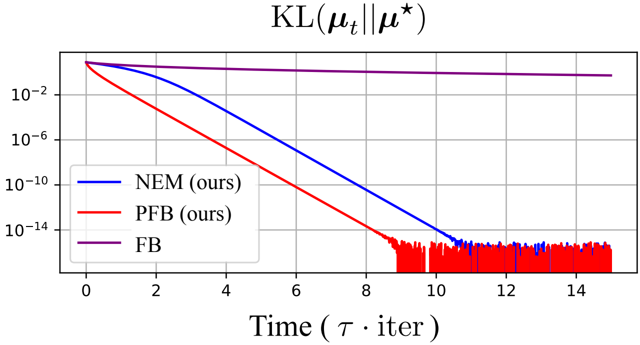
Goal:

$$\min_{\mu}\ \mathcal{F}(\mu) = \int V \mathrm{d}\mu + \mathcal{H}(\mu) \quad \text{with} \quad V(x) = \frac{1}{2} x^T \Sigma^{-1} x$$

$\rightarrow$ minimum $\mu^\star = \mathcal{N}(0, \Sigma)$.

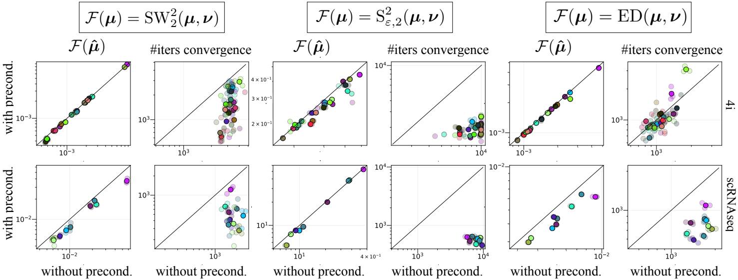
Comparison between:

- Forward-Backward (FB) on the Bures-Wasserstein space (Diao et al., 2023)
- Preconditioned Forward-Backward (PFB) scheme with $\phi(\mu) = \int V \mathrm{d}\mu$
- NEM: MD with $\phi(\mu) = \mathcal{H}(\mu)$ and restriction to Gaussian



Preconditioned GD on Single-Cells

Goal: $\min_\mu \ \mathcal{F}(\mu) = D(\mu, \nu)$ with μ_0 untreated cell and ν perturbed cell
Use PGD with $h^*(x) = (\|x\|_2^a + 1)^{1/a} - 1$ with $a \in \{1.25, 1.5, 1.75\}$, which is well suited to minimize functions growing in $\|x - x^*\|^{a/(a-1)}$ near x^*.



- Rows: 2 profiling technologies
- Columns/subcolumns: Different objectives $\mathcal{F}$/measure of convergence and number of iterations to converge
- Points: For treatment i, $z_i = (x_i, y_i)$ with x_i value of $\mathcal{F}(\hat{\mu}) = D(\hat{\mu}, \nu)$ (1st subcolumn) or number of iterations (2nd subcolumn) without preconditioning and y_i with preconditioning
- Colors: treatments

$\rightarrow$ **Points below the diagonal: PGD provides a better minimum or converges faster**

Conclusion

Conclusion:

- Mirror Descent on $\mathcal{P}_2(\mathbb{R}^d)$
- Preconditioned Gradient Descent on $\mathcal{P}_2(\mathbb{R}^d)$
- Convergence analysis of the discrete schemes
- Also in the paper: analysis of the Bregman Forward-Backward scheme

Perspectives:

- Better understand sufficient conditions of convergence for PGD
- Find more examples satisfying the conditions
- Analyze the Gaussian MD scheme

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Thank you for your attention!

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