Convex discretization of functionals involving the Monge-Ampère operator

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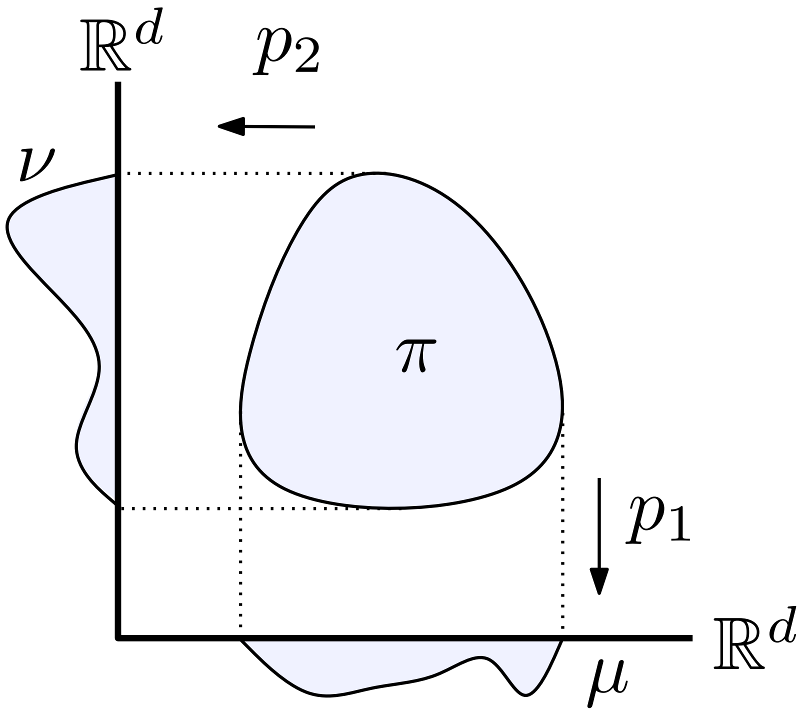
Joint work with J.D. Benamou, G. Carlier and É. Oudet

1. Motivation: Gradient flows in Wasserstein space

Background: Optimal transport

$\mathcal{P}_2(\mathbb{R}^d) = \{\mu \in \mathcal{P}(\mathbb{R}^d); \int \|x\|^2 \,\mathrm{d}\,\mu(x) < +\infty\}$

$\mathcal{P}_2^{\mathrm{ac}}(\mathbb{R}^d) = \mathcal{P}_2(\mathbb{R}^d) \cap \mathrm{L}^1(\mathbb{R}^d)$



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Definition: $\mathrm{W}_2^2(\mu, \nu) := \min_{\pi \in \Gamma(\mu,\nu)} \int \|x - y\|^2 \,\mathrm{d}\,\pi(x, y)$.

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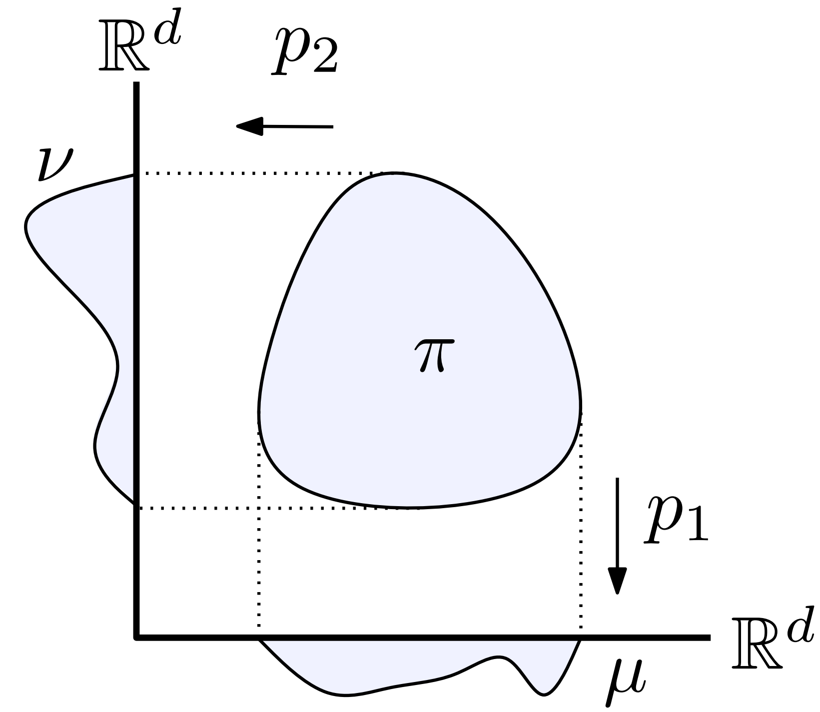

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- Relation to convex functions:

Def: $\mathcal{K} :=$ finite convex functions on $\mathbb{R}^d$

Theorem (Brenier): Given $\mu \in \mathcal{P}_2^{\mathrm{ac}}(\mathbb{R}^d)$ and $\nu \in \mathcal{P}_2(\mathbb{R}^d)$, [Brenier '91]
$\exists \phi \in \mathcal{K}$ such that $\nabla\phi_{\#}\mu = \nu$, and $\mathrm{W}_2^2(\mu,\nu) = \int_{\mathbb{R}^d} \|x - \nabla\phi(x)\|^2 \,\mathrm{d}\,\mu(x)$

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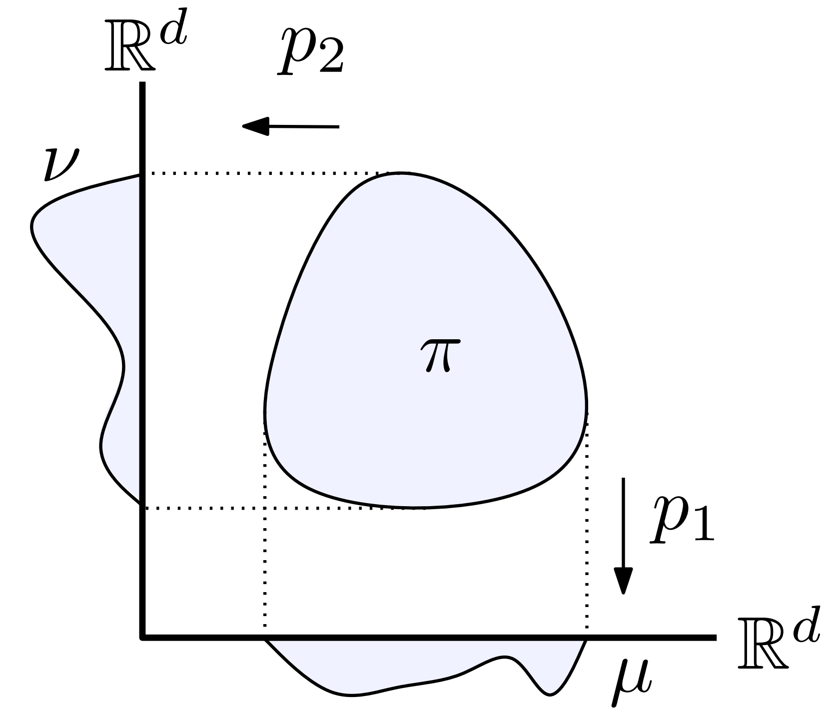

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Given any $\mu \in \mathcal{P}_2^{\mathrm{ac}}(\mathbb{R}^d)$, we get a "parameterization" of $\mathcal{P}_2(\mathbb{R}^d)$, or more precisely, an onto map $\mathcal{K} \mapsto \mathcal{P}_2(\mathbb{R}^d)$, $\phi \mapsto \nabla\phi_{\#}\mu$.

Gas equilibrium and displacement convexity

- Equilibrium states of gazes: $\min_{\nu\in\mathcal{P}_2(\mathbb{R}^d)} \mathcal{U}(\nu)+\mathcal{E}(\nu)$

$$\mathcal{U}(\nu) := \begin{cases} \int_{\mathbb{R}^d} U(\sigma(x))\,\mathrm{d}\,x \text{ if } \mathrm{d}\,\nu = \sigma\,\mathrm{d}\,\mathcal{H}^d \\ +\infty \text{ if not} \end{cases}$$

internal energy

ν = particle distribution

$$\mathcal{E}(\nu) := \int_{\mathbb{R}^d} V(x)\,\mathrm{d}\,\nu(x) + \int_{\mathbb{R}^d} W(x-y)\,\mathrm{d}[\nu\otimes\nu](x,y)$$

potential energy   interaction energy

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- Displacement convexity

Definition: $\mathcal{F}$ is displacement-convex if for any W_2-geodesic (ν_t) in $\mathcal{P}_2^{\mathrm{ac}}(\mathbb{R}^d)$, the function $t \mapsto \mathcal{F}(\nu_t)$ is convex.

Theorem: $V, W : \mathbb{R}^d \to \mathbb{R}$ are convex functions $\Longrightarrow$ $\mathcal{E}$ is displacement-convex

$r^d U(r^{-d})$ is convex non-increasing, $U(0) = 0 \Longrightarrow \mathcal{U}$ is displacement-convex

$\longrightarrow$ strict convexity $\Longrightarrow$ uniqueness of minimum

[McCann '94]

Convexity under generalized displacements

- Generalized displacement convexity

Definition: $\mathcal{F}$ is convex under generalized displacement (u.g.d.) if for any μ in $\mathcal{P}_2^{\mathrm{ac}}(\mathbb{R}^d)$, the function $\phi \in \mathcal{H} \mapsto \mathcal{F}(\nabla\phi_{\#}\mu)$ is convex.

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- **Proof:** Non-smooth change of variable formula:

$$\mathcal{E}(\nabla\phi_{\#}\rho) = \int V(\nabla\phi(x))\rho(x)\,\mathrm{d}\,x + \int W(\nabla\phi(x) - \nabla\phi(z))\rho(z)\rho(y)\,\mathrm{d}\,x\,\mathrm{d}\,y$$

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$$\mathcal{U}(\nabla\phi_{\#}\rho) = \int U\left(\frac{\rho(x)}{\mathrm{MA}[\phi](x)}\right)\mathrm{MA}[\phi](x)\,\mathrm{d}\,x$$

$$\mathrm{MA}[\phi](x) := \det(\mathrm{D}^2\phi(x))$$

Minkowski determinant inequality: $A \in \mathrm{SDP}(\mathbb{R}^d) \to \det(A)^{1/d}$ is concave

Heat equation as a Wasserstein gradient flow

Heat equation $$\boxed{\frac{\partial \rho}{\partial t} = \Delta \rho \qquad \rho(0,.) = \rho_0} \qquad \rho(t,.) \in \mathcal{P}^{\mathrm{ac}}(\mathbb{R}^d)$$

- Solution $\rho(t,.) =$ gradient flow in $\mathrm{L}^2(\mathbb{R}^d)$ of $\mathcal{D}(\rho) := \frac{1}{2} \int \|\nabla \rho(x)\|^2 \,\mathrm{d}\, x$.

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$$\rho^\tau_{k+1} = \arg\min_{\sigma \in \mathcal{P}^{\mathrm{ac}}(\mathbb{R}^d)} \frac{1}{2\tau} \|\rho^\tau_k - \sigma\|^2_{\mathrm{L}^2(\mathbb{R}^d)} + \mathcal{D}(\sigma).$$

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- Convergence analysis for the linear Fokker-Planck equation.

[Jordan, Kinderlehrer, Otto '99]

Diffusive PDEs as Wasserstein gradient flows

- Generalization to some evolution PDEs, where $\rho(t,.) \in \mathcal{P}^{\mathrm{ac}}(\mathbb{R}^d)$

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- Many applications: porous medium equation, cell movement via chemotaxis, crowd motion with congestion, models of cities in economy, etc.

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- Plan of the talk:

  Part 2: Convex discretization of the problem $(*_Y)$ under McCann's hypotheses.

  Part 3: Γ-convergence results from the discrete problem to the continuous one.

  Part 4: Numerical simulations: non-linear diffusion, crowd motion.

2. Convex discretization of a JKO step

Prior work: functionals involving the gradient

$$\min_{\phi \in \mathcal{K}} \int_X F(\phi(x), \nabla\phi(x)) \,\mathrm{d}\,\mu(x)$$

$\mathcal{K} :=$ finite convex functions on $\mathbb{R}^d$

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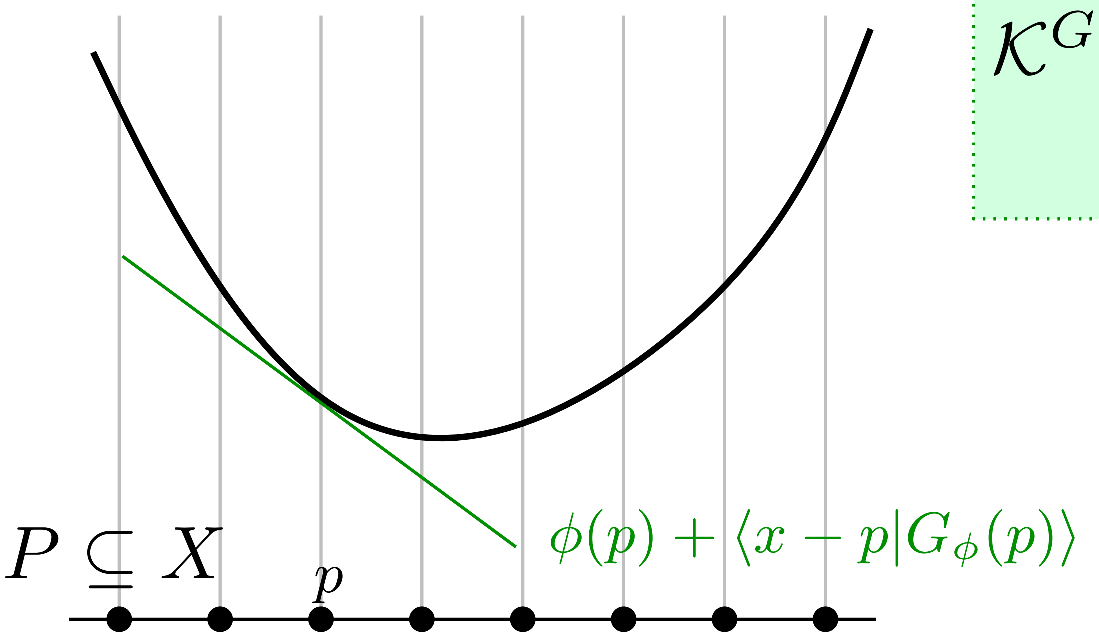

$\mathcal{K}^G(P) := \{(\phi, G_\phi) : P \to \mathbb{R} \times \mathbb{R}^d$ such that $\forall p, q \in P,\ \phi(q) \geq \phi(p) + \langle q - p | G_\phi(p) \rangle\}$

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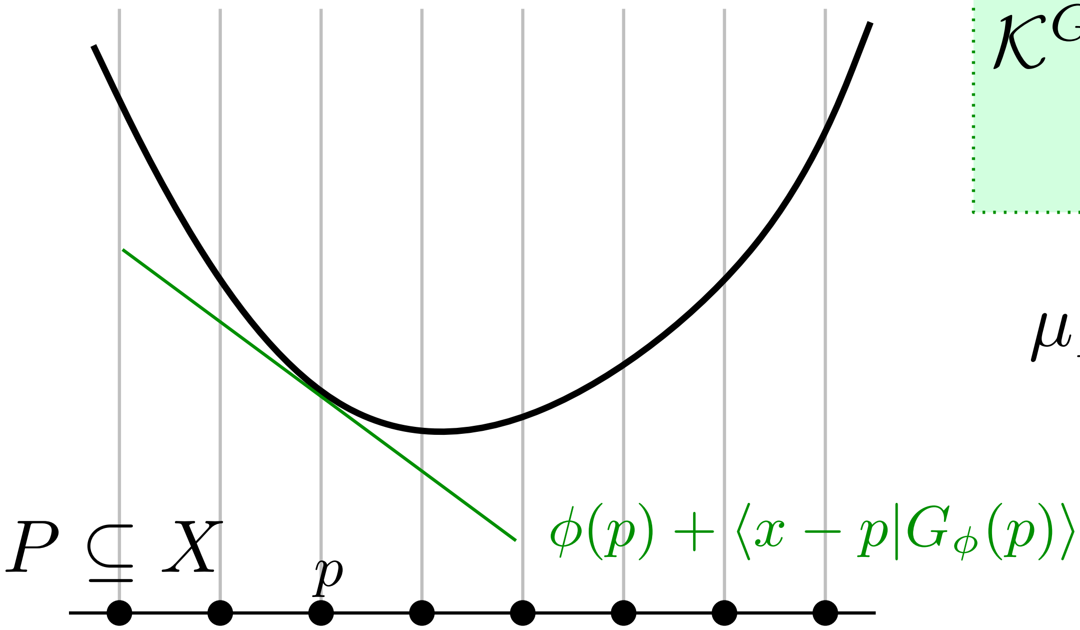

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$\mu_P := \sum_{p \in P} \mu_p \delta_p$, discretization of the measure μ

$$\min_{\phi \in \mathcal{K}^G(P)} \sum_{p \in P} F(\phi(p), G_\phi(p))\mu_p$$

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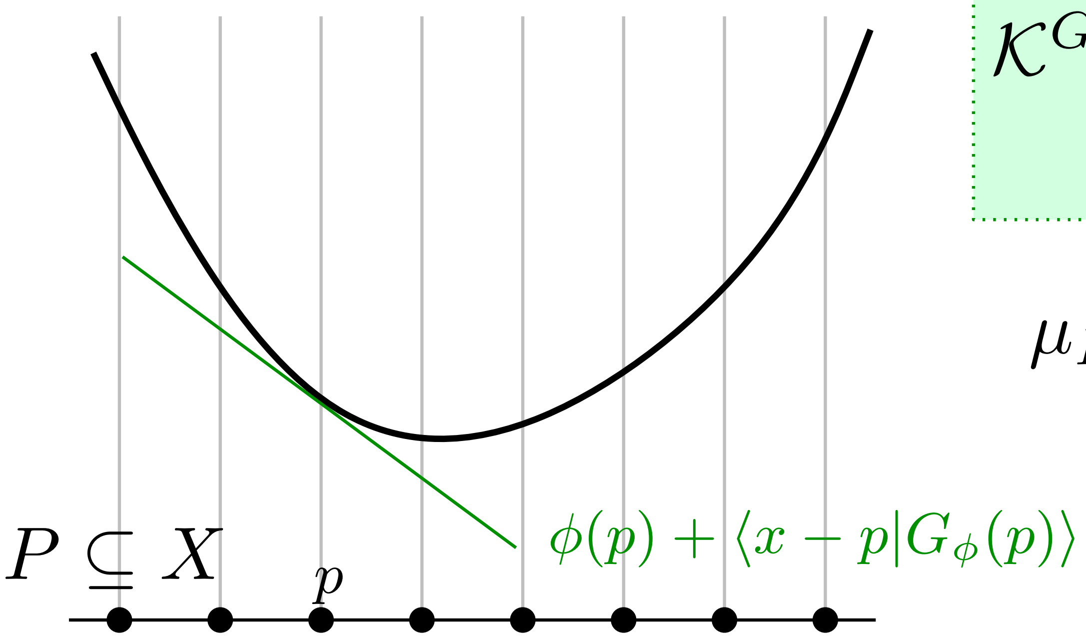

$\mathcal{K}^G(P) := \{(\phi, G_\phi) : P \to \mathbb{R}\times\mathbb{R}^d$ such that $\forall p, q \in P,\ \phi(q) \geq \phi(p) + \langle q - p | G_\phi(p)\rangle\}$

$\mu_P := \sum_{p\in P} \mu_p \delta_p$, discretization of the measure μ

$$\min_{\phi\in\mathcal{K}^G(P)} \sum_{p\in P} F(\phi(p), G_\phi(p))\mu_p$$

$|P|^2$ linear constraints $\longrightarrow$ adaptive method [Mirebeau '14]

$\longrightarrow$ exterior parameterization [Oberman '14][Oudet-M. '14]

Convex functions with constrained gradient

- Let X, Y be bounded convex domains, and $\mu \in \mathcal{P}^{\mathrm{ac}}(X)$ with density ρ,

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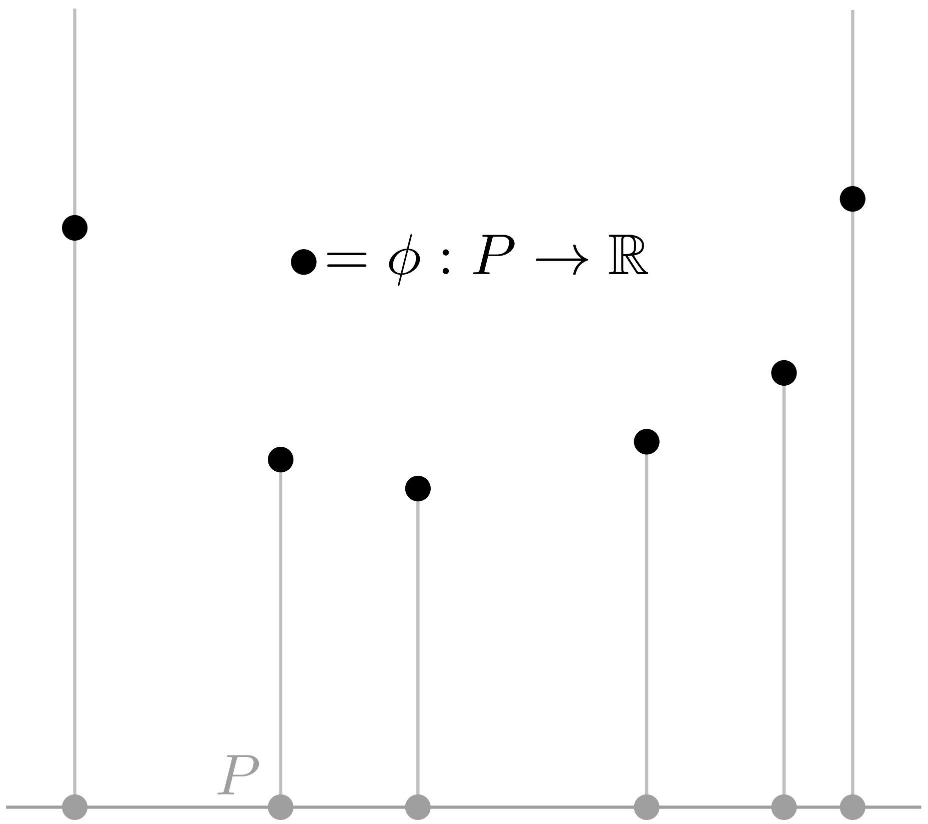
$\longrightarrow$ finite-dimensional polyhedron



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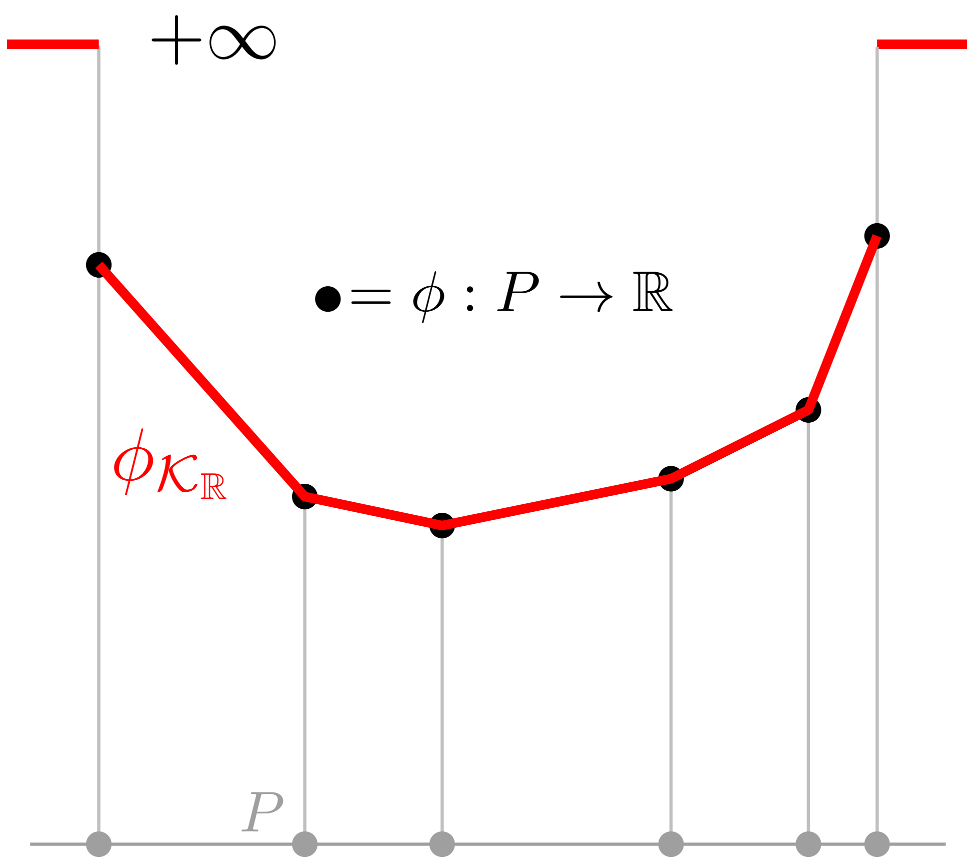

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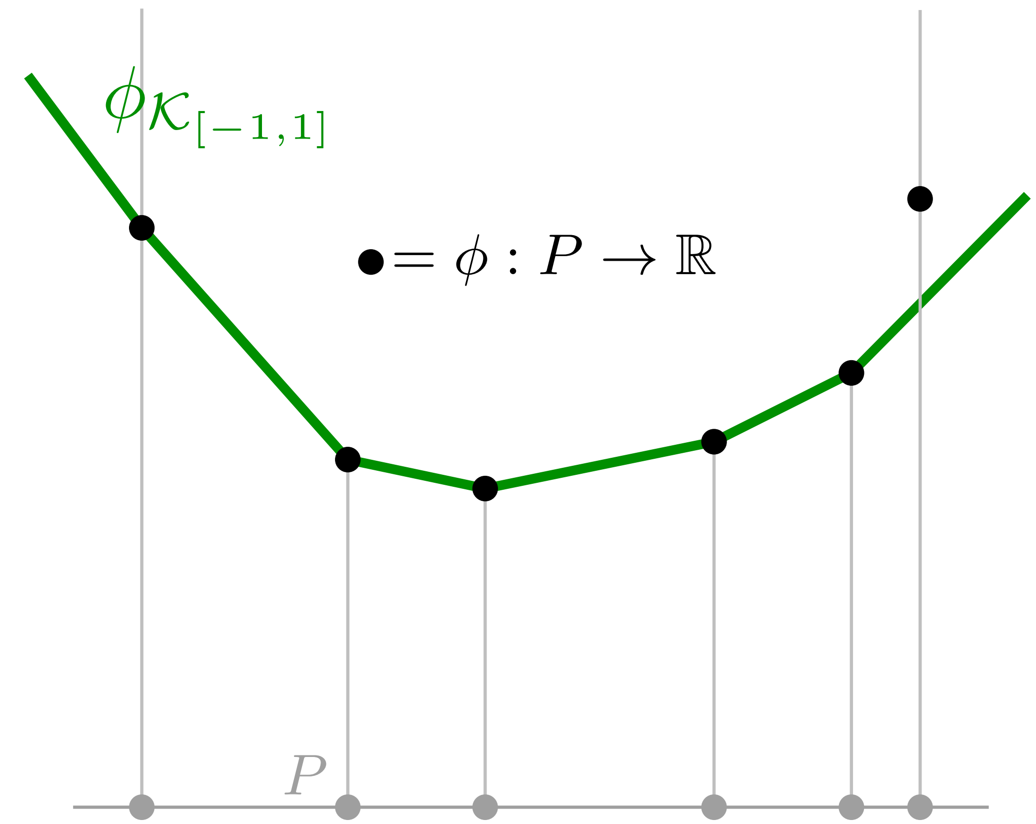

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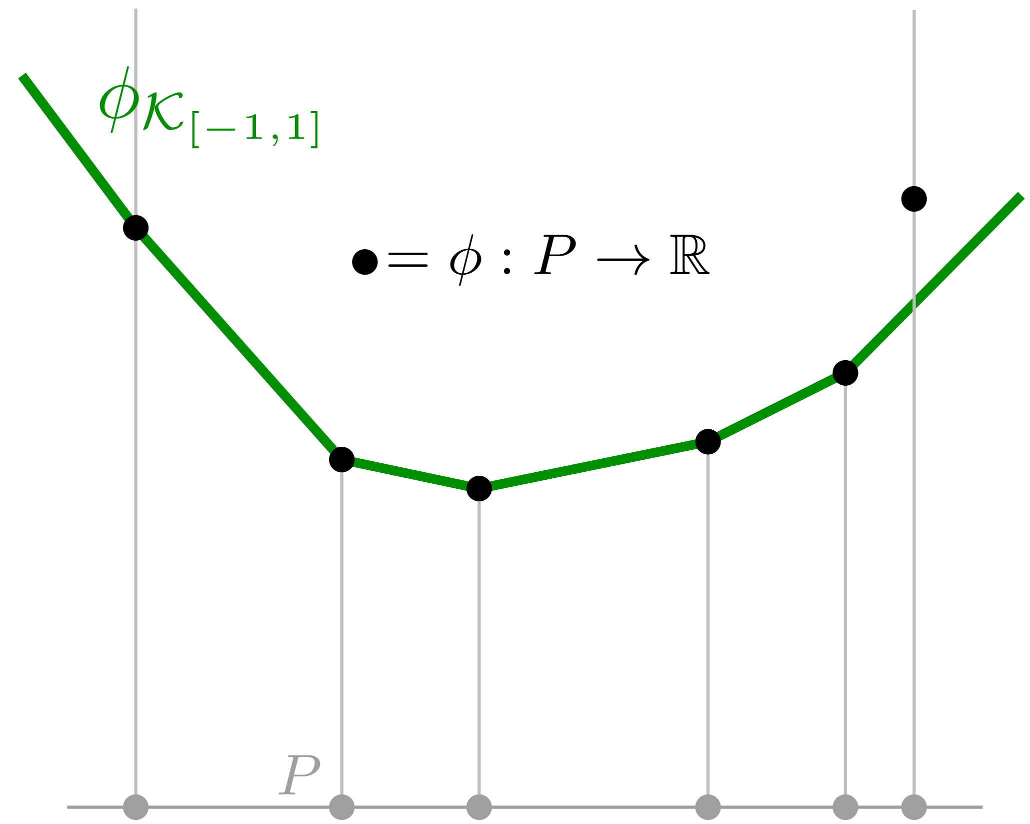

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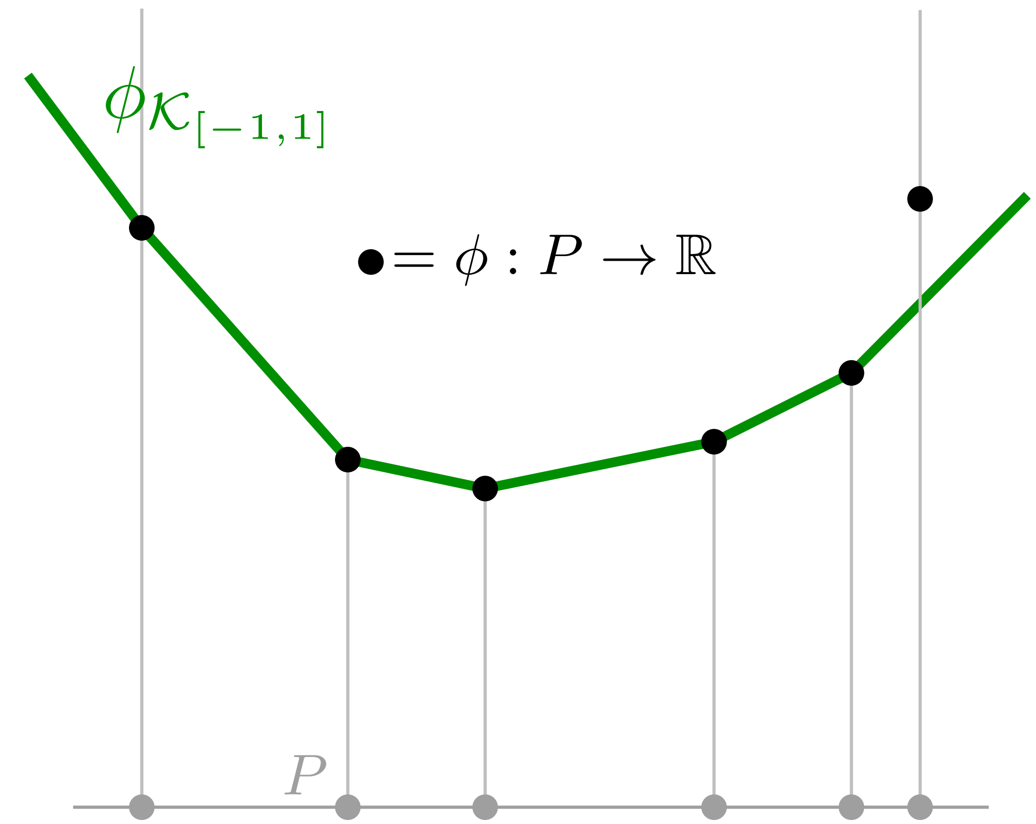

$$\min_{\phi\in\mathcal{K}_Y(P)} \frac{1}{2\tau}\mathrm{W}_2^2(\mu_P, "\nabla\phi_{\mathcal{K}_Y\#}\mu_P") + \mathcal{U}("\nabla\phi_{\mathcal{K}_Y\#}\mu_P") + \mathcal{E}("\nabla\phi_{\mathcal{K}_Y\#}\mu_P")$$

Absolutely continuous pushforward by $\partial\phi_{\mathcal{K}_Y}$

- Given $\phi \in \mathcal{K}_Y(P)$, the function $\psi = \phi_{\mathcal{K}_Y}$ is usually non-smooth at $p \in P$
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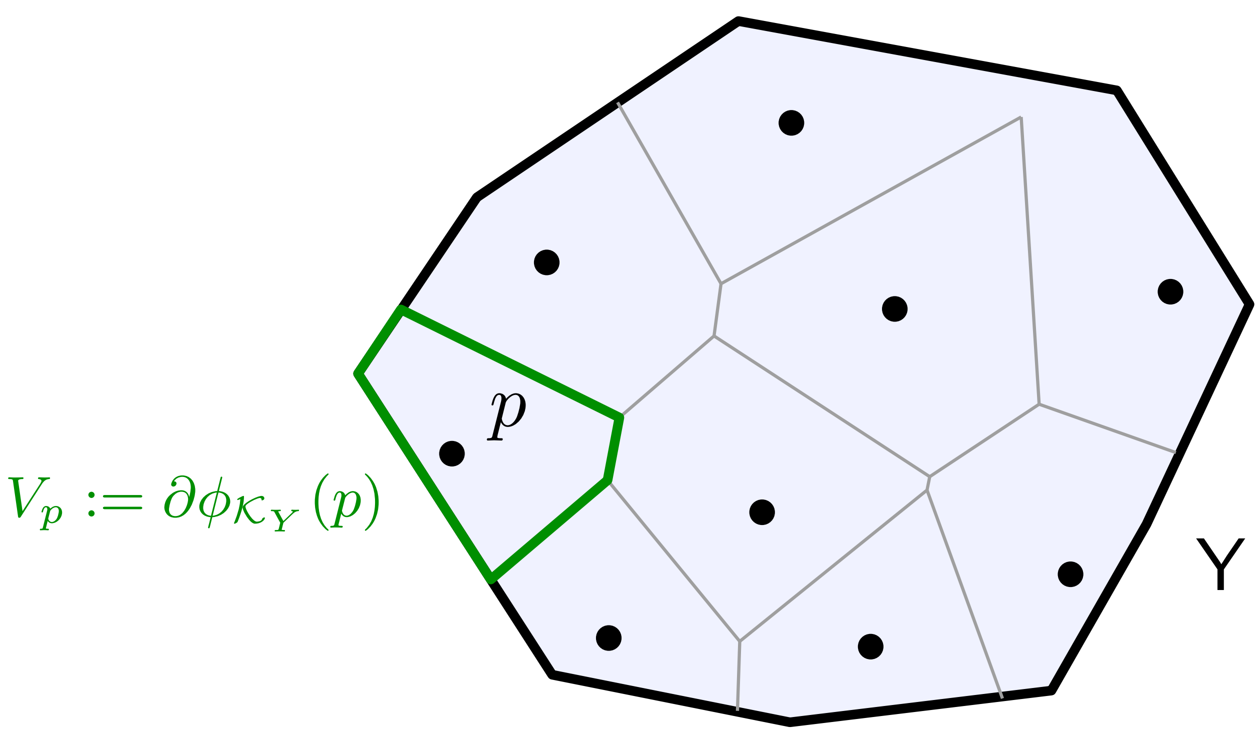

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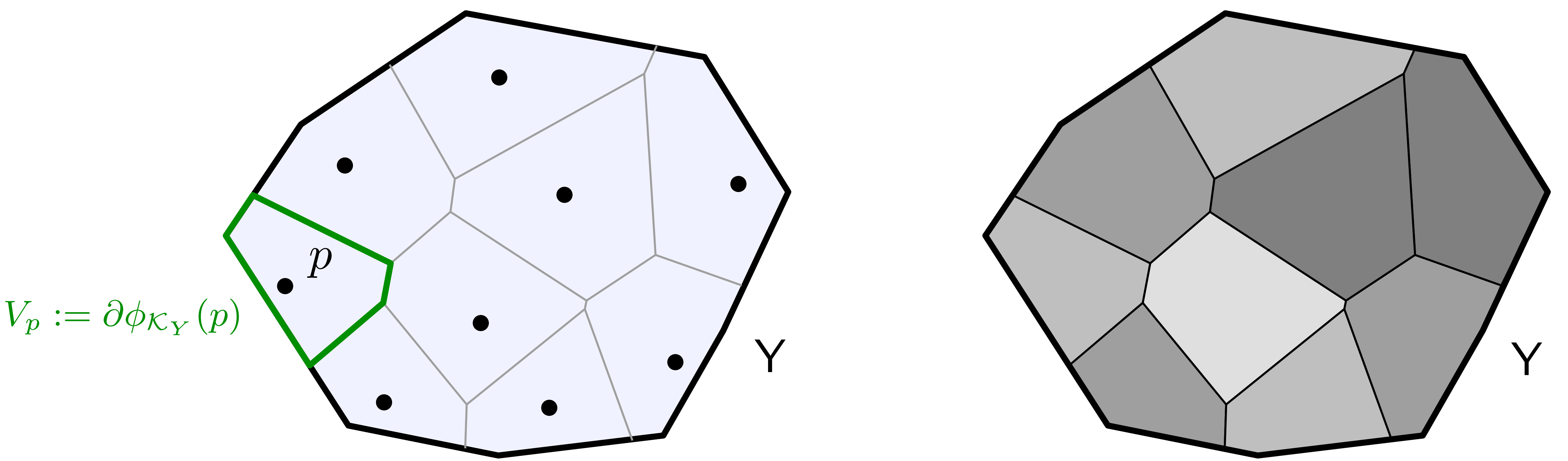
Definition: For $\phi \in \mathcal{K}_Y(P)$ and $\mu_P = \sum_{p \in P} \mu_p \delta_p$, we let $V_p := \partial\phi_{\mathcal{K}_Y}(p)$ and define $G^{\mathrm{ac}}_{\phi\#}\mu_P$ as the probability measure on Y whose density σ satisfies:

(i) σ is constant on the subdifferentials $\{V_p\}_{p \in P}$;

(ii) for $p \in P$, $\int_{V_p} \sigma(x) \,\mathrm{d}\, x = \mu_p$.

Explicit formula: $\sigma = \sum_{p \in P} \frac{\mu_p}{\mathcal{H}^d(V_p)} \mathbf{1}_{V_p}$

piecewise-constant density σ of $G^{\mathrm{ac}}_{\phi\#}\mu_P$



Convex discretization of the internal energy

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$$\mathcal{U}(G^{\mathrm{ac}}_{\phi\#}\mu_P) = \sum_{p\in P} U\left(\mu_p/\mathrm{MA}_Y[\phi](p)\right)\mathrm{MA}_Y[\phi](p)$$

NB: similarity with $\mathcal{U}(\nabla\phi_{\#}\rho) = \int U\left(\frac{\rho(x)}{\mathrm{MA}[\phi](x)}\right)\mathrm{MA}[\phi](x)\,\mathrm{d}\,x$

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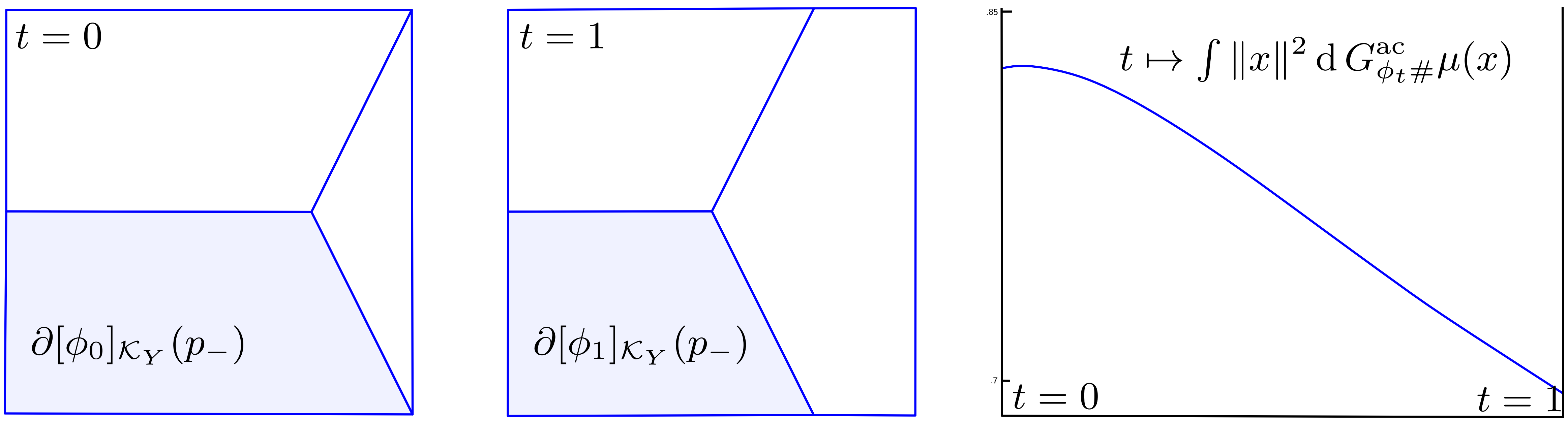
Convex discretization of the potential energy

- **Difficulty:** Lack of convexity of $\phi \in \mathcal{K}_Y(P) \mapsto \mathcal{E}(G^{\mathrm{ac}}_{\phi\#}\mu_P)$.



E.g. $P = \{p_\pm, q\}, p_\pm = (0, \pm 1), q = (2, 0))$, $Y = [-1, 1]^2$, $\phi_t = (1-t)\mathbf{1}_q$, $\mu_P = 0.1(\delta_{p_+} + \delta_{p_-}) + 0.8\delta_q$.

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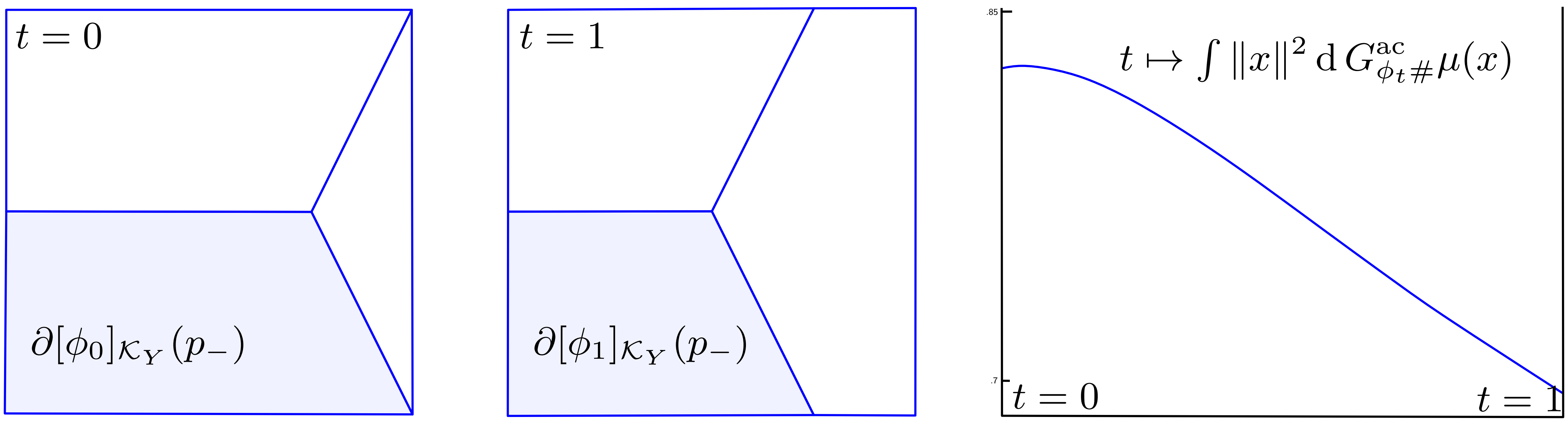

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- We follow Ekeland-Moreno '10, and include the gradient as an unknown:

Def: $\mathcal{K}^G_Y(P) = \{(\phi, G_\phi) : P \to \mathbb{R} \times \mathbb{R}^d; \phi \in \mathcal{K}_Y(P),\ \forall p, G_\phi(p) \in \partial\phi_{\mathcal{K}_Y}(p)\}$.

Def: Given $(\phi, G_\phi) \in \mathcal{K}^G_Y(P)$, we define $G_{\phi\#}\mu_P = \sum_{p \in P} \mu_p \delta_{G_\phi(p)}$.

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Summary of the convex discretization

Theorem: Assume that $V, W : \mathbb{R}^d \to \mathbb{R}$ are convex functions and $r^d U(r^{-d})$ is convex non-increasing, $U(0) = 0$.

Then, the following optimization problem is convex:

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The minimum is unique if e.g. V and $r^d U(r^{-d})$ are strictly convex.

[Carlier-Benamou-M.-Oudet]

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- Generalization to non-negatively cross-curved cost functions [Figalli-Kim-McCann]

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NB: $|P|$ non-linear constraints vs $|P|^2$ linear constraints

- Generalization to non-negatively cross-curved cost functions [Figalli-Kim-McCann]
- Other convex discretization using wide-stencils. Convergence is unclear.

3. A Γ-convergence result

Convergence theorem

JKO step: X, Y bounded and convex, $\mu \in \mathcal{P}^{\mathrm{ac}}(X)$ with density $c^{-1} \leq \rho \leq c$

$$(*) \quad \min_{\nu \in \mathcal{P}(Y)} \frac{1}{2\tau} \mathrm{W}_2^2(\mu, \nu) + \mathcal{E}(\nu) + \mathcal{U}(\nu)$$

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example: $U(r) = r \log r$, $U(r) = r^m/(m-1)$ with $m > 0$.

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Theorem: Let $P_n \subseteq X$ finite, $\mu_n \in \mathcal{P}(P_n)$ with $\lim \mathrm{W}_2(\mu_n, \mu) = 0$, and:

$$(*)_n \quad \min_{\phi \in \mathcal{K}_Y^G(P_n)} \frac{1}{2\tau} \mathrm{W}_2(\mu_n, G_{\phi\#}\mu_n) + \mathcal{E}(G_{\phi\#}\mu_n) + \mathcal{U}(G_{\phi\#}^{\mathrm{ac}}\mu_n)$$

If ϕ_n minimizes $(*)_n$, then $\nu_n := G_{\phi_n\#}^{\mathrm{ac}}\mu_n$ is a minimizing sequence for $(*)$.

[Carlier-Benamou-M.-Oudet]

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Proof of the convergence theorem: Lower bound

JKO step: X, Y bounded and convex, $\mu \in \mathcal{P}^{\mathrm{ac}}(X)$ with density $c^{-1} \leq \rho \leq c$

Let $m := \min_{\sigma \in \mathcal{P}(Y)} \mathcal{F}(\sigma)$ $\qquad \mathcal{F}(\sigma) := \mathrm{W}_2^2(\mu, \sigma) + \mathcal{E}(\sigma) + \mathcal{U}(\sigma)$

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Using **(C2)** and a convolution argument

$\Longleftarrow$ Given any probability density $\sigma \in \mathcal{C}^0(Y)$ with $\varepsilon < \sigma < \varepsilon^{-1}$, $\exists \phi_n \in \mathcal{K}_Y(P_n)$ s.t. $\lim_{n \to \infty} \|\sigma - \sigma_n\|_{\mathrm{L}^\infty(Y)} = 0$, where $\sigma_n := \frac{\mathrm{d}\, G^{\mathrm{ac}}_{\phi \#}\mu_n}{\mathrm{d}\, \mathcal{H}^d}$.

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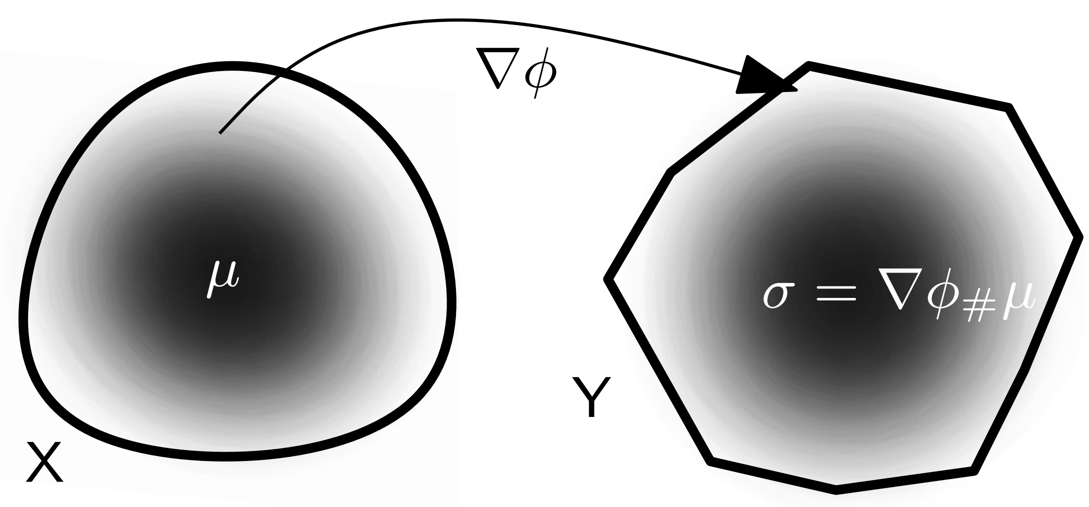

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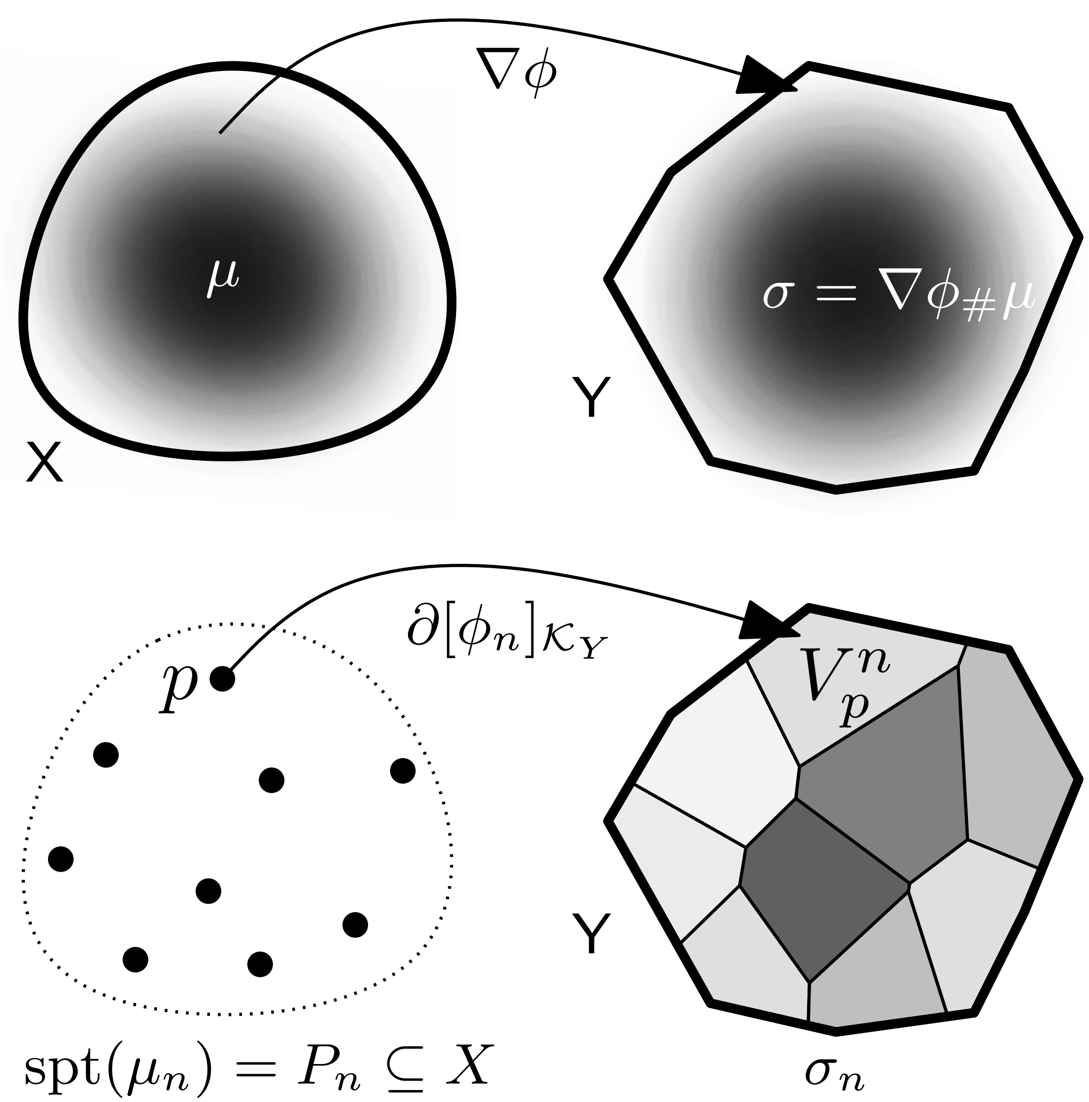

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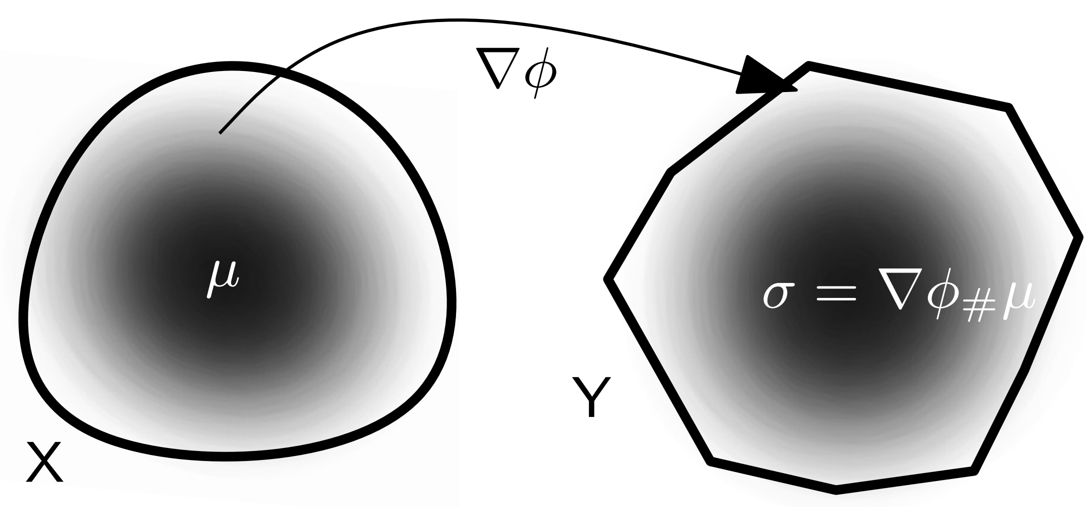

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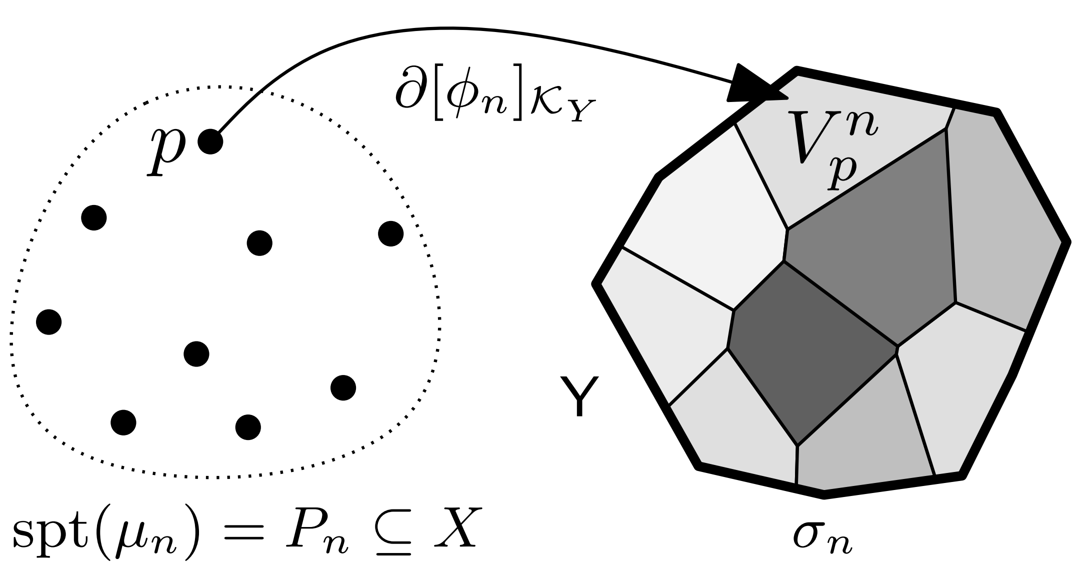

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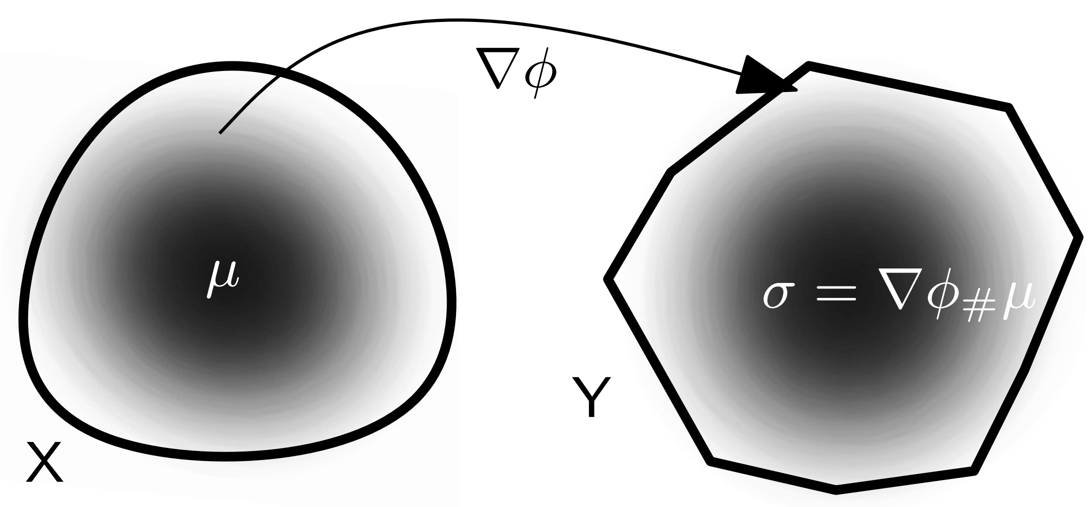

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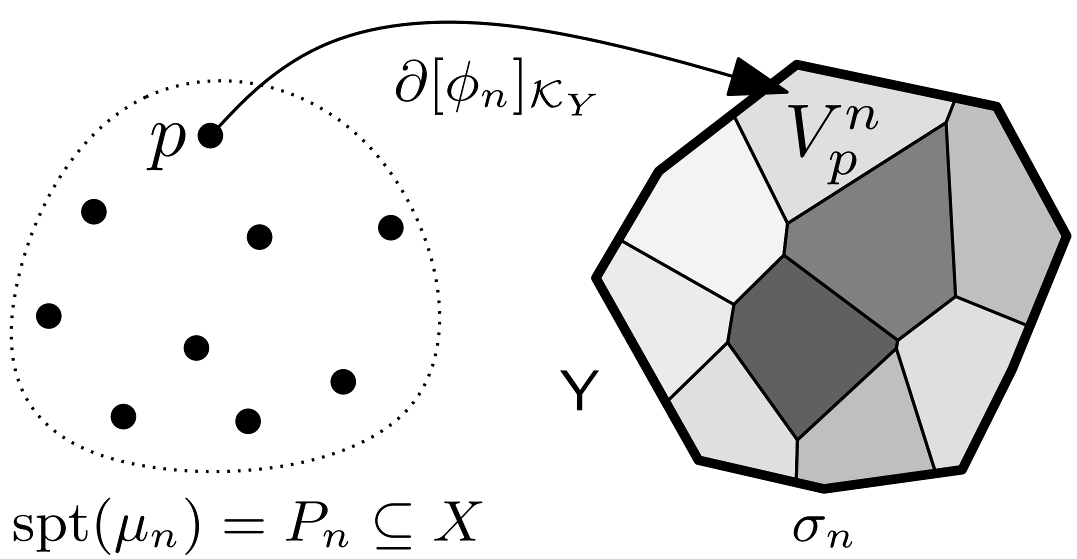

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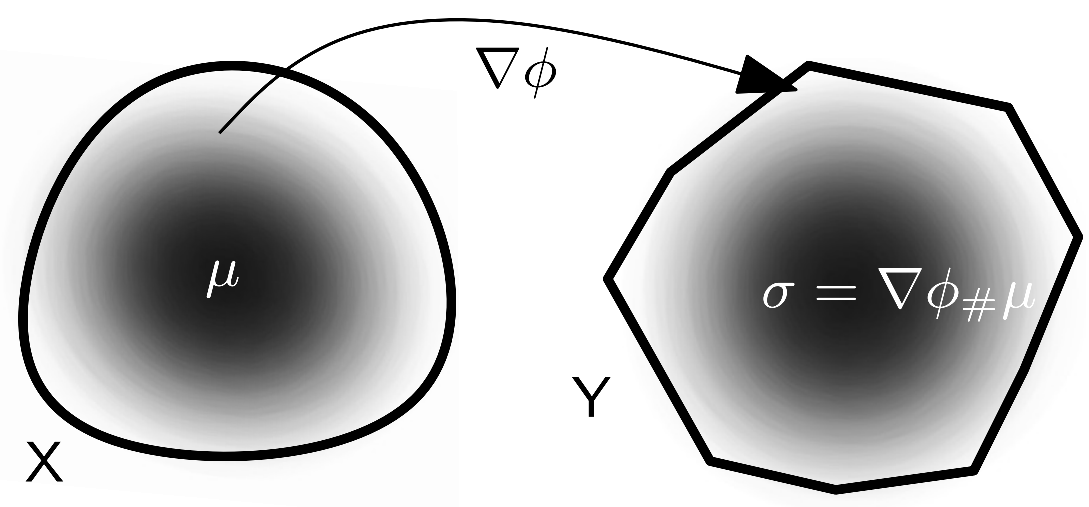

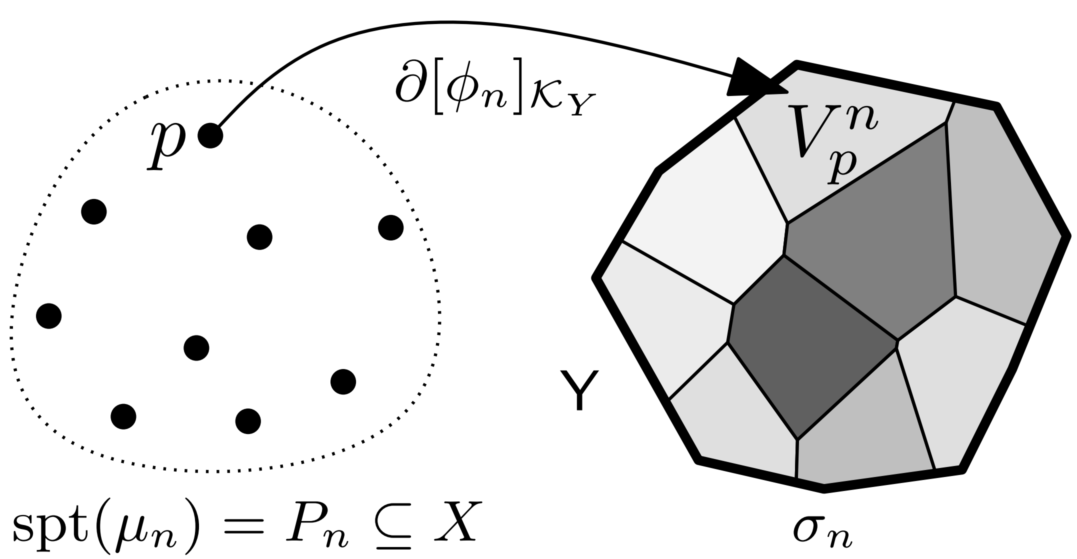

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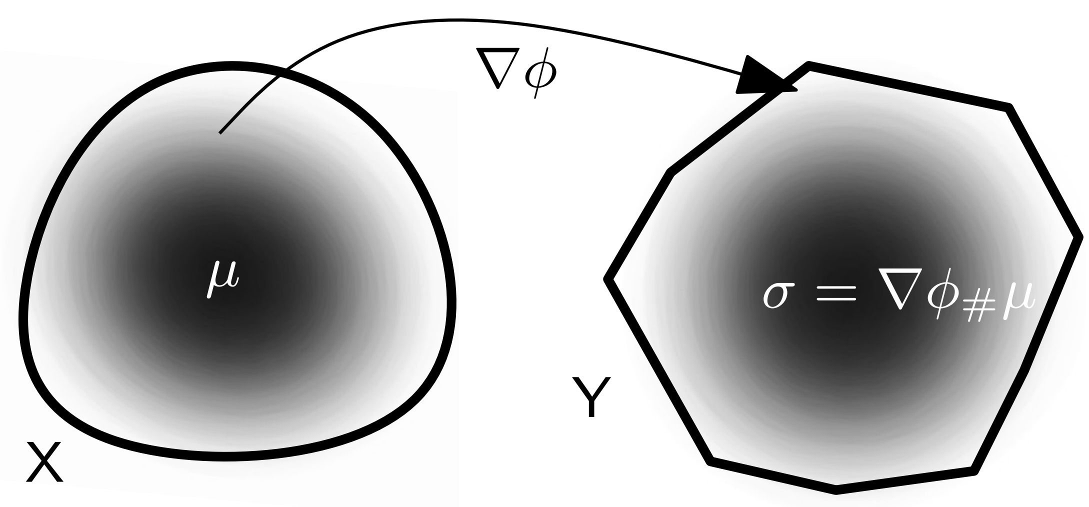

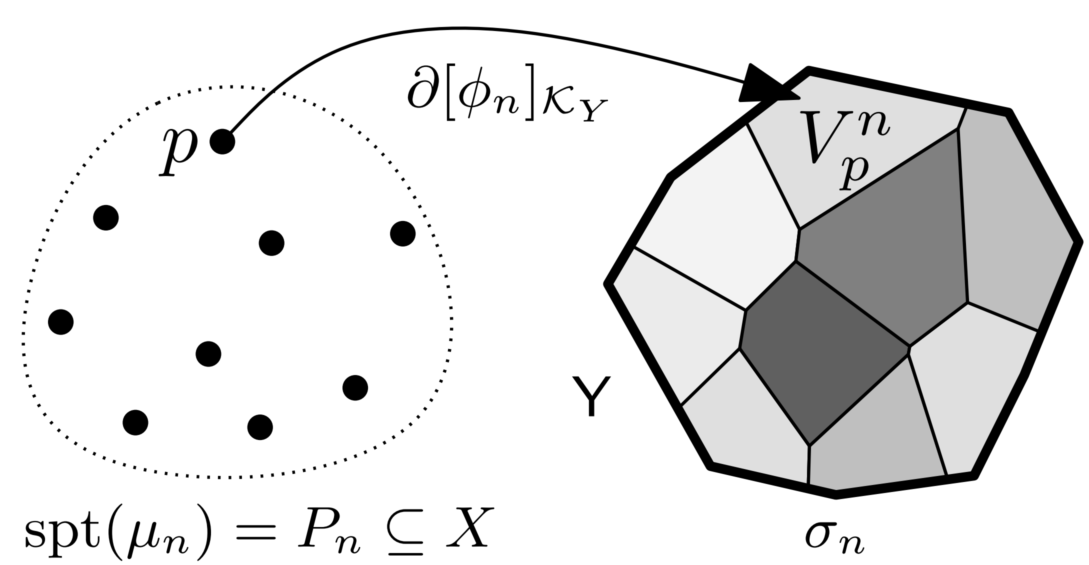

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(d) Moreover, $\nabla\phi_{\#}\rho = \sigma$. By Caffarelli's regularity theorem, $\phi \in \mathcal{C}^1$: Contradiction of (2).

4. Numerical results

Computing the discrete Monge-Ampère operator

$$\mathcal{U}(G^{\mathrm{ac}}_{\phi\#}\mu_P) = \sum_{p\in P} U\left(\mu_p/\mathrm{MA}_Y[\phi](p)\right)\mathrm{MA}_Y[\phi](p)$$

with $\mathrm{MA}_Y[\phi](p) := \mathcal{H}^d(\partial\phi_{\mathcal{K}_Y}(p)).$

- **Goal:** fast computation of $\mathrm{MA}_Y[\phi](p)$ and its 1st/2nd derivatives w.r.t ϕ

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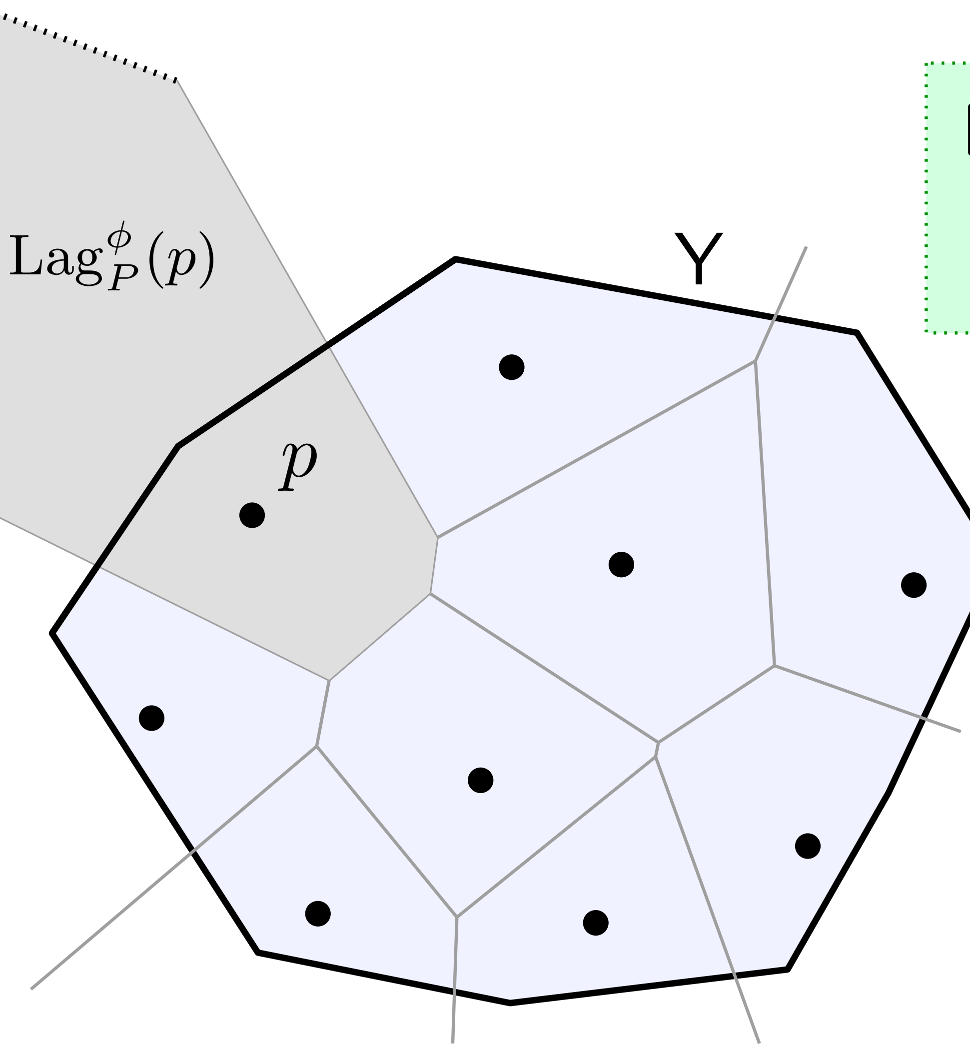
- We rely on the notion of **Laguerre (or power) cell** in computational geometry



Definition: Given a function $\phi : P \to \mathbb{R}$,

$$\mathrm{Lag}^{\phi}_{P}(p) := \{y \in \mathbb{R}^d; \forall q \in P, \phi(q) \geq \phi(p) + \langle q - p | y\rangle\}$$

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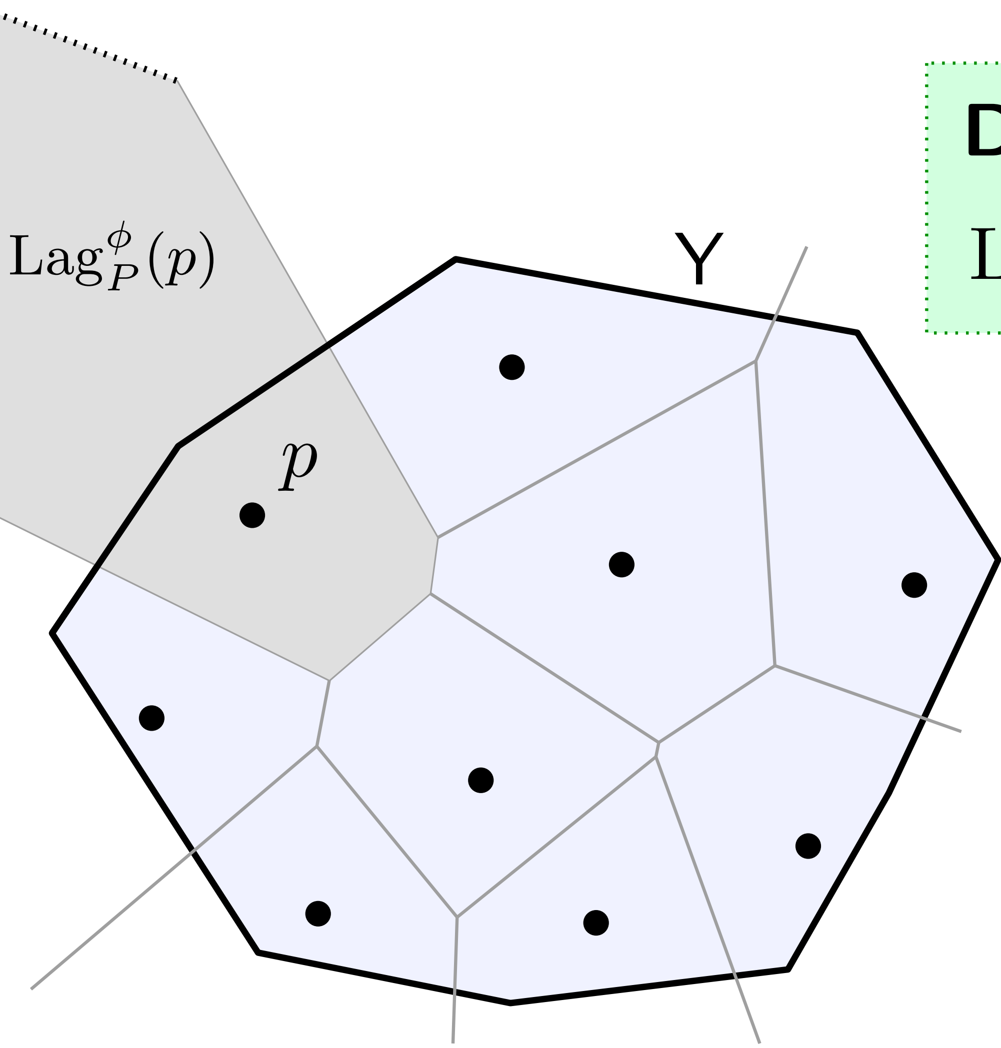

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$\longrightarrow$ Decomposition of $\mathbb{R}^d$ into convex polyhedra

$\longrightarrow$ For $\phi(p) = \|p\|^2/2$, one gets the Voronoi cell:

$$\mathrm{Lag}_P^\phi(p) := \{y; \forall q \in P, \|q-y\|^2 \geq \|p-y\|^2\}$$

$\longrightarrow$ Computation in time $O(|P|\log|P|)$ in 2D

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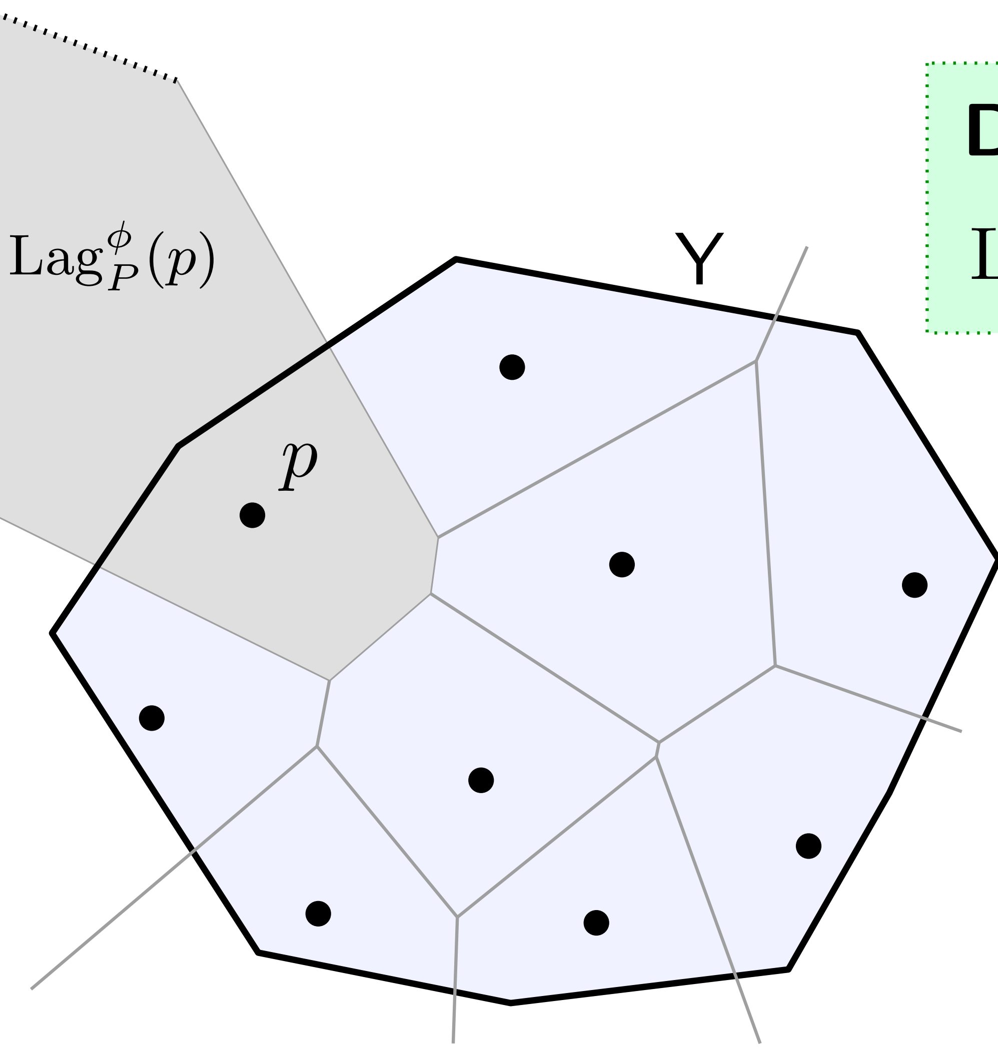

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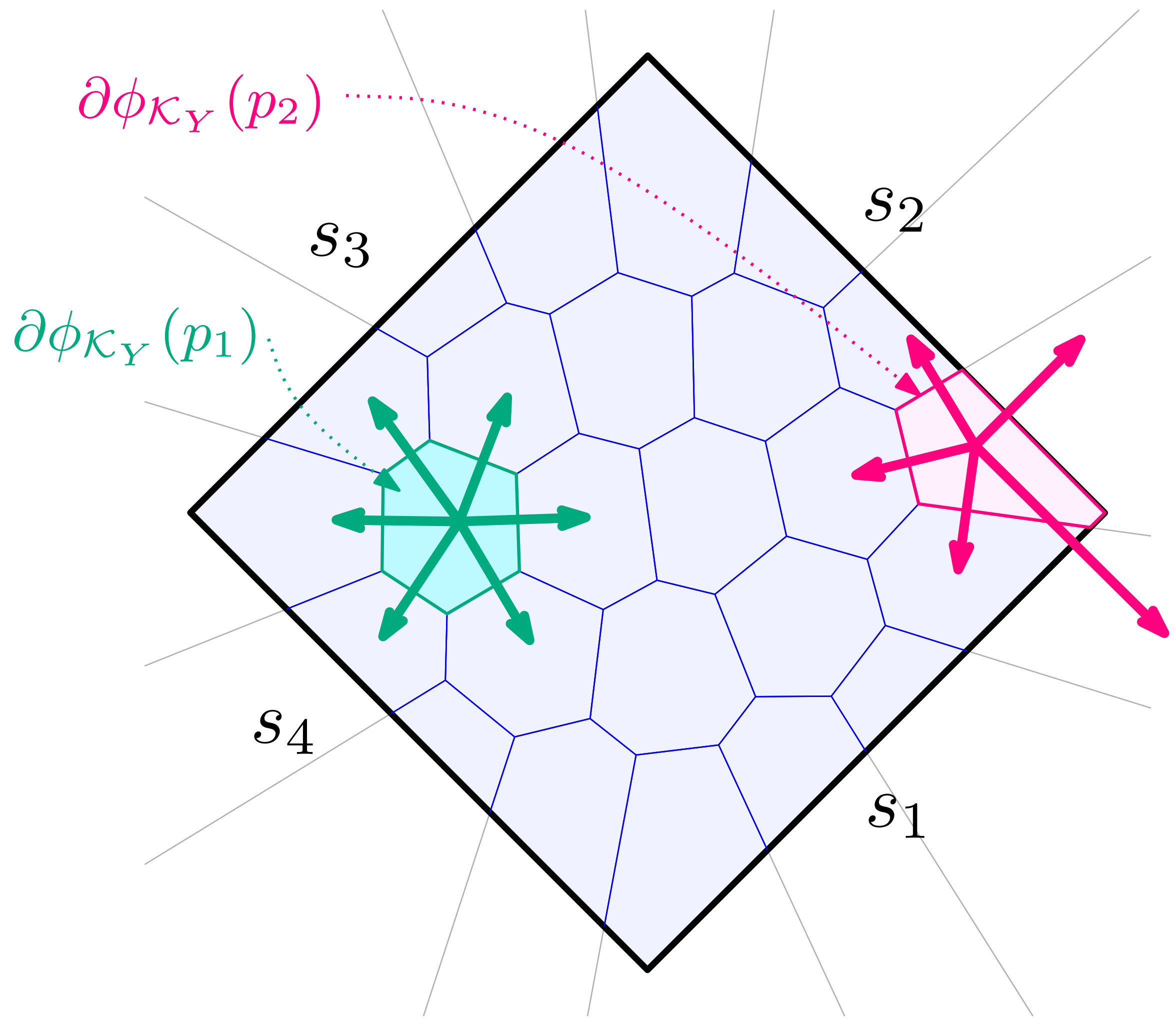
Lemma: For $\phi \in \mathcal{K}_Y(P)$ and $p \in P$, $\partial\phi_{\mathcal{K}_Y}(p) = \mathrm{Lag}^\phi_P(p) \cap Y$.

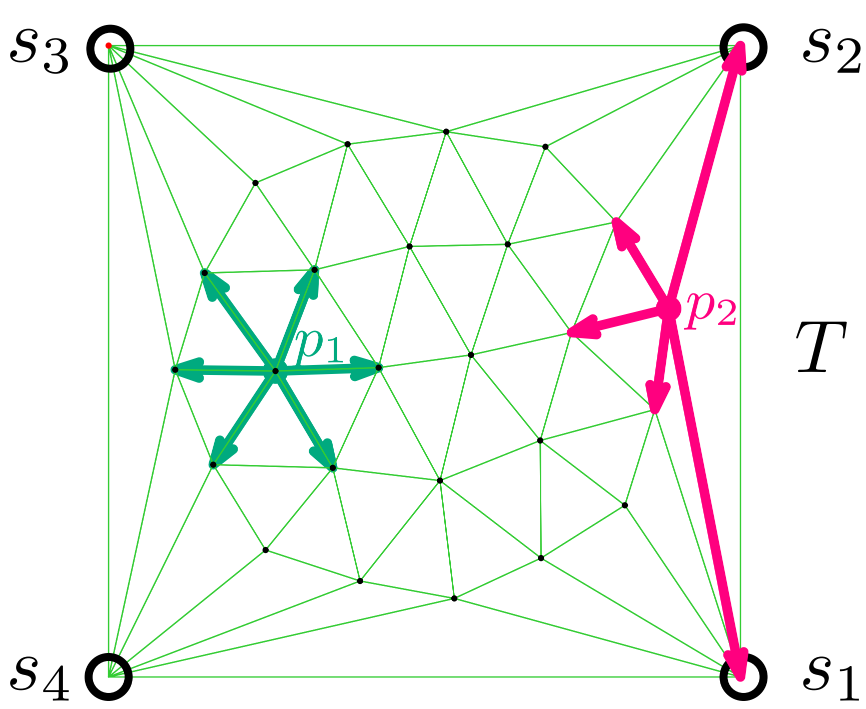
Computing the discrete Monge-Ampère operator

- Global construction of the intersections $(\mathrm{Lag}_P^\phi(p) \cap Y)_{p \in P}$ in 2D.



Assumption: $\partial Y = \cup_{s \in S} s$,

with S = finite family of segments.



- Combinatorics stored as an (abstract) triangulation T of the finite set $P \cup S$, i.e.

$(p_1, p_2, p_3) \in T$ iff $(\mathrm{Lag}_P^\phi(p_1) \cap \mathrm{Lag}_P^\phi(p_2) \cap \mathrm{Lag}_P^\phi(p_3)) \cap Y \neq \emptyset$

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Computation in time $O(|P| \log |P| + |S|)$ in 2D.

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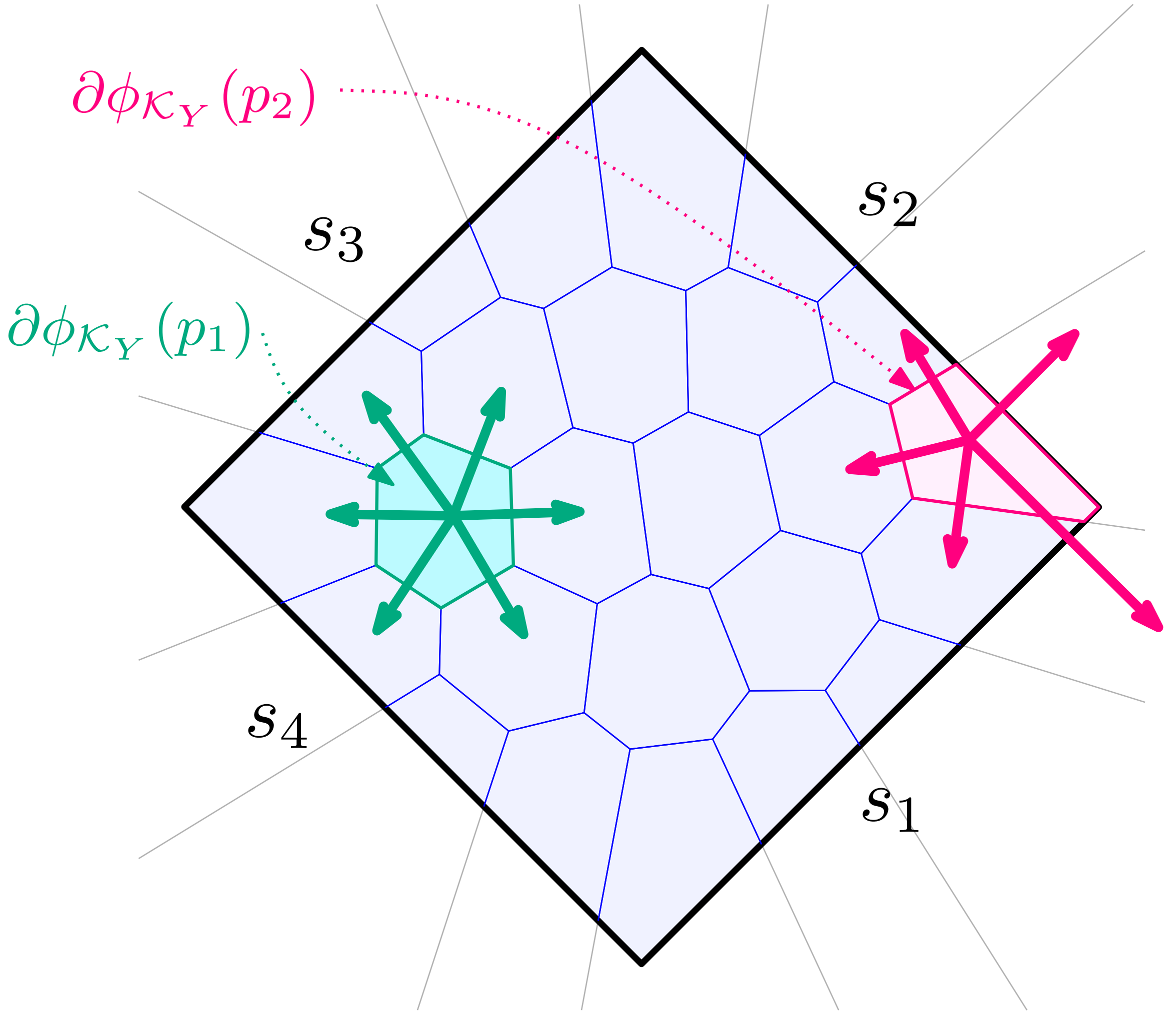

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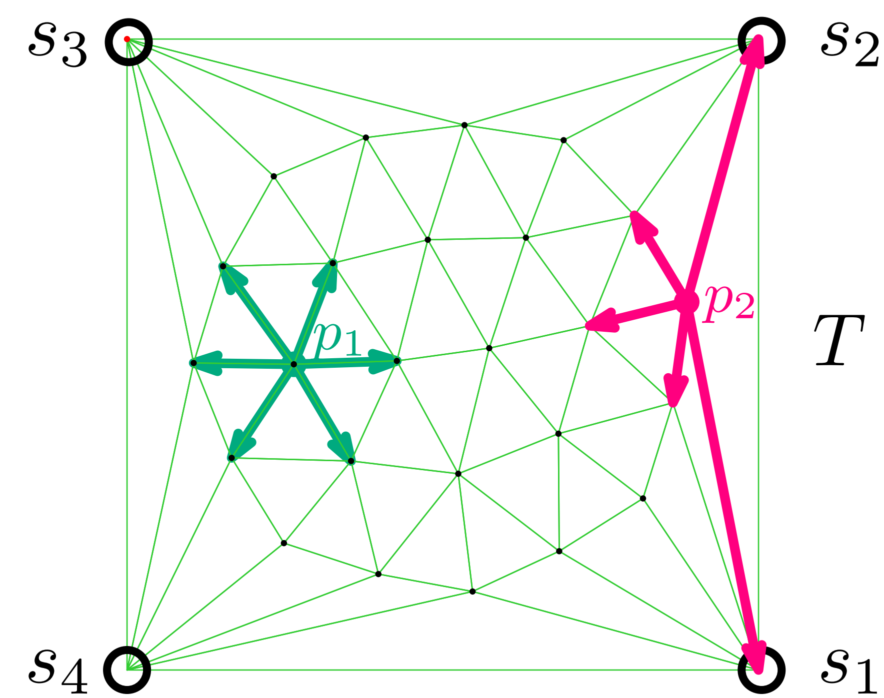

- Computation of $\mathrm{MA}_Y(p) = \mathcal{H}^2(\mathrm{Lag}^{\phi}_{P}(p) \cap Y)$ and its derivatives.

  The **sparsity structure** of the Jacobian/Hessian is encoded in T:

$$\frac{\partial \mathrm{MA}_Y(p)}{\partial \phi(q)} \neq 0 \Longrightarrow (p, q) \text{ is an edge of } T$$

$$\frac{\partial^2 \mathrm{MA}_Y(p)}{\partial \phi(r) \partial \phi(q)} \neq 0 \Longrightarrow (p, q, r) \text{ is a triangle of } T$$

Example 1: Nonlinear diffusion on point clouds

$$(*) \quad \begin{cases} \dfrac{\partial \rho}{\partial t} = \Delta \rho^m & \text{on } X \\ \nabla \rho \perp \mathbf{n}_X & \text{on } \partial X \end{cases}$$

fast diffusion equation: $m \in [1 - 1/d, 1)$

porous medium equation: $m > 1$

Gradient flow in $(\mathcal{P}(X), \mathrm{W}_2)$. for $\mathcal{U}(\rho) = \int U(\rho(x))\,\mathrm{d}\,x$ with $U(r) = \frac{r^m}{m-1}$ [Otto]

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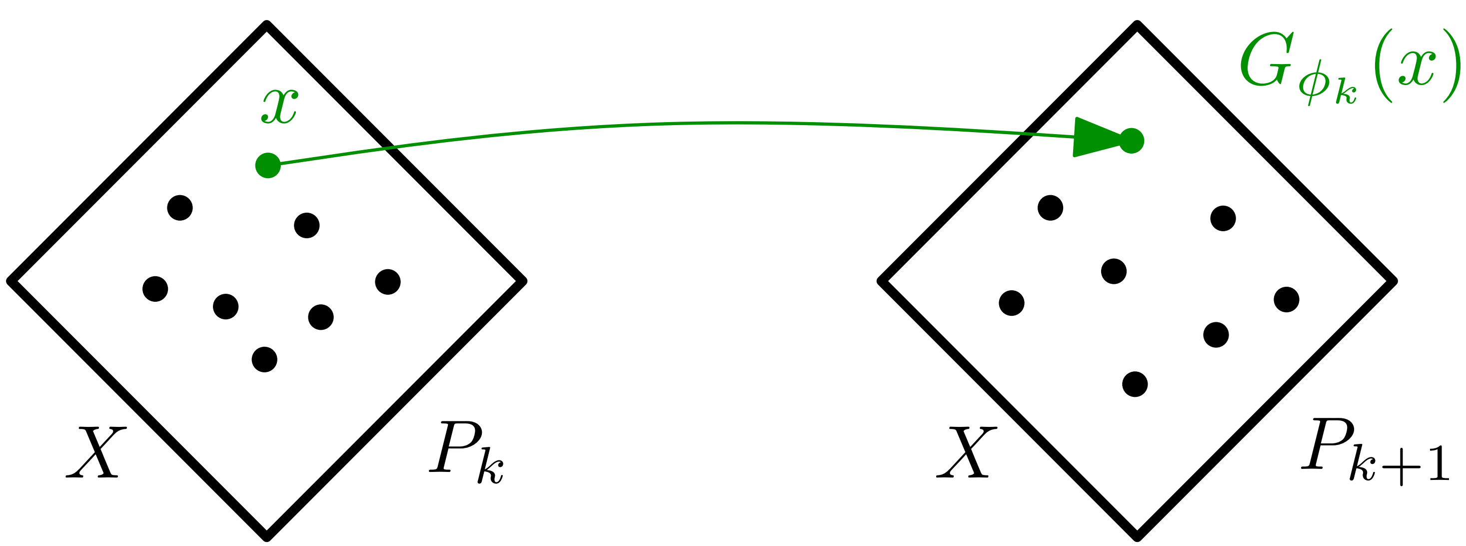
Algorithm: Input: $\mu_0 := \sum_{x \in P_0} \frac{\delta_x}{|P_0|}$, $\tau > 0$

For $k \in \{0, ..., T\}$

$\phi \leftarrow \arg\min_{\phi \in \mathcal{K}_X^G(P_k)} \frac{1}{2\tau} \mathrm{W}_2^2(\mu_k, G_{\phi\#}\mu_k) + \mathcal{U}(G^{\mathrm{ac}}_{\phi\#}\mu_k)$ ← Newton's method

$\mu_{k+1} \leftarrow G_{\phi\#}\mu_k$; $P_{k+1} \leftarrow \mathrm{spt}(\mu_{k+1})$



Example 2: Crowd motion and congestion

- Gradient flow model of crowd motion with congestion, with a JKO scheme:
  [Maury-Roudneff-Chupin-Santambrogio 10]

$$\mu_{k+1} = \min_{\nu \in \mathcal{P}(X)} \frac{1}{2\tau} \mathrm{W}_2^2(\mu_k, \nu) + \mathcal{E}(\nu) + \mathcal{U}(\nu)$$

$$\mathcal{E}(\nu) := \int_X V(x) \, \mathrm{d}\,\nu(x)$$

$$\mathcal{U}(\nu) := \begin{cases} 0 \text{ if } \mathrm{d}\,\nu / \mathrm{d}\,\mathcal{H}^d \leq 1, \\ +\infty \text{ if not} \end{cases}$$

Prop: The congestion term $\mathcal{U}$ is convex under generalized displacements.

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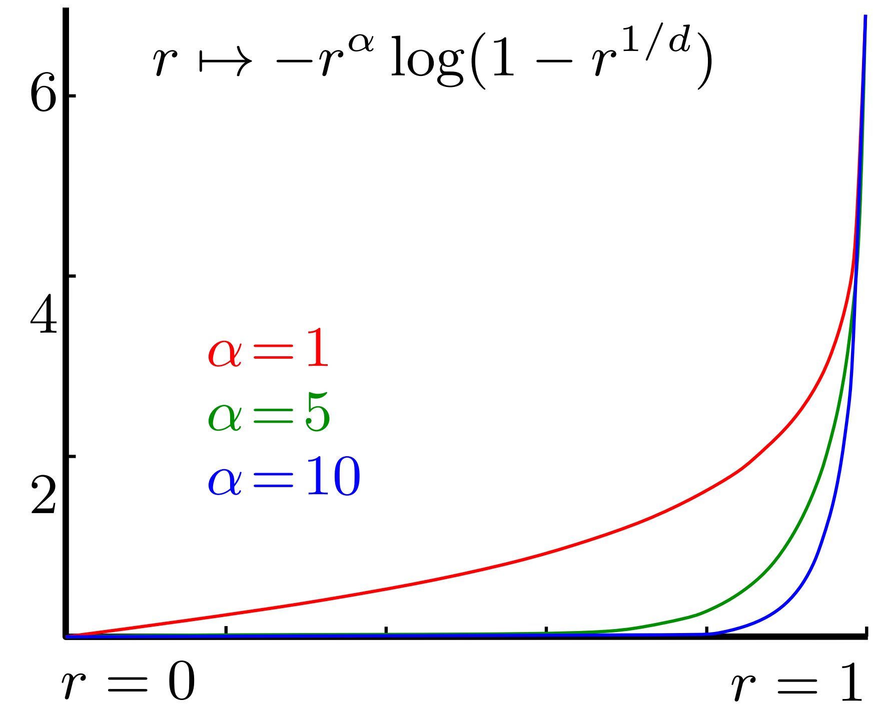
- Convex optimization problem if V is λ-convex ($V + \lambda\|.\|^2$ convex) and $\tau \leq \lambda/2$.
  We solve this problem with a relaxed hard congestion term:

$$\boxed{\mathcal{U}_\alpha(\rho) := -\int \rho(x)^\alpha \log(1-\rho(x)^{1/d})\,\mathrm{d}\,x}$$

Prop: (i) $\mathcal{U}_\alpha$ is convex under gen. displacements

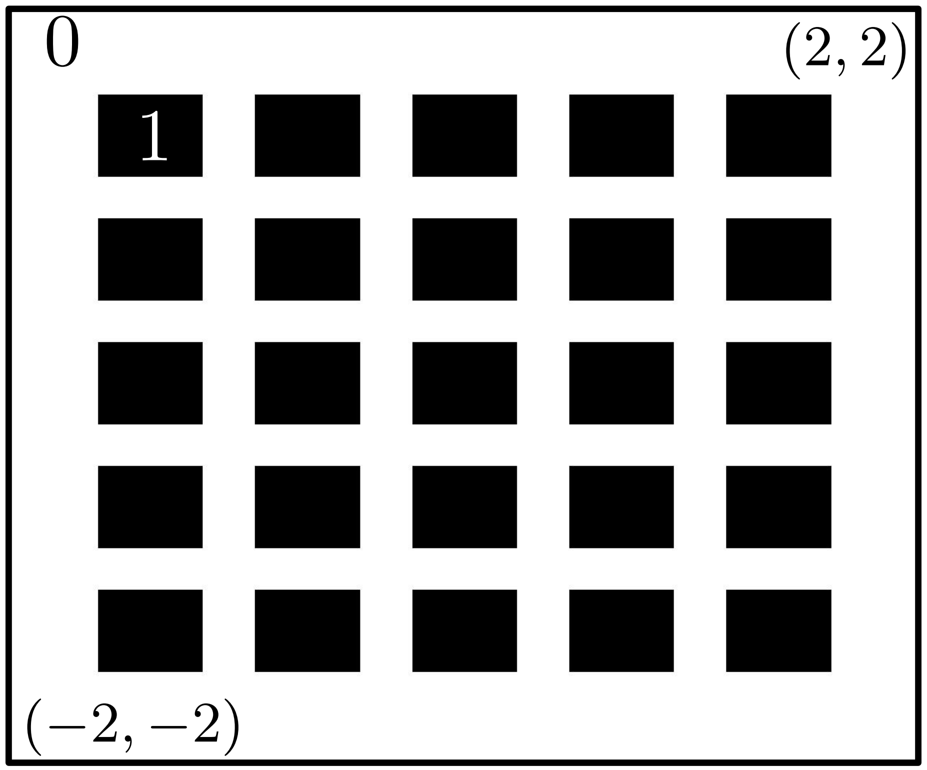
(ii) $\mathcal{U}_\alpha \xrightarrow{\Gamma} \mathcal{U}$ as $\alpha \to \infty$.

$\beta\mathcal{U}_1 \xrightarrow{\Gamma} \mathcal{U}$ as $\beta \to 0$.



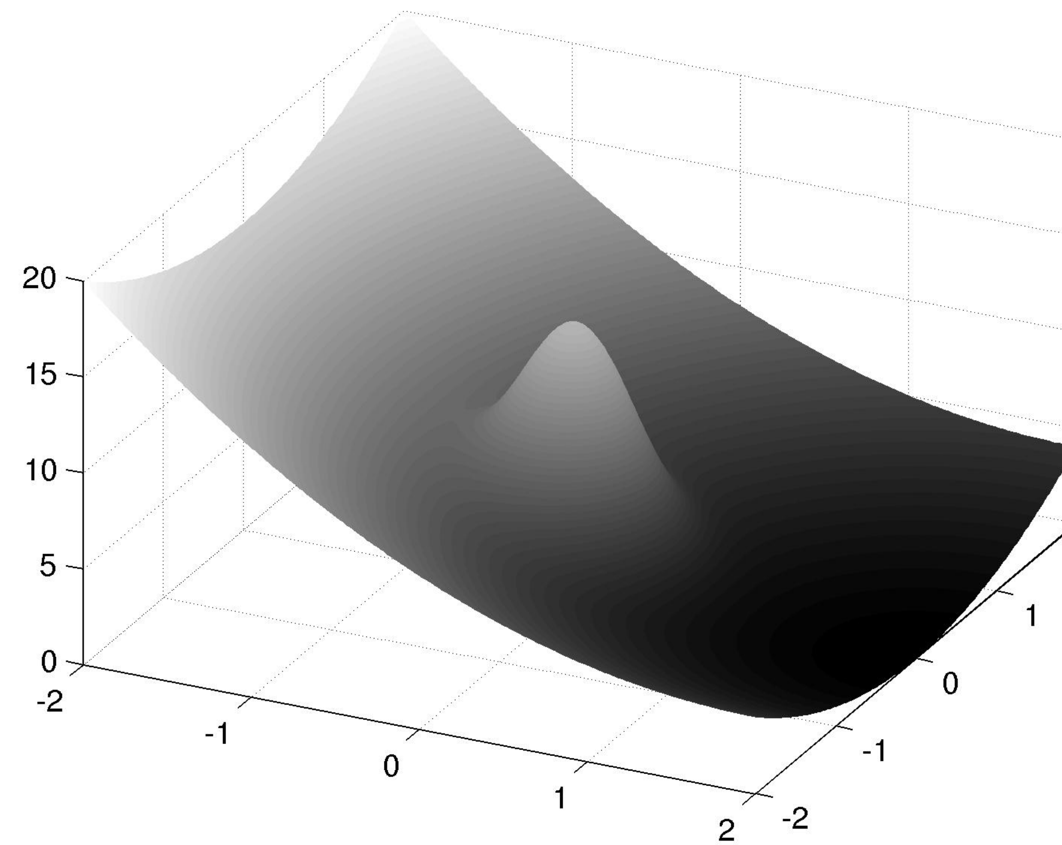
Example 2: Crowd motion and congestion

Initial density on $X = [-2,2]^2$



$P = 200 \times 200$ regular grid.

Potential



$V(x) = \|x - (2,0)\|^2 + 5\exp(-5\|x\|^2/2)$

Algorithm: Input: $\mu_0 \in \mathcal{P}(P), \tau > 0,\ \alpha > 0,\ \beta \geq 1.$

For $k \in \{0, ..., T\}$

$\phi \leftarrow \arg\min_{\phi \in \mathcal{K}_X^G(P_k)} \frac{1}{2\tau} \mathrm{W}_2^2(\mu_k, G_{\phi\#}\mu_k) + \mathcal{E}(G_{\phi\#}\mu_k) + \alpha \mathcal{U}_\beta(G_{\phi\#}^{\mathrm{ac}}\mu_k)$

$\nu \leftarrow G_{\phi\#}\mu_k$; $\mu_{k+1} \leftarrow$ projection of $\nu|_{[-2,2)\times[-2,2]}$ on P.