A comparison principle for variational problems with application to OT

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What is submodularity?

History of submodularity

A function $E: \mathbb{R}^d \to \mathbb{R}$ is submodular if:

$$E(x \wedge y) + E(x \vee y) \leq E(x) + E(y)$$

where
$$x \wedge y = (\min(x_i, y_i))_i$$
 and $x \vee y = (\max(x_i, y_i))_i$.

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Economics [Lorentz, 1953, Topkis, 1978] to derive monotone comparative statics in \mathbb{R}^d ,

Optimization On discrete domains [Bach, 2013], then in \mathbb{R}^d [Bach, 2018],

Calculus of variations [Alter et al., 2005] to derive comparison principles for optimizers of the perimeter.

Examples of lattices

- $ightharpoonup \mathbb{R}^n$ where $x \leq y \iff x_i \leq y_i$ for all i.
- ▶ Sobolev space: If $U \subset \mathbb{R}^n$ is open then $H^1(U)$, with $u \leq v$ if $u(x) \leq v(x)$ for almost every $x \in U$, is a lattice.

$$u \vee v(x) = u(x) \vee v(x), \nabla(u \vee v)(x) = \nabla u(x) \chi_{u(x) \geq v(x)} + \nabla v(x) \chi_{u(x) < v(x)}$$

- ▶ Continuous functions: $C(\Omega)$ is a lattice with $\phi \leq \psi$ if $\phi(x) \leq \psi(x)$ for all $x \in \Omega$.
- ▶ Radon measures: $\mathcal{M}(\Omega)$ is a lattice with

$$\mu \leq \nu \iff \forall \phi \in C(\Omega), \phi \geq 0, \int \phi d\mu \leq \int \phi d\nu$$

Examples of submodular functionals

▶ Dirichlet's energy on $H^1(U)$

$$u \mapsto \int_U \|\nabla u(x)\|^2 dx.$$

► Kantorovich functional in optimal transport

$$(\phi \in C(\Omega)) \mapsto \int \phi^c d\nu$$

where $\nu \in M_+(\Omega)$ and $(\phi^c(y) = \sup_x \phi(x) - c(x, y)$.

(Entropic) Optimal Transport

Let Ω be a compact metric space, $c \in C(\Omega \times \Omega)$ a cost function, $\epsilon \geq 0$, and $\alpha \in \mathcal{M}_+(\Omega)$ a nonzero reference measure.

For $\mu, \nu \in \mathcal{M}_+(\Omega)$ with $\mu(\Omega) = \nu(\Omega) > 0$, the entropic optimal transport problem is:

$$OT_{c,\epsilon}(\mu,\nu) = \inf_{\pi \in \Pi(\mu,\nu)} \int c \, d\pi + \epsilon \, \mathsf{KL}(\pi \mid \alpha \otimes \nu) = \sup_{\phi \in \mathcal{C}(\Omega)} \left[\int \phi \, d\mu - K_{\epsilon,\nu}(\phi) \right]$$

where the Kullback-Leibler divergence is

$$\mathsf{KL}(\pi \mid \alpha \otimes \nu) = \int \log \left(\frac{d\pi}{d(\alpha \otimes \nu)} \right) d\pi.$$

Kantorovich functional

The semidual/Kantorovich functional is

$$K_{\epsilon,\nu}(\phi) = \int \epsilon \log \left(\int e^{[\phi(x) - c(x,y)]/\epsilon} d\alpha(x) \right) d\nu(y) \xrightarrow[\epsilon \to 0]{} K_{0,\nu}(\phi) = \int \phi^{c} d\nu$$

The functional $K_{\epsilon,\nu}$ is convex and submodular.

JKO Scheme (Jordan-Kinderlehrer-Otto)

Let $\mu_0 \in \mathcal{M}_+(\Omega)$ be an initial measure.

The JKO scheme defines recursively a sequence $(\mu_n^{\tau})_{n\in\mathbb{N}}$ by solving:

$$\mu_{n+1}^{ au} = \operatorname*{arg\,min}_{
u \in \mathcal{M}_+(\Omega)} \left\{ rac{1}{ au} \, \mathit{OT}_{\mathsf{c},\epsilon}(\mu_n^{ au},
u) + \mathit{H}(
u)
ight\}$$

where H is a functional over $\mathcal{M}_+(\Omega)$ typically, an internal energy functional.

Comparison principle

Theorem

Let $c \in C(\Omega \times \Omega)$ and $h \colon [0, +\infty) \to \mathbb{R}$ denote a strictly convex, l.s.c., and superlinear function. Define $H_m \colon (\nu \in \mathcal{M}_+(\Omega)) \mapsto \int h(\frac{d\nu}{dm}) \, dm$ where $m \in \mathcal{M}_+(\Omega)$ is a fixed reference measure. If $\mu_1 \leq \mu_2$, then

$$u_1 \leq \nu_2, \quad \text{where } \nu_i = \operatorname*{arg\,min}_{\nu} OT_{c,\epsilon}(\mu_i, \nu) + H_m(\nu).$$

A similar result for $\epsilon=0$ was obtained in [Jacobs et al., 2020] by leveraging the existence of a transport map when c is C^1_{loc} and twisted.

Submodularity and duality

Banach lattices

Definition

Let $(X, \|\cdot\|)$ be a Banach space equipped with a partial ordering \leq . X is a Banach lattice if

- (i) (X, \leq) is a lattice: $\phi_1 \wedge \phi_2$ and $\phi_1 \vee \phi_2$ exist in X,
- (ii) $\phi_1 \leq \phi_2$ implies $\phi_1 + \phi_3 \leq \phi_2 + \phi_3$ for $\phi_3 \in X$, and $\phi_1 \leq \phi_2$ implies $\lambda \phi_1 \leq \lambda \phi_2$ for $\lambda \geq 0$,
- (iii) $|\phi_1| \le |\phi_2|$ implies $||\phi_1|| \le ||\phi_2||$ where $|\phi| = \phi^+ + \phi^-$ with $\phi^+ = \phi \lor 0$ and $\phi^- = -(\phi \land 0)$.

 $L^p(\mathbb{R}^n)$, $C(\Omega)$ and $\mathcal{M}(\Omega)$ are Banach lattices. $H^1(U)$ is a sublattice of the Banach lattice $L^2(U)$.

Submodularity and P-dominance

Definition

Let E_1 , E_2 : $X \to \mathbb{R}$. We say that E_1 is P-dominated by E_2 denoted $E_1 \ll_P E_2$ if for any $\phi_1, \phi_2 \in X$ we have

$$E_1(\phi_1 \wedge \phi_2) + E_2(\phi_1 \vee \phi_2) \leq E_1(\phi_1) + E_2(\phi_2).$$

If $E \ll_{\mathbf{P}} E$, then E is submodular.

Observe that if $E_1 \ll_P E_2$, $E_3 \ll_P E_4$, then $E_1 + E_3 \ll_P E_2 + E_4$

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- ▶ $E: (u \in \mathbb{R}^I) \mapsto \max_i u_i$. In particular $(\phi \in C(\Omega)) \mapsto \max_{x \in \Omega} \phi(x) - c(x, y)$ is submodular.

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- ▶ $E: ((a,b) \in \mathbb{R}^2) \mapsto h(a-b)$ where h is a convex function.
- ▶ If $E_i : (\phi \in C(\Omega)) \mapsto -\langle \phi, \mu_i \rangle$ for $\mu_i \in \mathcal{M}(\Omega)$, then for $\mu_1 \leq \mu_2$ we have $E_1 \ll_P E_2$.

P-dominance for sets

Let A_1 , A_2 be two subsets of X. We say that A_1 is P-dominated by A_2 denoted $A_1 \ll_P A_2$ if for any $\phi_1 \in A_1$, $\phi_2 \in A_2$ we have

$$\phi_1 \wedge \phi_2 \in A_1$$
 and $\phi_1 \vee \phi_2 \in A_2$.

This is equvialent to the P-dominance of their indicator functions: $\iota_{A_1} \ll_P \iota_{A_2}$ where ι_A is the indicator function of A. We recover Veinott's order or the strong set order.

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Lemma

Let $\phi_1, \phi_2 \in X$ then $\{\phi_1\} \ll_P \{\phi_2\}$ if and only if $\phi_1 \leq \phi_2$.

P-dominance implies comparison principle

Theorem

Let $E_1, E_2 \colon X \to \mathbb{R}$. If $E_1 \ll_{\mathrm{P}} E_2$ then

 $\text{arg min } E_1 \ll_{\mathrm{P}} \text{arg min } E_2.$

Take $\phi_1 \in \arg \min E_1$ and $\phi_2 \in \arg \min E_2$ then by P-dominance we have

$$E_1(\phi_1 \wedge \phi_2) + E_2(\phi_1 \vee \phi_2) \leq E_1(\phi_1) + E_2(\phi_2).$$

Which implies that $\phi_1 \land \phi_2 \in \arg \min E_1$ and $\phi_1 \lor \phi_2 \in \arg \min E_2$.

Duality

The following two results are extensions of [Galichon et al., 2024] to Banach lattices.

Theorem

Let $E_1, E_2 \colon X \to \mathbb{R}$ be two convex l.s.c. proper functions.

Then, $E_1 \ll_{\mathrm{P}} E_2$ if and only if $E_2^* \ll_{\mathrm{Q}} E_1^*$.

In particular E is submodular if and only if $E^* \ll_{\mathbb{Q}} E^*$ (we say that E^* is exchangeable).

Recall that $E^*(\mu) = \sup_{\phi} \langle \phi, \mu \rangle - E(\phi)$ is the convex conjugate of E.

Exchangeability and Q-dominance

Definition

Let $F_1, F_2 \colon X^* \to \mathbb{R}$. We say that F_1 is Q-dominated by F_2 ($F_1 \ll_{\mathbb{Q}} F_2$) if : for any $\mu_1, \mu_2 \in X^*$ and $t_{12} \in [0, (\mu_1 - \mu_2)^+]$ there is $t_{21} \in [0, (\mu_1 - \mu_2)^-]$ such that

$$F_1(\mu_1-(t_{12}-t_{21}))+F_2(\mu_2+(t_{12}-t_{21}))\leq F_1(\mu_1)+F_2(\mu_2).$$

If $F \ll_{\mathbb{Q}} F$ then F is said to be exchangeable. Exchangeability is stronger than convexity.

Exchangeability and Q-dominance

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$$F_1(\mu_1 - (t_{12} - t_{21})) + F_2(\mu_2 + (t_{12} - t_{21})) \le F_1(\mu_1) + F_2(\mu_2).$$

If $F \ll_{\mathbb{Q}} F$ then F is said to be exchangeable. Exchangeability is stronger than convexity.

Variations of this definition were introduced : M^{\natural} -convexity in discrete convex analysis [Murota, 2003], S-convexity in \mathbb{R}^n [Chen and Li, 2020].

Q-dominance for sets

Let B_1 , B_2 be two subsets of X^* . We say that B_1 is Q-dominated by B_2 denoted $B_1 \ll_Q B_2$ if for any $\mu_1 \in B_1$, $\mu_2 \in B_2$ and any $t_{12} \in [0, (\mu_1 - \mu_2)^+]$ there is $t_{21} \in [0, (\mu_1 - \mu_2)^-]$ such that

$$\mu_1 - (t_{12} - t_{21}) \in B_1 \text{ and } \mu_2 + (t_{12} - t_{21}) \in B_2.$$

This is equivalent to the Q-dominance of their indicator functions: $\iota_{B_1} \ll_{\mathrm{Q}} \iota_{B_2}$.

Probabilities are exchangeable

Lemma

The set $\mathcal{P}(\Omega)$ is exchangeable.

Let $\mu_1, \mu_2 \in \mathcal{P}(\Omega)$. For $t_{12} \in [0, (\mu_1 - \mu_2)^+]$ set $t_{21} = \frac{t_{12}(\Omega)}{(\mu_1 - \mu_2)^+(\Omega)} (\mu_1 - \mu_2)^-$. We have $t_{21} \in [0, (\mu_1 - \mu_2)^-]$ thus

$$\mu_1' = \mu_1 - (t_{12} - t_{21}) \ge \mu_1 - t_{12} \ge \mu_1 \land \mu_2 \ge 0$$

and
$$\mu'_1(\Omega) = \mu_1(\Omega) - t_{12}(\Omega) + t_{12}(\Omega) = 1$$
.

Q-dominance for singletons

Lemma

Let $\mu_1, \mu_2 \in X^*$ then $\{\mu_1\} \ll_{\mathrm{Q}} \{\mu_2\}$ if and only if $\mu_1 \leq \mu_2$.

Assume $\{\mu_1\} \ll_{\mathbf{Q}} \{\mu_2\}$ then for any $t_{12} \in [0, (\mu_1 - \mu_2)^+]$ there is $t_{21} \in [0, (\mu_1 - \mu_2)^-]$ such that $\mu_1 - (t_{12} - t_{21}) \in \{\mu_1\}$. Which implies that $(t_{12} - t_{21}) = 0$ and in particular $t_{12} = (t_{12} - t_{21})^+ = 0$. Thus $(\mu_1 - \mu_2)^+ = 0$ which is equivalent to $\mu_1 \leq \mu_2$.

Q-dominance implies comparison principle

Proposition

Let $F_1, F_2 \colon X^* \to \mathbb{R}$. If $F_1 \ll_{\mathrm{Q}} F_2$ then

 $\operatorname{arg\,min} F_1 \ll_{\mathrm{Q}} \operatorname{arg\,min} F_2.$

Take $\mu_1 \in \arg \min F_1, \mu_2 \in \arg \min F_2$. By Q-dominance for any $t_{12} \in [0, (\mu_1 - \mu_2)^+]$ there is $t_{21} \in [0, (\mu_1 - \mu_2)^-]$

$$F_1(\mu_1 - (t_{12} - t_{21})) + F_2(\mu_2 + (t_{12} - t_{21})) \le F_1(\mu_1) + F_2(\mu_2).$$

Thus as before we have $\mu_1 - (t_{12} - t_{21}) \in \arg \min F_1$, $\mu_2 + (t_{12} - t_{21}) \in \arg \min F_2$.

Q-dominance and sum

Given $F_1 \ll_{\mathrm{Q}} F_2$ we will be interested in comparing

$$\mathop{\mathrm{arg\,min}}_{\nu} F_1(\nu) + H(\nu) \quad \text{and} \quad \mathop{\mathrm{arg\,min}}_{\nu} F_2(\nu) + H(\nu).$$

However H exchangeable is not sufficient to imply $F_1 + H \ll_{\mathbb{Q}} F_2 + H$. We need a stronger assumption on H: total exchangeability.

Total exchangeability

Definition

H is totally exchangeable if for any μ_1 , μ_2 and any $t_{12} \in [0, (\mu_1 - \mu_2)^+]$, $t_{21} \in [0, (\mu_1 - \mu_2)^-]$ we have

$$H(\mu_1-(t_{12}-t_{21}))+H(\mu_2+(t_{12}-t_{21}))\leq H(\mu_1)+H(\mu_2).$$

If H is totally exchangeable then H is exchangeable and if $F_1 \ll_{\mathbb{Q}} F_2$ then $F_1 + H \ll_{\mathbb{Q}} F_2 + H$.

Internal energies $H_m: \nu \mapsto \int h(\frac{d\nu}{dm})dm$ where $h: \mathbb{R}_+ \to \mathbb{R}_+ \cup \{+\infty\}$ is a proper convex function are totally exchangeable.

Submodularity of Log-Laplace

Lemma

Let $m\in\mathcal{M}_+(\Omega)$ then $\mathcal{L}_m:\phi\mapsto\log\left(\int e^\phi dm\right)$ is submodular.

Since $KL(\cdot \mid m)$ is totally exchangeable and $\mathcal{P}(\Omega)$ is exchangeable we have that $KL(\cdot \mid m) + \iota_{\mathcal{P}(\Omega)}$ is exchangeable. Since $\mathcal{L}_m = (KL(\cdot \mid m) + \iota_{\mathcal{P}(\Omega)})^*$ we get the result by duality.

Application to Optimal transport

Reminder OT

For $\mu, \nu \in \mathcal{M}_+(\Omega)$ such that $\mu(\Omega) = \nu(\Omega)$, the entropic optimal transport problem is

$$OT_{c,\epsilon}(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int cd\pi + \epsilon \operatorname{\mathsf{KL}}(\pi \mid \alpha \otimes \nu) = \sup_{\phi \in C(\Omega)} \int \phi d\mu - K_{\epsilon, \nu}(\phi)$$

where

$$K_{\epsilon,\nu}(\phi) = \int \epsilon \log \left(\int e^{[\phi(x) - c(x,y)]/\epsilon} d\alpha(x) \right) d\nu(y), \quad K_{0,\nu}(\phi) = \int \phi^c d\nu.$$

We also have the following duality formula

$$OT_{c,\epsilon}(\mu,\nu) = \sup_{\phi,\psi} \int \phi d\mu - \int \psi d\nu - \epsilon \int e^{[\phi(x)-\psi(y)-c(x,y)]/\epsilon} d\alpha \otimes \nu(x,y)$$

Comparison principle on the potentials

For $\mu, \nu \in \mathcal{P}(\Omega)$ define the set of Kantorovich potentials

$$\Phi_{c,\epsilon}(\mu,\nu) = rg \max_{\phi} \int \phi d\mu - K_{\epsilon,\nu}(\phi)$$

Theorem

Let U be a Borel subset of Ω , then

$$\begin{cases} \mu_1 \leq \mu_2 & \text{ on } U \\ \phi_1 \leq \phi_2 & \text{ on } \Omega \setminus U \end{cases} \implies \phi_1 \wedge \phi_2 \in \Phi_{c,\epsilon}(\mu_1,\nu), \phi_1 \vee \phi_2 \in \Phi_{c,\epsilon}(\mu_2,\nu)$$

And $\phi_1 \leq \phi_2$ on the support of $\mu_2 - \mu_1$.

Comparison principle on the potentials

For $\mu, \nu \in \mathcal{P}(\Omega)$ define the set of Kantorovich potentials

$$\Phi_{c,\epsilon}(\mu,
u) = rg \max_{\phi} \int \phi d\mu - K_{\epsilon,
u}(\phi)$$

Theorem

Let U be a Borel subset of Ω , then

$$\begin{cases} \mu_1 \leq \mu_2 & \text{ on } U \\ \phi_1 \leq \phi_2 & \text{ on } \Omega \setminus U \end{cases} \implies \phi_1 \wedge \phi_2 \in \Phi_{c,\epsilon}(\mu_1,\nu), \phi_1 \vee \phi_2 \in \Phi_{c,\epsilon}(\mu_2,\nu)$$

And $\phi_1 \leq \phi_2$ on the support of $\mu_2 - \mu_1$.

When ϕ_i is determined up to a constant we have $\phi_1 \leq \phi_2$.

For $\epsilon=0$ and c quadratic we recover the comparison principle for the Monge–Ampère equation.

Submodularity in dual OT

Lemma

Let $\nu \in \mathcal{M}_+(\Omega)$, $\epsilon \geq 0$. Then $\mathcal{K}_{\epsilon,\nu}$ is submodular.

Since $f \mapsto \log(\int e^f d\alpha)$ is submodular we have for any $y \in \Omega$

$$\begin{split} &\log\left(\int e^{\phi_1(x)-c(x,y)}d\alpha(x)\right) + \log\left(\int e^{\phi_2(x)-c(x,y)}d\alpha(x)\right) \geq \\ &\log\left(\int e^{\phi_1\vee\phi_2(x)-c(x,y)}d\alpha(x)\right) + \log\left(\int e^{\phi_1\wedge\phi_2(x)-c(x,y)}d\alpha(x)\right). \end{split}$$

Result follows by integration.

Proof of comparison principle on potentials

The submodularity of $K_{\epsilon,\nu}$ grants

$$\int \phi_1 d\mu_1 - K_{\epsilon,\nu}(\phi_1) + \int \phi_2 d\mu_2 - K_{\epsilon,\nu}(\phi_2)
\leq \int \phi_1 d\mu_1 - K_{\epsilon,\nu}(\phi_1 \wedge \phi_2) + \int \phi_2 d\mu_2 - K_{\epsilon,\nu}(\phi_1 \vee \phi_2)
\leq \int \phi_1 \wedge \phi_2 d\mu_1 - K_{\epsilon,\nu}(\phi_1 \wedge \phi_2) + \int \phi_1 \vee \phi_2 d\mu_2 - K_{\epsilon,\nu}(\phi_1 \vee \phi_2)
- \int (\phi_1 - \phi_2)^+ d(\mu_2 - \mu_1).$$

Then optimality of ϕ_1, ϕ_2 ensures $\phi_1 \wedge \phi_2 \in \Phi_{c,\epsilon}(\mu_1, \nu), \phi_1 \vee \phi_2 \in \Phi_{c,\epsilon}(\mu_2, \nu)$ as well as $\int (\phi_1 - \phi_2)^+ d(\mu_2 - \mu_1) = 0$.

Comparison principle for JKO

Theorem

Let $c \in C(\Omega \times \Omega)$ and $h \colon [0, +\infty) \to \mathbb{R}$ denote a strictly convex l.s.c. and superlinear function. Define $H_m \colon (\nu \in \mathcal{M}_+(\Omega)) \mapsto \int h(\frac{d\nu}{dm}) \, dm$ where $m \in \mathcal{M}_+(\Omega)$ is a fixed reference measure. If $\mu_1 \leq \mu_2$ then

$$\nu_1 \leq \nu_2$$
, where $\nu_i = \operatorname*{arg\,min}_{\nu} OT_{c,\epsilon}(\mu_i,\nu) + H_m(\nu)$.

Exchangeability in primal OT

Lemma

The following functional defined over $\mathcal{M}_+(\Omega) \times \mathcal{M}_-(\Omega)$ is exchangeable

$$F:(\mu,\tau)\mapsto OT_{c,\epsilon}(\mu,-\tau)$$

Indeed

$$F(\mu,\tau) = OT_{c,\epsilon}(\mu,-\tau) = \sup_{\phi,\psi} \int \phi d\mu + \int \psi d\tau - \epsilon \int e^{[\phi(x)-\psi(y)-c(x,y)]/\epsilon} d\alpha \otimes \nu(x,y)$$

is the Legendre-Fenchel conjugate of a submodular function.

Application to JKO

Take $\mu_1 \leq \mu_2$ then $OT_{c,\epsilon}(\mu_1,\cdot) \ll_{\mathbb{Q}} OT_{c,\epsilon}(\mu_2,\cdot)$. Since H_m is totally exchangeable then

$$\arg\min_{\nu} OT_{c,\epsilon}(\mu_1,\nu) + H_m(\nu) \ll_{\mathbb{Q}} \arg\min_{\nu} OT_{c,\epsilon}(\mu_2,\nu) + H_m(\nu).$$

We conclude using the strict convexity of H_m which ensures the uniqueness of the minimizers.

Outlook

- ► The framework allows to derive comparison principles for a wide class of variational problems : in PDEs it allows for local or non local operators, in OT we also obtain results for unbalanced optimal transport.
- ▶ Proofs of the JKO comparison principle are often based on the properties of the transport map. Here we fully bypassed the use of the transport map or the Monge-Ampère equation.

Thank you for your attention!

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