Submodular Functions: from Discrete to Continuous Domains

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INRIA - Ecole Normale Supérieure

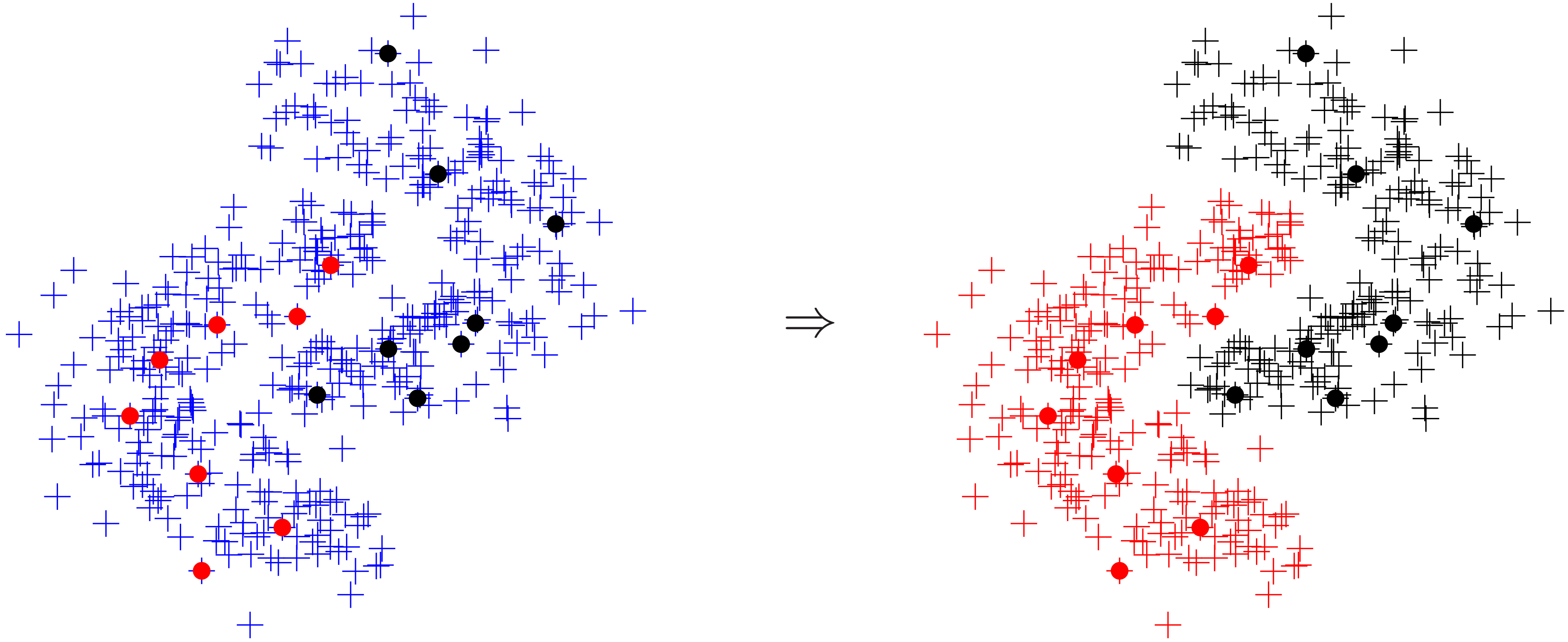
Optimization Without Borders, dedicated to Yuri Nesterov's 60$^{\text{th}}$ birthday - Les Houches - February 2016

Submodular functions
From discrete to continuous domains
Summary

- **Which functions can be minimized in polynomial time?**
  - Beyond convex functions
- **Submodular functions**
  - Not convex, ... but "equivalent" to convex functions
  - Usually defined on $\{0,1\}^n$
  - Extension to continuous domains
- **Preprint available on arXiv**

Submodularity (almost) everywhere
Clustering

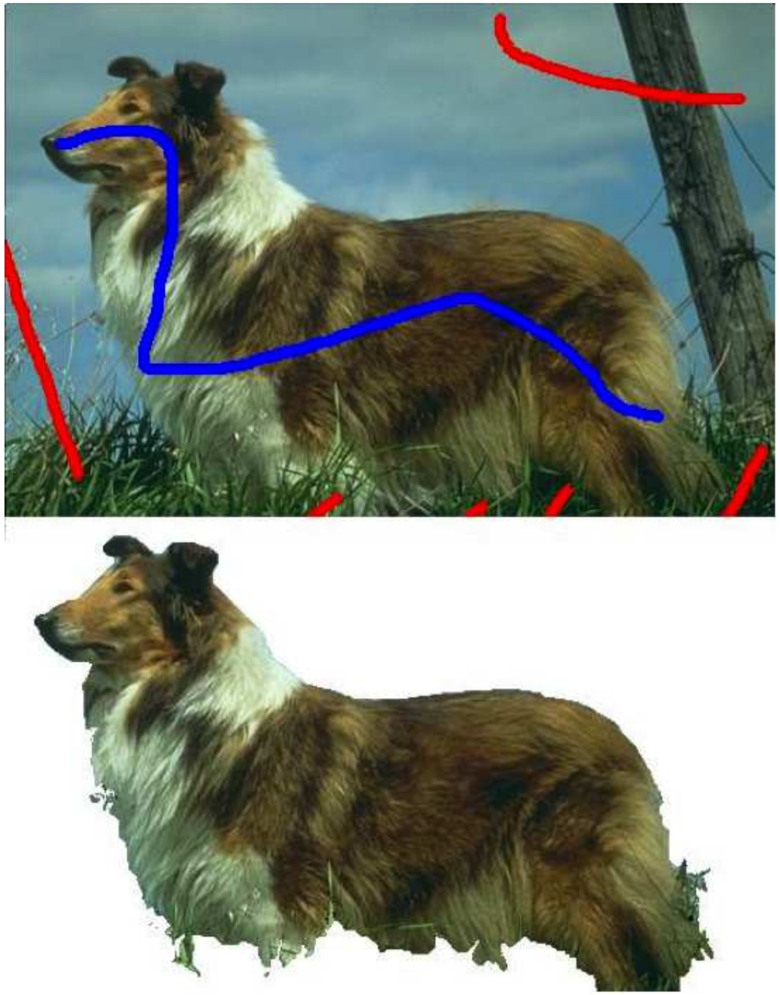
- Semi-supervised clustering



- Submodular function minimization

Submodularity (almost) everywhere

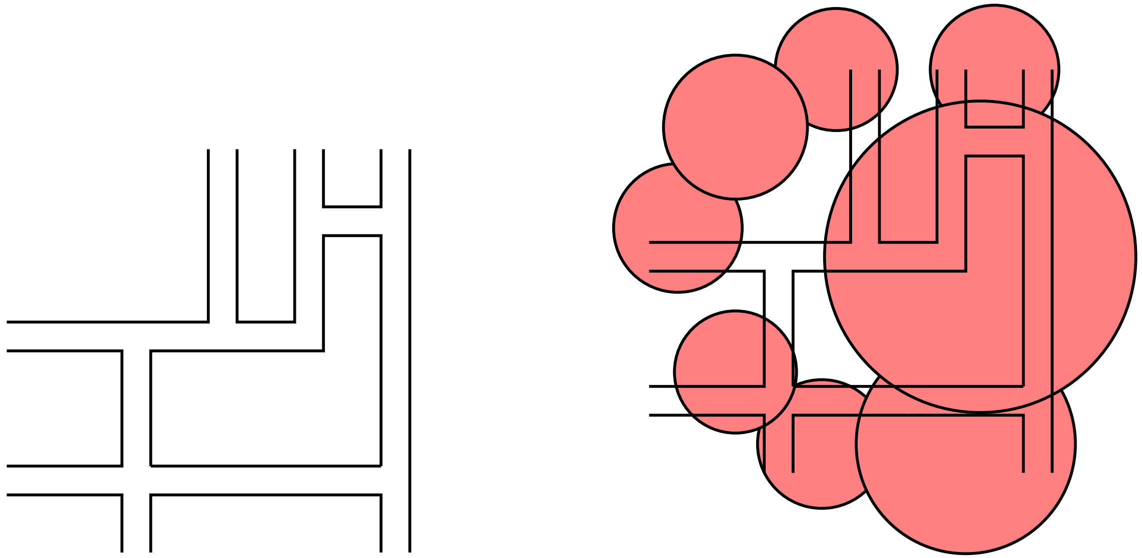
Graph cuts and image segmentation



- Submodular function minimization

Submodularity (almost) everywhere
Sensor placement

- Each sensor covers a certain area (Krause and Guestrin, 2005)
  - Goal: maximize coverage



- Submodular function maximization
- Extension to experimental design (Seeger, 2009)

Submodularity (almost) everywhere
Image denoising

- Total variation denoising (Chambolle, 2005)


- Submodular convex optimization problem

Submodularity (almost) everywhere
Combinatorial optimization problems

- Set $V = \{1, \dots, n\}$
- Power set 2^V = set of all subsets, of cardinality 2^n
- Minimization/maximization of a set-function $F : 2^V \to \mathbb{R}$.

$$\min_{A \subset V} F(A) = \min_{A \in 2^V} F(A)$$

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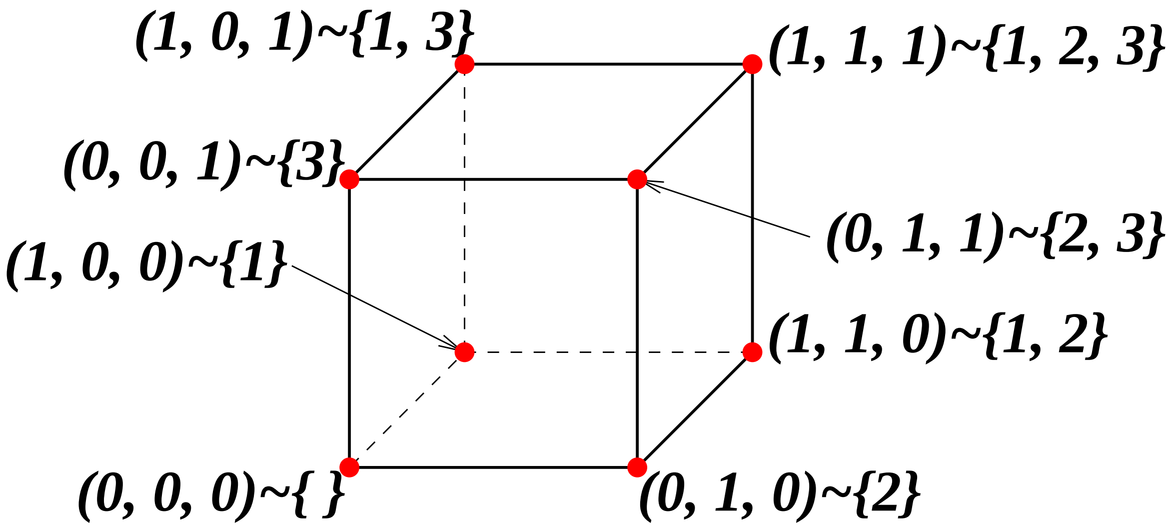
- Reformulation as (pseudo) Boolean function

$$\boxed{\min_{x \in \{0,1\}^n} H(x)}$$

with $H : \{0,1\}^n \to \mathbb{R}$
and $\forall A \subset V,\ H(1_A) = F(A)$



Outline

1. Submodular set-functions

– Definitions, examples
– Links with convexity through Lovász extension
– Minimization by convex optimization

2. From discrete to continuous domains

– Nonpositive second-order derivatives
– Invariances and examples
– Extensions on product measures through optimal transport

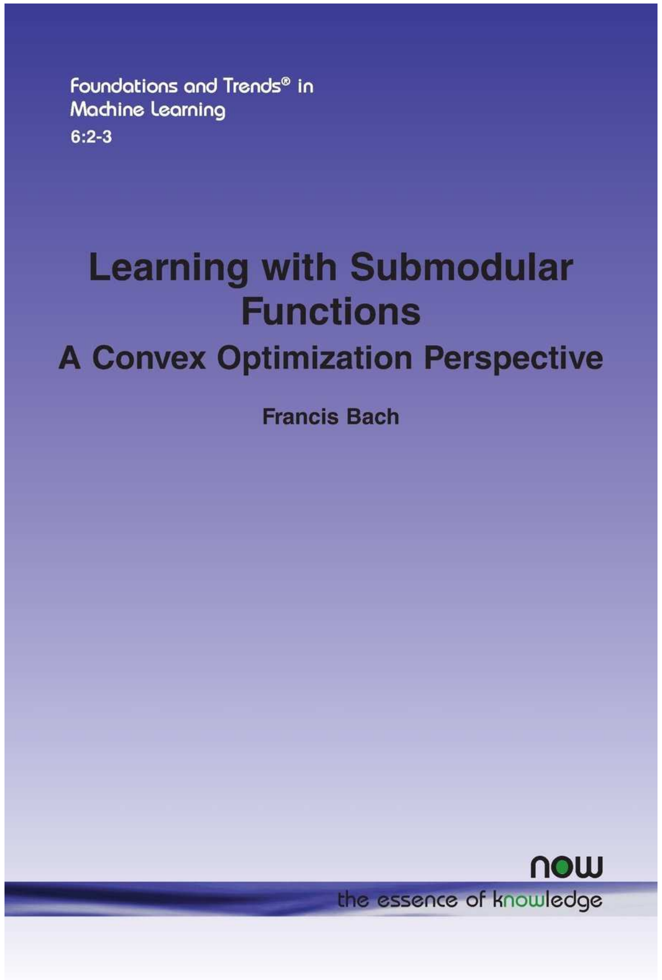
3. Minimization of continuous submodular functions

– Subgradient descent
– Frank-Wolfe optimization

Submodular functions - **References**

- **Reference book based on combinatorial optimization**
  - *Submodular Functions and Optimization* (Fujishige, 2005)

- **Tutorial monograph based on convex optimization** (Bach, 2013)
  - *Learning with submodular functions: a convex optimization perspective*



Submodular functions
Definitions

- **Definition**: $H : \{0,1\}^n \to \mathbb{R}$ is **submodular** if and only if

$$\forall x, y \in \{0,1\}^n, \quad H(x) + H(y) \geqslant H(\max\{x,y\}) + H(\min\{x,y\})$$

  - NB: equality for *modular* functions (linear functions of x)
  - Always assume $H(0) = 0$

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- **Equivalent definition**: (with $e_i \in \mathbb{R}^n$ i-th canonical basis vector)

$$\forall i \in \{1,\dots,n\}, \quad x \mapsto H(x+e_i) - H(x) \text{ is non-increasing}$$

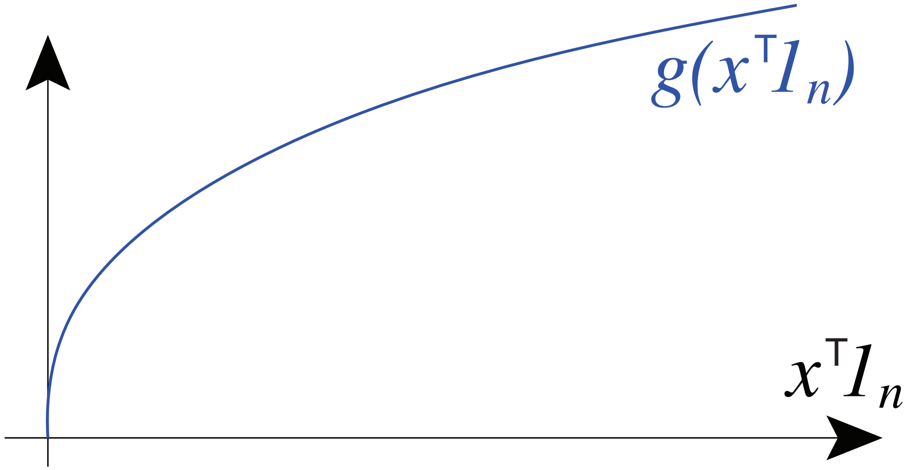
  - "Concave property": Diminishing returns

Submodular functions - Examples (see, e.g., Fujishige, 2005; Bach, 2013)

- Concave functions of the cardinality
- Cuts
- Entropies
  - Joint entropy of $(X_k)_{x_k=1}$, from n random variables $X_1, \dots, X_n$
- Functions of eigenvalues of sub-matrices
- Network flows
- Rank functions of matroids

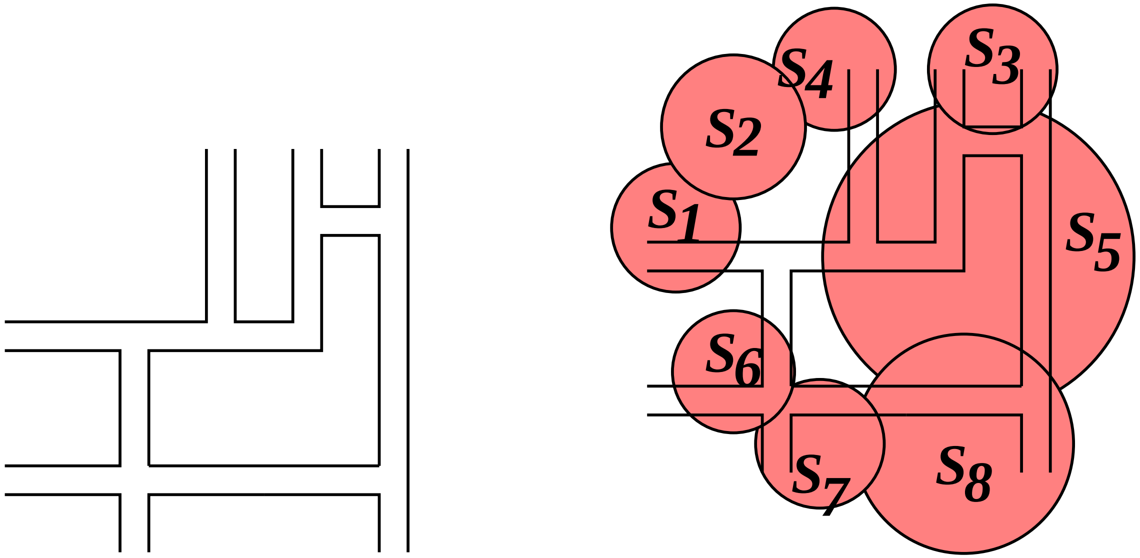
Examples of submodular functions
Cardinality-based functions

- Modular function: $H(x) = w^\top x$ for $w \in \mathbb{R}^n$
  - Cardinality example: If $w = 1_n$, then $H(x) = 1_n^\top x$
- If g is a concave function, then $H : x \mapsto g(1_n^\top x)$ is submodular
  - Diminishing return property



Examples of submodular functions

Covers

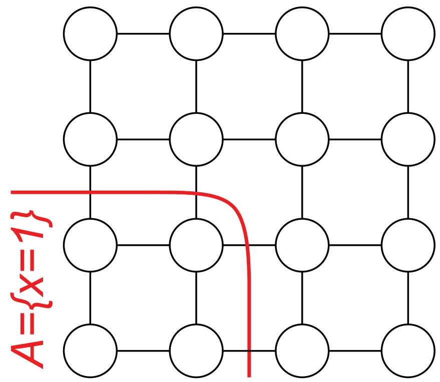


- Let W be any "base" set, and for each $k \in V$, a set $S_k \subset W$
- Set cover defined as $H(x) = \left| \bigcup_{x_k=1} S_k \right|$

Examples of submodular functions

Cuts

- Given a (un)directed graph, with vertex set $V = \{1, \ldots, n\}$ and edge set $E \subset V \times V$
  - $H(x)$ is the total number of edges going from $\{x = 1\}$ to $\{x = 0\}$.

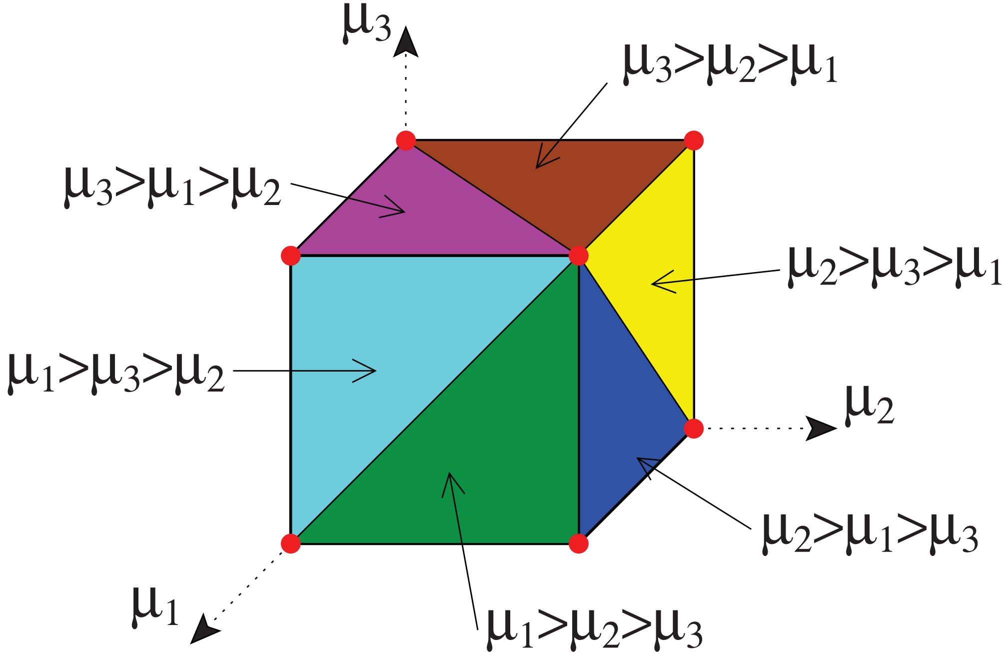


- Generalization with $d : \{1, \ldots, n\} \times \{1, \ldots, n\} \to \mathbb{R}_+$

$$H(x) = \sum_{j,k} d(k, j)(x_k - x_j)_+$$

Choquet integral (Choquet, 1954) - Lovász extension

- Subsets may be identified with elements of $\{0,1\}^n$
- Given any function H and $\mu \in \mathbb{R}^n$ such that $\mu_{j_1} \geqslant \cdots \geqslant \mu_{j_n}$



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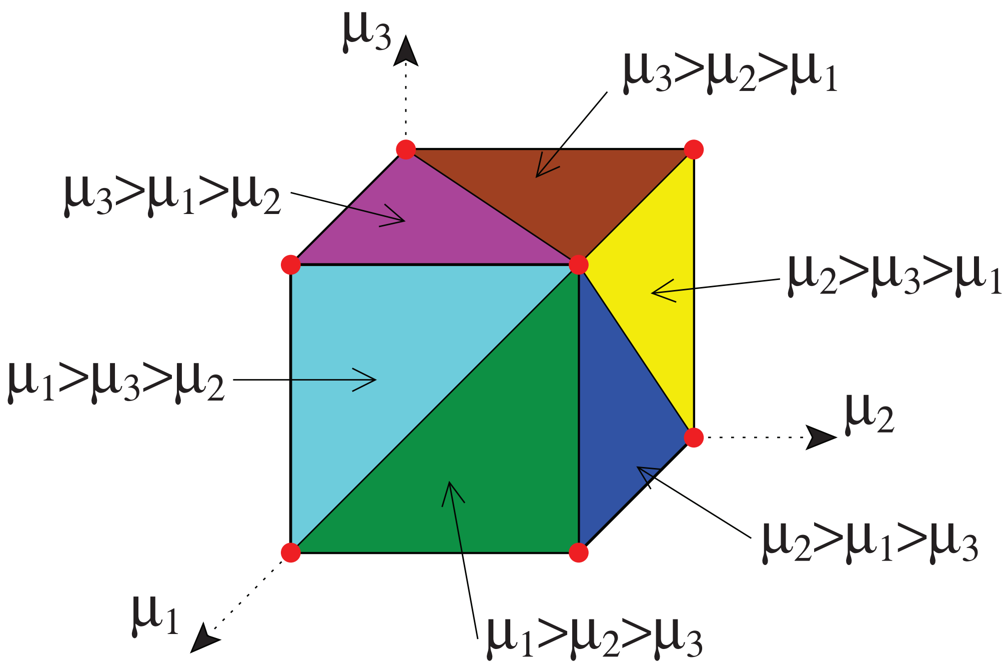
$$h(\mu) \;=\; \sum_{k=1}^{n} \mu_{j_k} [H(e_{j_1} + \cdots + e_{j_k}) - H(e_{j_1} + \cdots + e_{j_{k-1}})]$$



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- For $H(x) = w^\top x$, then $h(\mu) = w^\top \mu$
- For cuts, $h(\mu) = \sum_{k,j \in V} d(k,j)|\mu_k - \mu_j|$ is the *total variation*

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- For cuts, $h(\mu) = \sum_{k,j \in V} d(k,j)|\mu_k - \mu_j|$ is the *total variation*
- For any set-function H (even not submodular)
  - h is piecewise-linear and positively homogeneous
  - If $x \in \{0,1\}^n$, $h(x) = H(x) \Rightarrow$ extension from $\{0,1\}^n$ to $[0,1]^n$

Submodular set-functions
Links with convexity (Lovász, 1982)

1. **H is submodular if and only if h is convex**

2. **If H is submodular, then**

$$\min_{x\in\{0,1\}^n} H(x) = \min_{\mu\in\{0,1\}^n} h(\mu) = \min_{\mu\in[0,1]^n} h(\mu)$$

3. **If H is submodular, then a subgradient of h at any μ may be computed by the "greedy algorithm"**
   - Order the components of $\mu \in \mathbb{R}^n$ as $\mu_{j_1} \geqslant \cdots \geqslant \mu_{j_n}$
   - Define $w_{j_k} = H(e_{j_1} + \cdots + e_{j_k}) - H(e_{j_1} + \cdots + e_{j_{k-1}})$ for all k
   - Moreover $h(\mu) = w^\top \mu$

Submodular set-functions

Links with convexity (Lovász, 1982)

1. H **is submodular if and only if** h **is convex**

2. **If** H **is submodular, then**

$$\min_{x \in \{0,1\}^n} H(x) = \min_{\mu \in \{0,1\}^n} h(\mu) = \min_{\mu \in [0,1]^n} h(\mu)$$

3. **If** H **is submodular, then a subgradient of** h **at any** μ **may be computed by the "greedy algorithm"**

- **Consequences**
  - Submodular function minimization may be done in polynomial time
  - Ellipsoid algorithm in $O(n^5)$ (Grötschel et al., 1981)

Exact submodular function minimization
Combinatorial algorithms

- Algorithms based on $\min_{\mu \in [0,1]^n} h(\mu)$ and its dual problem

- Output the subset A and a dual certificate of optimality

- Best algorithms have polynomial complexity (Schrijver, 2000; Iwata et al., 2001; Orlin, 2009)
  - Typically $O(n^6)$ or more

- **Not practical for large problems...**

Submodular function minimization
Through convex optimization

- Convex non-smooth optimization problem

$$\min_{x \in \{0,1\}^n} H(x) = \min_{\mu \in \{0,1\}^n} h(\mu) = \min_{\mu \in [0,1]^n} h(\mu)$$

- **Important properties of h for convex optimization**
  - Polyhedral function
  - Known subgradients obtained from greedy algorithm

- **Generic algorithms** (blind to submodular structure)
  - Some with complexity bounds, some without
  - Subgradient, Frank-Wolfe, simplex, cutting-plane (ACCPM)
  - See Bach (2013)

Submodular function minimization
Through convex optimization

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- **Important properties of h for convex optimization**
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- **Generic algorithms** (blind to submodular structure)

- **Algorithms for sums of simple submodular functions**
  - Using alternating reflections (Jegelka, Bach, and Sra, 2013)

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   - Nonpositive second-order derivatives
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   - Subgradient descent
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From discrete to continuous domains

- **Main insight**: $\{0, 1\}$ **is totally ordered!**

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- **Extension to** $\{0,\ldots,k-1\}$: $H : \{0,\ldots,k-1\}^n \to \mathbb{R}$

$$\forall x, y, \quad H(x) + H(y) \geqslant H(\min\{x,y\}) + H(\max\{x,y\})$$

  – Equivalent definition: with $(e_i)_{i\in\{1,\ldots,n\}}$ canonical basis of $\mathbb{R}^n$

$$\forall x, i, j, \quad H(x+e_i) + H(x+e_j) \geqslant H(x) + H(x+e_i+e_j)$$

  – See Lorentz (1953); Topkis (1978)

From discrete to continuous domains

- **Main insight**: $\{0,1\}$ **is totally ordered!**

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  - See Lorentz (1953); Topkis (1978)

- **Generalization to all totally ordered sets**: $\mathcal{X}_i \subset \mathbb{R}$

  intervals $+\, H$ twice differentiable: $\forall x \in \prod_{i=1}^{n} \mathcal{X}_i, \quad \frac{\partial^2 H}{\partial x_i \partial x_j}(x) \leqslant 0$

A "new" class of continuous functions

- Assume each $\mathcal{X}_i \subset \mathbb{R}$ is a compact interval, and (for simplicity) H twice differentiable:

$$\textbf{Submodularity}: \ \forall x \in \prod_{i=1}^{n} \mathcal{X}_i, \quad \frac{\partial^2 H}{\partial x_i \partial x_j}(x) \leqslant 0$$

- **Invariance** by
  - individual increasing smooth change of variables $H(\varphi_1(x_1), \dots, \varphi_n(x_n))$
  - adding arbitrary (smooth) separable functions $\sum_{i=1}^{n} v_i(x_i)$

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- **Examples**
  - Quadratic functions with Hessians with non-negative off-diagonal entries (Kim and Kojima, 2003)
  - $\varphi(x_i - x_j)$, φ convex; $\varphi(x_1 + \cdots + x_n)$, φ concave; $\log\det$, etc...
  - Monotone of order two (Carlier, 2003), Spence-Mirrlees condition (Milgrom and Shannon, 1994)

Extensions to the space of product measures

- **Set-function:** $\mathcal{X}_i = \{0,1\}$
  - $[0,1] \approx$ set of probability distributions on $\{0,1\}$: $\mu_i = \mathbb{P}(X_i = 1)$
  - Lovász extension: for $\mu \in [0,1]^n$ such that $\mu_{j_1} \geqslant \cdots \geqslant \mu_{j_n}$

$$
\begin{aligned}
h(\mu) &= \sum_{k=1}^{n} \mu_{j_k} [H(e_{j_1} + \cdots + e_{j_k}) - H(e_{j_1} + \cdots + e_{j_{k-1}}\})] \\
&= (1 - \mu_{j_1}) H(0) + \sum_{k=1}^{n-1} (\mu_{j_k} - \mu_{j_{k+1}}) H(e_{j_1} + \cdots + e_{j_k}) + \mu_{j_n} H(1_n) \\
&= \mathbb{E}\big[H\big(1_{\mu \geqslant t}\big)\big] \text{ for } t \text{ uniform in } [0,1]
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- Relaxation on product measures
  - Continuous variable $\mu = (\mu_1, \dots, \mu_n) \in \prod_{i=1}^n [0, 1]$
  - Based on inverse cumulative distribution functions: $[0, 1] \to \mathcal{X}_i$

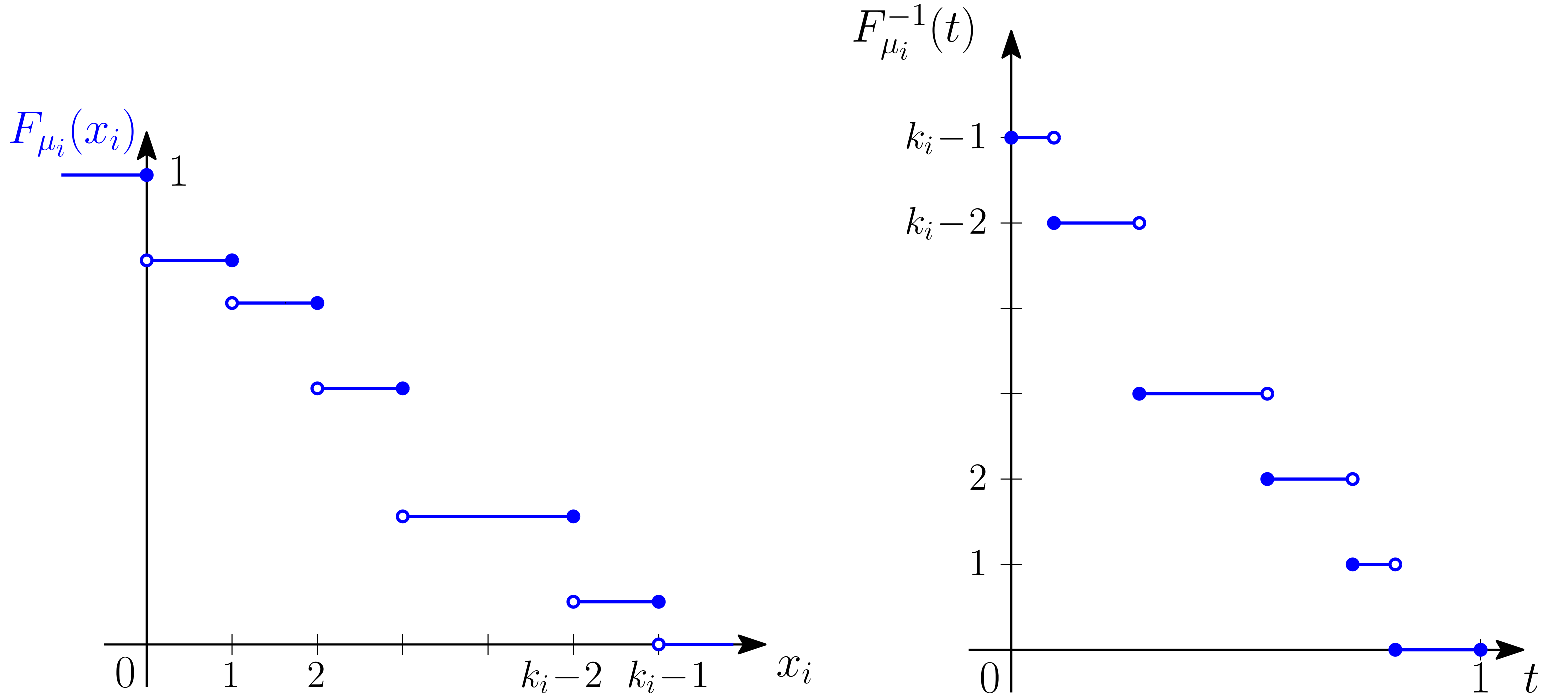
Extensions to the space of product measures

View 1: thresholding cumulative distrib. functions

- Given a probability distribution $\mu_i \in \mathcal{P}(\mathcal{X}_i)$
  - (reversed) cumulative distribution function $F_{\mu_i} : \mathcal{X}_i \to [0,1]$ as

$$F_{\mu_i}(x_i) = \mu_i\big(\{y_i \in \mathcal{X}_i, y_i \geqslant x_i\}\big) = \mu_i\big([x_i, +\infty)\big) \in [0,1]$$

  - and its "inverse": $F_{\mu_i}^{-1}(t) = \inf\{x_i \in \mathcal{X}_i,\ F_{\mu_i}(x_i) \leqslant t\} \in \mathcal{X}_i$



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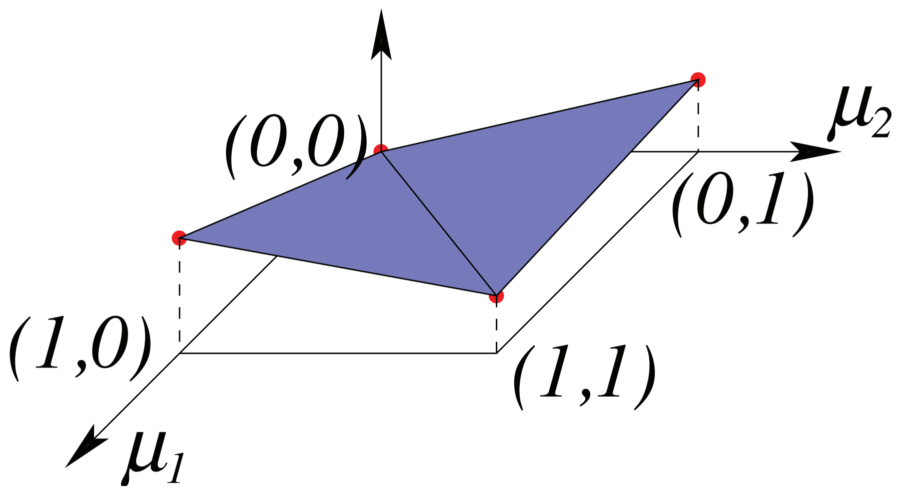
- **"Continuous" extension**

$$\forall \mu \in \prod_{i=1}^{n} \mathcal{P}(\mathcal{X}_i), \quad h(\mu_1, \dots, \mu_n) = \int_0^1 H\big[F_{\mu_1}^{-1}(t), \dots, F_{\mu_n}^{-1}(t)\big] dt$$

  - For finite sets, can be computed by sorting *all* values of $F_{\mu_i}(x_i)$
  - Equal to the Lovász extension for set-functions

Extensions to the space of product measures
View 2: convex closure

- Given any function H on $\mathcal{X} = \prod_{i=1}^n \mathcal{X}_i$
  - Known value $H(x)$ for any "extreme points" of product measures (i.e., all Diracs δ_x at any $x \in \mathcal{X}$)
  - Convex closure $\tilde{h}$ = largest convex lower bound
  - Minimizing H and its convex closure $\tilde{h}$ is equivalent



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- Need to compute the bi-conjugate of

$$a : \mu \mapsto H(x) \text{ if } \mu = \delta_x \text{ for some } x \in \mathcal{X}, \text{ and } +\infty \text{ otherwise}$$

Computation of the convex envelope

- Need to compute the bi-conjugate of

$$a : \mu \mapsto H(x) \text{ if } \mu = \delta_x \text{ for some } x \in \mathcal{X}, \text{ and } +\infty \text{ otherwise}$$

- Step 1: compute $a^*(w)$ for $w \in \prod_{i=1}^n \mathbb{R}^{\mathcal{X}_i}$

$$\begin{aligned} a^*(w) &= \sup_{x \in \mathcal{X}} \sum_{i=1}^n w_i(x_i) - H(x) = \sup_{\gamma \in \mathcal{P}(\mathcal{X})} \sum_{x \in \mathcal{X}} \gamma(x) \Big\{ \sum_{i=1}^n w_i(x_i) - H(x) \Big\} \\ &= \sup_{\gamma \in \mathcal{P}(\mathcal{X})} \left\{ \sum_{i=1}^n \sum_{x_i \in \mathcal{X}_i} w_i(x_i) \gamma_i(x_i) - \sum_{x \in \mathcal{X}} \gamma(x) H(x) \right\} \end{aligned}$$

  - with $\gamma_i(x_i) = \sum_{x_j, j \neq i} \gamma(x_1, \dots, x_n)$ the i-th marginal of γ

Computation of the convex envelope

- Step 1: $a^*(w) = \sup_{\gamma\in\mathcal{P}(\mathcal{X})} \left\{ \sum_{i=1}^{n} \sum_{x_i\in\mathcal{X}_i} w_i(x_i)\gamma_i(x_i) - \sum_{x\in\mathcal{X}} \gamma(x)H(x) \right\}$

- Step 2: compute $a^{**}(\mu) = \sup_w \langle w,\mu\rangle - a^*(w)$ for $\mu \in \prod_{i=1}^n \mathcal{P}(\mathcal{X}_i)$

$$
\begin{aligned}
a^{**}(\mu) &= \sup_w \langle w,\mu\rangle - \sup_{\gamma\in\mathcal{P}(\mathcal{X})} \left\{ \sum_{i=1}^{n} \sum_{x_i\in\mathcal{X}_i} w_i(x_i)\gamma_i(x_i) - \sum_{x\in\mathcal{X}} \gamma(x)H(x) \right\} \\
&= \inf_{\gamma\in\mathcal{P}(\mathcal{X})} \sup_w \sum_{i=1}^{n} \sum_{x_i\in\mathcal{X}_i} w_i(x_i)\big(\gamma_i(x_i) - \mu_i(x_i)\big) - \sum_{x\in\mathcal{X}} \gamma(x)H(x)
\end{aligned}
$$

- Thus $a^{**}(\mu) = \inf_{\gamma\in\mathcal{P}(\mathcal{X})} \int_{\mathcal{X}} H(x)d\gamma(x)$ such that $\forall i,\ \gamma_i(x_i) = \mu_i(x_i)$

Extensions to the space of product measures
View 2: convex closure

- Given any function H on $\mathcal{X} = \prod_{i=1}^{n} \mathcal{X}_i$
  - Known value $H(x)$ for any "extreme points" of product measures (i.e., all Diracs δ_x at any $x \in \mathcal{X}$)
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- "Closed-form" formulation: $\tilde{h}(\mu_1, \dots, \mu_n) = \inf_{\gamma \in \mathcal{P}(\mathcal{X})} \int_{\mathcal{X}} H(x) d\gamma(x)$,
  - with respect to all prob. measures γ on $\mathcal{X}$ such that $\gamma_i(x_i) = \mu_i(x_i)$
  - Multi-marginal optimal transport

Extensions to the space of product measures
Combining the two views

- **View 1: thresholding cumulative distribution functions**

  \+ closed form computation for any H, always an extension

  − not convex

- **View 2: convex closure**

  \+ convex for any H, allows minimization of H

  − not computable, may not be an extension

Extensions to the space of product measures
Combining the two views

- **View 1: thresholding cumulative distribution functions**
  + closed form computation for any H, always an extension
  − not convex

- **View 2: convex closure**
  + convex for any H, allows minimization of H
  − not computable, may not be an extension

- **Submodularity**
  – The two views are equivalent
  – Direct proof through optimal transport
  – All results from submodular set-functions go through

Kantorovich optimal transport in one dimension

- **Theorem** (Carlier, 2003): If H is submodular, then

$$\inf_{\gamma \in \mathcal{P}(\mathcal{X})} \int_{\mathcal{X}} H(x) d\gamma(x) \text{ such that } \forall i, \gamma_i = \mu_i$$

is equal to $\displaystyle\int_0^1 H\left[F_{\mu_1}^{-1}(t), \dots, F_{\mu_n}^{-1}(t)\right] dt$

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- **Proof/intuition for $n = 2$ for the Monge problem**

(a) Assume for simplicity atomless measures
(b) The following increasing map is natural $F_{\mu_2}^{-1} \circ F_{\mu_1} : \mathcal{X}_1 \to \mathcal{X}_2$
(c) This is the only increasing map
(d) Transport maps always increasing when H submodular
  – If $x_1 < x_1'$ mapped to $x_2 > x_2'$, then exchanging x_2 and x_2' would increase the cost by $c(x_1, x_2') + c(x_1', x_2) - c(x_1, x_2) - c(x_1', x_2') \leqslant 0$

Duality - Subgradients of extension

- General duality

$$h(\mu) = \sup_w \sum_{i=1}^n \sum_{x_i \in \mathcal{X}_i} w_i(x_i)\mu_i(x_i) - \sup_{x \in \mathcal{X}} \left\{ \sum_{i=1}^n w_i(x_i) - H(x) \right\}$$

- Subgradients from "greedy algorithm"
  - Sort all values of $F_{\mu_i}(x_i)$ for $i \in \{1, \ldots, n\}$ and $x_i \in \mathcal{X}_i$
  - Get a subgradient w by taking differences of values of H
  - See Bach (2015) for more details

Submodular functions
Links with convexity (Bach, 2015)

1. H **is submodular if and only if** h **is convex**

2. **If** H **is submodular, then**

$$\min_{x \in \prod_{i=1}^{n} \mathcal{X}_i} H(x) = \min_{\mu \in \prod_{i=1}^{n} \mathcal{P}(\mathcal{X}_i)} h(\mu)$$

3. **If** H **is submodular, then a subgradient of** h **at any** μ **may be computed by a "greedy algorithm"**

Outline

1. **Submodular set-functions**
   - Definitions, examples
   - Links with convexity through Lovász extension
   - Minimization by convex optimization

2. **From discrete to continuous domains**
   - Nonpositive second-order derivatives
   - Invariances and examples
   - Extensions on product measures through optimal transport

3. **Minimization of continuous submodular functions**
   - Subgradient descent
   - Frank-Wolfe optimization

Minimization of submodular functions
Projected subgradient descent

- **For simplicity**: discretizing all sets $\mathcal{X}_i$, $i = 1, \dots, n$ to k elements
- Assume **Lispschitz-continuity**: $\forall x, e_i,\ |H(x + e_i) - H(x)| \leqslant B$
  - Fact: subgradients of h bounded by B in ℓ_∞-norm
- **Projected subgradient descent**
  - Convergence rate of $O(nkB/\sqrt{t})$ after t iterations
  - Cost of each iteration $O(nk \log(nk))$
  - Reasonable scaling with respect to discretization

Minimization of submodular functions
Frank-Wolfe / conditional gradient

- **Submodular set-functions**: $\mathcal{X}_i = \{0, 1\}$
  - (C) : $\min_{\mu \in [0,1]^n} h(\mu)$ non-smooth convex
  - Solve instead (S) : $\min_{\mu \in \mathbb{R}^n} h(\mu) + \frac{1}{2}\|\mu\|^2$ (strongly convex)
  - Fact: level sets of (S) obtained from minimizers of $H(x) + \lambda x^\top 1_n$

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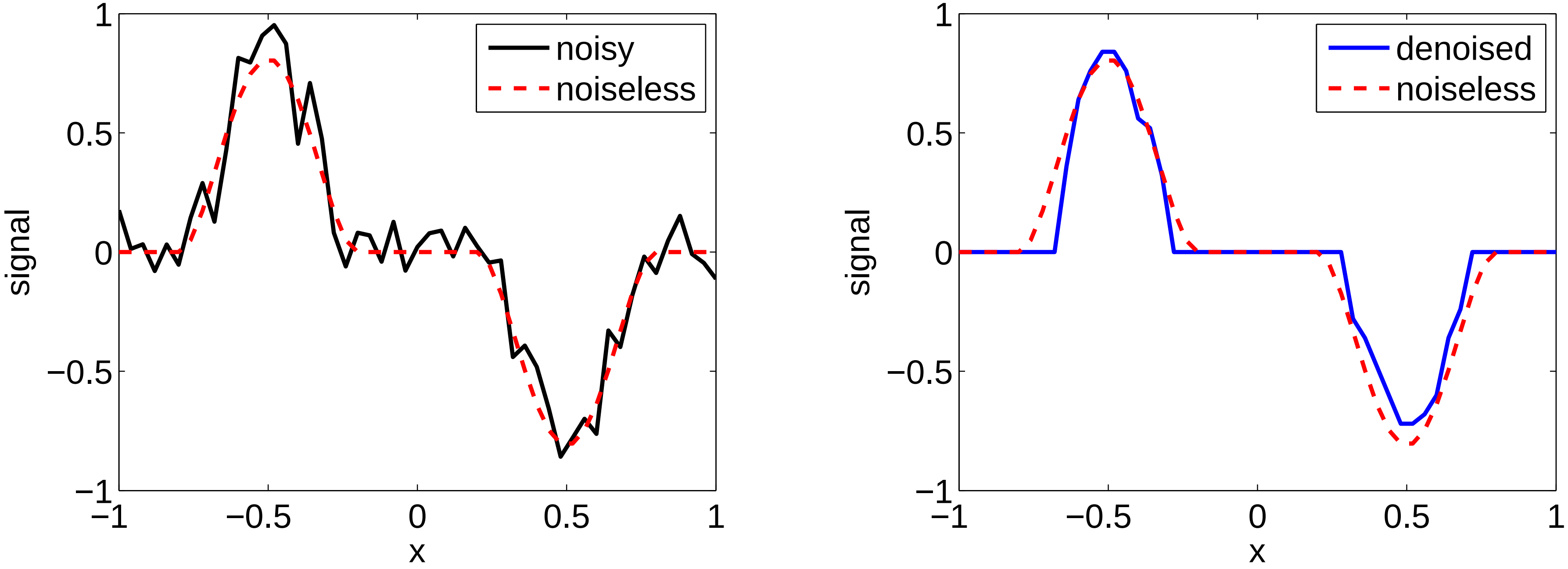
- **Extension to all submodular functions**
  - (C) : $\min_{\mu \in \prod_{i=1}^n \mathcal{P}(\mathcal{X}_i)} h(\mu)$
  - Solve instead (S) : $\min_{\mu \in \prod_{i=1}^n \mathcal{P}(\mathcal{X}_i)} f(\mu) + \sum_{i=1}^n \varphi_i(\mu_i)$
  - $\varphi(\mu_i)$ defined through optimal transport with a submodular cost $c_i(x_i, t)$ between μ_i and the uniform distribution on $[0, 1]$
  - $\varphi(\mu_i)$ can be strongly convex
  - Level sets of (S) obtained from minimizers of $H(x) + \sum_{i=1}^n c_i(x_i, t)$

Empirical simulations

- Signal processing example: $H : [-1, 1]^n \to \mathbb{R}$

$$H(x) = \frac{1}{2}\sum_{i=1}^{n}(x_i - z_i)^2 + \lambda \sum_{i=1}^{n} |x_i|^\alpha + \mu \sum_{i=1}^{n-1}(x_i - x_{i+1})^2$$



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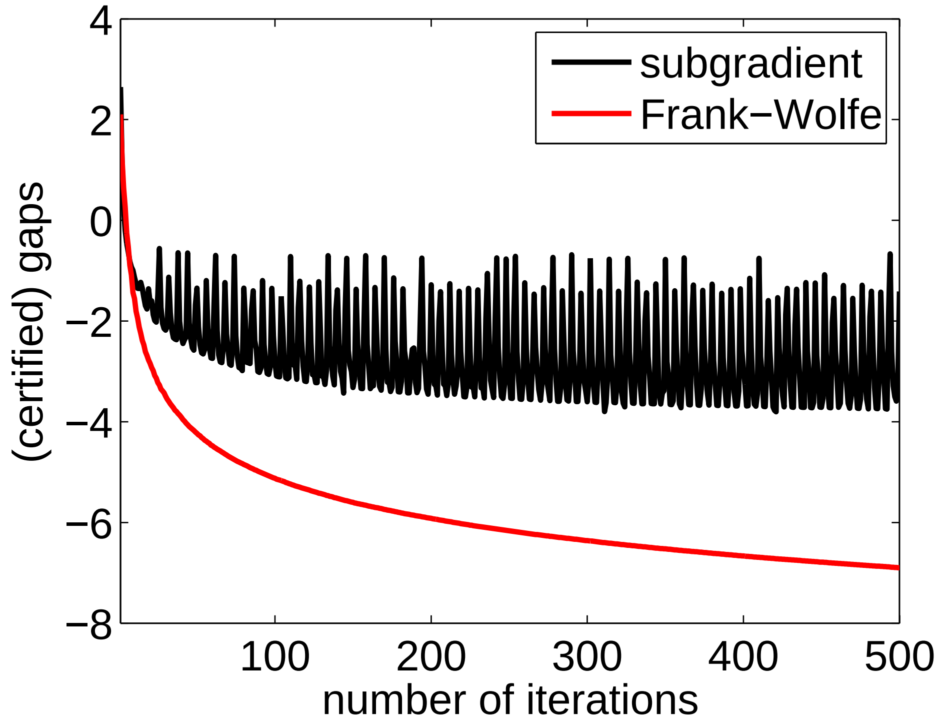

Conclusion

- **Submodular function and convex optimization**
  - From discrete to continuous domains
  - Extensions to product measures
  - Direct link with one-dimensional multi-marginal optimal transport

Conclusion

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  - From discrete to continuous domains
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- **On-going work**
  - Optimal transport beyond submodular functions
  - Beyond discretization
  - Beyond minimization
  - Sums of submodular functions and convex functions

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