A derivative-free algorithm for continuous submodular optimization

Clément Royer

Joint work with Marc Kaspar

COCANA Seminar - July 29, 2025





Story of an internship in Dauphine

Timeline

- Fall 2023: Marc follows my Master 1 course.
- May 2024: Starts an internship with me.
- August 2024: The internship ends.
- July 2025: This talk!

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The topic: Submodular optimization

- Popular in ML recently (part of my department).
- Originally a discrete maths concept (the other part of my department).
- \rightarrow Goal: Apply what I do (derivative-free optimization) to this setting!

Outline

- Continuous submodular optimization
- 2 Derivative-free optimization and direct search
- 3 Submodular optimization with direct search
- 4 Conclusion

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Submodular functions

Definition (Edmonds '70?)

 $f: \mathbf{2}^n \to \mathbb{R}$ is submodular if for every $A \subset B \subset \{1, \dots, n\}$ and $\mathbf{v} \notin B$, one has

$$f(A \cup \{\mathbf{v}\}) - f(A) \ge f(B \cup \{\mathbf{v}\}) - f(B).$$

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$$f(\mathbf{w}) - f(\mathbf{w}) \ge f(\mathbf{w}) - f(\mathbf{w})$$

- J. Bilmes, Submodular Functions, Optimization and Machine Learning (2020).
 - Discrete concept for set-valued functions.
 - Sometimes called diminishing returns (DR).
 - Arises in economics, network/graph theory, etc.

Discrete submodular optimization

A submodular optimization problem (for today)

- f submodular function.
- $\mathcal{C} \subset 2^n$ constraint set.
- \rightarrow NP-hard problem in general!
- \rightarrow Optimal value can be approximated up to a certain factor.

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Example: Cardinality constraint

- f nonnegative monotone, $C = \{|X| \le k\}, k < n$.
- Can compute X_k such that $f(X_k) \ge \left(1 \frac{1}{e}\right) \max_{|X| \le k} f(X)$ in polynomial time!

Continuous submodular functions

Continuous submodularity

• Discrete submodularity $(f: 2^n \to \mathbb{R})$

$$\forall (X,Y) \in 2^n, \qquad f(X) + f(Y) \ge f(X \cup Y) + f(X \cap Y).$$

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• Continuous submodularity $(f:[0,1]^n \to \mathbb{R})$

$$\forall (\mathbf{x}, \mathbf{y}) \in [0, 1]^n, \quad f(\mathbf{x}) + f(\mathbf{y}) \geq f(\mathbf{x} \vee \mathbf{y}) + f(\mathbf{x} \wedge \mathbf{y}),$$

 \vee/\wedge componentwise max/min.

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 \lor/\land componentwise max/min.

- Several other concepts of submodularity exist, with connections to concavity (An Bian et al '17, Bilmes '22).
- Applications in information theory and natural language processing.

Case study: Topic modeling and summarization

Topic modeling

- Data: Text documents.
- Goal: Identify topics through occurrences of certain words.

Alies De Dolomer Maire et redomation of habitane de la sinte de Dagmer de la la sinte de Dagmer de la la sinte de la sinte de

Example: Grievances from France's 1789 cahiers!

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Collins Be Dolman & Homer et restamation of Collins Be hadden be la view de la grand dellarie Commandation de la collins de la c
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Topic summarization (Lin & Bilmes '11)

- Input: Documents and probabilistic topic model for each document.
- Goal: Select a subset of documents to maximize the probabilistic coverage of topics.
 - Discrete: Select a subset of documents.
 - Continuous: Select document i with probability $x_i \in [0,1]$.
- → Submodular maximization problem!

From submodular to a internship

- Continuous submodular optimization
 - Continuous submodular replaces discrete submodular.
 - Cool applications in natural language processing.

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- Solving those problems
 - Algorithms with various approximation guarantees and complexity (An Bian et al '17).
 - Derivative-free optimization techniques (Chen et al '20).

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My internship proposal

Given a submodular optimization problem and my favorite (derivative-free) algorithm,

- What can we prove in theory?
- Does it work in practice?

- Continuous submodular optimization
- 2 Derivative-free optimization and direct search
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Derivative-free optimization

Today's problem class

```
 \left\{ \begin{array}{ll} \mathsf{maximize}_{\pmb{x} \in \mathbb{R}^n} & f(\pmb{x}) \\ \mathsf{subject to} & \pmb{x} \in \mathcal{F} = \{ \pmb{\ell} \leq \pmb{x} \leq \pmb{u}, \pmb{A}\pmb{x} \leq \pmb{b} \}. \end{array} \right.
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with $f: \mathbb{R}^n \to \mathbb{R}$, \mathcal{F} polytope.

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Derivative-free/Black-box optimization setup

- Derivatives of f not available for algorithmic purposes.
- Algorithm must use only function values.

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Two algorithmic paradigms in derivative-free optimization

- Build a model of f.
- Explore the space through directions→Direct search.

Direct search for maximization

Problem maximize_{$\mathbf{x} \in \mathbb{R}^n$} $f(\mathbf{x})$ s.t. $\mathbf{x} \in \mathcal{F} = \{\ell \leq \mathbf{x} \leq \mathbf{u}, \ \mathbf{A}\mathbf{x} \leq \mathbf{b}\}.$

Inputs: $\mathbf{x}_0 \in \mathcal{F}$, $\alpha_0 > 0$.

Iteration k: Given (\mathbf{x}_k, α_k) ,

- Choose a set $\mathcal{D}_k \subset \mathbb{R}^n$ of m vectors.
- If $\exists \ d_k \in \mathcal{D}_k$ such that

$$\mathbf{x}_k + \alpha_k \mathbf{d}_k \in \mathcal{F}$$
 and $f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) > f(\mathbf{x}_k) + \alpha_k^2$

set
$$\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{d}_k$$
, $\alpha_{k+1} := 2\alpha_k$.

• Otherwise, set $x_{k+1} := x_k$, $\alpha_{k+1} := \alpha_k/2$.

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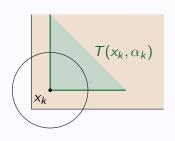
Key for theory and pratice: Choice of \mathcal{D}_k .

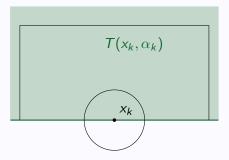
Choosing the directions \mathcal{D}_k

Assumptions on directions \mathcal{D}_k

- \mathcal{D}_k consists of m unit vectors.
- ullet \mathcal{D}_k is a κ -descent set for the constraints

$$\min_{\substack{\boldsymbol{v} \in T(\boldsymbol{x}_k, \alpha_k) \\ \boldsymbol{v} \neq 0}} \max_{\boldsymbol{d} \in \mathcal{D}_k} \frac{\boldsymbol{v}^{\mathrm{T}} \boldsymbol{d}}{\|\boldsymbol{v}\|} \geq \kappa.$$





Complexity result for maximize $x \in \mathcal{F} f(x)$

Assumptions

- f is C^1 , ∇f Lipschitz continuous.
- f is concave, has a maximum f^* .
- Distance to maxima is bounded (technical condition).
- \mathcal{D}_k κ -descent, $|\mathcal{D}_k| = m \ \forall k$.

Theorem (from Dodangeh & Vicente '14, Gratton et al '19)

Direct search reaches x_k such that $f^* - f(x_k) \le \epsilon$ in at most

- $\mathcal{O}(\kappa^{-2}\epsilon^{-1})$ iterations.
- $\mathcal{O}(m\kappa^{-2}\epsilon^{-1})$ evaluations of f.

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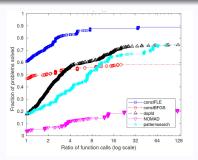
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- $ightarrow \epsilon^{-1}$: on par with derivative-based methods.
- $\rightarrow m \kappa^{-2}$: cost of being derivative-free.

What about practice?

My code: dspfd

- Deterministic and randomized techniques for choosing directions in linearly-constrained problems.
- MATLAB code from 2017, still works off the shelf!
- Still beats MATLAB's *patternsearch* (and sometimes Polytechnique Montréal's *nomad*).



Experiments on CUTEst linearly-constrained problems (Royer et al '24).

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Same problem, different assumptions

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Key: Suppose f is (DR)-submodular!

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Definition

f is DR-submodular if

$$\forall \mathbf{x}, \mathbf{y} \in \mathcal{F}^2, \quad \mathbf{x} \geq \mathbf{y} \Rightarrow \nabla f(\mathbf{x}) \geq \nabla f(\mathbf{y}).$$

 $\mathbf{x} \geq \mathbf{y} \Leftrightarrow \mathbf{x}_i \geq \mathbf{y}_i \ \forall i = 1, \ldots, n.$

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- Continuous submodularity+concavity along positive directions.
- Example Nonconvex quadratics

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} + \mathbf{b}^{\mathrm{T}}\mathbf{x}, \quad A_{ij} \leq 0 \ \forall (i,j).$$

Assumptions on f and previous complexity

Assume f is

- DR-submodular.
- Monotone: $f(x) \ge f(y)$ if $x \ge y$.

Goal: Approach the value $(1 - \frac{1}{e})f^*$.

Derivative-based Frank-Wolfe method (Bian et al '17)

After K iterations, get \mathbf{x}_{K}^{FW} such that

$$f(\mathbf{x}_{K}^{FW}) \geq (1 - e^{-\delta})f^* - \frac{L}{2} \sum_{k=0}^{K-1} \gamma_k^2 + e^{-\delta} f(\mathbf{x}_0).$$

- γ_k : Stepsize, predefined (constant).
- $\delta \in (0,1)$.
- Translates in complexity $\mathcal{O}(\epsilon^{-1})$ to get within ϵ of $(1-\frac{1}{e})$ f^* .

Direct search for maximization on $[\ell, u]$

Inputs: $x_0 \in \mathcal{F}$, $\alpha_0 > 0$. Iteration k: Given (x_k, α_k) ,

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- Otherwise, set $x_{k+1} := x_k$, $\alpha_{k+1} := \alpha_k/2$.
- Difference from before: complete polling.
- Needed for the analysis, not in practice.

Direction quality

Classical assumption: \mathcal{D}_k has m unit vectors.

Main assumption on \mathcal{D}_k

At every iteration k,

$$\max_{\boldsymbol{d} \in D_k} \boldsymbol{d}^{\mathrm{T}} \nabla f(\boldsymbol{x}_k) \ \geq \ \kappa \max_{\boldsymbol{v} \in \mathcal{F}, \|\boldsymbol{v}\| \leq 1} \boldsymbol{v}^{\mathrm{T}} \nabla f(\boldsymbol{x}_k) \quad \text{where} \quad \kappa \in (0,1].$$

- Stronger than the assumption from the concave case.
- Link to Frank-Wolfe requirements.

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The case $\mathcal{F} = \{0 \le \mathbf{x} \le 1\}$

Natural choice: $\mathcal{D}_k = [\mathbf{I}_n - \mathbf{I}_n]$.

- Concave case: κ -descent with $\kappa = \frac{1}{\sqrt{n}}$.
- Submodular case: $\kappa = \frac{1}{n}$ (worse!).

Results in the submodular case

Theorem (Kaspar, R. '24-25)

After $K \geq 1$ successful iterations j_1, \ldots, j_K , the method satisfies

$$f(x_{j_K}) \geq f^* - \left(1 - e^{-\mathcal{O}(\kappa^2)\sum_{i=1}^K \alpha_{j_i}^2}\right) (f^* - f(\mathbf{x}_0)) - \frac{L}{2} \sum_{i=1}^K \alpha_{j_i}^2.$$

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Corollary

Reaches x_k such that $f(x_k) \ge (1 - \frac{1}{e})f^* + \epsilon$ in at most

- $\tilde{\mathcal{O}}(\kappa^{-2} \epsilon^{-1})$ iterations.
- $\tilde{\mathcal{O}}(m \kappa^{-2} \epsilon^{-1})$ iterations.
- $ightarrow \epsilon^{-1}$: On par with (derivative-based) Frank-Wolfe approach
- ightarrow $m\,\kappa^{-2}$: Similar to concave maximization (but values of m/κ may differ!)

Other stepsize choices

- Previous work: Predefined stepsizes (fixed, adaptive).
- Variant of direct search without distinction between success/failure.

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 α_k Guarantee after K iterations

Complexity (its/evals)

$$\frac{1}{K} \quad f(\boldsymbol{x}_K) \geq (1 - \mathrm{e}^{-\kappa}) f(\boldsymbol{x}^*) - \frac{L}{2K} + \mathrm{e}^{-\kappa} f(\boldsymbol{x}_0) \quad \mathcal{O}(\kappa^{-1} \epsilon^{-1}) / \mathcal{O}(m\kappa^{-1} \epsilon^{-1})$$

$$\frac{1}{\kappa K} \quad f(\boldsymbol{x}_K) \geq (1 - \mathrm{e}^{-1}) f(\boldsymbol{x}^*) - \frac{L\kappa}{2K} + \mathrm{e}^{-1} f(\boldsymbol{x}_0) \quad \mathcal{O}(\kappa^{-1} \epsilon^{-1}) / \mathcal{O}(m\kappa^{-1} \epsilon^{-1}).$$

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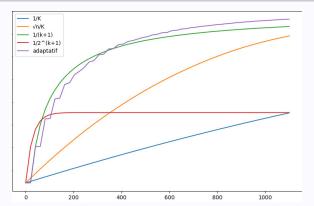
$$\frac{1}{\kappa K} \quad f(\mathbf{x}_{K}) \geq (1 - e^{-1}) f(\mathbf{x}^{*}) - \frac{L\kappa}{2K} + e^{-1} f(\mathbf{x}_{0}) \quad \mathcal{O}(\kappa^{-1} \epsilon^{-1}) / \mathcal{O}(m\kappa^{-1} \epsilon^{-1}).$$

- Better complexities than before (factor κ^{-1}).
- Should we use those instead?

The best stepsize choice

Two variants of direct search

- Fixed/Decreasing step sizes.
- adaptatif (pardon my French): Classical updating rule.



Run on a submodular quadratic over $[0,1]^{10}$ using 100 simplex gradients.

A topic summarization problem

Data

- 40 lectures that I gave on optimization for machine learning.
- 4 courses (1-8, 9-16, 17-24, 25-40).
- Discrete probability distribution of the lectures around 4 topics (derivatives/convexity/algorithms/applications).
- \rightarrow A matrix of topic probabilities $T \in [0, 1]^{40 \times 1}$.

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Topic summarization in this setting

- Find a subset of lectures that covers the four topics as best as possible.
- Constraints: At most two lectures from the first three courses, four from the last course.

A topic summarization problem ('ed)

The problem

$$\begin{cases} \text{ maximize}_{\mathbf{x} \in \mathbb{R}^{40}} & \frac{1}{4} \sum_{t=1}^{4} \left(1 - \prod_{i=1}^{40} (1 - p_i(t) x_i) \right) \\ \text{s.t.} & \sum_{i=1}^{8} x_i \le 2, \sum_{i=9}^{16} x_i \le 2 \\ & \sum_{i=17}^{24} x_i \le 2, \sum_{i=25}^{40} x_i \le 4 \\ & 0 \le \mathbf{x} \le 1. \end{cases}$$

- Continuous submodular optimization problem!
- Probabilities explicit here, could result from a blackbox process.

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Comparison

- Deterministic and randomized direct-search variants (dspfd).
- Budget: 200n evaluations (n = 40).

Results: Deterministic VS Randomized approach

- Best function value: Deterministic (0.96 VS 0.94).
- Sparser solution: Randomized (10 nonzero VS 25).
 ⇒ Randomized better at finding integer solutions!

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Lectures selected by randomized approach

- Course 1: Basics of Optimization, Gradient descent.
- Course 2: Basics of Optimization, Last year's exam.
- Course 3: Basics of Optimization, Lab gradient descent.
- Course 4: Optimality conditions, Advanced gradient descent, Stochastic gradient, Course homework.

Good coverage of the four topics (derivatives/convexity/algorithms/applications).

Summing up

Submodular optimization

- Discrete and continuous concepts!
- Applications in machine learning.

Summing up

Submodular optimization

- Discrete and continuous concepts!
- Applications in machine learning.

Direct search and concave maximization

- Existing algorithms for linearly constrained problems.
- Guarantees for concave and non-concave maximization.

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Our method for submodular optimization

- Guarantees even with adaptive stepsizes (under complete polling?)
- Encouraging behavior of randomized variants.

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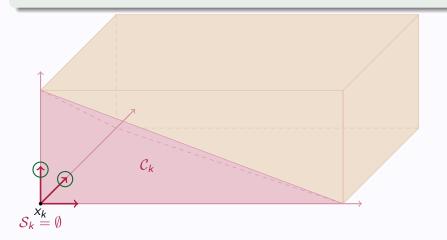
Thank you!

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Bonus: Randomized strategy for direct search

Decomposition $T(\mathbf{x}_k, \alpha_k) = C_k + S_k$

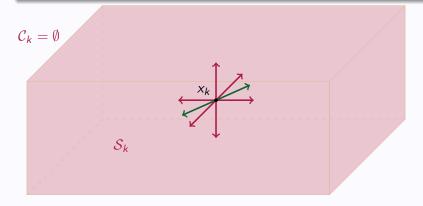
• In C_k : Random subset of generators.



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