Away-step Frank-Wolfe Method for Convex Optimization Involving a Log-Homogeneous Barrier

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where the stepsize $\alpha_k \geq 0$ is given by exact line-search.

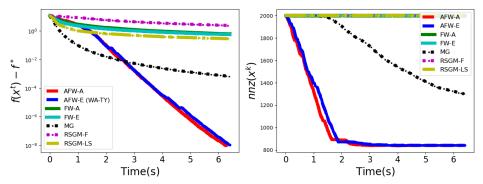
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- ▷ Excellent numerical performance:



ASFW-A & ASFW-E (this work): Away-step FW methods for LHB FW-A & FW-E [Fed72; Kha96; ZFce]: Generalized FW methods for LHB RSGM-F & RSGM-LS [BBT17; LFN18]: Relatively smooth gradient method MG [STT78]: Multiplicative gradient method

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- ▷ Some deeper questions:
 - What is the essential structure of (D-OPT) that drives the linear convergence of the WA-TY method (or the AFW method)?
 - Can it help us develop and analyze a new type of AFW methods for an "unconventional" class of problems?

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- ▶ In this work, we will provide affirmative answers to the questions above.

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Away-step FW for Log-Homogeneous Barrier

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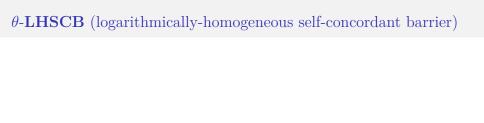
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- \triangleright Besides D-optimal design, other applications include
 - Budget-constrained D-optimal design
 - Positron emission tomography
 - (Reformulated) Poisson image deblurring with TV-regularization



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 - $|D^3 f(y)[w, w, w]| \le 2||w||_y^3 \quad \forall y \in \text{int } \mathcal{K}, \forall w \in \mathbb{Y},$
 - $(y_k) \to +\infty$ for any $\{y_k\}_{k\geq 1} \subseteq \operatorname{int} \mathcal{K}$ such that $y_k \to u \in \operatorname{bd} \mathcal{K}$,
 - 3 $f(ty) = f(y) \theta \ln(t) \quad \forall y \in \text{int } \mathcal{K}, \ \forall t > 0.$

where $||w||_y := \langle \nabla^2 f(y)w, w \rangle^{1/2}$ denotes the local norm of w at $y \in \operatorname{int} \mathcal{K}$.

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 - $(FW \text{ direction}) \text{ Compute } v^k \in \arg\min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle, \ d_F^k := v^k x^k \text{ and } G_k := \langle -\nabla F(x^k), d_F^k \rangle. \text{ If } G_k = 0, \text{ then STOP.}$

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- ▷ If $|\mathcal{V}| = \omega(n)$, we may prefer to maintain a compact representation of \mathcal{S}_k such that $|\mathcal{S}_k| = O(n)$ for $k \ge 0$, at computational cost of $O(n^2)$ per iteration [BS17].

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- ▷ For all applications of interest, computing $D_k = \|\mathsf{A}d^k\|_{y^k} = \langle \nabla^2 F(x^k)d^k, d^k \rangle^{1/2}$ takes O(n) times, instead of $O(n^2)$ time.

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Global linear convergence of $\{\delta_k\}_{k\geq 0}$:

- \triangleright $\{\delta_k\}_{k>0}$ is strictly decreasing (until termination).
- For all $k \geq 0$, define $k_{\text{eff}} := \lceil \max\{(k |\mathcal{S}_0| + q)/2, 0\} \rceil \approx k/2$, and then

$$\delta_k \le (1-\rho)^{k_{\text{eff}}} \delta_0$$
, where $\rho := \min \left\{ \frac{1}{5 \cdot 3(\delta_0 + \theta + B)}, \frac{\mu \Phi(\mathcal{X}, \mathcal{X}^*)^2}{42 \cdot 4(\theta + B)^2} \right\}$,

where

- μ is the quadratic-growth constant of f on \mathcal{Y} that only depends on $R_{\mathcal{Y}}(y^*)$
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- $\,\rhd\,$ All the quantities defining ρ are affine-invariant and norm-independent.

Global linear convergence of $\{G_k\}_{k\geq 0}$:

For some (affine-invariant) $\bar{D} < +\infty$ and all $k \geq 0$, we have

$$G_k \le \begin{cases} 4(1-\rho)^{k_{\text{eff}}} \delta_0 \max\{\bar{D}, 1\}, & \text{if } \delta_k > 1\\ 4\sqrt{1-\rho^{k_{\text{eff}}}} \sqrt{\delta_0} \max\{\bar{D}, 1\}, & \text{if } \delta_k \le 1 \end{cases}.$$

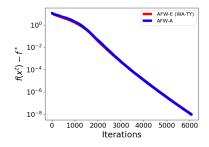
Essentially, this means $\{G_k\}_{k\geq 0}$ converges at the linear rate $\sqrt{1-\rho}$, which is worse than the rate of $\{\delta_k\}_{k\geq 0}$, namely $(1-\rho)$.

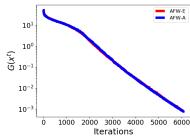
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Land on \mathcal{F} in finite iterations:

Let $\bar{k} \geq 0$ satisfy that

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For all $k \geq \bar{k}$, if $x^k \notin \mathcal{F}$, then

- $\triangleright \mathcal{S}_{k+1} \subseteq \mathcal{S}_k$, when either exact line-search or adaptive stepsize is used in Step 7,
- $\triangleright \mathcal{S}_{k+1} = \mathcal{S}_k \setminus \{a^k\}$ for some $a^k \in \mathcal{S}_k \cap \bar{\mathcal{V}}_{\mathcal{F}}$, when exact line-search is used in Step 7; otherwise, if $x^k \in \mathcal{F}$, then $x^l \in \mathcal{F}$ for all $l \geq k$.

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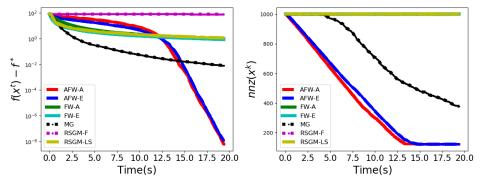
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Thank you!

References

- [BBT17] Heinz H. Bauschke, Jérôme Bolte, and Marc Teboulle. "A Descent Lemma Beyond Lipschitz Gradient Continuity: First-Order Methods Revisited and Applications". In: *Math. Oper. Res.* 42.2 (2017), pp. 330–348.
- [BS17] A. Beck and S. Shtern. "Linearly convergent away-step conditional gradient for non-strongly convex functions". In: Math. Program. 164 (2017), 1–27.
- [Cov84] T. Cover. "An algorithm for maximizing expected log investment return". In: IEEE Trans. Inf. Theory 30.2 (1984), pp. 369–373.
- [Dvu23] P. Dvurechensky et al. "Generalized self-concordant analysis of Frank-Wolfe algorithms". In: Math. Program. 198 (2023), 255—323.
- [Fed72] V. V. Fedorov. Theory of Optimal Experiments. Academic Press, 1972.
- [Kha96] Leonid G. Khachiyan. "Rounding of Polytopes in the Real Number Model of Computation". In: Math. Oper. Res. 21.2 (1996), pp. 307–320.
- [LFN18] Haihao. Lu, Robert M. Freund, and Yurii. Nesterov. "Relatively Smooth Convex Optimization by First-Order Methods, and Applications". In: SIAM J. Optim. 28.1 (2018), pp. 333–354.
- [LJJ15] Simon Lacoste-Julien and Martin Jaggi. "On the Global Linear Convergence of Frank-Wolfe Optimization Variants". In: Proc. NeurIPS. Montreal, Canada, 2015, 496—504.
- [PR19] Javier Peña and Daniel Rodríguez. "Polytope Conditioning and Linear Convergence of the Frank-Wolfe Algorithm". In: Math. Oper. Res. 44.1 (2019), pp. 1–18.
- [STT78] S.D. Silvey, D.H. Titterington, and B. Torsney. "An algorithm for optimal designs on a design space". In: Commun. Stat. Theory Methods 7.14 (1978), pp. 1379–1389.

References

- $[ZFce] & Renbo Zhao and Robert M. Freund. "Analysis of the Frank-Wolfe Method for Convex Composite Optimization involving a Logarithmically-Homogeneous Barrier". In: \\ \underline{Math.\ Program.\ (accepted,\ 2022)}.$
- [ZZS13] Ke Zhou, Hongyuan Zha, and Le Song. "Learning Social Infectivity in Sparse Low-rank Networks Using Multi-dimensional Hawkes Processes". In: Proc. AISTATS. 2013, pp. 641–649.