Approximate Frank-Wolfe Algorithms over Graph-structured Support Sets

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Graph-structured set:

 $\mathcal{D}(\mathcal{C}, \mathbb{M}) \triangleq \operatorname{conv} \{ \mathbf{x} : \|\mathbf{x}\|_2 \leq \mathcal{C}, \operatorname{supp}(\mathbf{x}) \in \mathbb{M} \}$ is a convex hull of interesting support sets described by \mathbb{M} , which contains a collection of allowed structures of the problem.

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Applications: Graph-structured compressive sensing, Gene-pathway finding, etc...

FW-type algorithm: $\mathbf{x}_{t+1} = \mathbf{x}_t + \eta_t (\rho \mathbf{v}_t - \mathbf{x}_t)$, where \mathbf{v}_t is the minimizer of *graph-structured LMO*

LMO:
$$\mathbf{v}_t \in \underset{\mathbf{v} \in \mathcal{D}(C, \mathbb{M})}{\operatorname{argmin}} \langle a\mathbf{x}_t + b\nabla f(\mathbf{x}_t), \mathbf{v} \rangle$$
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Fact: LMO is NP-hard to solve when $\mathcal{D}(C, \mathbb{M})$ is complex.

Approximate LMOs and adversarial examples

Additive approximate LMO[Dunn and Harshbarger, 1978] finds $\bar{\mathbf{v}}_t$: $\langle \nabla f(\mathbf{x}_t), \bar{\mathbf{v}}_t \rangle \leq \min_{\mathbf{v} \in \mathcal{D}} \langle \nabla f(\mathbf{x}_t), \mathbf{v} \rangle + \mathcal{O}(\frac{\epsilon}{t})$

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Multiplicative approximate LMO[Locatello et al., 2017] returns $\bar{\mathbf{v}}_t: \underbrace{\langle \nabla f(\mathbf{x}_t), \bar{\mathbf{v}}_t - \mathbf{x}_t \rangle}_{\bar{g}_t(\mathbf{x}_t)} \leq \delta \underbrace{\min_{\mathbf{v} \in \mathcal{D}} \langle \nabla f(\mathbf{x}_t), \mathbf{v} - \mathbf{x}_t \rangle}_{g_t(\mathbf{x}_t)}, \text{ where } \delta \in (0, 1].$

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$$\begin{split} \textbf{Multiplicative approximate LMO}[\text{Locatello et al., 2017}] \text{ returns} \\ \bar{\boldsymbol{v}}_t: \underbrace{\langle \nabla f(\boldsymbol{x}_t), \bar{\boldsymbol{v}}_t - \boldsymbol{x}_t \rangle}_{\bar{g}_t(\boldsymbol{x}_t)} \leq \delta \cdot \underbrace{\min_{\boldsymbol{v} \in \mathcal{D}} \langle \nabla f(\boldsymbol{x}_t), \boldsymbol{v} - \boldsymbol{x}_t \rangle}_{g_t(\boldsymbol{x}_t)}, \text{ where } \delta \in (0, 1]. \end{split}$$

Adversarial examples setup: We show that these two popular approximate LMOs are generally impractical to obtain. Suppose $\tau \in (0, 1/2)$ and $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\top}\mathbf{x} - \mathbf{x}^{\top}\mathbf{b}$, $\mathbf{b} = [1, 1, 1, 1, \tau, \cdots, \tau]^{\top}$. Take C = 1 and then the solution is $\mathbf{x}^* = [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, \dots, 0]^{\top}$ with $\nabla f(\mathbf{x}^*) = -[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \tau, \cdots, \tau]^{\top}$. When $\mathbf{x}_t = \mathbf{x}^*$, $\mathbf{v}_t = \mathbf{x}^*$, and the duality gap $g_t(\mathbf{x}^*) = 0$.

Gap-additive bound cannot decay properly: Any suboptimal \bar{v}_t gives $g_t(\mathbf{x}^*) - \bar{g}_t(\mathbf{x}^*) = 1 - \sqrt{\frac{3}{4} + \tau^2} > 0$, which is strictly positive and constant in t, hence violating additive approximate LMO.

Inner Product Operator (IPO): Given $z \in \mathbb{R}^d$, $\mathcal{D} \subseteq \mathbb{R}^d$, and approximation factor $\delta \in (0, 1]$, it returns v such that

$$(\delta, \boldsymbol{z}, \mathcal{D})$$
-IPO : $\langle \boldsymbol{z}, \boldsymbol{v} \rangle \leq \delta \cdot \min_{\boldsymbol{s} \in \mathcal{D}} \langle \boldsymbol{z}, \boldsymbol{s} \rangle$.

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Dual Maximization Oracle(DMO) finds an $S \in \mathbb{M}$ such that

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-DMO : $\|\boldsymbol{z}_{\mathcal{S}}\|_{2} \geq \delta \cdot \max_{\boldsymbol{S}' \in \mathbb{M}} \|\boldsymbol{z}_{\mathcal{S}'}\|_{2}.$

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Theorem (IPO ⇔ DMO)

Given the set \mathcal{D} and suppose $S \in (\delta, \mathbf{z}, \mathcal{D})$ -DMO. Define the approximate supporting vector $\tilde{\mathbf{v}}_t \triangleq -C \cdot \mathbf{z}_S / \|\mathbf{z}_S\|_2$. Then, $\tilde{\mathbf{v}}_t \in (\delta, \mathbf{z}, \mathcal{D})$ -IPO.

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DMO is easy to obtain: The method of **Top**-g + neighbor visiting provides $\delta = \sqrt{1/\lceil s/g \rceil}$.

Approximated DMO-FW

DMO-FW-I:

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \eta_t \left(\frac{C \cdot (\mathbf{z}_t)_{S_t}}{\|(\mathbf{z}_t)_{S_t}\|_2} - \mathbf{x}_t \right), S_t = (\delta, \nabla f(\mathbf{x}_t), \mathcal{D})$$
-DMO
DMO-FW-II $(\mathbf{x}_t \in \mathcal{D}/\delta)$: $\mathbf{x}_{t+1} = \mathbf{x}_t + \eta_t \left(\frac{C \cdot (\mathbf{z}_t)_{S_t}}{\delta \cdot \|(\mathbf{z}_t)_{S_t}\|_2} - \mathbf{x}_t \right)$.

Theorem (Convergence Rate of DMO-FW)

Let $s = \max_{S \in \mathbb{M}} |S|$ be the maximal allowed sparsity. Suppose $\nu \in (0, 1]$ and $\|\nabla f(\mathbf{x})\|_{\infty} \leq B$, DMO-FW-I admits

$$h(\boldsymbol{x}_t) \triangleq f(\boldsymbol{x}_t) - f(\boldsymbol{x}^*) \leq \begin{cases} \mathcal{O}\left(\frac{BC\sqrt{s}}{t^{\nu}}\right), & \|\nabla f(\boldsymbol{x}_t)\|_{\infty} \leq \frac{B}{t^{\nu}} \\ \mathcal{O}\left(\frac{BC\sqrt{s}(1-\delta)}{\delta}\right), & Otherwise. \end{cases}$$

Furthermore,

DMO-FW-II
$$(\mathbf{x}_t \in \mathcal{D}/\delta)$$
 : $h(\mathbf{x}_t) \leq \frac{8LC^2}{\delta^2(t+2)}$.

Acceleration: DMO-AccFW

DMO-AccFW (Inspired from Garber and Wolf [2021]):

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Quadratic Growth Condition: Exist a constant $\mu > 0$ such that

$$f(\mathbf{x}) - f(\mathbf{x}^*) \geq \frac{\mu}{2} \|\mathbf{x} - [\mathbf{x}]_{\mathcal{X}^*}\|_2^2, \forall \mathbf{x} \in \mathcal{D}, [\mathbf{x}]_{\mathcal{X}^*} \triangleq \operatorname*{argmin}_{\mathbf{z} \in \mathcal{X}^*} \|\mathbf{z} - \mathbf{x}\|_2^2.$$

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Theorem (Main result)

Assume further that \mathbf{x}^* is on the boundary and $\delta = 1$, for all $t \ge 1$, the primal error of DMO-AccFW satisfies

$$h(\mathbf{x}_t) \leq \frac{4e^{4L/\mu}h(\mathbf{x}_0)}{(t+2)^2}$$



Experimental evaluation

Graph-structured linear sensing: Recover a graph-sparse model \tilde{x}^* using measurements generated as

$$\mathbf{y} = \langle \mathbf{A}, \tilde{\mathbf{x}}^* \rangle + \mathbf{e}, \qquad \mathbf{e} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_d).$$

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- We prove that the DMO is equivalent to the IPO. The standard FW admits $\mathcal{O}((1-\delta)\sqrt{s}/\delta)$ in worst case and our accelerated version has rate $\mathcal{O}(1/t^2)$.
- Initial experiments indicate that inexact FW-type methods are attractive for this type of problems and one is encouraged to find faster methods based on fully-corrective or other methods.

Code and datasets: https://github.com/baojian/dmo-fw