~~Breaking the cycle~~: Flexible block-iterative analysis for the Frank-Wolfe algorithm

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Flexible Block-Coordinate Frank-Wolfe Algorithm

1. Motivation
2. Our approach
3. Analysis
4. Numerical experiments

Problem setting

Given m nonempty closed convex sets $C_i \subset \mathbb{R}^{n_i}$ with $i \in \{1, \ldots, m\} =: I$ and a smooth function $f: \mathbb{R}^N \to \mathbb{R}$ with $N = \sum_{i \in I} n_i$, solve

$$\underset{\boldsymbol{x} \in C_1 \times \ldots \times C_m}{\text{minimize}} \quad f(\boldsymbol{x}). \tag{1}$$

Applications: matrix factorization, SVM training, sequence labeling, splitting, ...

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Two families of first-order methods to solve (1): projection methods and Frank-Wolfe AKA "CG" methods, which use linear minimization oracles.

$$\mathrm{proj}_C(\boldsymbol{x}) = \underset{\boldsymbol{v} \in C}{\mathrm{Argmin}} \, \|\boldsymbol{x} - \boldsymbol{v}\|^2 \qquad \mathrm{LMO}_C(\boldsymbol{x}) \in \underset{\boldsymbol{v} \in C}{\mathrm{Argmin}} \, \langle \boldsymbol{x} \mid \boldsymbol{v} \rangle \tag{2}$$

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[Combettes/Pokutta, '21]: For many $\underbrace{\text{constraints}}$, C, proj_C is **more expensive** than LMO_C.
(e.g., nuclear norm ball, ℓ_1 ball, probability simplex, Birkhoff polytope, general LP, ...)

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For $\boldsymbol{x} \in \mathbb{R}^N$ with components $\boldsymbol{x} = (\boldsymbol{x}^1, \ldots, \boldsymbol{x}^m)$ $(\boldsymbol{x}_i \in \mathbb{R}^{n_i})$,

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"Let's avoid computing so many LMOs per iteration!" (paraphrased)

– [Patriksson, '98], [Lacoste-Julien et al., 2013], [Beck et al., 2015], [Wang et al., 2016], [Osokin et al., 2016], [Bomze et al., 2024], ...

(Generic) BCFW Algorithm

Known modes of convergence:

for $t = 0, 1$ **to** $\dots$ **do**
  Select $I_t \subset \{1, \dots, m\}$
  $\boldsymbol{g}_t \leftarrow \nabla f(\boldsymbol{x}_t)$
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    if $i \in I_t$ **then**
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- [Patriksson, 1998]:
  - Asymptotic convergence if f convex
  - Exact and Armijo linesearches fixed across all components $\gamma_t^i = \gamma_t$
  - Full update $(I_t = \{1, \ldots, m\})$
  - Deterministic essentially cyclic $(\exists K > 0)$:

$$I_t = \{\mathrm{i}_t\}, \text{ with } \{\mathrm{i}_t, \ldots, \mathrm{i}_{t+K}\} = \{1, \ldots, m\}$$

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- [Beck et al., 2015]:
  - $\mathcal{O}(1/t)$ convergence (f convex)
  - open-loop, short-step, and backtracking γ_t^i
  - Deterministic cyclic updates

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- Stochastic variants:
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- [Bomze et al., 2024]:
  - Linear convergence (KL condition $+ \cdots$)
  - Short-Step Chain (SSC) procedure: γ_t^i, $\boldsymbol{v}_t^i$
  - Full updates ($I_t = \{1, \ldots, m\}$)
  - Uniform singleton selection ($I_t = \{\mathrm{i}_t\}$)
  - Gauss-Southwell “greedy” singleton updates (based on suboptimality criterion).

Let's recap. . .

- Singleton updates:

  $\rightarrow$ cyclic, essentially cyclic, Gauss-Southwell, (uniform or non-uniform) random

- Parallel updates:

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- **deterministic** parallel updates?
- blocks with **different sizes**?
- **cost-aware** methodologies? (e.g., if some LMOs are numerically expensive, and others are cheap)

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A bit of history

Assumption

There exists a positive integer K such that, for every iteration t,

$$(\forall 1 \leqslant i \leqslant m) \quad i \in \bigcup_{n=t}^{t+K-1} I_n. \tag{$\star$}$$

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  $\rightarrow$ We can set the ratio of $\dfrac{\text{(expensive LMO evals)}}{\text{(cheap LMO evals)}} = \dfrac{1}{K}$ arbitrarily small.

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Apparently **never considered for F-W algorithms** before!?

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Goals

Under Assumption $(\star)$, establish competitive convergence rates.

What we did:

- f convex: $\mathcal{O}(K/t)$ rate (for primal gap) using:
  - Short-step γ_t^i
  - An adaptive stepsize scheme γ_t^i
- f nonconvex: $\mathcal{O}(K/\sqrt{t})$ rate (for F-W optimality gap) using short-step γ_t^i
- Some conjectures and interesting analysis along the way. . .

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Frank Wolfe gaps

Recall $I = \{1, \ldots, m\}$. The **Frank-Wolfe gap** at $\boldsymbol{x} \in \mathbb{R}^N$ is

$$G_I(\boldsymbol{x}) = \langle \nabla f(\boldsymbol{x}) \mid \boldsymbol{x} - \mathrm{LMO}_{\times_{i \in I} C_i}(\nabla f(\boldsymbol{x})) \rangle$$

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Fact

(A) If $\boldsymbol{x} \in \times_{i\in I} C_i$, then $(\forall J \subset I) \quad G_J(\boldsymbol{x}) \geqslant 0$.

(B) $\boldsymbol{x}$ is a stationary point of (1) if and only if $\boldsymbol{x} \in \times_{i\in I} C_i$ and $G_I(x) = 0$.

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$\Rightarrow$ nonconvex convergence results typically show **first order criticality**: $G_I(\boldsymbol{x}_t) \to 0$.

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Smoothness and short-steps

For $L_f > 0$, the function f is L_f-**smooth** on a convex set C if

$$(\forall \boldsymbol{x}, \boldsymbol{y} \in C) \quad f(\boldsymbol{y}) - f(\boldsymbol{x}) \leqslant \langle \nabla f(\boldsymbol{x}) \mid \boldsymbol{y} - \boldsymbol{x} \rangle + \frac{L_f}{2} \|\boldsymbol{y} - \boldsymbol{x}\|^2.$$

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For BCFW, this means

$$f(\boldsymbol{x}_{t+1}) - f(\boldsymbol{x}_t) \leqslant \sum_{i \in I_t} \gamma_t^i \underbrace{\langle \nabla^i f(\boldsymbol{x}_t) \mid \boldsymbol{v}_t^i - \boldsymbol{x}_t^i \rangle}_{-G_i(\boldsymbol{x}_t)} + \frac{L_f}{2} (\gamma_t^i)^2 \|\boldsymbol{v}_t^i - \boldsymbol{x}_t^i\|^2.$$

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To tighten the inequality, the stepsize

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is known as the componentwise **short step**. Downside: requires upper-estimate of L_f.

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Fact (Hazan & Luo, 2016)

Let f be convex and L_f-smooth. Then,

$$(\forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^N) \quad f(\boldsymbol{x}) - f(\boldsymbol{y}) - \langle \nabla f(\boldsymbol{y}) \mid \boldsymbol{x} - \boldsymbol{y} \rangle \geqslant \frac{\|\nabla f(\boldsymbol{x}) - \nabla f(\boldsymbol{y})\|^2}{2L_f}.$$

Adaptive step-size algorithm for convex functions

Typical adaptive setup [Pedregosa et al., 2020], [Pokutta, 2023]:

1. Update γ_t^i based on an estimated the smoothness constant $\widetilde{M}$.
2. If (2*) holds between $\boldsymbol{x}_t$ and $\boldsymbol{x}_{t+1}$: done.
3. Else, increase $\widetilde{M} \leftarrow \tau\widetilde{M}$ by $\tau > 1$ and recompute $\boldsymbol{x}_{t+1}$ until (2*) holds.

Pros: No a-priori knowledge of L_f; sometimes we get larger steps.

Cons: Extra function and/or gradient evaluations.

Fact (Hazan & Luo, 2016)

Let f be convex and L_f-smooth. Then, for $\widetilde{M}$ sufficiently large,

$$f(\boldsymbol{x}_t) - f(\boldsymbol{x}_{t+1}) - \langle \nabla f(\boldsymbol{x}_{t+1}) \mid \boldsymbol{x}_t - \boldsymbol{x}_{t+1} \rangle \geqslant \frac{\|\nabla f(\boldsymbol{x}_t) - \nabla f(\boldsymbol{x}_{t+1})\|^2}{2\widetilde{M}}. \tag{2*}$$

Progress lemma

Lemma (Progress bound via smoothness and convexity, short-step)

Let $\bigtimes_{i\in I} C_i \subset \mathcal{H}$ be a product of m nonempty compact convex sets, let f be convex and L_f-smooth, let D be the diameter of $\bigtimes_{i\in I} C_i$, and assume $(\star)$. Let $\boldsymbol{x}^*$ solve (1), and set $H_t = f(\boldsymbol{x}_t) - f(\boldsymbol{x}^*)$. Then

$$H_t - H_{t+K} \geqslant \begin{cases} H_t + A_t - \frac{KL_f D^2}{2}, & \text{if } H_t + A_t \geqslant KL_f D^2; \\ \dfrac{(H_t + A_t)^2}{2KL_f D^2}, & \text{if } H_t + A_t \leqslant KL_f D^2, \end{cases} \text{ where}$$

$$A_t = \sum_{k=1}^{K-1} G_{\underbrace{I_{t+k-1} \cap (I_{t+k} \cup \cdots \cup I_{t+K-1})}_{J_k}}(\boldsymbol{x}_{t+k}) \geqslant 0$$

A_t describes partial F-W gaps for **all re-activated components**.

Progress lemma

Lemma (Progress bound via smoothness and convexity, short-step)

Let $\bigtimes_{i\in I} C_i \subset \mathcal{H}$ be a product of m nonempty compact convex sets, let f be convex and L_f-smooth, let D be the diameter of $\bigtimes_{i\in I} C_i$, and assume $(\star)$. Let $\boldsymbol{x}^*$ solve (1), and set $H_t = f(\boldsymbol{x}_t) - f(\boldsymbol{x}^*)$. Then

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A_t may explain good behavior in experiments.

Progress lemma

Lemma (Progress bound via smoothness and convexity, short-step)

Let $\times_{i\in I} C_i \subset \mathcal{H}$ be a product of m nonempty compact convex sets, let f be convex and L_f-smooth, let D be the diameter of $\times_{i\in I} C_i$, and assume $(\star)$. Let $\boldsymbol{x}^*$ solve (1), and set $H_t = f(\boldsymbol{x}_t) - f(\boldsymbol{x}^*)$. Then

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$$A_t = \sum_{k=1}^{K-1} G_{\underbrace{I_{t+k-1} \cap (I_{t+k} \cup \cdots \cup I_{t+K-1})}_{J_k}}(\boldsymbol{x}_{t+k}) \geqslant \sum_{k=1}^{K-1} f(\boldsymbol{x}_{t+k}) - \min_{\substack{\boldsymbol{x}\in\times_{i\in I} C_i \\ \boldsymbol{x}^{I\setminus J_k} = \boldsymbol{x}_{t+k}^{I\setminus J_k}}} f(\boldsymbol{x}) \geqslant 0.$$

We don't know how to leverage A_ts for an improved rate!

Progress lemma

Lemma (Progress bound via smoothness and convexity, adaptive step size strategy)

Let $\bigtimes_{i\in I} C_i \subset \mathcal{H}$ be a product of m nonempty compact convex sets, let f be convex and L_f-smooth, let D be the diameter of $\bigtimes_{i\in I} C_i$, let $0 < \eta \leqslant 1 < \tau$ and $M_0 > 0$, and assume $(\star)$. Let $\boldsymbol{x}^*$ solve (1), and set $H_t = f(\boldsymbol{x}_t) - f(\boldsymbol{x}^*)$. Then

$$H_t - H_{t+K} \geqslant \begin{cases} H_t + A_t - \frac{K\max\{\eta^t M_0, \tau L_f\} D^2}{2}, & \text{if } H_t + A_t \geqslant K\max\{\eta^t M_0, \tau L_f\} D^2; \\ \frac{(H_t + A_t)^2}{2K\max\{\eta^t M_0, \tau L_f\} D^2}, & \text{if } H_t + A_t \leqslant K\max\{\eta^t M_0, \tau L_f\} D^2, \end{cases}$$

$$A_t = \sum_{k=1}^{K-1} G_{\underbrace{I_{t+k-1} \cap (I_{t+k} \cup \cdots \cup I_{t+K-1})}_{J_k}}(\boldsymbol{x}_{t+k}) \geqslant \sum_{k=1}^{K-1} f(\boldsymbol{x}_{t+k}) - \min_{\substack{\boldsymbol{x}\in \bigtimes_{i\in I} C_i \\ \boldsymbol{x}^{I\setminus J_k} = \boldsymbol{x}_{t+k}^{I\setminus J_k}}} f(\boldsymbol{x}) \geqslant 0.$$

A_t describes partial F-W gaps for **all re-activated components**.

Convex setting: flexible stepsizes

Theorem

Let $\bigtimes_{i\in I} C_i \subset \mathcal{H}$ be a product of m nonempty compact convex sets, let f be convex and L_f-smooth, let $\tau > 1 \geqslant \eta$ and $M_0 > 0$ be approximation parameters, let D be the diameter of $\bigtimes_{i\in I} C_i$, let $\boldsymbol{x}_0 \in \mathbb{R}^N$, let $\boldsymbol{x}^*$ solve (1), and assume ($\star$). Set $n_0 := \max\{\lceil \log(\tau L_f/(\eta M_0))/(K \log \eta)\rceil, 0\}$. Then,

$$f(\boldsymbol{x}_{nK}) - f(\boldsymbol{x}^*) \leqslant \begin{cases} \min\limits_{0\leqslant p\leqslant n-1} \left\{ \dfrac{K\eta^{pK} M_0 D^2}{2} - A_{pK} \right\} & \text{if } 1 \leqslant n \leqslant n_0 + 1 \\ \dfrac{2K\tau L_f D^2}{n - n_0 + \sum_{p=n_0}^{n} \frac{2A_{pK}}{f(\boldsymbol{x}_{n_0}) - f(\boldsymbol{x}^*)} + \left(\frac{A_{pK}}{f(\boldsymbol{x}_{n_0}) - f(\boldsymbol{x}^*)}\right)^2} & \text{if } n > n_0 + 1. \end{cases}$$

After t iterations, Adaptive-BCFW has evaluated f and ∇f at-most $2 + \lceil \log_\tau(L_f/\eta^t M_0)\rceil$ times.

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After t iterations, Adaptive-BCFW has evaluated f and ∇f at-most $2 + \lceil \log_\tau (L_f/\eta^t M_0)\rceil$ times.

$\rightarrow$ After t iterations, matches $\mathcal{O}(K/t)$ rate for convex cyclic setting

Corollary: Parallelized short-step BCFW

Corollary

Let $\bigtimes_{i \in I} C_i \subset \mathcal{H}$ be a product of m nonempty compact convex sets, let f be convex and L_f-smooth, let D be the diameter of $\bigtimes_{i \in I} C_i$, let $\boldsymbol{x}^*$ solve (1), and assume ($\star$). Then,

$$(\forall n \in \mathbb{N}) \quad f(\boldsymbol{x}_{nK}) - f(\boldsymbol{x}^*) \leqslant \begin{cases} \dfrac{KL_f D^2}{2} - A_0 & \text{if } n = 1 \\ \dfrac{2KL_f D^2}{n - 1 + \sum_{p=1}^{n} \frac{2A_{pK}}{f(\boldsymbol{x}_1) - f(\boldsymbol{x}^*)} + \left(\frac{A_{pK}}{f(\boldsymbol{x}_1) - f(\boldsymbol{x}^*)}\right)^2} & \text{if } n \geqslant 2. \end{cases}$$

Furthermore, Short-step BCFW requires one gradient evaluation per iteration.

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Furthermore, Short-step BCFW requires one gradient evaluation per iteration.

→ Matches rate **and** constant for non-block Short-step FW.

→ Easier to parallelize than Adaptive BCFW.

Nonconvex convergence

Theorem (Nonconvex convergence)

Let $\bigtimes_{i\in I} C_i \subset \mathcal{H}$ be a product of m nonempty compact convex sets with diameter D. Let ∇f be L_f-Lipschitz continuous on $\bigtimes_{i\in I} C_i$, set $H_0 = f(\boldsymbol{x}_0) - \inf f(\bigtimes_{i\in I} C_i)$. Suppose that $(\star)$ holds. Then, for every $n \in \mathbb{N}$, Short-step BCFW guarantees

$$\min_{0\leqslant p\leqslant n-1} G_I(\boldsymbol{x}_{pK}) \leqslant \frac{1}{n}\sum_{p=0}^{n-1} G_I(\boldsymbol{x}_{pK}) \leqslant \begin{cases} \frac{2H_0 - \sum_{p=0}^{n-1} A_{pK}}{n} + \frac{KL_f D^2}{2} & \text{if } n \leqslant \frac{2H_0}{KL_f D^2} \\ 2D\sqrt{\frac{H_0 K L_f}{n}} - \frac{\sum_{p=0}^{n-1} A_{pK}}{n} & \text{otherwise.} \end{cases}$$

In particular, there exists a subsequence $(n_k)_{k\in\mathbb{N}}$ such that $G_I(\boldsymbol{x}_{n_k K}) \to 0$, and every accumulation point of $(\boldsymbol{x}_{n_k K})_{k\in\mathbb{N}}$ is a stationary point of (1).

$\to$ Reactivated gap terms reappear!

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$\to$ Reactivated gap terms reappear!

$\to$ After t iterations, minimal F-W gap converges like $\mathcal{O}(K/\sqrt{t})$.

Flexible Block-Coordinate Frank-Wolfe Algorithm

Experiments

Toy intersection problem (convex)

Find a matrix in the intersection of the spectrahedron $C_1 = \{X \in \mathbb{S}_+^{r\times r} \mid \mathrm{Trace}(X) = 1\}$ and the hypercube $C_2 = [-5, \mu]^{r\times r}$ ($\mu = 1/r$).

$$\underset{\boldsymbol{x}\in C_1\times C_2}{\text{minimize}} \ \frac{1}{2}\|\boldsymbol{x}^1 - \boldsymbol{x}^2\|^2$$

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$$\underset{\boldsymbol{x}\in C_1\times C_2}{\text{minimize}} \ \frac{1}{2}\|\boldsymbol{x}^1 - \boldsymbol{x}^2\|^2$$

→ LMO_{C_1} is far more expensive than LMO_{C_2}.

→ We use Short-step BCFW to compare the following block activations: full, cyclic, permuted-cyclic, and "q-lazy":

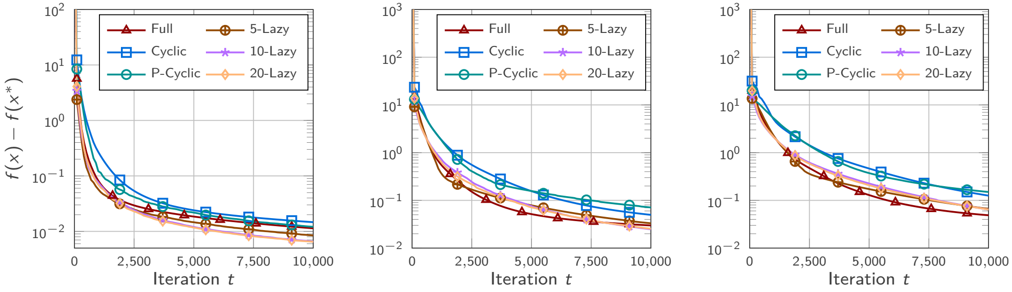
$$(\forall t \in \mathbb{N}) \quad I_t = \begin{cases} \{1,2\} & \text{if } t \equiv 0 \mod q; \\ \{2\} & \text{otherwise.} \end{cases} \tag{q-Lazy}$$

Experiments

Toy intersection problem (convex)

comparing block-activations: full, cyclic, permuted-cyclic, and

$$\underset{\boldsymbol{x}\in C_1\times C_2}{\text{minimize}} \ \frac{1}{2}\|\boldsymbol{x}^1-\boldsymbol{x}^2\|^2 \qquad (\forall t\in\mathbb{N}) \quad I_t=\begin{cases}\{1,2\} & \text{if } t\equiv 0 \mod q;\\ \{1\} & \text{otherwise.}\end{cases} \qquad (q\text{-lazy})$$



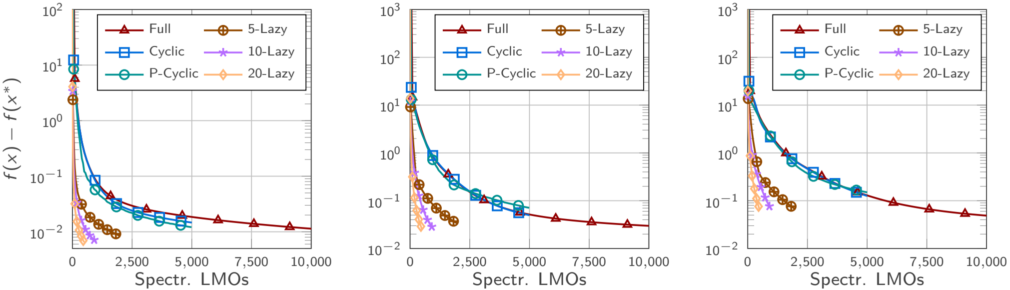
(a) $r=100$ (b) $r=300$ (c) $r=500$

Experiments

Toy intersection problem (convex)

comparing block-activations: full, cyclic, permuted-cyclic, and

$$\underset{\boldsymbol{x}\in C_1\times C_2}{\text{minimize}}\ \frac{1}{2}\|\boldsymbol{x}^1-\boldsymbol{x}^2\|^2 \qquad (\forall t\in\mathbb{N})\quad I_t=\begin{cases}\{1,2\} & \text{if } t\equiv 0 \mod q;\\ \{1\} & \text{otherwise.}\end{cases} \qquad (q\text{-lazy})$$



(d) $r=100$ (e) $r=300$ (f) $r=500$

Experiments

Toy intersection problem (convex)

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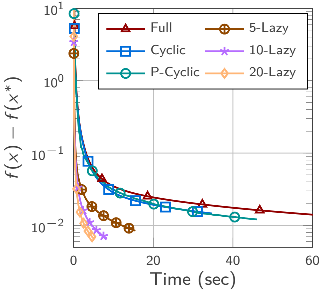
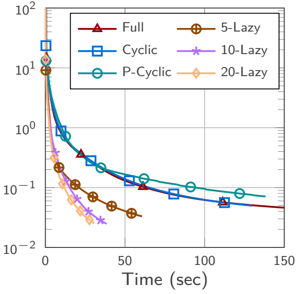
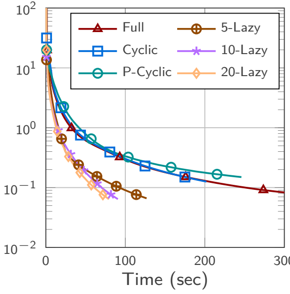
$$\underset{\boldsymbol{x}\in C_1\times C_2}{\text{minimize}} \ \frac{1}{2}\|\boldsymbol{x}^1-\boldsymbol{x}^2\|^2 \qquad (\forall t\in\mathbb{N}) \quad I_t=\begin{cases}\{1,2\} & \text{if } \ t\equiv 0 \mod q;\\ \{1\} & \text{otherwise.}\end{cases} \qquad (q\text{-lazy})$$



(g) $r=100$



(h) $r=300$



(i) $r=500$

Experiments

Toy Difference-of-Convex quadratic problem

Find a $2r \times r$ matrix such that its first $r \times r$ submatrix satisfies $\|X\|_\infty \leqslant 1$, and its second submatrix satisfies $\|X\|_{\text{nuc}} \leqslant 1$. To investigate BCFW when the number of components is large, we set $C_1 = \ldots = C_r = \{x \in \mathbb{R}^r \mid \|x\|_\infty \leqslant 1\}$ and $C_{r+1} = \{X \in \mathbb{R}^{r \times r} \mid \|X\|_{\text{nuc}} \leqslant 1\}$. For PSD $2r \times r$ matrices A and B, we seek to solve

$$\underset{\boldsymbol{x} \in \bigtimes_{1 \leqslant i \leqslant r+1} C_i}{\text{minimize}} \ \langle [x] \mid [x]A \rangle - \langle [x] \mid [x]B \rangle$$

$\rightarrow$ For each instance, we verify $A - B$ is indefinite.

$\rightarrow$ Problem is nonseparable

Experiments

Toy Difference-of-Convex quadratic problem

→ $\mathrm{LMO}_{C_{r+1}}$ is far more expensive than $(\mathrm{LMO}_{C_i})_{1\leqslant i\leqslant r}$.

→ We use Short-step BCFW to compare the following block activations: full, cyclic, permuted-cyclic, and "(p, q)-lazy":

$$(\forall t \in \mathbb{N}) \quad I_t = \begin{cases} I & \text{if } \; t \equiv 0 \pmod{q} \\ \{i_1, \ldots, i_p\} \subset_R I \setminus \{r+1\} & \text{otherwise.} \end{cases} \qquad ((p,q)\text{-Lazy})$$

Full update every q iterations; otherwise, update a random subset of p "cheap" coordinates in parallel.

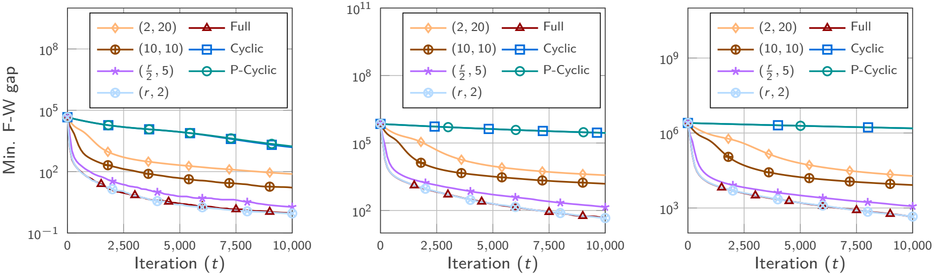
Experiments

Toy Difference-of-Convex quadratic problem

comparing full, cyclic, perm.-cyclic, and "(p, q)-lazy":

$$\underset{x \in \times_{1 \leqslant i \leqslant r+1} C_i}{\text{minimize}} \ \langle [x] \mid [x]A \rangle - \langle [x] \mid [x]B \rangle$$

$$I_t = \begin{cases} I & \text{if } t \equiv 0 \pmod{q} \\ \{i_1, \dots, i_p\} \subset_R I \setminus \{r+1\} & \text{otherwise.} \end{cases}$$



(j) $r = 100$ (k) $r = 300$ (l) $r = 500$

Experiments

Toy Difference-of-Convex quadratic problem

comparing full, cyclic, perm.-cyclic, and "(p, q)-lazy":

$$\underset{\boldsymbol{x} \in \bigtimes_{1 \leqslant i \leqslant r+1} C_i}{\text{minimize}} \ \langle [x] \mid [x]A \rangle - \langle [x] \mid [x]B \rangle$$

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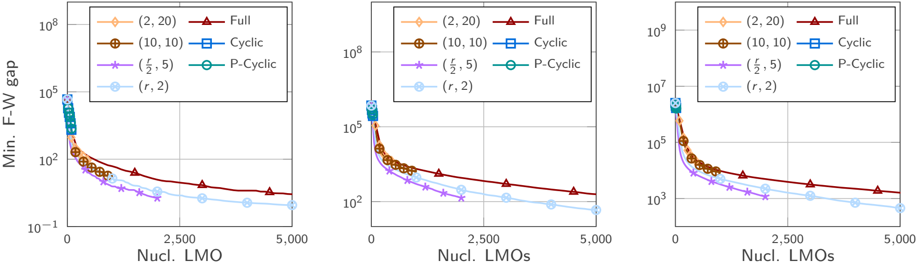

(m) $r = 100$ (n) $r = 300$ (o) $r = 500$

Experiments

Toy Difference-of-Convex quadratic problem

comparing full, cyclic, perm.-cyclic, and "(p, q)-lazy":

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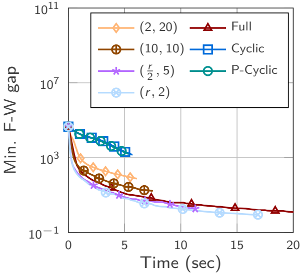
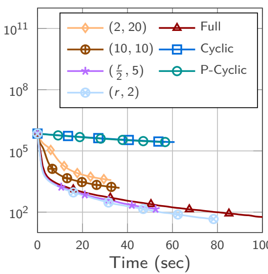
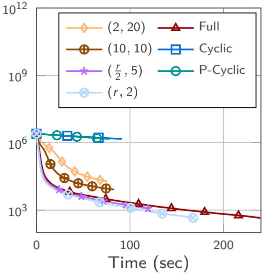


(p) $r = 100$



(q) $r = 300$



(r) $r = 500$

Thank you for your attention!

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