Frank-Wolfe with New and Practical Descent Directions

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Zuse Institute Berlin and TU Berlin
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Outline

Introduction

Consider

$$\begin{aligned} &\min\ f(x) \\ &\text{s.t. } x \in \mathcal{C} \end{aligned}$$

where

- $\mathcal{C} \subset \mathbb{R}^n$ is a compact convex set
- $f : \mathbb{R}^n \to \mathbb{R}$ is a smooth convex function

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Example

- Sparse logistic regression

$$\min_{x \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^{m} \ln(1 + \exp(-y_i \langle a_i, x \rangle))$$
$$\text{s.t. } \|x\|_1 \leqslant \tau$$

- Low-rank matrix completion

$$\min_{X \in \mathbb{R}^{m \times n}} \frac{1}{2|\mathcal{I}|} \sum_{(i,j) \in \mathcal{I}} (Y_{i,j} - X_{i,j})^2$$
$$\text{s.t. } \|X\|_{\text{nuc}} \leqslant \tau$$

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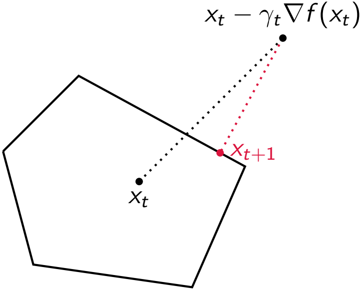

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Feasible region $\mathcal{C}$	**Linear minimization**	**Projection**
$\ell_1/\ell_2/\ell_\infty$-ball	$\mathcal{O}(n)$	$\mathcal{O}(n)$
ℓ_p-ball, $p \in \,]1, \infty[\, \setminus \{2\}$	$\mathcal{O}(n)$	N/A
Nuclear norm-ball	$\mathcal{O}(\text{nonzeros})$	$\mathcal{O}(mn \min\{m, n\})$
Flow polytope	$\mathcal{O}(n)$	$\mathcal{O}(n^{3.5})$
Birkhoff polytope	$\mathcal{O}(n^3)$	N/A
Matroid polytope	$\mathcal{O}(n \ln(n))$	$\mathcal{O}(\text{poly}(n))$

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- Can we avoid projections?

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The Frank-Wolfe algorithm (Frank & Wolfe, 1956) a.k.a. conditional gradient algorithm (Levitin & Polyak, 1966):

Algorithm Frank-Wolfe (FW)

Input: $x_0 \in \mathcal{C}$, $\gamma_t \in [0, 1]$.

1: **for** $t = 0$ **to** $T - 1$ **do**

2: $\quad v_t \leftarrow \arg\min_{v \in \mathcal{C}} \langle \nabla f(x_t), v \rangle$

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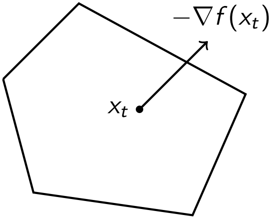

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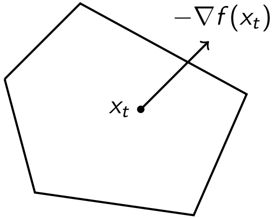

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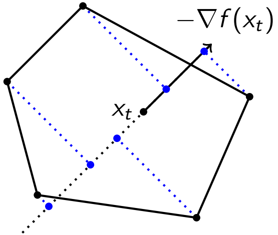

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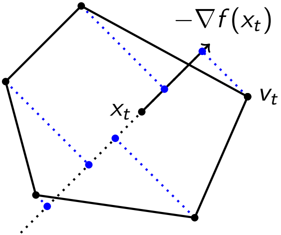

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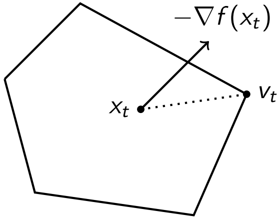

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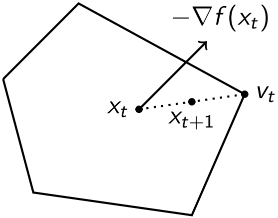

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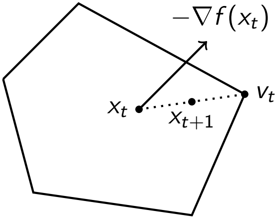

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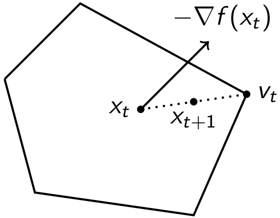

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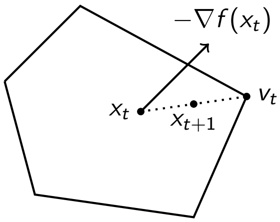

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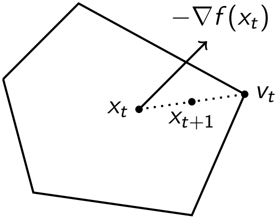

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- Successfully applied to: traffic assignment, computer vision, optimal transport, adversarial learning, etc.

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Theorem (Levitin & Polyak, 1966; Jaggi, 2013)

Let $\mathcal{C} \subset \mathbb{R}^n$ *be a compact convex set with diameter* D *and* $f : \mathbb{R}^n \to \mathbb{R}$ *be a* L*-smooth convex function, and let* $x_0 \in \arg\min_{v \in \mathcal{C}} \langle \nabla f(y), v \rangle$ *for some* $y \in \mathcal{C}$*. If* $\gamma_t = \frac{2}{t+2}$ *(default) or* $\gamma_t = \min\left\{\frac{\langle \nabla f(x_t), x_t - v_t \rangle}{L\|x_t - v_t\|^2}, 1\right\}$ *("short step"), then*

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- Why?

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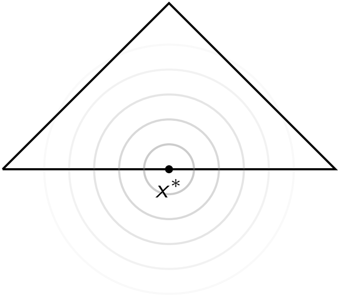
and $x^* = \begin{pmatrix}0\\0\end{pmatrix}$



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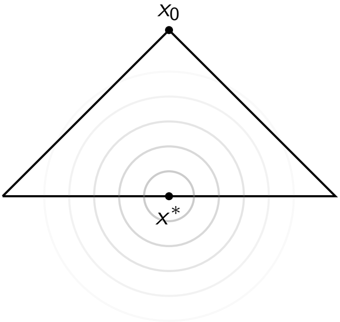

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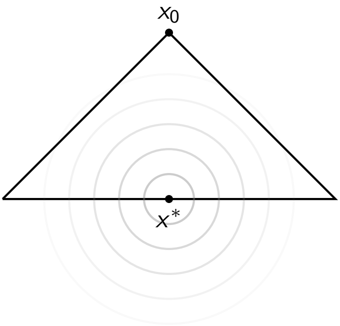

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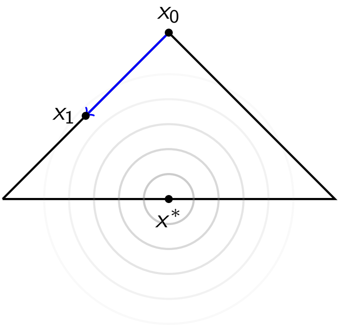

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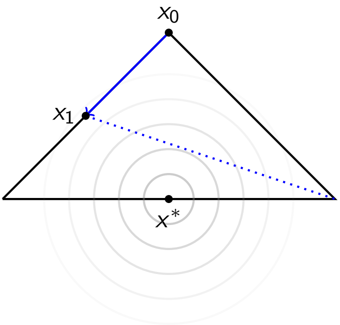

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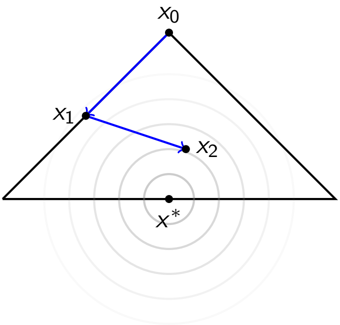

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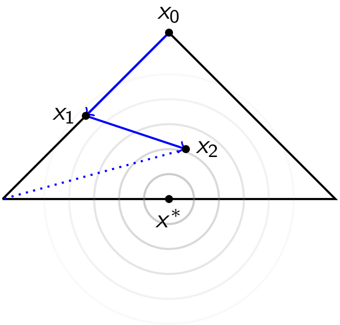

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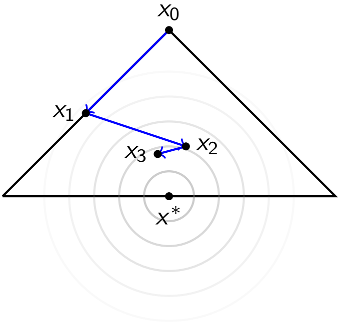

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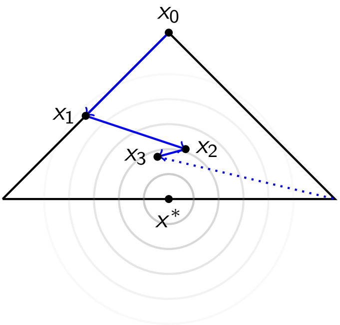

- Let $x_0 = \begin{pmatrix}0\\1\end{pmatrix}$
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The Frank-Wolfe algorithm

Consider the simple problem

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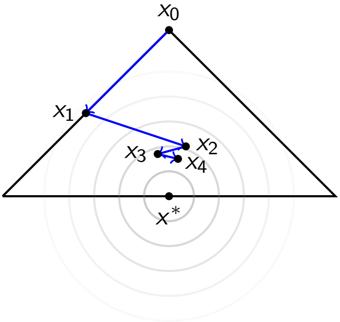

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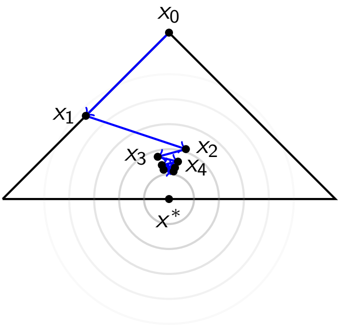

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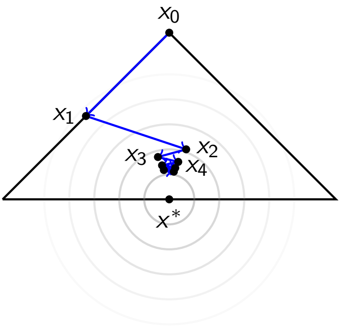

- Let $x_0 = \begin{pmatrix}0\\1\end{pmatrix}$
- FW tries to reach x^* by moving towards vertices
- This yields an inefficient zig-zagging trajectory

Improved Frank-Wolfe variants

- Away-Step Frank-Wolfe (AFW) (Wolfe, 1970; Lacoste-Julien & Jaggi, 2015): enhances FW by allowing to move away from vertices

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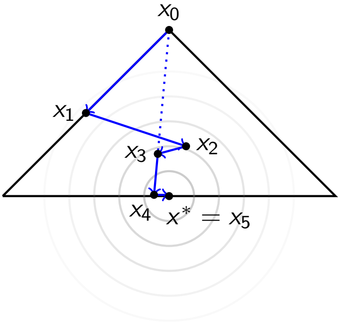

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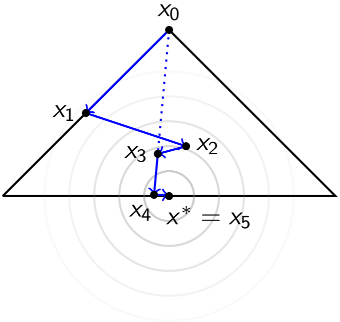

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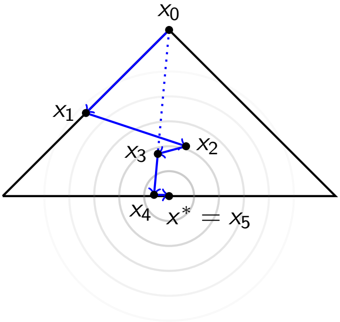

- Decomposition-Invariant Pairwise Conditional Gradient (DICG) (Garber & Meshi, 2016): memory-free variant of AFW
- Blended Conditional Gradients (BCG) (Braun et al., 2019): blends FCFW and FW

Boosting Frank-Wolfe

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Idea (C & Pokutta, 2020):

- Speed up FW by moving in a direction better aligned with $-\nabla f(x_t)$
- Build this direction by using $\mathcal{C}$ to maintain the projection-free property

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- How can we build a direction better aligned with $-\nabla f(x_t)$ and that allows to update x_{t+1} without projection?

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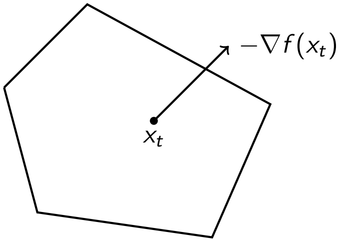

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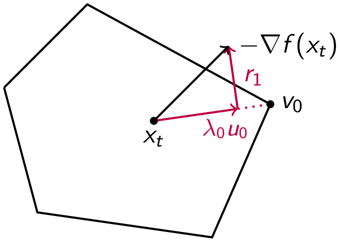

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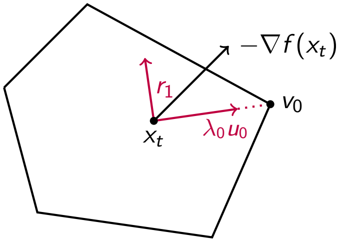

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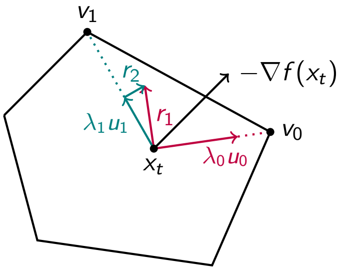

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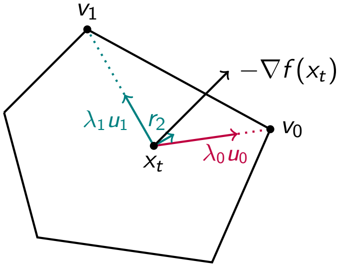

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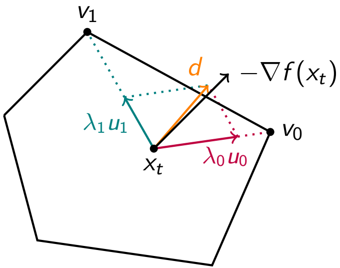

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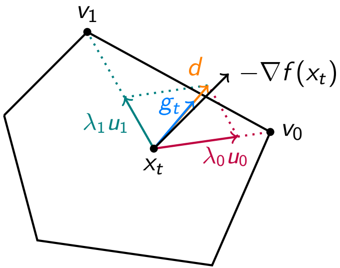

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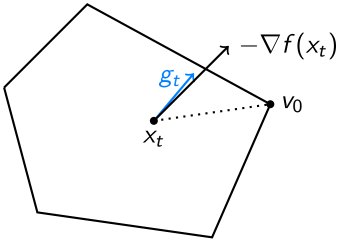

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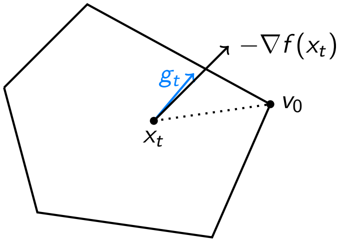

- The boosted direction g_t is better aligned with $-\nabla f(x_t)$ than is the FW direction $v_0 - x_t$ and satisfies $[x_t, x_t + g_t] \subseteq \mathcal{C}$ so we can update

$$x_{t+1} = x_t + \gamma_t g_t \quad \text{for any } \gamma_t \in [0, 1]$$

Boosting Frank-Wolfe

Why $[x_t, x_t + g_t] \subseteq \mathcal{C}$? Let K_t be the number of alignment rounds. We have

$$d = \sum_{k=0}^{K_t-1} \lambda_k (v_k - x_t) \quad \text{where } \lambda_k > 0 \text{ and } v_k \in \mathcal{C}$$

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Thus, $x_t + g_t \in \mathcal{C}$ so $[x_t, x_t + g_t] \subseteq \mathcal{C}$ by convexity

Boosting Frank-Wolfe

Algorithm Finding a direction g *well* aligned with ∇ from a reference point z

Input: $z \in \mathcal{C}$, $\nabla \in \mathbb{R}^n$, $K \in \mathbb{N}\backslash\{0\}$, $\delta \in]0,1[$.

$d_0 \leftarrow 0$, $\Lambda \leftarrow 0$
for $k = 0$ **to** $K - 1$ **do**
  $r_k \leftarrow \nabla - d_k$ ▷ k-th residual
  $v_k \leftarrow \arg\max_{v \in \mathcal{C}} \langle r_k, v \rangle$ ▷ FW oracle
  $u_k \leftarrow \arg\max_{u \in \{v_k - z, -d_k/\|d_k\|\}} \langle r_k, u \rangle$
  $\lambda_k \leftarrow \langle r_k, u_k \rangle / \|u_k\|^2$
  $d'_k \leftarrow d_k + \lambda_k u_k$
  if $\operatorname{align}(\nabla, d'_k) - \operatorname{align}(\nabla, d_k) \geqslant \delta$ **then**
    $d_{k+1} \leftarrow d'_k$
    $$\Lambda_t \leftarrow \begin{cases} \Lambda + \lambda_k & \textbf{if } u_k = v_k - z \\ \Lambda(1 - \lambda_k/\|d_k\|) & \textbf{if } u_k = -d_k/\|d_k\| \end{cases}$$
  else
    break ▷ exit k-loop
$g \leftarrow d_k/\Lambda$ ▷ normalization

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- Technicality to ensure convergence of the procedure (Locatello et al., 2017)

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- Technicality to ensure convergence of the procedure (Locatello et al., 2017)
- The stopping criterion is an alignment improvement condition (typically $\delta = 10^{-3}$ and $K = +\infty$)

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Input: $x_0 \in \mathcal{C}$, $\gamma_t \in [0,1]$.

1: **for** $t = 0$ **to** $T-1$ **do**

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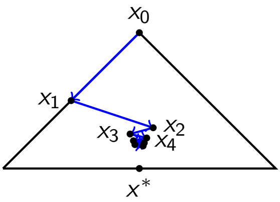

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Input: $x_0 \in \mathcal{C}$, $\gamma_t \in [0,1]$, $K \in \mathbb{N} \backslash \{0\}$, $\delta \in]0,1[$.

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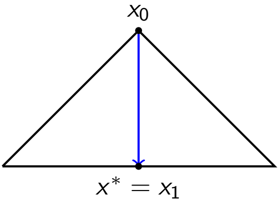

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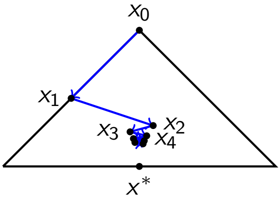

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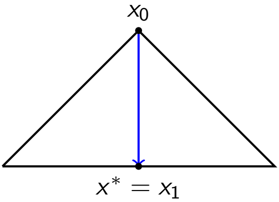

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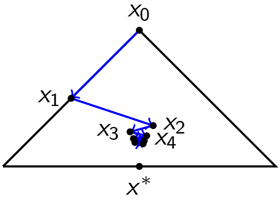

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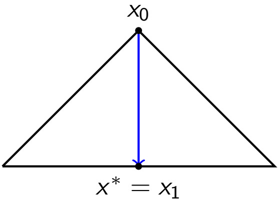

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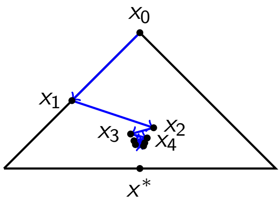

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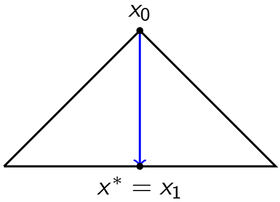

- What is the convergence rate of BoostFW?
- Is BoostFW expensive in practice?
- How does it compare to the state-of-the-art?

Boosting Frank-Wolfe

- Let N_t be the number of iterations up to t where at least 2 rounds of alignment were performed (FW = always 1 round)

Theorem (C & Pokutta, 2020)

Let $\mathcal{C} \subset \mathbb{R}^n$ be a compact convex set with diameter D and $f : \mathbb{R}^n \to \mathbb{R}$ be a L-smooth, convex, and μ-gradient dominated function, and let $x_0 \in \arg\min_{v \in \mathcal{C}} \langle \nabla f(y), v \rangle$ for some $y \in \mathcal{C}$. Set $\gamma_t = \min\left\{\frac{\langle -\nabla f(x_t), g_t \rangle}{L\|g_t\|^2}, 1\right\}$ ("short step") and suppose that $N_t \geqslant \omega t$. Then

$$f(x_t) - \min_{\mathcal{C}} f \leqslant \frac{LD^2}{2} \exp\left(-\delta^2 \frac{\mu}{L} \omega t\right)$$

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- Else, BoostFW reduces to FW and the convergence rate is $\frac{4LD^2}{t+2}$
- In practice, $N_t \approx t$ (so $\omega \lesssim 1$)

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$$\begin{aligned} \min_{x\in\mathbb{R}^{|\mathcal{A}|}} \;& \sum_{a\in\mathcal{A}} \tau_a x_a \left(1+0.03\left(\frac{x_a}{c_a}\right)^4\right) && \\ \text{s.t. } x_a &= \sum_{r\in\mathcal{R}} \mathbb{1}_{\{a\in r\}} y_r && a\in\mathcal{A} \\ & \sum_{r\in\mathcal{R}_{i,j}} y_r = d_{i,j} && (i,j)\in\mathcal{S} \\ & y_r \geqslant 0 && r\in\mathcal{R}_{i,j},\ (i,j)\in\mathcal{S} \end{aligned}$$

$$\begin{aligned} \min_{x\in\mathbb{R}^n} \;& \frac{1}{m}\sum_{i=1}^{m} \ln(1+\exp(-y_i\langle a_i,x\rangle)) \\ \text{s.t. } & \|x\|_1 \leqslant \tau \end{aligned}$$

$$\begin{aligned} \min_{X\in\mathbb{R}^{m\times n}} \;& \frac{1}{|\mathcal{I}|}\sum_{(i,j)\in\mathcal{I}} h_\rho(Y_{i,j}-X_{i,j}) \\ \text{s.t. } & \|X\|_{\text{nuc}} \leqslant \tau \end{aligned}$$

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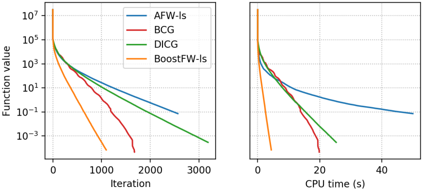
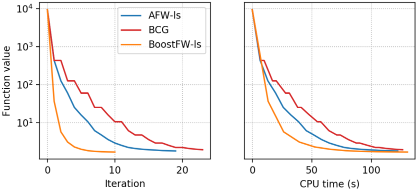
- For BoostFW and AFW we also run the line search-free variants (the "short step" strategy) and label them with an "L"

Computational experiments

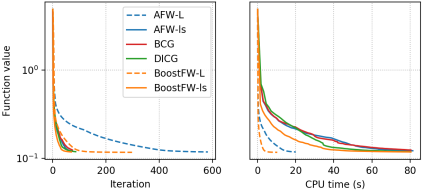
- Sparse signal recovery



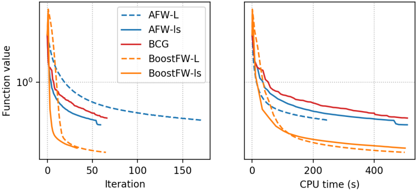
- Traffic assignment



- Sparse logistic regression on the Gisette dataset

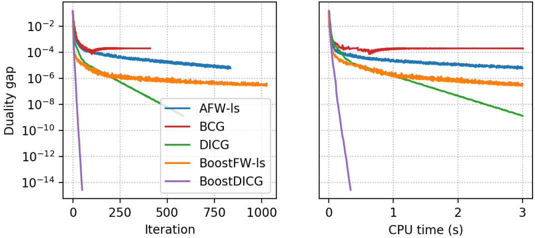


- Collaborative filtering on the MovieLens 100k dataset



Boosting DICG

- DICG is known to perform particularly well on the video co-localization experiment (YouTube-Objects dataset)
- BoostDICG: application of our method to DICG



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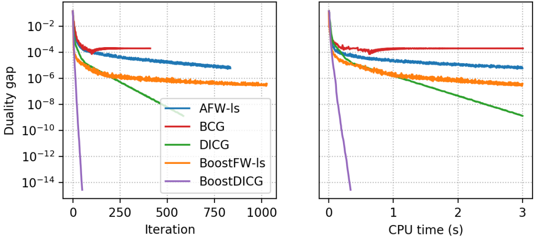

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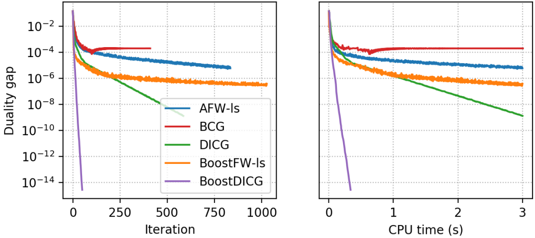

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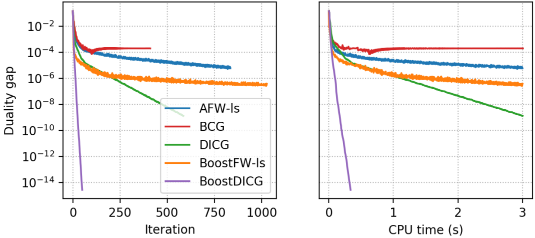

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- Although it performs more linear minimizations per iteration, the progress obtained greatly overcomes their cost
- The boosting procedure can be applied to any descent direction $-d_t$ (obtained from, e.g., momentum acceleration, stochasticity, etc.):

$$
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Large-scale optimization

Consider

$$\min \left\{ f(x) := \frac{1}{m} \sum_{i=1}^{m} f_i(x) \right\}$$
$$\text{s.t. } x \in \mathcal{C}$$

where

- $\mathcal{C} \subset \mathbb{R}^n$ is a compact convex set
- $f_1, \ldots, f_m \colon \mathbb{R}^n \to \mathbb{R}$ are smooth (non)convex functions
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Computing $f(x)$ or $\nabla f(x)$ is too expensive

- Cannot use line search
- More efficient to use an estimator $\tilde{\nabla} f(x)$ to get approximate (but cheap) gradient information

Stochastic Frank-Wolfe algorithms

Template Stochastic Frank-Wolfe

Input: $x_0 \in \mathcal{C}$, $\gamma_t \in [0, 1]$.

1: **for** $t = 0$ **to** $T - 1$ **do**

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Typical analysis: let $\varepsilon_t := f(x_t) - \min_{\mathcal{C}} f$, then by smoothness, convexity, and Cauchy-Schwarz,

$$\mathrm{E}[\varepsilon_{t+1}] \leqslant (1 - \gamma_t)\mathrm{E}[\varepsilon_t] + \gamma_t \mathrm{E}[\|\tilde{\nabla} f(x_t) - \nabla f(x_t)\|] D + \frac{L}{2}\gamma_t^2 D^2$$

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To obtain $\mathrm{E}[\varepsilon_t] = \mathcal{O}(1/t)$, we need $\mathrm{E}[\|\tilde{\nabla} f(x_t) - \nabla f(x_t)\|^2] = \mathcal{O}(1/t^2)$

Stochastic Frank-Wolfe algorithms

- The *vanilla* Stochastic Frank-Wolfe algorithm (SFW) estimates the gradient by averaging over a minibatch of size b_t:

$$\tilde{\nabla} f(x_t) \leftarrow \frac{1}{b_t} \sum_{i=i_1}^{i_{b_t}} \nabla f_i(x_t) \quad \text{where} \quad i_1, \ldots, i_{b_t} \overset{\text{i.i.d.}}{\sim} \mathcal{U}([\![1, m]\!])$$

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This estimator is unbiased and its variance is bounded by

$$\mathrm{E}[\|\tilde{\nabla} f(x_t) - \nabla f(x_t)\|^2] \leqslant \frac{G^2}{b_t} \quad \text{where} \quad G := \max_{i \in [\![1,m]\!]} \max_{x \in \mathcal{C}} \|\nabla f_i(x)\|$$

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- See also, e.g., Shen et al. (2019), Yurtsever et al. (2019), Xie et al. (2020), Zhang et al. (2020), Négiar et al. (2020)

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CSFW	$\tilde{\nabla} f(x_{t-1}) + \sum_{i=i_1}^{i_{b_t}} \left(\frac{1}{m} f_i'(\langle a_i, x_t\rangle) - [\alpha_{t-1}]_i\right) a_i$
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Simultaneously proposed by Duchi et al. (2011) and McMahan & Streeter (2010):

Algorithm Adaptive Gradient (AdaGrad)

Input: $x_0 \in \mathcal{C}$, $\delta > 0$, $\eta > 0$.

1: **for** $t = 0$ **to** $T - 1$ **do**

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Larger step-sizes are given to infrequent (but potentially very informative) features whenever they appear so that they do not go unnoticed. This adjusts the trajectory of the iterates

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as did FW for unconstrained gradient descent (for which $G_t = \nabla f(x_t)$)?

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  as did FW for unconstrained gradient descent (for which $G_t = \nabla f(x_t)$)?

- We would likely lose the precious properties of the descent directions of AdaGrad

Frank-Wolfe with adaptive gradients

- Instead, consider the constrained subproblem occurring at every iteration:

$$x_{t+1} \leftarrow \arg\min_{x \in \mathcal{C}} \eta \langle \tilde{\nabla} f(x_t), x \rangle + \frac{1}{2} \|x - x_t\|_{H_t}^2$$

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- We claim that leveraging just a small amount of information from the adaptive metric H_t is enough

Frank-Wolfe with adaptive gradients

Template Frank-Wolfe with adaptive gradients

Input: $x_0 \in \mathcal{C}$, $0 < \lambda_t^- \leqslant \lambda_{t+1}^- \leqslant \lambda_{t+1}^+ \leqslant \lambda_t^+$, $K \in \mathbb{N}\backslash\{0\}$, $\eta > 0$, $\gamma_t \in [0,1]$.

for $t = 0$ **to** $T-1$ **do**
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- AdaX depending on the strategy for $\tilde{\nabla} f(x_t)$: AdaSFW, AdaSVRF, etc.

Frank-Wolfe with adaptive gradients

Theorem (C et al., 2020)

Let $\mathcal{C} \subset \mathbb{R}^n$ be a compact convex set with diameter D and $f_1, \ldots, f_m \colon \mathbb{R}^n \to \mathbb{R}$ be L-smooth convex functions. Then AdaSFW with $b_t \leftarrow \big(G(t+2)/(LD)\big)^2$, $\eta_t \leftarrow \lambda_t^-/L$, and $\gamma_t \leftarrow 2/(t+2)$ satisfies

$$\mathbb{E}[f(x_t)] - \min_{\mathcal{C}} f \leqslant \frac{2LD^2(K+1+\kappa)}{t+1}$$

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- Also no need for λ_t^-, λ_t^+ and can set η_t to a constant value
- AdaSVRF and AdaCSFW also yield $\mathcal{O}(1/t)$ convergence
- If $f_1, \ldots, f_m$ are nonconvex, then AdaSFW converges to a stationary point at a rate $\mathcal{O}(1/\sqrt{t})$

Computational experiments

- We compare our method to SFW, SVRF, SPIDER-FW, ORGFW, and CSFW on a wide range of experiments

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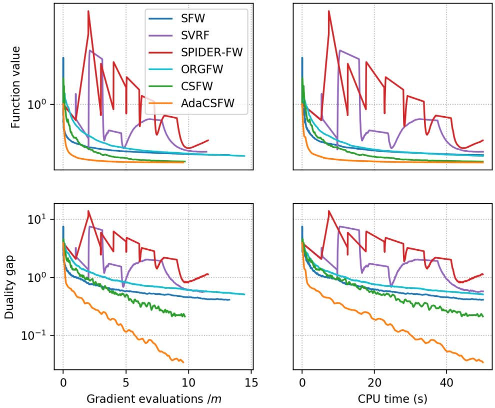
- We set $K \sim 5$

Support vector classification on a synthetic dataset

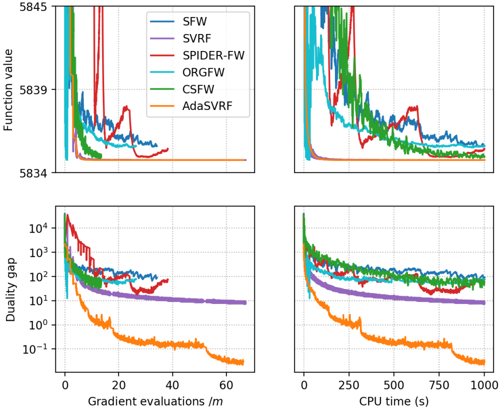
$$\min_{x \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^{m} \max\{0, 1 - y_i \langle a_i, x \rangle\}^2$$

$$\text{s.t. } \|x\|_\infty \leqslant \tau$$



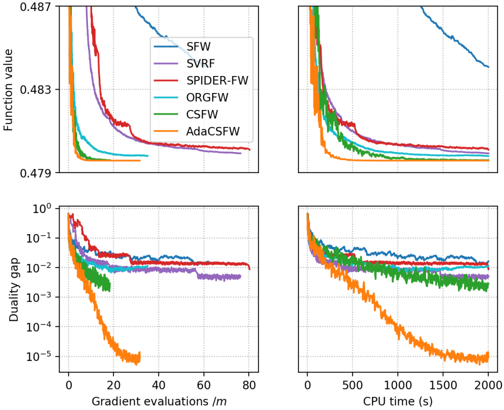
Linear regression on the YearPredictionMSD dataset

$$\min_{x\in\mathbb{R}^n} \frac{1}{m}\sum_{i=1}^{m}(y_i - \langle a_i, x\rangle)^2$$
$$\text{s.t. } \|x\|_1 \leqslant \tau$$



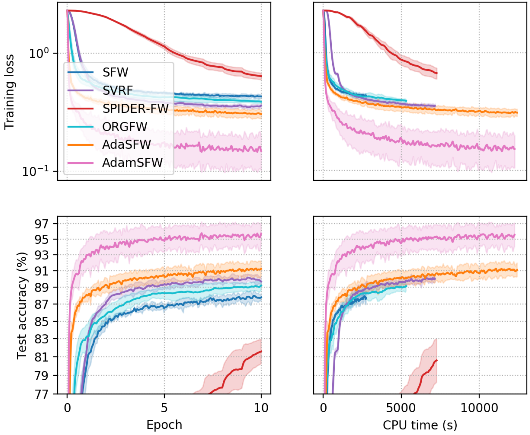
Logistic regression on the RCV1 dataset

$$\min_{x \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^{m} \ln(1 + \exp(-y_i \langle a_i, x \rangle))$$
$$\text{s.t. } \|x\|_1 \leqslant \tau$$



Convolutional neural network on the MNIST dataset

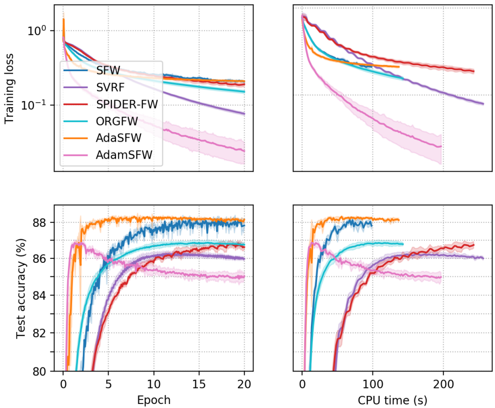
- Each layer of the neural network is constrained into an ℓ_1-ball



- AdamSFW strongly outperforms the other methods

Neural network with one hidden layer on the IMDB dataset

- Each layer is constrained into an ℓ_∞-ball



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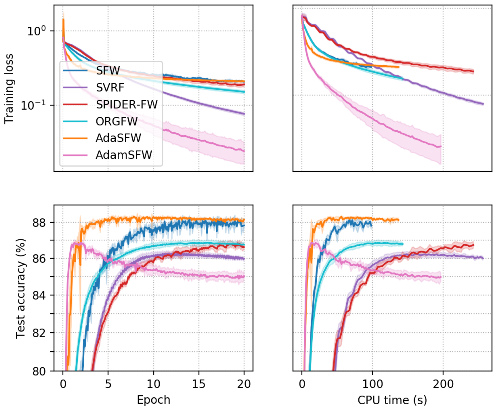

- AdaSFW and AdamSFW are the only ones to outperform SFW

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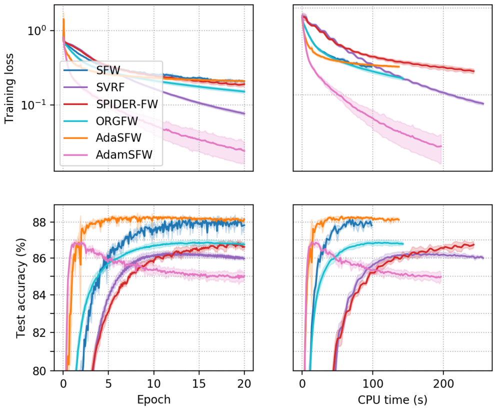

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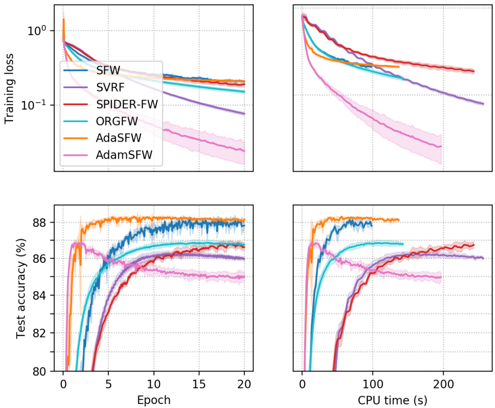

- AdaSFW and AdamSFW are the only ones to outperform SFW
- AdamSFW reaches its maximum test accuracy very fast (good for early stopping)
- AdaSFW yields the best test performance, despite optimizing slowly over the training set

Convolutional network on the CIFAR-10 dataset

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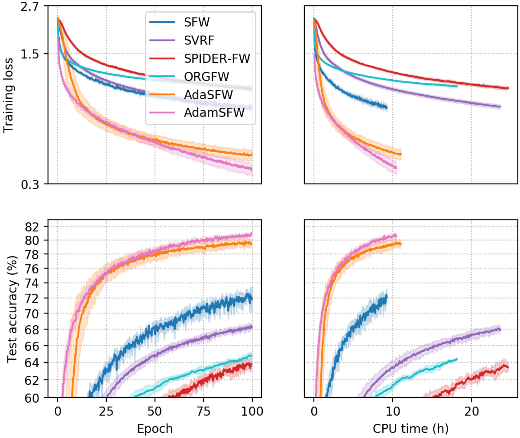

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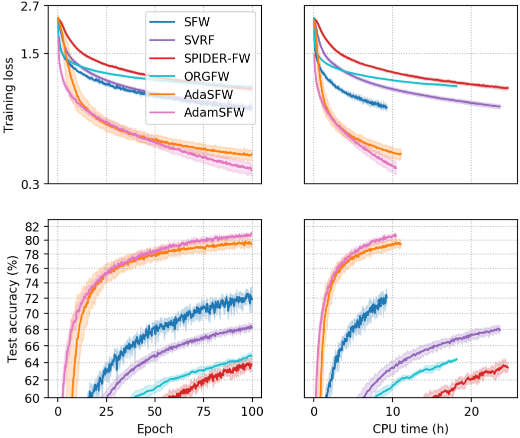

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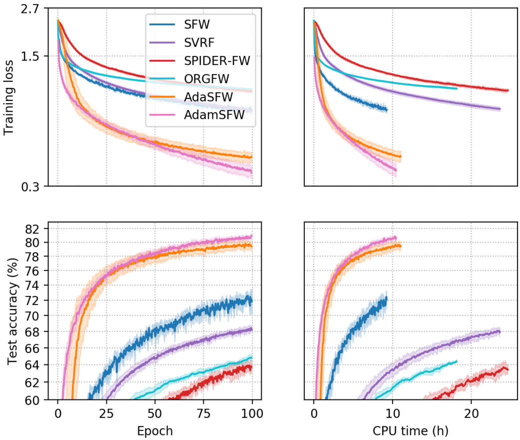

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Thank you!

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