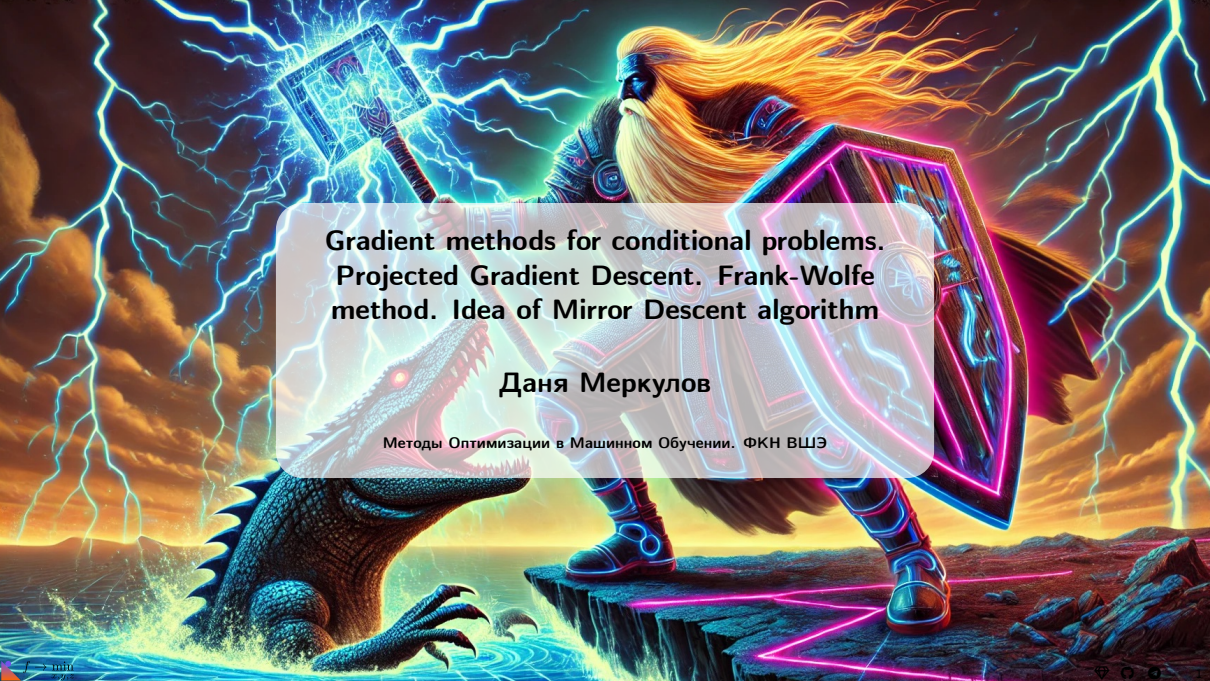

Gradient methods for conditional problems. Projected Gradient Descent. Frank-Wolfe method. Idea of Mirror Descent algorithm

Даня Меркулов

Методы Оптимизации в Машинном Обучении. ФКН ВШЭ

Conditional methods

Constrained optimization

Unconstrained optimization

$$\min_{x \in \mathbb{R}^n} f(x)$$

- Any point $x_0 \in \mathbb{R}^n$ is feasible and could be a solution.

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Gradient Descent is a great way to solve unconstrained problem

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k) \tag{GD}$$

Is it possible to tune GD to fit constrained problem?

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Is it possible to tune GD to fit constrained problem?

Yes. We need to use projections to ensure feasibility on every iteration.

Example: White-box Adversarial Attacks

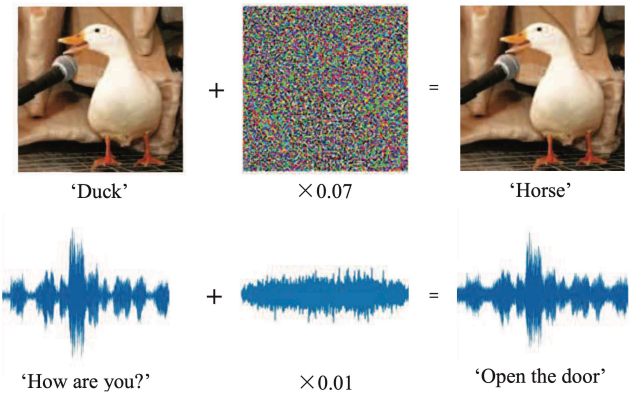

Figure 1: Source

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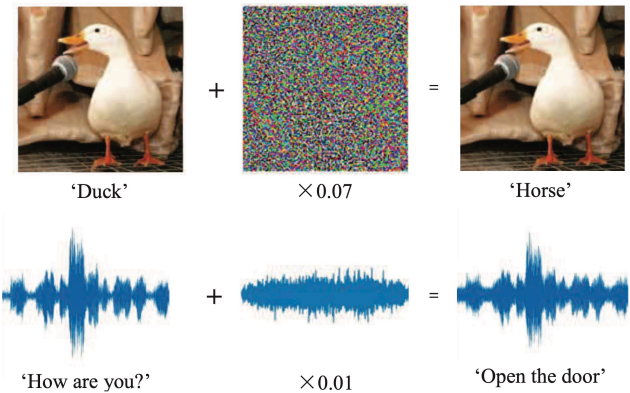

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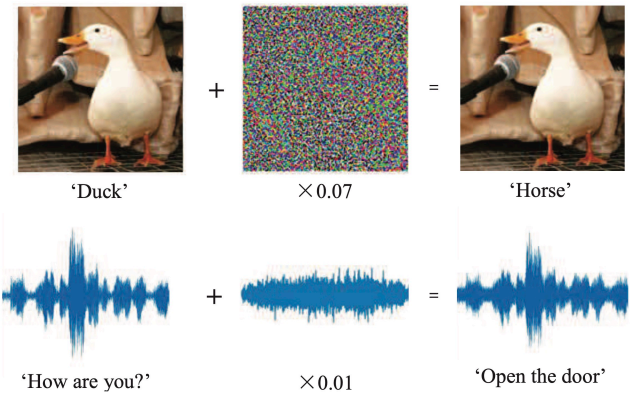

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- Mathematically, a neural network is a function $f(w; x)$
- Typically, input x is given and network weights w optimized
- Could also freeze weights w and optimize x, adversarially!

$$\min_{\delta} \text{size}(\delta) \quad \text{s.t.} \quad \text{pred}[f(w; x+\delta)] \neq y$$

or

$$\max_{\delta} l(w; x+\delta, y) \text{ s.t. } \text{size}(\delta) \leq \epsilon,\ 0 \leq x+\delta \leq 1$$

Idea of Projected Gradient Descent

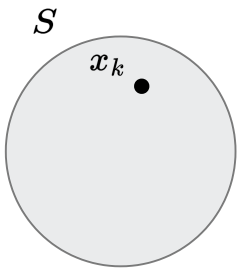

Figure 2: Suppose, we start from a point x_k.

Idea of Projected Gradient Descent

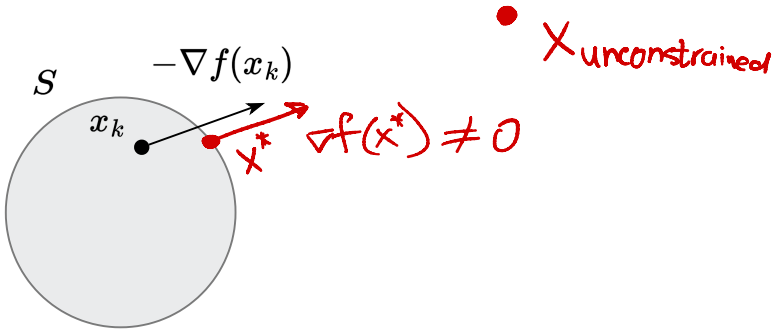

Figure 3: And go in the direction of $-\nabla f(x_k)$.

Idea of Projected Gradient Descent

$$y_k = x_k - \alpha_k \nabla f(x_k)$$

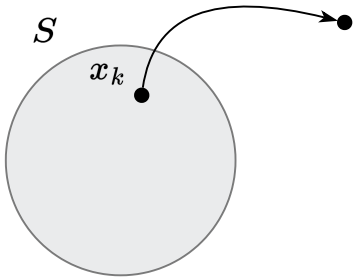

Figure 4: Occasionally, we can end up outside the feasible set.

Idea of Projected Gradient Descent

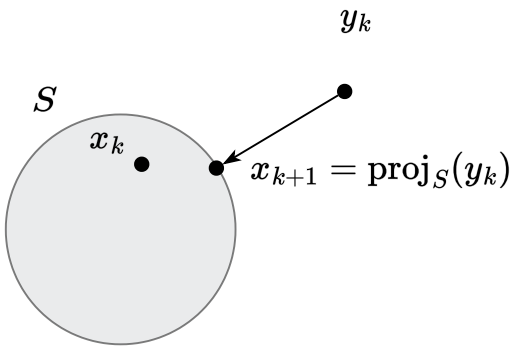

Figure 5: Solve this little problem with projection!

Idea of Projected Gradient Descent

$$x_{k+1} = \text{proj}_S\left(x_k - \alpha_k \nabla f(x_k)\right) \quad \Leftrightarrow \quad \begin{aligned} y_k &= x_k - \alpha_k \nabla f(x_k) \\ x_{k+1} &= \text{proj}_S\left(y_k\right) \end{aligned}$$

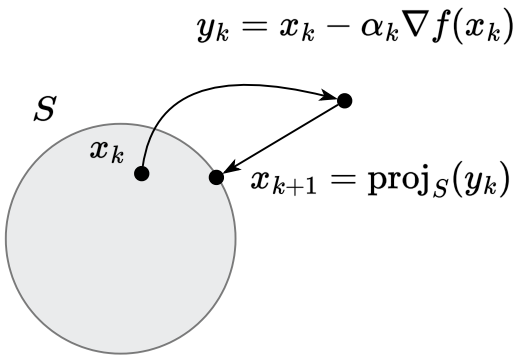

Figure 6: Illustration of Projected Gradient Descent algorithm

Projection

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The distance d from point $\mathbf{y} \in \mathbb{R}^n$ to closed set $S \subset \mathbb{R}^n$:

$$d(\mathbf{y}, S, \|\cdot\|) = \inf\{\|x - y\| \mid x \in S\}$$

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$$\text{proj}_S(\mathbf{y}) = \arg\min_{\mathbf{x} \in S} \frac{1}{2}\|x - y\|_2^2$$

если это не так, см. зеркальный спуск Mirror Descent

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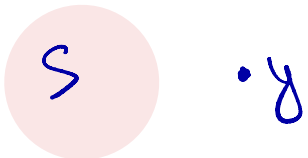

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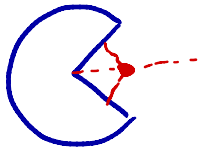

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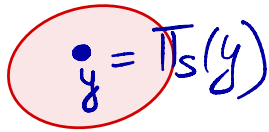

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Projection criterion (Bourbaki-Cheney-Goldstein inequality)

Theorem

Let $S \subseteq \mathbb{R}^n$ be closed and convex, $\forall x \in S, y \in \mathbb{R}^n$. Then

$$\langle y - \text{proj}_S(y), \mathbf{x} - \text{proj}_S(y) \rangle \leq 0 \tag{1}$$

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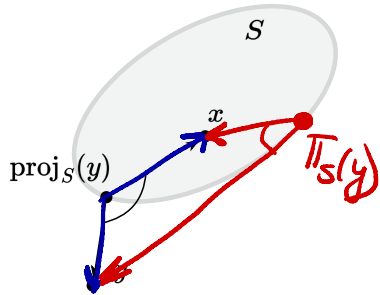

Figure 7: Obtuse or straight angle should be for any point $x \in S$

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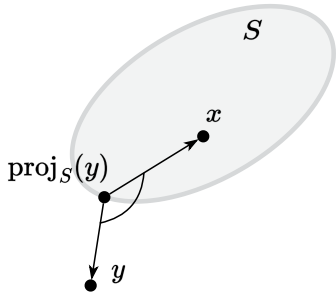

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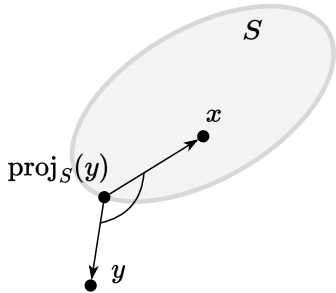

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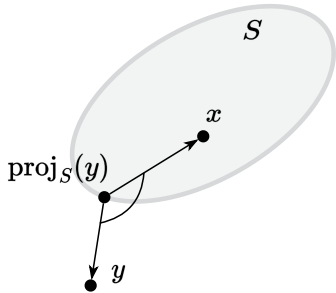

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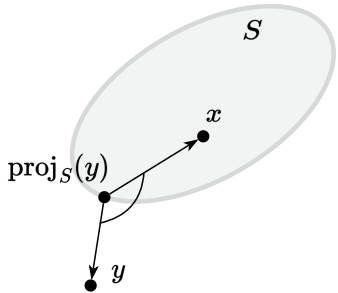

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$x^T y = \|x\| \cdot \|y\| \cdot \cos\alpha$

$\cos\alpha = \dfrac{\|x\|^2 + \|y\|^2 - \|x-y\|^2}{\|x\| \cdot \|y\|}$

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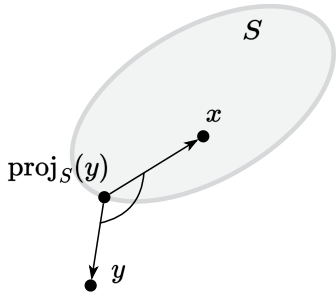

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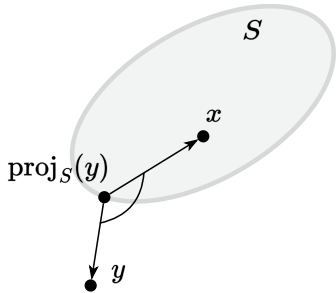

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Projection operator is non-expansive

- A function f is called non-expansive if f is L-Lipschitz with $L \leq 1$ [1]. That is, for any two points $x, y \in \mathrm{dom} f$,

$$\|f(x) - f(y)\| \leq L\|x - y\|, \text{ where } L \leq 1.$$

It means the distance between the mapped points is possibly smaller than that of the unmapped points.

$\forall x, y \quad \|\Pi(x) - \Pi(y)\| \leq \|x - y\|$

[1] Non-expansive becomes contractive if $L < 1$.

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$$\langle \pi(x) - x, \pi(x) - \pi(y) \rangle \leq 0. \tag{6}$$

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$$\begin{aligned}
\langle y - \pi(y) + \pi(x) - x, \pi(x) - \pi(y) \rangle &\leq 0 \\
\langle y - x, \pi(x) - \pi(y) \rangle &\leq -\langle \pi(x) - \pi(y), \pi(x) - \pi(y) \rangle \\
\langle y - x, \pi(y) - \pi(x) \rangle &\geq \|\pi(x) - \pi(y)\|_2^2 \\
\|(y - x)^\top (\pi(y) - \pi(x))\|_2 &\geq \|\pi(x) - \pi(y)\|_2^2
\end{aligned}$$

Projection operator is non-expansive

$\forall x, y \in \mathbb{R}^n : \|\Pi_S(x) - \Pi_S(y)\| \leq \|x - y\|$

S-ben. zárvány.

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\langle y - x, \pi(y) - \pi(x) \rangle &\geq \|\pi(x) - \pi(y)\|_2^2 \\
\|(y - x)^\top (\pi(y) - \pi(x))\|_2 &\geq \|\pi(x) - \pi(y)\|_2^2
\end{aligned}$$

By Cauchy-Schwarz inequality, the left-hand-side is upper bounded by $\|y - x\|_2 \|\pi(y) - \pi(x)\|_2$, we get $\|y - x\|_2 \|\pi(y) - \pi(x)\|_2 \geq \|\pi(x) - \pi(y)\|_2^2$. Cancels $\|\pi(x) - \pi(y)\|_2$ finishes the proof.

Example: projection on the ball

Find $\pi_S(y) = \pi$, if $S = \{x \in \mathbb{R}^n \mid \|x - x_0\| \leq R\}$, $y \notin S$

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$$\left(x_0 - y + R\frac{y - x_0}{\|y - x_0\|}\right)^T \left(x - x_0 - R\frac{y - x_0}{\|y - x_0\|}\right) =$$

$$\left(\frac{(y - x_0)(R - \|y - x_0\|)}{\|y - x_0\|}\right)^T \left(\frac{(x - x_0)\|y - x_0\| - R(y - x_0)}{\|y - x_0\|}\right) =$$

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The first factor is negative for point selection y. The second factor is also negative, which follows from the Cauchy-Bunyakovsky inequality:

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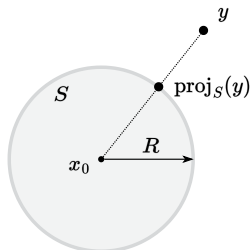
The first factor is negative for point selection y. The second factor is also negative, which follows from the Cauchy-Bunyakovsky inequality:

$$(y - x_0)^T (x - x_0) \leq \|y - x_0\| \|x - x_0\|$$

$$\frac{(y - x_0)^T (x - x_0)}{\|y - x_0\|} - R \leq \frac{\|y - x_0\| \|x - x_0\|}{\|y - x_0\|} -$$



Example: projection on the halfspace

Find $\pi_S(y) = \pi$, if $S = \{x \in \mathbb{R}^n \mid c^T x = b\}$, $y \notin S$. Build a hypothesis from the figure: $\pi = y + \alpha c$. Coefficient α is chosen so that $\pi \in S$: $c^T \pi = b$, so:

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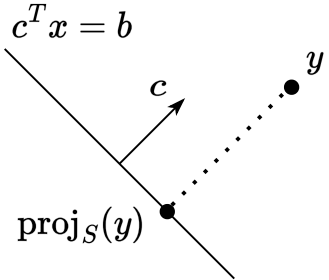

Figure 9: Hyperplane

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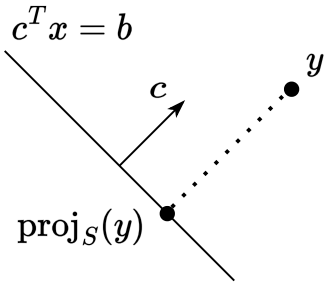

Figure 9: Hyperplane

$$c^T(y + \alpha c) = b$$
$$c^T y + \alpha c^T c = b$$
$$c^T y = b - \alpha c^T c$$

Check the inequality for a convex closed set:
$(\pi - y)^T (x - \pi) \geq 0$

$$(y + \alpha c - y)^T (x - y - \alpha c) =$$
$$\alpha c^T (x - y - \alpha c) =$$
$$\alpha(c^T x) - \alpha(c^T y) - \alpha^2 (c^T c) =$$
$$\alpha b - \alpha(b - \alpha c^T c) - \alpha^2 c^T c =$$
$$\alpha b - \alpha b + \alpha^2 c^T c - \alpha^2 c^T c = 0 \geq 0$$

Projected Gradient Descent (PGD)

Idea

$$x_{k+1} = \text{proj}_S\left(x_k - \alpha_k \nabla f(x_k)\right) \quad \Leftrightarrow \quad \begin{aligned} y_k &= x_k - \alpha_k \nabla f(x_k) \\ x_{k+1} &= \text{proj}_S\left(y_k\right) \end{aligned}$$

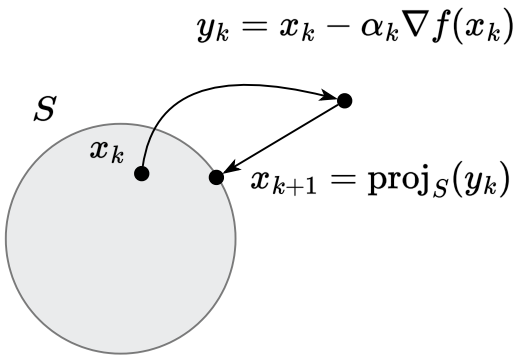

Figure 10: Illustration of Projected Gradient Descent algorithm

Convergence rate for smooth and convex case

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex and differentiable. Let $S \subseteq \mathbb{R}^n$d be a closed convex set, and assume that there is a minimizer x^* of f over S; furthermore, suppose that f is smooth over S with parameter L. The Projected Gradient Descent algorithm with stepsize $\frac{1}{L}$ achieves the following convergence after iteration $k > 0$:

$$f(x_k) - f^* \leq \frac{L\|x_0 - x^*\|_2^2}{2k}$$

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1. Let's prove sufficient decrease lemma, assuming, that $y_k = x_k - \frac{1}{L}\nabla f(x_k)$ and cosine rule $2x^T y = \|x\|^2 + \|y\|^2 - \|x - y\|^2$:

(7)

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   Smoothness: $f(x_{k+1}) \leq f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{L}{2}\|x_{k+1} - x_k\|^2$

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& = f(x_k) - \frac{1}{2L}\|\nabla f(x_k)\|^2 + \frac{L}{2}\|y_k - x_{k+1}\|^2
\end{aligned} \tag{7}$$

Convergence rate for smooth and convex case

2. Now we do not immediately have progress at each step. Let's use again cosine rule:

$$\left\langle \frac{1}{L}\nabla f(x_k), x_k - x^* \right\rangle = \frac{1}{2}\left(\frac{1}{L^2}\|\nabla f(x_k)\|^2 + \|x_k - x^*\|^2 - \|x_k - x^* - \frac{1}{L}\nabla f(x_k)\|^2\right)$$

$$\langle \nabla f(x_k), x_k - x^* \rangle = \frac{L}{2}\left(\frac{1}{L^2}\|\nabla f(x_k)\|^2 + \|x_k - x^*\|^2 - \|y_k - x^*\|^2\right)$$

$$x^T y = \frac{1}{2}\left(\|x\|_2^2 + \|y\|_2^2 - \|x-y\|_2^2\right)$$

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3. We will use now projection property: $\|x - \text{proj}_S(y)\|^2 + \|y - \text{proj}_S(y)\|^2 \leq \|x - y\|^2$ with $x = x^*, y = y_k$:

$$\|x^* - \text{proj}_S(y_k)\|^2 + \|y_k - \text{proj}_S(y_k)\|^2 \leq \|x^* - y_k\|^2$$

$$\|y_k - x^*\|^2 \geq \|x^* - x_{k+1}\|^2 + \|y_k - x_{k+1}\|^2$$

$\pi_S(y_k) = x_{k+1}$

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$$\|y_k - x^*\|^2 \geq \|x^* - x_{k+1}\|^2 + \|y_k - x_{k+1}\|^2$$

4. Now, using convexity and previous part:

Convergence rate for smooth and convex case

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$$\left\langle \frac{1}{L}\nabla f(x_k), x_k - x^* \right\rangle = \frac{1}{2}\left(\frac{1}{L^2}\|\nabla f(x_k)\|^2 + \|x_k - x^*\|^2 - \|x_k - x^* - \frac{1}{L}\nabla f(x_k)\|^2 \right)$$

$$\langle \nabla f(x_k), x_k - x^* \rangle = \frac{L}{2}\left(\frac{1}{L^2}\|\nabla f(x_k)\|^2 + \|x_k - x^*\|^2 - \|y_k - x^*\|^2 \right)$$

3. We will use now projection property: $\|x - \text{proj}_S(y)\|^2 + \|y - \text{proj}_S(y)\|^2 \leq \|x - y\|^2$ with $x = x^*, y = y_k$:

$$\|x^* - \text{proj}_S(y_k)\|^2 + \|y_k - \text{proj}_S(y_k)\|^2 \leq \|x^* - y_k\|^2$$

$$\|y_k - x^*\|^2 \geq \|x^* - x_{k+1}\|^2 + \|y_k - x_{k+1}\|^2$$

4. Now, using convexity and previous part:

Convexity: $f(x_k) - f^* \leq \langle \nabla f(x_k), x_k - x^* \rangle$

Convergence rate for smooth and convex case

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Convergence rate for smooth and convex case

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Sum for $i = 0, k-1$
$$\sum_{i=0}^{k-1}[f(x_i) - f^*] \leq \sum_{i=0}^{k-1}\frac{1}{2L}\|\nabla f(x_i)\|^2 + \frac{L}{2}\|x_0 - x^*\|^2 - \frac{L}{2}\sum_{i=0}^{i-1}\|y_i - x_{i+1}\|^2$$

Convergence rate for smooth and convex case

5. Bound gradients with sufficient decrease lemma 7:

Convergence rate for smooth and convex case

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$$\sum_{i=0}^{k-1}[f(x_i)-f^*] \leq \sum_{i=0}^{k-1}\left[f(x_i)-f(x_{i+1})+\frac{L}{2}\|y_i-x_{i+1}\|^2\right]+\frac{L}{2}\|x_0-x^*\|^2-\frac{L}{2}\sum_{i=0}^{i-1}\|y_i-x_{i+1}\|^2$$

Convergence rate for smooth and convex case

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Convergence rate for smooth and convex case

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\sum_{i=0}^{k-1}f(x_i)-kf^* &\leq f(x_0)-f(x_k)+\frac{L}{2}\|x_0-x^*\|^2
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Convergence rate for smooth and convex case

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Convergence rate for smooth and convex case

6. From the sufficient decrease inequality

$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2L}\|\nabla f(x_k)\|^2 + \frac{L}{2}\|y_k - x_{k+1}\|^2,$$

Convergence rate for smooth and convex case

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Convergence rate for smooth and convex case

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Substitute back into $(*)$:

$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2L}\|\nabla f(x_k)\|^2 + \frac{1}{2L}\|\nabla f(x_k)\|^2 = f(x_k).$$

$-\frac{1}{2}$ $+\frac{1}{2}$

Convergence rate for smooth and convex case

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Hence

$$\boxed{f(x_{k+1}) \leq f(x_k)} \quad \text{for each } k,$$

so $\{f(x_k)\}$ is a monotonically nonincreasing sequence.

Convergence rate for smooth and convex case

7. Final convergence bound From step 5, we have already established

$$\sum_{i=0}^{k-1}[f(x_i) - f^*] \leq \frac{L}{2}\|x_0 - x^*\|_2^2.$$

Convergence rate for smooth and convex case

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$$k\,[f(x_k) - f^*] \leq \sum_{i=0}^{k-1}[f(x_i) - f^*] \leq \frac{L}{2}\|x_0 - x^*\|_2^2,$$

$k \cdot f_3 \leq f_1 + f_2 + f_3$

$k = 3$

Convergence rate for smooth and convex case

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which immediately gives

$$\boxed{f(x_k) - f^* \leq \frac{L\|x_0 - x^*\|_2^2}{2k}.}$$

This completes the proof of the $\mathcal{O}(\frac{1}{k})$ convergence rate for convex and L-smooth f under projection constraints.

Convergence rate for smooth strongly convex case

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ be μ-strongly convex (or, PL-function with parameter μ) and L-smooth. Let $S \subseteq \mathbb{R}^n$ be a closed convex set, and assume that there is a minimizer x^* of f over S; The Projected Gradient Descent algorithm with stepsize $\frac{1}{L}$ achieves the following convergence after iteration $k > 0$:

$$f(x_k) - f^* \leq \left(1 - \frac{\mu}{L}\right)^k (f(x_0) - f^*)$$

$\left(\frac{L-\mu}{L}\right)$

1. We will use the notation $x_{k+1} = \text{proj}_S\left(x_k - \frac{1}{L}\nabla f(x_k)\right) = \pi(y_k)$. Since projection is nonexpansive, we have:

$$\|x_{k+1} - x_k\| = \|\pi(y_k) - \pi(x_k)\| \leq \|y_k - x_k\| = \frac{1}{L}\|\nabla f(x_k)\| \quad \Rightarrow \quad \|x_{k+1} - x_k\|^2 \leq \frac{1}{L^2}\|\nabla f(x_k)\|^2 \qquad (8)$$

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$$\begin{aligned} f(x_{k+1}) - f(x_k) &\leq \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{L}{2}\|x_{k+1} - x_k\|^2 \\ &\leq \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{1}{2L}\|\nabla f(x_k)\|^2 \end{aligned} \tag{9}$$

Convergence rate for smooth strongly convex case

3. By first-order optimality for that Euclidean projection problem, $\langle y_k - x_{k+1}, z - x_{k+1} \rangle \leq 0 \quad \forall z \in S$. In particular, for $z = x_k$,

Convergence rate for smooth strongly convex case

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Convergence rate for smooth strongly convex case

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Convergence rate for smooth strongly convex case

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Convergence rate for smooth strongly convex case

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$$\begin{aligned}
\langle y_k - x_{k+1}, x_k - x_{k+1} \rangle &\leq 0 \\
\langle x_k - \tfrac{1}{L}\nabla f(x_k) - x_{k+1}, x_k - x_{k+1} \rangle &\leq 0 \\
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\end{aligned}$$

4. Returning back to the smoothness inequality (9) we obtain sufficient decrease property:

$$\begin{aligned}
f(x_{k+1}) &\leq f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{1}{2L}\|\nabla f(x_k)\|^2 \\
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Convergence rate for smooth strongly convex case

5. If we have a PL-function, we can use the following inequality: $\|\nabla f(x_k)\|^2 \geq 2\mu\,(f(x_k) - f^*)$. Thus, we can write:

$$f(x_{k+1}) \leq f(x_k) - \frac{\mu}{L}\,(f(x_k) - f^*)$$

$$f(x_{k+1}) - f^* \leq f(x_k) - f^* - \frac{\mu}{L}\,(f(x_k) - f^*)$$

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6. Now we can use induction to get the following bound:

$$f(x_k) - f^* \leq \left(1 - \frac{\mu}{L}\right)^k (f(x_0) - f^*)$$

Frank-Wolfe Method

Figure 11: Marguerite Straus Frank (1927-2024)

Figure 12: Philip Wolfe (1927-2016)

Idea

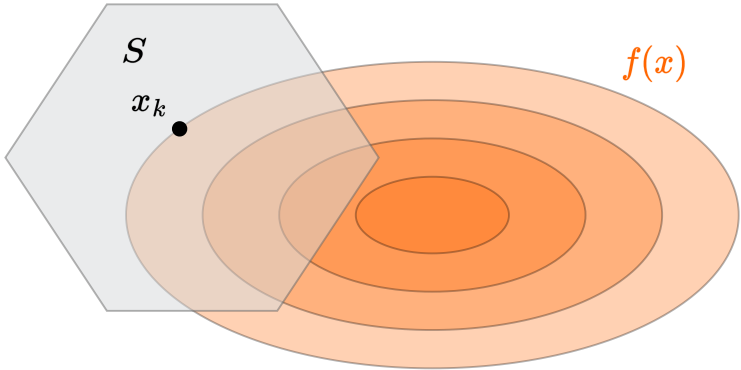

Figure 13: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

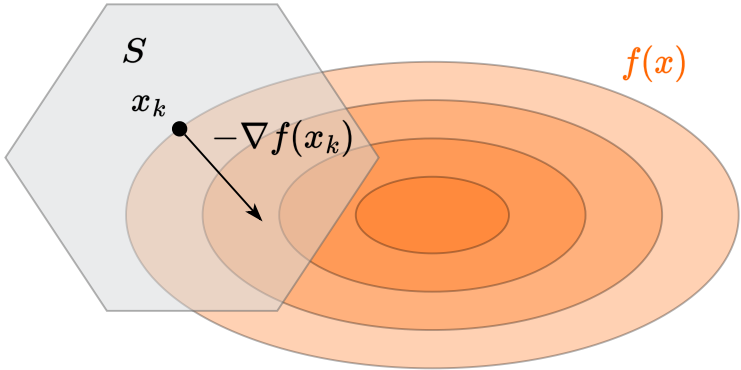

Figure 14: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

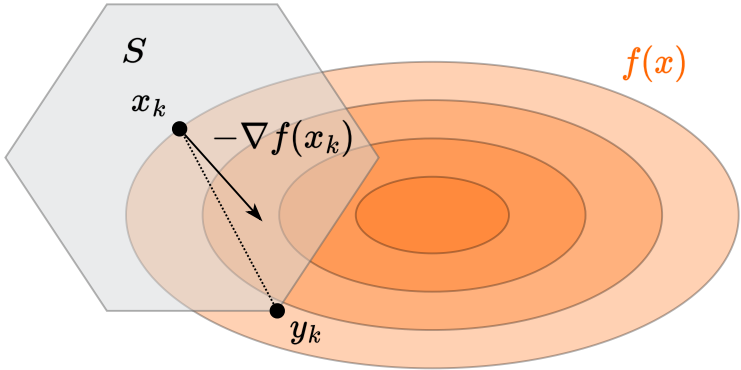

Figure 15: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

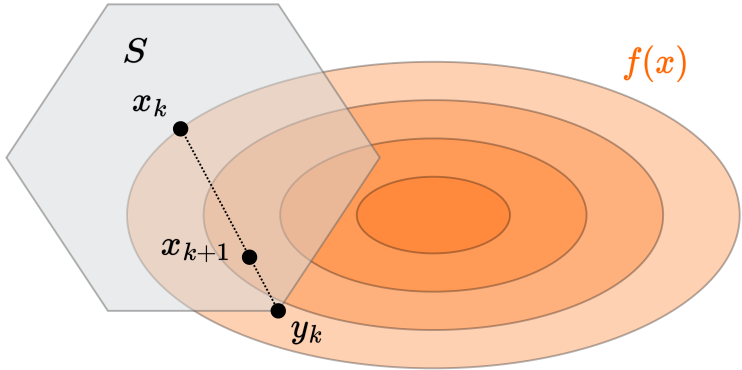

Figure 16: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

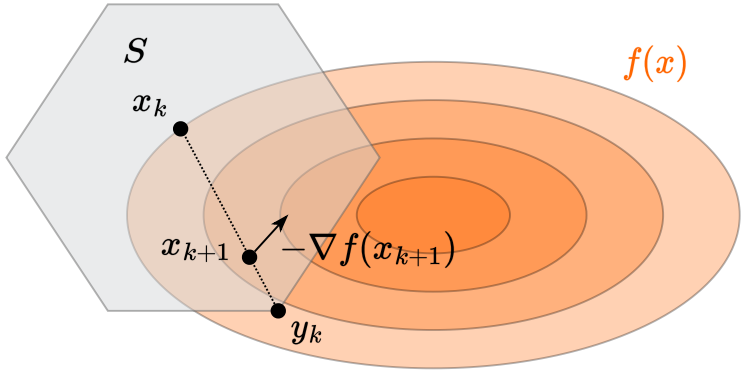

Figure 17: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

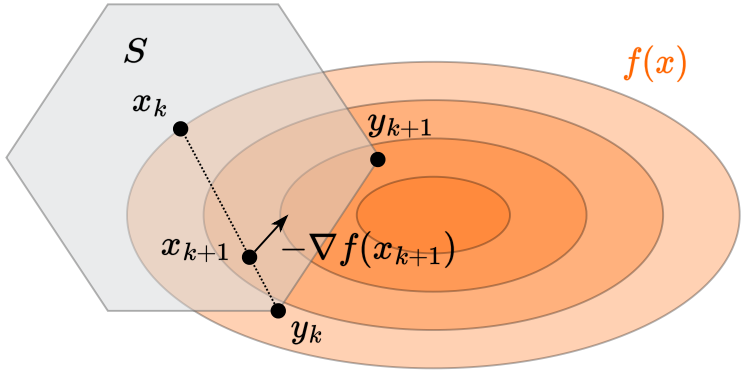

Figure 18: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

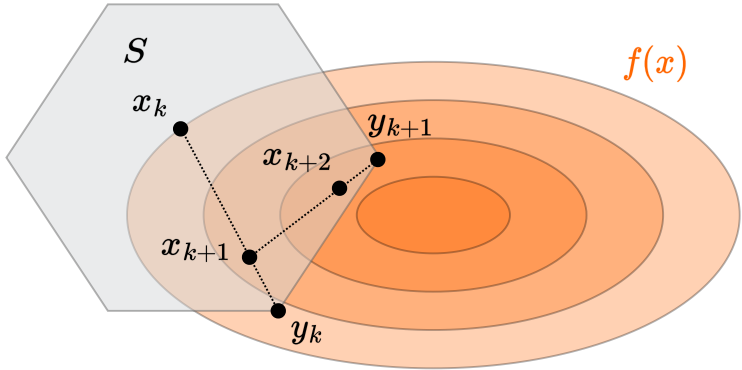

Figure 19: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

$$f_{x_k}^I(x) = f(x_k) + \langle \nabla f(x_k), x - x_k \rangle$$

$$y_k = \arg\min_{x \in S} f_{x_k}^I(x) = \arg\min_{x \in S} \langle \nabla f(x_k), x \rangle$$

$$x_{k+1} = \gamma_k x_k + (1 - \gamma_k) y_k$$

LMO
Linear
Minimizat.
Oracle

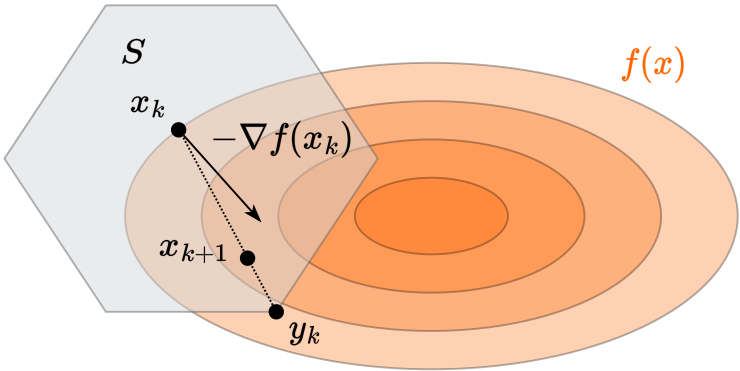

Figure 20: Illustration of Frank-Wolfe (conditional gradient) algorithm

Convergence rate for smooth and convex case

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex and differentiable. Let $S \subseteq \mathbb{R}^n$ be a closed convex set, and assume that there is a minimizer x^* of f over S; furthermore, suppose that f is smooth over S with parameter L. The Frank-Wolfe algorithm with step size $\gamma_k = \frac{k-1}{k+1}$ achieves the following convergence after iteration $k > 0$:

$$f(x_k) - f^* \leq \frac{2LR^2}{k+1}$$

where $R = \max_{x,y \in S} \|x - y\|$ is the diameter of the set S.

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where $R = \max_{x,y \in S} \|x - y\|$ is the diameter of the set S.

1. By L-smoothness of f, we have:

$$\begin{aligned} f(x_{k+1}) - f(x_k) &\leq \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{L}{2} \|x_{k+1} - x_k\|^2 \\ &= (1 - \gamma_k) \langle \nabla f(x_k), y_k - x_k \rangle + \frac{L(1-\gamma_k)^2}{2} \|y_k - x_k\|^2 \end{aligned}$$

Convergence rate for smooth and convex case

2. By convexity of f, for any $x \in S$, including x^*:

$$\langle \nabla f(x_k), x - x_k \rangle \leq f(x) - f(x_k)$$

In particular, for $x = x^*$:

$$\langle \nabla f(x_k), x^* - x_k \rangle \leq f(x^*) - f(x_k)$$

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4. Combining the above inequalities:

$$\begin{aligned} f(x_{k+1}) - f(x_k) &\leq (1-\gamma_k) \langle \nabla f(x_k), y_k - x_k \rangle + \frac{L(1-\gamma_k)^2}{2} \|y_k - x_k\|^2 \\ &\leq (1-\gamma_k)(f(x^*) - f(x_k)) + \frac{L(1-\gamma_k)^2}{2} R^2 \end{aligned}$$

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5. Rearranging terms:

$$f(x_{k+1}) - f(x^*) \leq \gamma_k (f(x_k) - f(x^*)) + (1-\gamma_k)^2 \frac{LR^2}{2}$$

Convergence rate for smooth and convex case

6. Denoting $\delta_k = \frac{f(x_k)-f(x^*)}{LR^2}$, we get:

$$\delta_{k+1} \leq \gamma_k \delta_k + \frac{(1-\gamma_k)^2}{2} = \frac{k-1}{k+1}\delta_k + \frac{2}{(k+1)^2}$$

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   - Then $\delta_{k+1} \leq \frac{k-1}{k+1} \cdot \frac{2}{k+1} + \frac{2}{(k+1)^2} = \frac{2k}{k^2+2k+1} < \frac{2}{k+2}$ 🎓

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В СИЛЬНО ВОГН. ТОЖЕ 1/K

Lower bound for Frank-Wolfe method [2]

Theorem

Consider any algorithm that accesses the feasible set $S \subseteq \mathbb{R}^n$ only via a linear minimization oracle (LMO). Let the diameter of the set S be R. There exists an L-smooth strongly convex function $f : \mathbb{R}^n \to \mathbb{R}$ such that this algorithm requires at least

$$\min\left(\frac{n}{2}, \frac{LR^2}{16\varepsilon}\right)$$

iterations (i.e., calls to the LMO) to construct a point $\hat{x} \in S$ with $f(\hat{x}) - \min_{x \in S} f(x) \leq \varepsilon$. The lower bound applies both for convex and strongly convex functions.

[2] The Complexity of Large-scale Convex Programming under a Linear Optimization Oracle

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Sketch of the proof. Consider the following optimization problem:

$$\min_{x \in S} f(x) = \min_{x \in S} \frac{1}{2}\|x\|_2^2$$

$$S = \left\{ x \in \mathbb{R}^n \mid x \geq 0, \sum_{i=1}^{n} x_i = 1 \right\}$$

Note, that:

- f is 1-smooth;
- the diameter of S is $R = 2$;
- f is strongly convex.

[2] The Complexity of Large-scale Convex Programming under a Linear Optimization Oracle

Lower bound for Frank-Wolfe method [3]

1. The optimal solution is

$$x^* = \frac{1}{n}\mathbf{1} = \frac{1}{n}\sum_{i=1}^{n} e_i, \quad \text{and} \quad f(x^*) = \frac{1}{2n},$$

where $e_i = (0, \dots, 0, \underset{\text{position } i}{1}, 0, \dots, 0)^\top$ is the i-th standard basis vector.

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2. A linear minimization oracle (LMO) over S returns a vertex e_i. After k iterations, the method will have discovered at most k different basis vectors $e_{i_1}, \dots, e_{i_k}$. The best convex combination one can form is

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4. To ensure that $f(\hat{x}) - f(x^*) \leq \varepsilon$, it is necessary that (full proof is in the paper):

$$k \geq \min\left\{\frac{n}{2}, \frac{1}{4\varepsilon}\right\} = \min\left\{\frac{n}{2}, \frac{LR^2}{16\varepsilon}\right\}.$$

[3] The Complexity of Large-scale Convex Programming under a Linear Optimization Oracle

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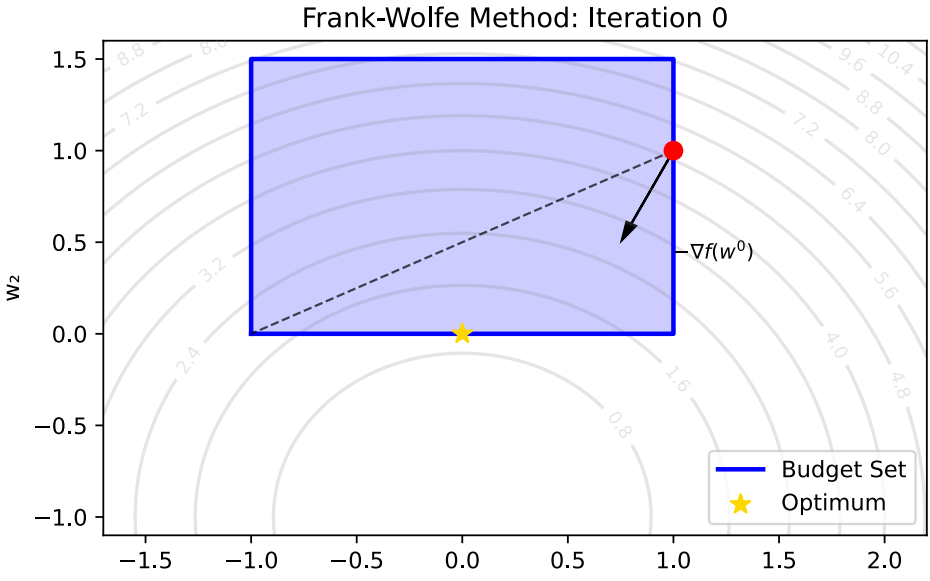
- Recent work showed the extension to non-smooth case (paper) with convergence rate $O\left(\frac{1}{\sqrt{k}}\right)$

Numerical experiments

2d example. Frank-Wolfe method



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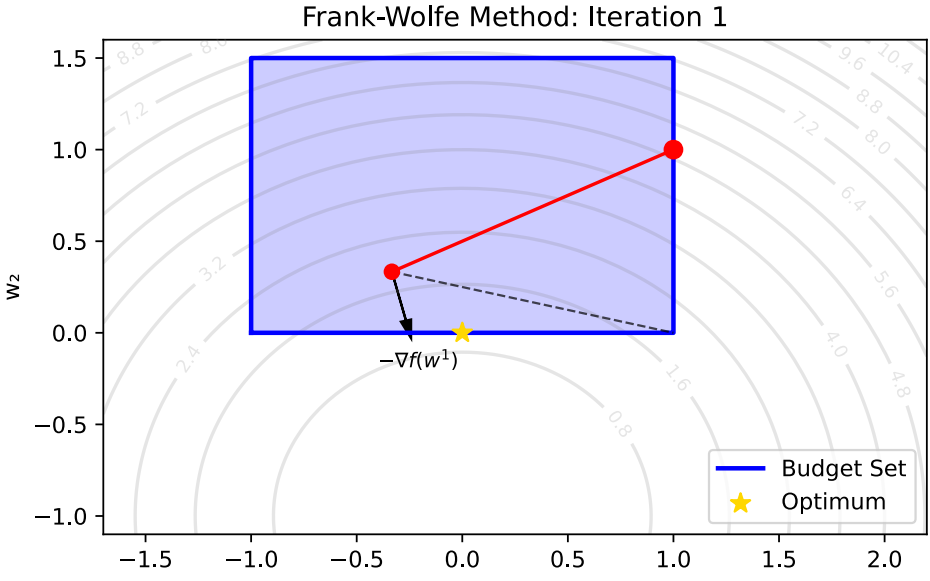

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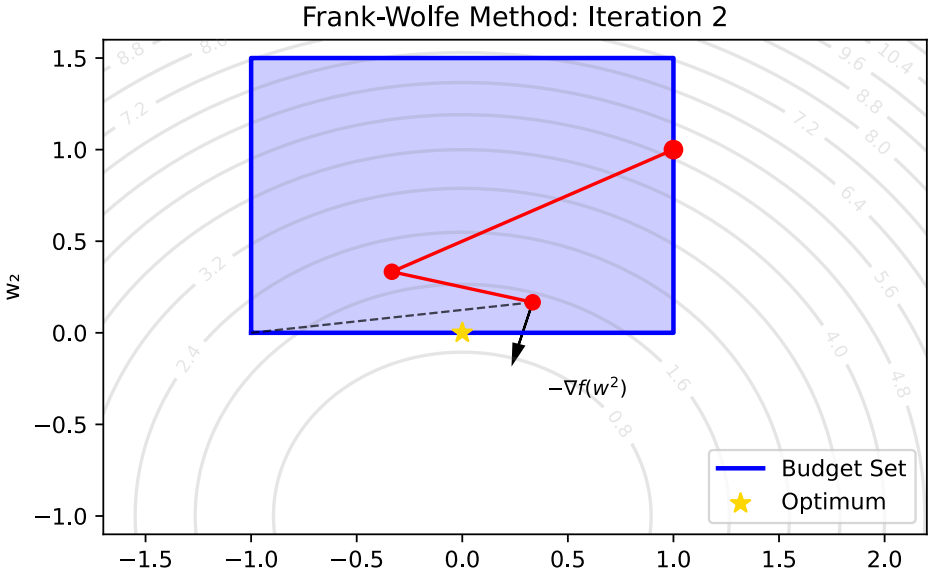

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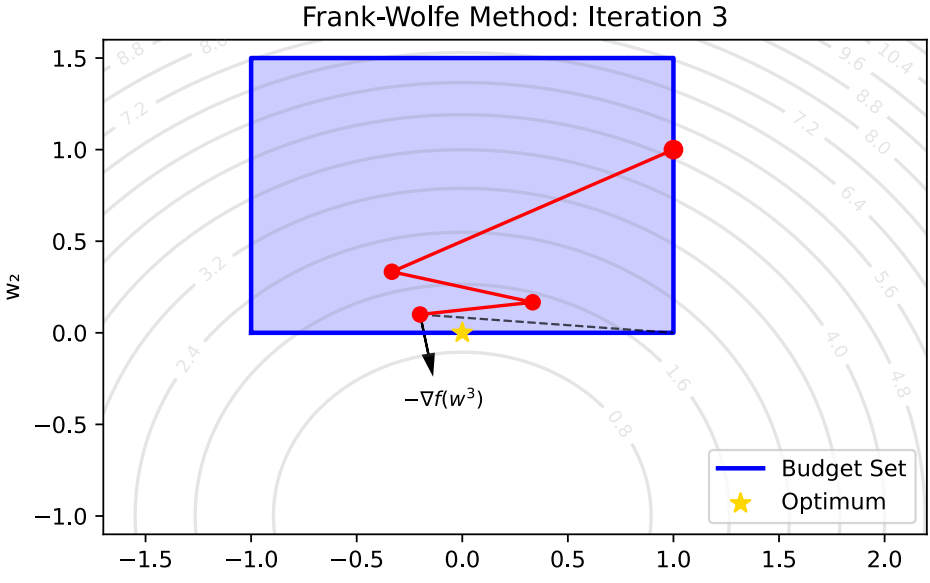

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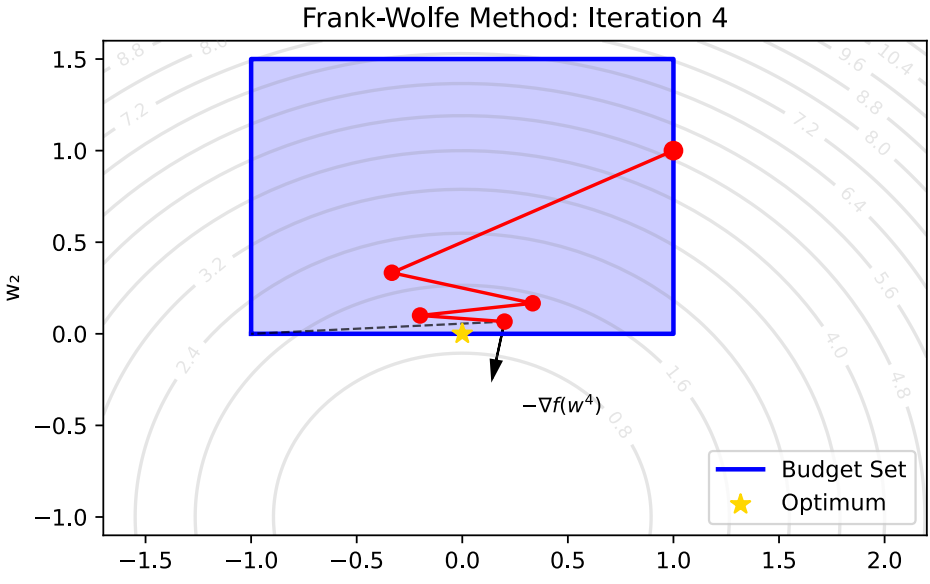
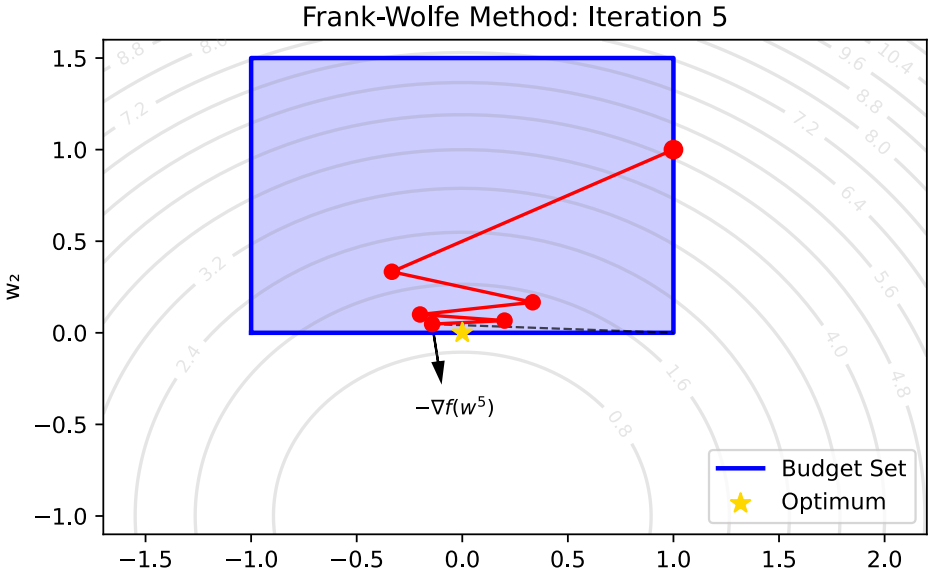
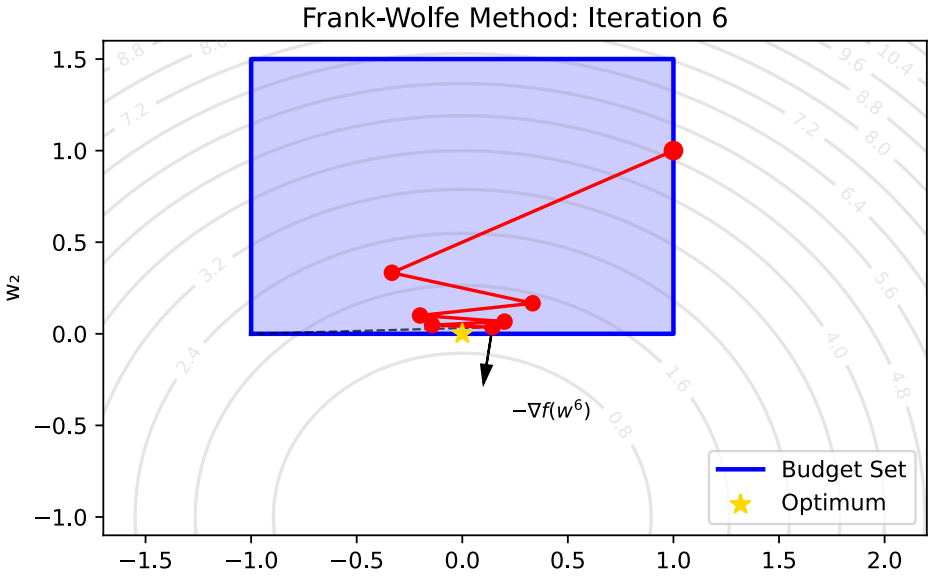


2d example. Frank-Wolfe method



2d example. Frank-Wolfe method



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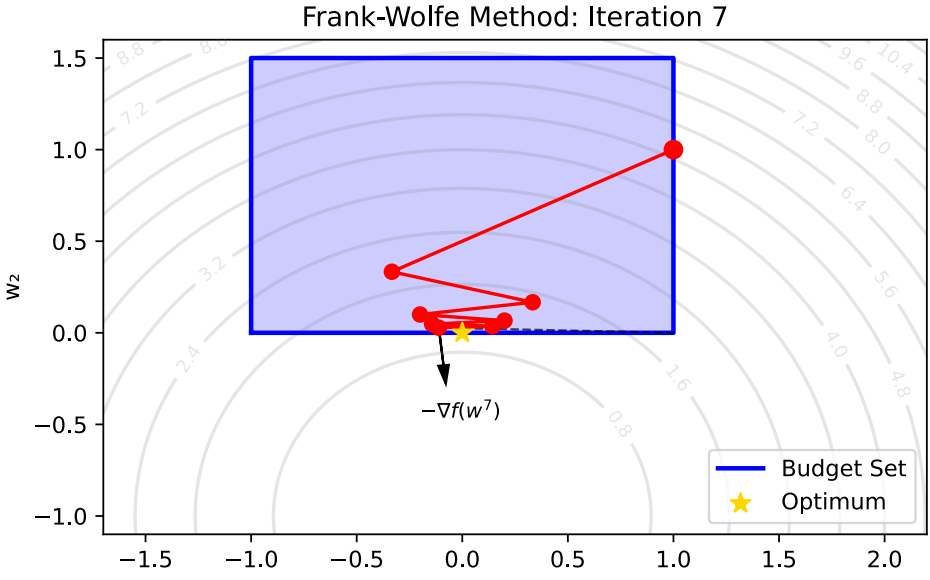
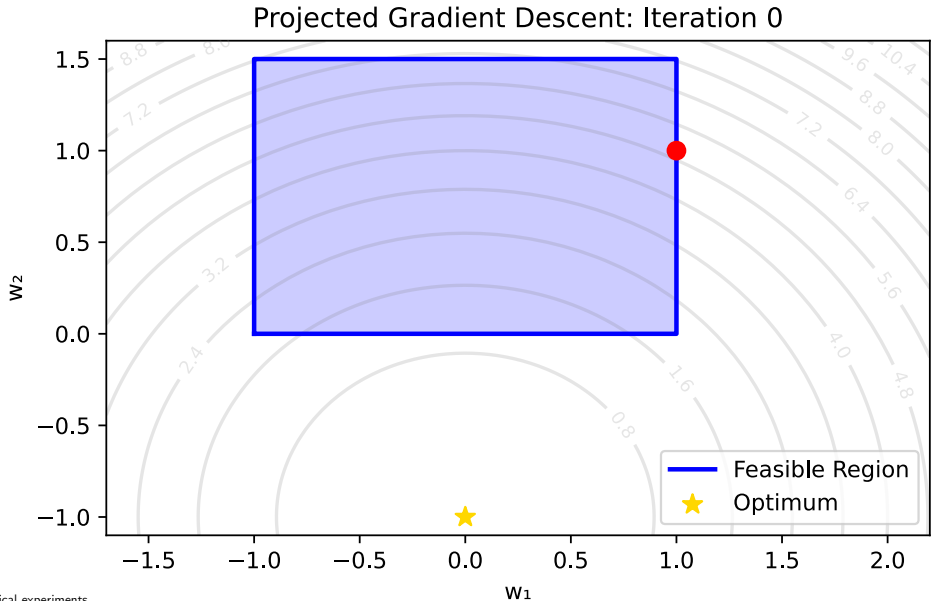


2d example. Projected gradient descent



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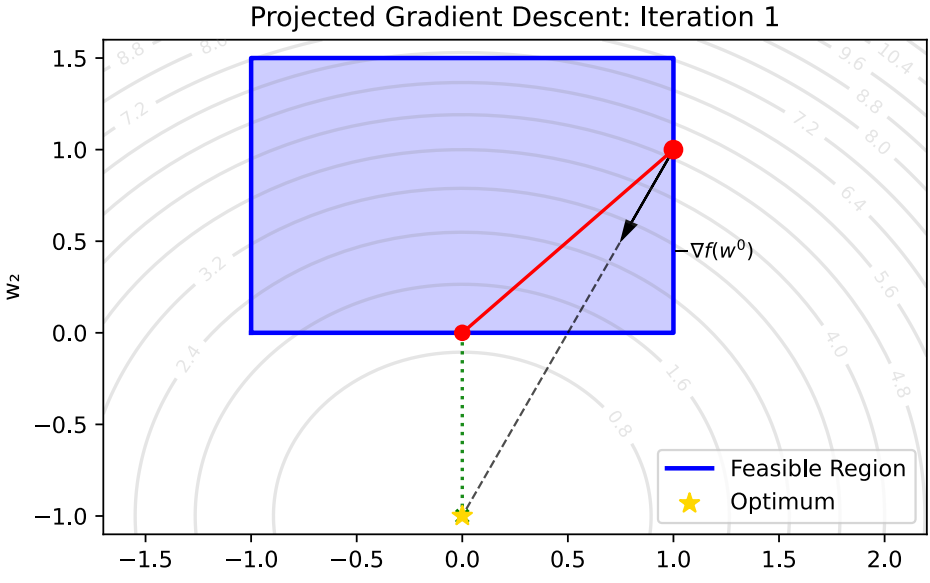
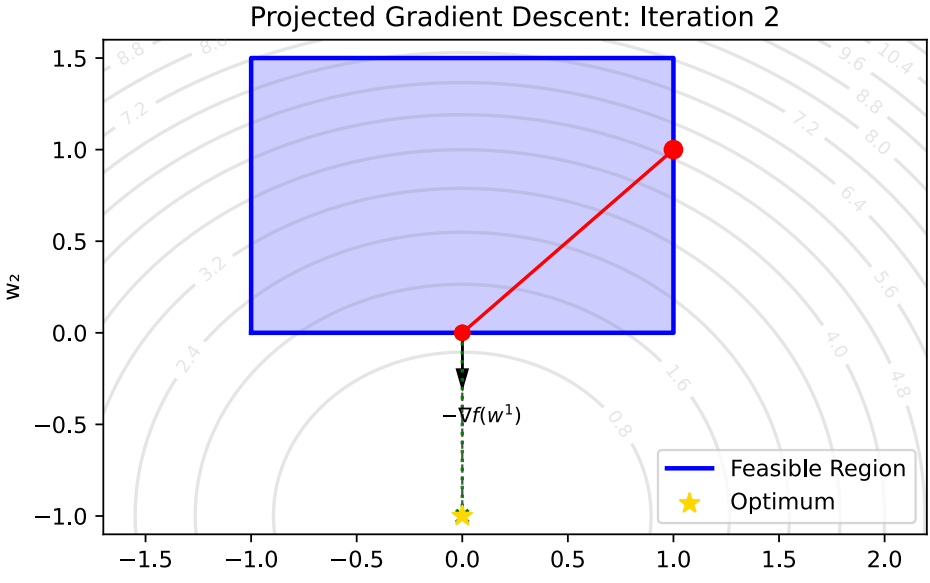


2d example. Projected gradient descent



Quadratic function. Box constraints

$$\min_{\substack{x\in\mathbb{R}^n \\ -\mathbf{1}\preceq x\preceq \mathbf{1}}} \frac{1}{2}x^\top Ax - b^\top x,$$

$$A \in \mathbb{R}^{n\times n}, \quad \lambda(A) \in [\mu; L].$$

The projection is simple:

$$\pi_S(x) = \text{clip}(x, -\mathbf{1}, \mathbf{1}).$$

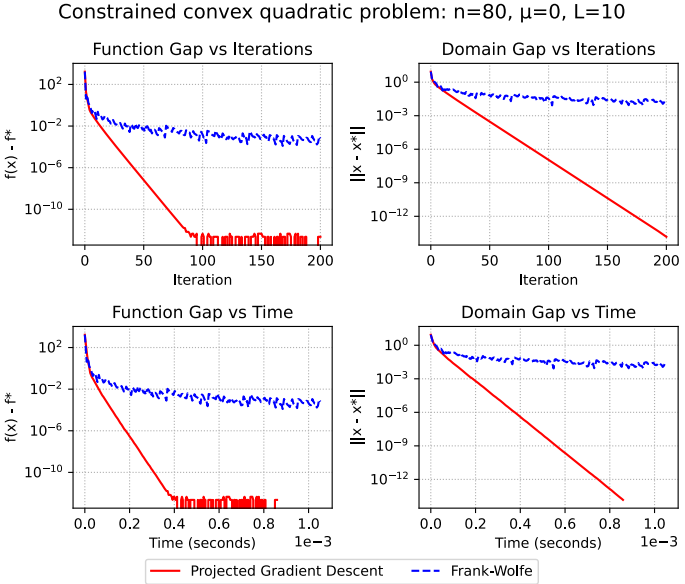
or

$$\pi_S(x) = \max\left(-\mathbf{1}, \min(\mathbf{1}, x)\right).$$

The linear minimization oracle (LMO) for a given gradient g is given by $y = \underset{z\in S}{\text{argmin}}\langle g, z\rangle$.

Since the feasible set is separable across coordinates, the solution is computed coordinate–wise as

$$y_i = \begin{cases} -1, & \text{if } g_i > 0, \\ 1, & \text{if } g_i \le 0. \end{cases}$$



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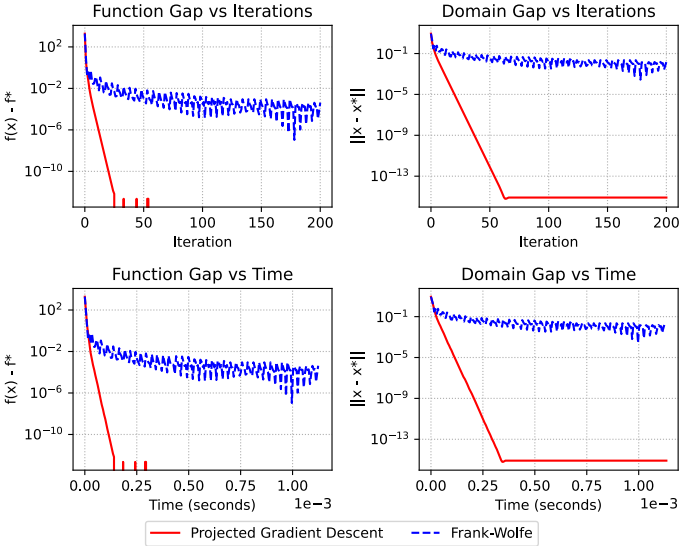
Constrained strongly Convex quadratic problem: n=80, μ=1, L=10



Quadratic function. Simplex constraints (Lucky problem with diagonal matrix)

$$\min_{\substack{x \in \mathbb{R}^n \\ x \geq 0, \mathbf{1}^T x = 1}} \frac{1}{2} x^T A x,$$

$$A \in \mathbb{R}^{n \times n}, \quad \lambda(A) \in [0; 100].$$

Method	Update time, ms	LMO/Projection
PGD	0.0069	0.0167
FW	0.0070	0.0066

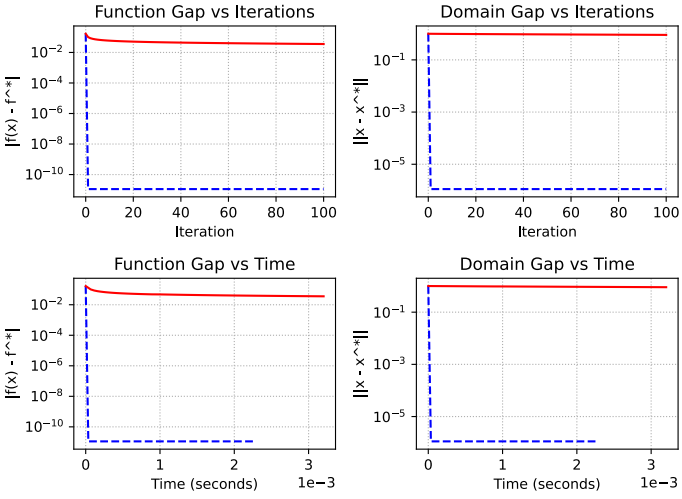
The projection onto the unit simplex $\pi_S(x)$ can be done in $\mathcal{O}(n \log n)$ or expected $\mathcal{O}(n)$ time. [a]

The LMO for a given gradient g is given by $y = \operatorname{argmin}_{z \in S} \langle g, z \rangle$. The solution corresponds to a vertex of the simplex:

$$y = e_j \quad \text{where} \quad j = \operatorname{argmin}_i g_i.$$

[a] Efficient Projections onto the ℓ_1-Ball for Learning in High Dimensions

$\min_{1^T x = 1, x \geq 0} 1/2 x^T A x, n = 200$



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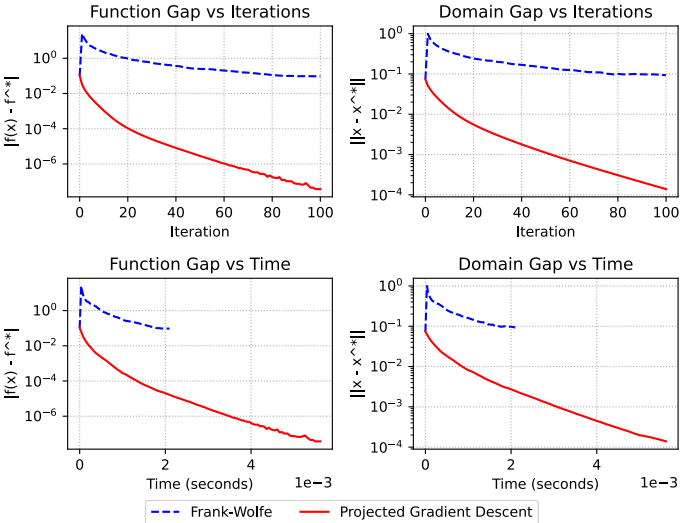
$$\min_{\substack{x \in \mathbb{R}^n \\ x \geq 0, \mathbf{1}^T x = 1}} \frac{1}{2} x^T A x,$$

$$A \in \mathbb{R}^{n \times n}, \quad \lambda(A) \in [0; 100].$$

Method	Update time, ms	LMO/Projection
PGD	0.0069	0.0420
FW	0.0069	0.0066

$$\min_{1^T x = 1, x \geq 0} 1/2 x^T A x, n = 200$$



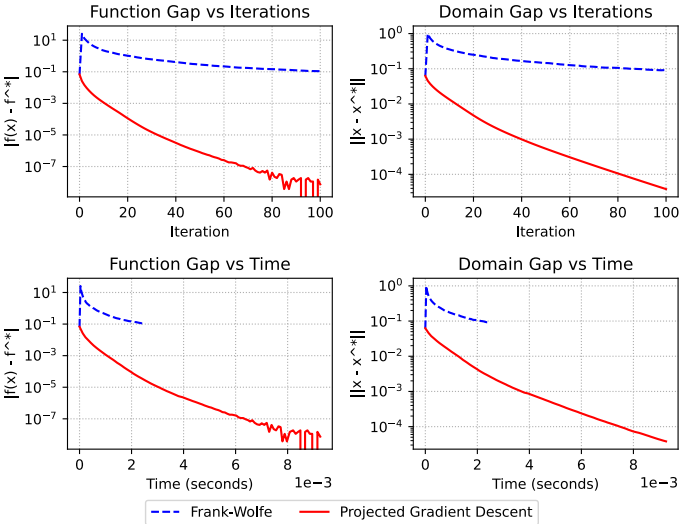
Quadratic function. Simplex constraints

$$\min_{\substack{x \in \mathbb{R}^n \\ x \geq 0, \mathbf{1}^T x = 1}} \frac{1}{2} x^T A x,$$

$$A \in \mathbb{R}^{n \times n}, \quad \lambda(A) \in [0; 100].$$

Method	Update time, ms	LMO/Projection
PGD	0.0068	0.0761
FW	0.0069	0.0070

$$\min_{1^T x = 1, x \geq 0} 1/2 x^T A x, n = 300$$



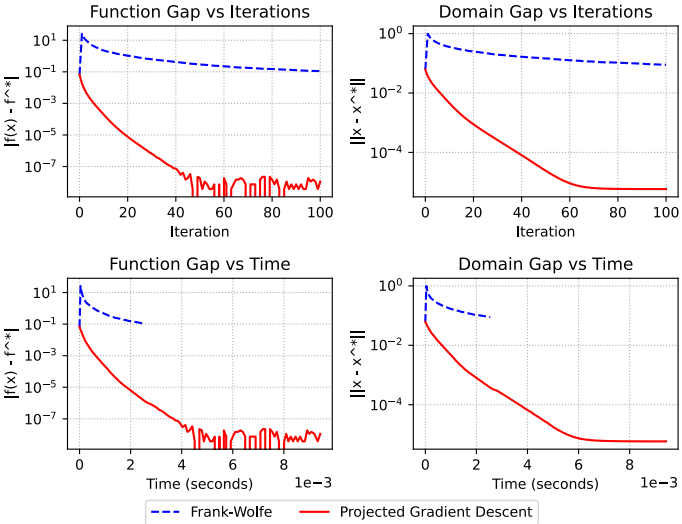
Quadratic function. Simplex constraints

$$\min_{\substack{x \in \mathbb{R}^n \\ x \geq 0, \mathbf{1}^T x = 1}} \frac{1}{2} x^T A x,$$

$$A \in \mathbb{R}^{n \times n}, \quad \lambda(A) \in [1; 100].$$

Method	Update time, ms	LMO/Projection
PGD	0.0068	0.0752
FW	0.0067	0.0068

$$\min_{1^T x = 1, x \geq 0} 1/2 x^T A x, n = 300$$



PGD vs Frank-Wolfe

The key difference between PGD and FW is that PGD requires projection, while FW needs only linear minimization oracle (LMO).

In a recent book authors presented the following comparison table with complexities of linear minimizations and projections on some convex sets up to an additive error ϵ in the Euclidean norm.

Set	**Linear minimization**	**Projection**
n-dimensional ℓ_p-ball, $p \neq 1, 2, \infty$	$\mathcal{O}(n)$	$\tilde{\mathcal{O}}(\frac{n}{\epsilon^2})$
Nuclear norm ball of $n \times m$ matrices	$\mathcal{O}\left(\nu \ln(m+n) \frac{\sqrt{\sigma_1}}{\sqrt{\epsilon}}\right)$	$\mathcal{O}(m\, n\, \min\{m, n\})$
Flow polytope on a graph with m vertices and n edges (capacity bound on edges)	$\mathcal{O}\Big((n \log m)(n + m \log m)\Big)$	$\tilde{\mathcal{O}}(\frac{n}{\epsilon^2})$ or $\mathcal{O}(n^4 \log n)$
Birkhoff polytope ($n \times n$ doubly stochastic matrices)	$\mathcal{O}(n^3)$	$\tilde{\mathcal{O}}(\frac{n^2}{\epsilon^2})$

When ϵ is missing, there is no additive error. The $\tilde{\mathcal{O}}$ hides polylogarithmic factors in the dimensions and polynomial factors in constants related to thedistancetothe optimum. For the nuclear norm ball, i.e., the spectrahedron, ν denotes the number of non-zero entries and σ_1 denotes the top singular value of the projected matrix.