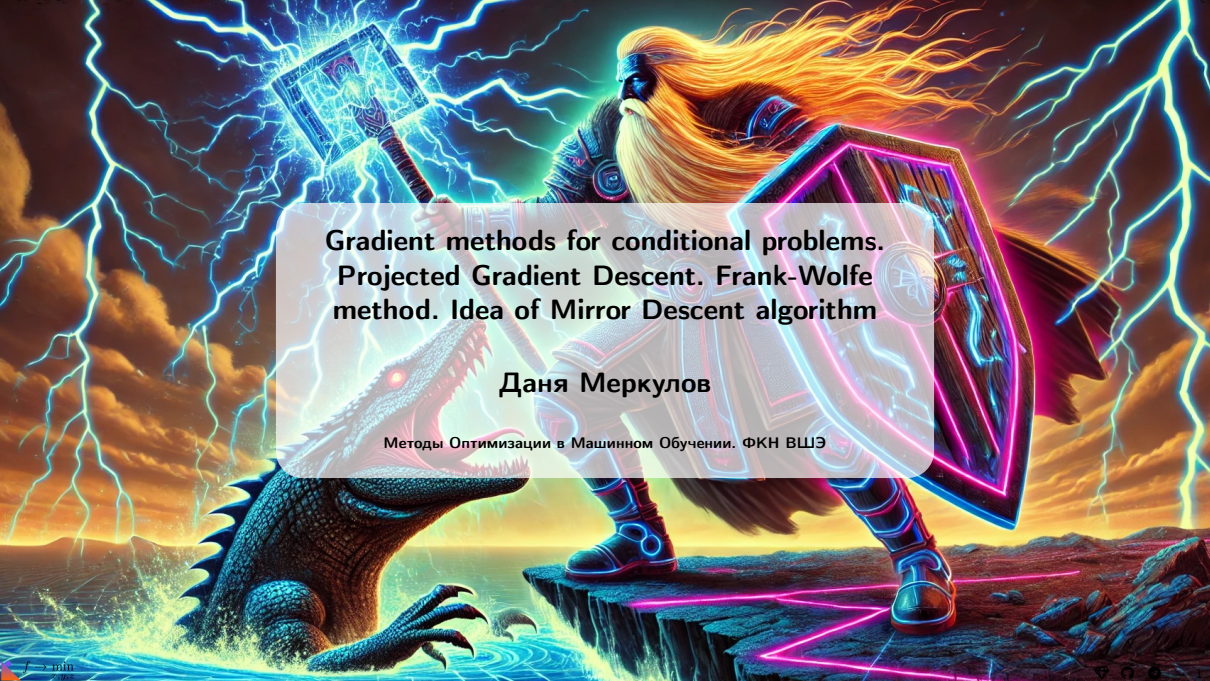

Gradient methods for conditional problems. Projected Gradient Descent. Frank-Wolfe method. Idea of Mirror Descent algorithm

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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$$\frac{1}{2}\|Ax - b\|_2^2 \to \min_{\|x\|_2^2 \leq 1}$$

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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

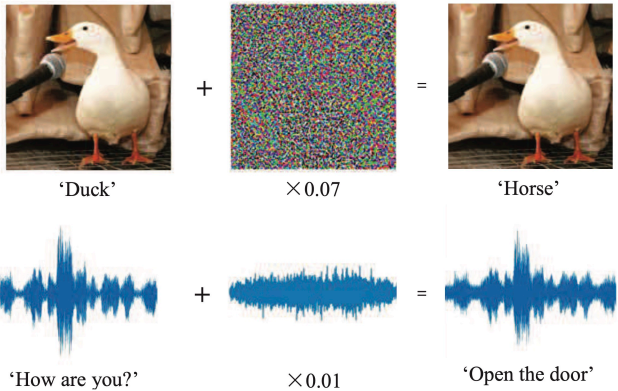

Рисунок 1: Source

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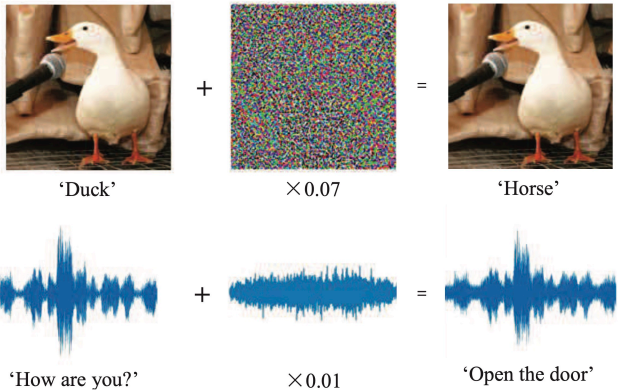

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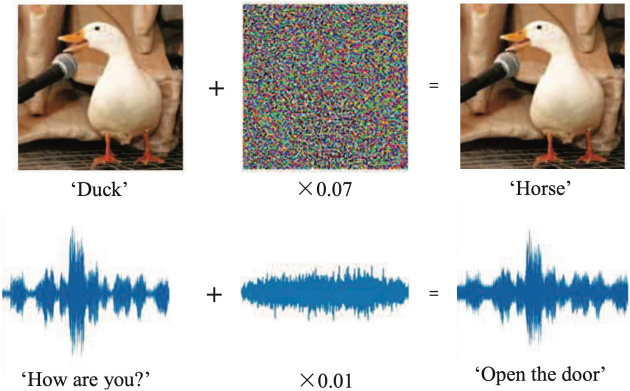

Рисунок 1: Source

- 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

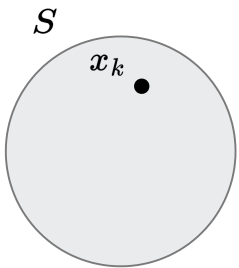

Рисунок 2: Suppose, we start from a point x_k.

Idea of Projected Gradient Descent

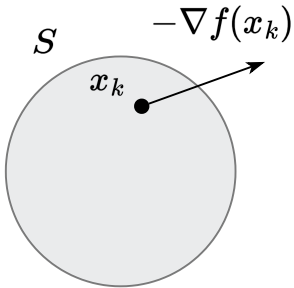

Рисунок 3: And go in the direction of $-\nabla f(x_k)$.

Idea of Projected Gradient Descent

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

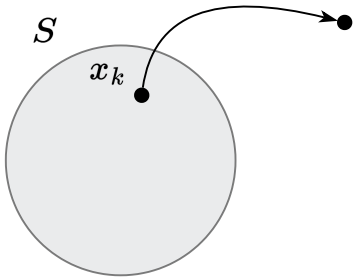

Рисунок 4: Occasionally, we can end up outside the feasible set.

Idea of Projected Gradient Descent

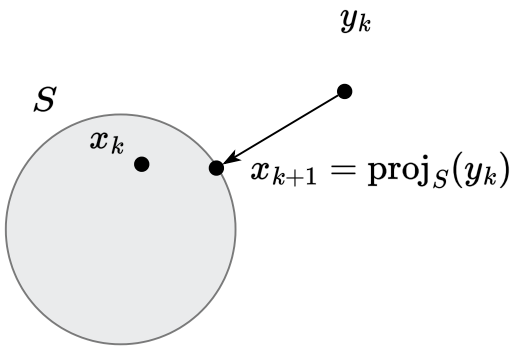

Рисунок 5: Solve this little problem with projection!

Idea of Projected Gradient Descent

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

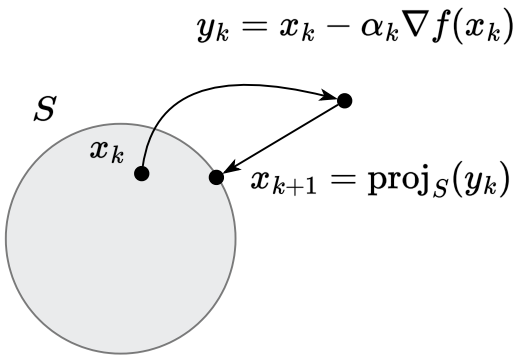

Рисунок 6: Illustration of Projected Gradient Descent algorithm

Projection

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

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We will focus on Euclidean projection (other options are possible) of a point $\mathbf{y} \in \mathbb{R}^n$ on set $S \subseteq \mathbb{R}^n$ is a point $\text{proj}_S(\mathbf{y}) \in S$:

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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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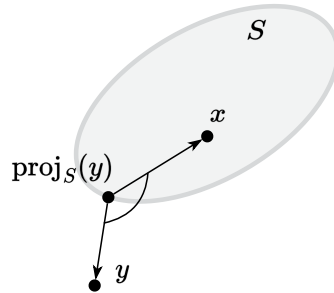

Рисунок 7: Obtuse or straight angle should be for any point $x \in S$

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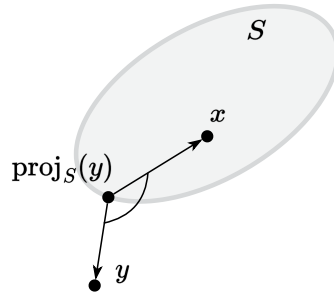

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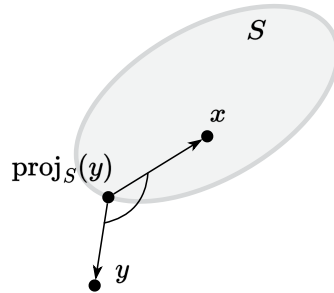

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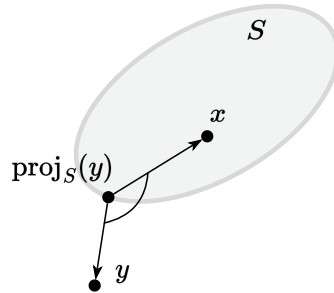

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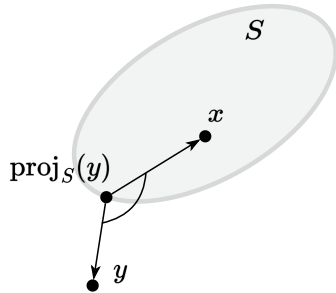

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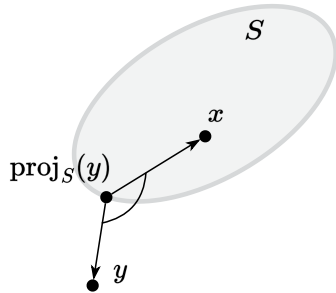

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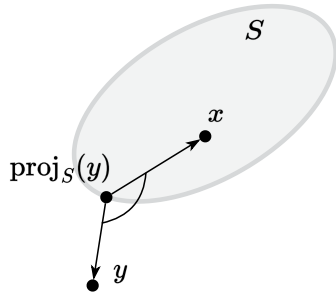

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Projection operator is non-expansive

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

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

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

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

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- Next: variational characterization implies non-expansiveness. i.e.,

$$\langle y - \mathsf{proj}(y), x - \mathsf{proj}(y)\rangle \leq 0 \quad \forall x \in S \qquad \Rightarrow \qquad \|\mathsf{proj}(x) - \mathsf{proj}(y)\|_2 \leq \|x - y\|_2.$$

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\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
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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

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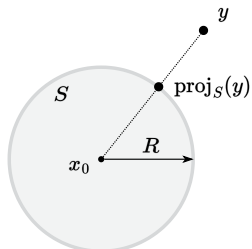
The first factor is negative for point selection y. The second factor is also negative, which follows from the Cauchy-Bunyakovsky inequality:

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

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



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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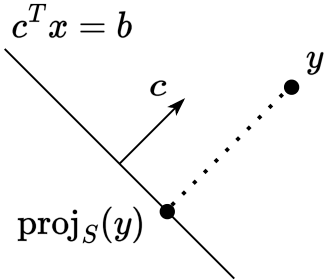

Рисунок 9: Hyperplane

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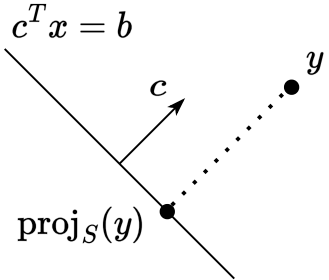

Рисунок 9: Hyperplane

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

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

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

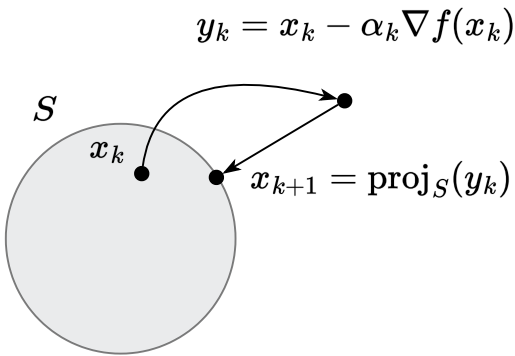

Рисунок 10: Illustration of Projected Gradient Descent algorithm

Convergence tools

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ be an L-smooth convex function. Then, for any $x, y \in \mathbb{R}^n$, the following inequality holds:

$$f(x) + \langle \nabla f(x), y - x \rangle + \frac{1}{2L} \|\nabla f(x) - \nabla f(y)\|_2^2 \leq f(y) \text{ or, equivalently,}$$

$$\|\nabla f(y) - \nabla f(x)\|_2^2 = \|\nabla f(x) - \nabla f(y)\|_2^2 \leq 2L \left(f(x) - f(y) - \langle \nabla f(y), x - y \rangle\right)$$

Proof

1. To prove this, we'll consider another function $\varphi(y) = f(y) - \langle \nabla f(x), y \rangle$. It is obviously a convex function (as a sum of convex functions). And it is easy to verify, that it is an L-smooth function by definition, since $\nabla \varphi(y) = \nabla f(y) - \nabla f(x)$ and $\|\nabla \varphi(y_1) - \nabla \varphi(y_2)\| = \|\nabla f(y_1) - \nabla f(y_2)\| \leq L \|y_1 - y_2\|$.

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2. Now let's consider the smoothness parabolic property for the $\varphi(y)$ function:

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2. Now let's consider the smoothness parabolic property for the $\varphi(y)$ function:

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$$\varphi\left(y - \frac{1}{L}\nabla \varphi(y)\right) \leq \varphi(y) - \frac{1}{2L}\|\nabla \varphi(y)\|_2^2$$

Convergence tools

3. From the first order optimality conditions for the convex function $\nabla\varphi(y) = \nabla f(y) - \nabla f(x) = 0$. We can conclude, that for any x, the minimum of the function $\varphi(y)$ is at the point $y = x$. Therefore:

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$$f(x) + \langle\nabla f(x), y - x\rangle + \frac{1}{2L}\|\nabla f(x) - \nabla f(y)\|_2^2 \leq f(y)$$

$$\|\nabla f(y) - \nabla f(x)\|_2^2 \leq 2L\left(f(y) - f(x) - \langle\nabla f(x), y - x\rangle\right)$$

switch x and y

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Convergence tools

3. From the first order optimality conditions for the convex function $\nabla\varphi(y) = \nabla f(y) - \nabla f(x) = 0$. We can conclude, that for any x, the minimum of the function $\varphi(y)$ is at the point $y = x$. Therefore:

$$\varphi(x) \leq \varphi\left(y - \frac{1}{L}\nabla\varphi(y)\right) \leq \varphi(y) - \frac{1}{2L}\|\nabla\varphi(y)\|_2^2$$

4. Now, substitute $\varphi(y) = f(y) - \langle\nabla f(x), y\rangle$:

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The lemma has been proved. From the first view it does not make a lot of geometrical sense, but we will use it as a convenient tool to bound the difference between gradients.

Convergence tools

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ be continuously differentiable on $\mathbb{R}^n$. Then, the function f is μ-strongly convex if and only if for any $x, y \in \mathbb{R}^d$ the following holds:

$$\text{Strongly convex case } \mu > 0 \quad \langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu \|x - y\|^2$$
$$\text{Convex case } \mu = 0 \quad \langle \nabla f(x) - \nabla f(y), x - y \rangle \geq 0$$

Proof

1. We will only give the proof for the strongly convex case, the convex one follows from it with setting $\mu = 0$. We start from necessity. For the strongly convex function

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} \|x - y\|_2^2$$
$$f(x) \geq f(y) + \langle \nabla f(y), x - y \rangle + \frac{\mu}{2} \|x - y\|_2^2$$
$$\text{sum} \quad \langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu \|x - y\|^2$$

Convergence tools

2. For the sufficiency we assume, that $\langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu \|x - y\|^2$. Using Newton-Leibniz theorem $f(x) = f(y) + \int_0^1 \langle \nabla f(y + t(x - y)), x - y \rangle dt$:

Convergence tools

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$$f(x) - f(y) - \langle \nabla f(y), x - y \rangle = \int_0^1 \langle \nabla f(y + t(x - y)), x - y \rangle dt - \langle \nabla f(y), x - y \rangle$$

Convergence tools

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$$\langle \nabla f(y), x - y \rangle = \int_0^1 \langle \nabla f(y), x - y \rangle dt$$

$$= \int_0^1 \langle \nabla f(y + t(x - y)) - \nabla f(y), (x - y) \rangle dt$$

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\langle \nabla f(y), x - y \rangle = \int_0^1 \langle \nabla f(y), x - y \rangle dt \quad &= \int_0^1 \langle \nabla f(y + t(x - y)) - \nabla f(y), (x - y) \rangle dt \\
y + t(x - y) - y = t(x - y) \quad &= \int_0^1 t^{-1} \langle \nabla f(y + t(x - y)) - \nabla f(y), t(x - y) \rangle dt
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Thus, we have a strong convexity criterion satisfied

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f(x) \geq f(y) + \langle \nabla f(y), x - y \rangle + \frac{\mu}{2} \|x - y\|_2^2
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$$

switch x and y

$$
- \langle \nabla f(x), x - y \rangle \leq - \left(f(x) - f(y) + \frac{\mu}{2} \|x - y\|_2^2 \right)
$$

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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$$\begin{aligned} \text{Smoothness:} \quad f(x_{k+1}) &\leq f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{L}{2}\|x_{k+1} - x_k\|^2 \\ \text{Method:} \quad &= f(x_k) - L\langle y_k - x_k, x_{k+1} - x_k \rangle + \frac{L}{2}\|x_{k+1} - x_k\|^2 \end{aligned} \tag{7}$$

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\text{Method:} \quad & = f(x_k) - L\langle y_k - x_k, x_{k+1} - x_k \rangle + \frac{L}{2}\|x_{k+1} - x_k\|^2 \\
\text{Cosine rule:} \quad & = f(x_k) - \frac{L}{2}\left(\|y_k - x_k\|^2 + \|x_{k+1} - x_k\|^2 - \|y_k - x_{k+1}\|^2\right) + \frac{L}{2}\|x_{k+1} - x_k\|^2
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\text{Smoothness:} \quad 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:

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

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

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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 $x = x^*, y = y_k$:

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

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

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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

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

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

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$$\|x^* - \text{proj}_S(y_k)\|^2 + \|y_k - \text{proj}_S(y_k)\|^2 \leq \|x^* - y_k\|^2$$
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$$f(x_k) - f^* \leq \langle \nabla f(x_k), x_k - x^* \rangle$$
$$\leq \frac{L}{2}\left(\frac{1}{L^2}\|\nabla f(x_k)\|^2 + \|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2 - \|y_k - x_{k+1}\|^2\right)$$

Convergence rate for smooth and convex case

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

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4. Now, using convexity and previous part:

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

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 inequality 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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$$\le f(x_0)-f(x_k)+\frac{L}{2}\sum_{i=0}^{i-1}\|y_i-x_{i+1}\|^2+\frac{L}{2}\|x_0-x^*\|^2-\frac{L}{2}\sum_{i=0}^{i-1}\|y_i-x_{i+1}\|^2$$

Convergence rate for smooth and convex case

5. Bound gradients with sufficient decrease inequality 7:

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

Convergence rate for smooth and convex case

5. Bound gradients with sufficient decrease inequality 7:

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

$$\le f(x_0)-f(x_k)+\frac{L}{2}\sum_{i=0}^{i-1}\|y_i-x_{i+1}\|^2+\frac{L}{2}\|x_0-x^*\|^2-\frac{L}{2}\sum_{i=0}^{i-1}\|y_i-x_{i+1}\|^2$$

$$\le f(x_0)-f(x_k)+\frac{L}{2}\|x_0-x^*\|^2$$

$$\sum_{i=0}^{k-1}f(x_i)-kf^* \le f(x_0)-f(x_k)+\frac{L}{2}\|x_0-x^*\|^2$$

Convergence rate for smooth and convex case

5. Bound gradients with sufficient decrease inequality 7:

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&\le f(x_0)-f(x_k)+\frac{L}{2}\sum_{i=0}^{i-1}\|y_i-x_{i+1}\|^2+\frac{L}{2}\|x_0-x^*\|^2-\frac{L}{2}\sum_{i=0}^{i-1}\|y_i-x_{i+1}\|^2 \\
&\le f(x_0)-f(x_k)+\frac{L}{2}\|x_0-x^*\|^2 \\
\sum_{i=0}^{k-1}f(x_i)-kf^* &\le f(x_0)-f(x_k)+\frac{L}{2}\|x_0-x^*\|^2 \\
\sum_{i=1}^{k}[f(x_i)-f^*] &\le \frac{L}{2}\|x_0-x^*\|^2
\end{aligned}$$

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

6. From the sufficient decrease inequality

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

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we use the fact that $x_{k+1} = \mathrm{proj}_S(y_k)$. By definition of projection,

$$\|y_k - x_{k+1}\| \leq \|y_k - x_k\|,$$

Convergence rate for smooth and convex case

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and recall that $y_k = x_k - \frac{1}{L}\nabla f(x_k)$ implies $\|y_k - x_k\| = \frac{1}{L}\|\nabla f(x_k)\|$. Hence

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

Convergence rate for smooth and convex case

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Substitute back into $(*)$:

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

Convergence rate for smooth and convex case

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

we use the fact that $x_{k+1} = \mathrm{proj}_S(y_k)$. By definition of projection,

$$\|y_k - x_{k+1}\| \leq \|y_k - x_k\|,$$

and recall that $y_k = x_k - \frac{1}{L}\nabla f(x_k)$ implies $\|y_k - x_k\| = \frac{1}{L}\|\nabla f(x_k)\|$. Hence

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

Substitute back into $(*)$:

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

Hence

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

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

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

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Convergence rate for smooth and convex case

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

Since $f(x_i)$ decreases in i, in particular $f(x_k) \leq f(x_i)$ for all $i \leq k$. Therefore

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

Convergence rate for smooth and convex case

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Since $f(x_i)$ decreases in i, in particular $f(x_k) \leq f(x_i)$ for all $i \leq k$. Therefore

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

which immediately gives

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

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. 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 $\alpha \leq \frac{1}{L}$ achieves the following convergence after iteration $k > 0$:

$$\|x_k - x^*\|_2^2 \leq (1 - \alpha\mu)^k \|x_0 - x^*\|_2^2$$

Proof

1. We first prove the stationary point property: $\text{proj}_S(x^* - \alpha\nabla f(x^*)) = x^*$.

   This follows from the projection criterion and the first-order optimality condition for x^*. Let $y = x^* - \alpha\nabla f(x^*)$. We need to show $\langle y - x^*, x - x^* \rangle \leq 0$ for all $x \in S$.

   $$\langle (x^* - \alpha\nabla f(x^*)) - x^*, x - x^* \rangle = -\alpha \langle \nabla f(x^*), x - x^* \rangle \leq 0$$

   The inequality holds because $\alpha > 0$ and $\langle \nabla f(x^*), x - x^* \rangle \geq 0$ is the optimality condition for x^*.

Convergence rate for smooth strongly convex case

1. Considering the distance to the solution and using the stationary point property:

Convergence rate for smooth strongly convex case

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$$\|x_{k+1} - x^*\|_2^2 = \|\text{proj}_S(x_k - \alpha \nabla f(x_k)) - x^*\|_2^2$$

Convergence rate for smooth strongly convex case

1. Considering the distance to the solution and using the stationary point property:

$$\|x_{k+1} - x^*\|_2^2 = \|\text{proj}_S(x_k - \alpha\nabla f(x_k)) - x^*\|_2^2$$
$$\text{stationary point property} = \|\text{proj}_S(x_k - \alpha\nabla f(x_k)) - \text{proj}_S(x^* - \alpha\nabla f(x^*))\|_2^2$$

Convergence rate for smooth strongly convex case

1. Considering the distance to the solution and using the stationary point property:

$$\begin{aligned}\|x_{k+1} - x^*\|_2^2 &= \|\mathsf{proj}_S(x_k - \alpha\nabla f(x_k)) - x^*\|_2^2 \\ \text{stationary point property} &= \|\mathsf{proj}_S(x_k - \alpha\nabla f(x_k)) - \mathsf{proj}_S(x^* - \alpha\nabla f(x^*))\|_2^2 \\ \text{nonexpansiveness} &\leq \|x_k - \alpha\nabla f(x_k) - (x^* - \alpha\nabla f(x^*))\|_2^2\end{aligned}$$

Convergence rate for smooth strongly convex case

1. Considering the distance to the solution and using the stationary point property:

$$
\begin{aligned}
\|x_{k+1} - x^*\|_2^2 &= \|\mathsf{proj}_S(x_k - \alpha\nabla f(x_k)) - x^*\|_2^2 \\
\text{stationary point property} &= \|\mathsf{proj}_S(x_k - \alpha\nabla f(x_k)) - \mathsf{proj}_S(x^* - \alpha\nabla f(x^*))\|_2^2 \\
\text{nonexpansiveness} &\leq \|x_k - \alpha\nabla f(x_k) - (x^* - \alpha\nabla f(x^*))\|_2^2 \\
&= \|x_k - x^*\|^2 - 2\alpha\langle\nabla f(x_k) - \nabla f(x^*), x_k - x^*\rangle + \alpha^2\|\nabla f(x_k) - \nabla f(x^*)\|_2^2
\end{aligned}
$$

Convergence rate for smooth strongly convex case

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&= \|x_k - x^*\|^2 - 2\alpha\langle\nabla f(x_k) - \nabla f(x^*), x_k - x^*\rangle + \alpha^2\|\nabla f(x_k) - \nabla f(x^*)\|_2^2
\end{aligned}
$$

2. Now we use smoothness from the convergence tools and strong convexity:

Convergence rate for smooth strongly convex case

1. Considering the distance to the solution and using the stationary point property:

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\|x_{k+1} - x^*\|_2^2 &= \|\mathsf{proj}_S(x_k - \alpha\nabla f(x_k)) - x^*\|_2^2 \\
\text{stationary point property} &= \|\mathsf{proj}_S(x_k - \alpha\nabla f(x_k)) - \mathsf{proj}_S(x^* - \alpha\nabla f(x^*))\|_2^2 \\
\text{nonexpansiveness} &\leq \|x_k - \alpha\nabla f(x_k) - (x^* - \alpha\nabla f(x^*))\|_2^2 \\
&= \|x_k - x^*\|^2 - 2\alpha\langle\nabla f(x_k) - \nabla f(x^*), x_k - x^*\rangle + \alpha^2\|\nabla f(x_k) - \nabla f(x^*)\|_2^2
\end{aligned}$$

2. Now we use smoothness from the convergence tools and strong convexity:

$$\text{smoothness} \quad \|\nabla f(x_k) - \nabla f(x^*)\|_2^2 \leq 2L\left(f(x_k) - f(x^*) - \langle\nabla f(x^*), x_k - x^*\rangle\right)$$

Convergence rate for smooth strongly convex case

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\|x_{k+1} - x^*\|_2^2 &= \|\mathsf{proj}_S(x_k - \alpha\nabla f(x_k)) - x^*\|_2^2 \\
\text{stationary point property} &= \|\mathsf{proj}_S(x_k - \alpha\nabla f(x_k)) - \mathsf{proj}_S(x^* - \alpha\nabla f(x^*))\|_2^2 \\
\text{nonexpansiveness} &\leq \|x_k - \alpha\nabla f(x_k) - (x^* - \alpha\nabla f(x^*))\|_2^2 \\
&= \|x_k - x^*\|^2 - 2\alpha\langle\nabla f(x_k) - \nabla f(x^*), x_k - x^*\rangle + \alpha^2\|\nabla f(x_k) - \nabla f(x^*)\|_2^2
\end{aligned}$$

2. Now we use smoothness from the convergence tools and strong convexity:

$$\begin{aligned}
\text{smoothness} \quad & \|\nabla f(x_k) - \nabla f(x^*)\|_2^2 \leq 2L\left(f(x_k) - f(x^*) - \langle\nabla f(x^*), x_k - x^*\rangle\right) \\
\text{strong convexity} \quad & -\langle\nabla f(x_k) - \nabla f(x^*), x_k - x^*\rangle \leq -\left(f(x_k) - f(x^*) + \frac{\mu}{2}\|x_k - x^*\|_2^2\right) - \langle\nabla f(x^*), x_k - x^*\rangle
\end{aligned}$$

Convergence rate for smooth strongly convex case

3. Substitute it:

Convergence rate for smooth strongly convex case

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$$\|x_{k+1} - x^*\|_2^2 \leq \|x_k - x^*\|^2 - 2\alpha \left(f(x_k) - f(x^*) + \frac{\mu}{2}\|x_k - x^*\|_2^2 \right) - 2\alpha\langle \nabla f(x^*), x_k - x^* \rangle + \\ + \alpha^2 2L \left(f(x_k) - f(x^*) - \langle \nabla f(x^*), x_k - x^* \rangle \right)$$

Convergence rate for smooth strongly convex case

3. Substitute it:

$$\begin{aligned}\|x_{k+1} - x^*\|_2^2 &\leq \|x_k - x^*\|^2 - 2\alpha\left(f(x_k) - f(x^*) + \frac{\mu}{2}\|x_k - x^*\|_2^2\right) - 2\alpha\langle\nabla f(x^*), x_k - x^*\rangle + \\ &+ \alpha^2 2L\left(f(x_k) - f(x^*) - \langle\nabla f(x^*), x_k - x^*\rangle\right) \\ &\leq (1 - \alpha\mu)\|x_k - x^*\|^2 + 2\alpha(\alpha L - 1)\left(f(x_k) - f(x^*) - \langle\nabla f(x^*), x_k - x^*\rangle\right)\end{aligned}$$

Convergence rate for smooth strongly convex case

3. Substitute it:

$$\begin{aligned}\|x_{k+1} - x^*\|_2^2 &\leq \|x_k - x^*\|^2 - 2\alpha\left(f(x_k) - f(x^*) + \frac{\mu}{2}\|x_k - x^*\|_2^2\right) - 2\alpha\langle\nabla f(x^*), x_k - x^*\rangle + \\ &+ \alpha^2 2L\left(f(x_k) - f(x^*) - \langle\nabla f(x^*), x_k - x^*\rangle\right) \\ &\leq (1 - \alpha\mu)\|x_k - x^*\|^2 + 2\alpha(\alpha L - 1)\left(f(x_k) - f(x^*) - \langle\nabla f(x^*), x_k - x^*\rangle\right)\end{aligned}$$

4. Due to convexity of f: $f(x_k) - f(x^*) - \langle\nabla f(x^*), x_k - x^*\rangle \geq 0$. Therefore, if we use $\alpha \leq \frac{1}{L}$:

$$\|x_{k+1} - x^*\|_2^2 \leq (1 - \alpha\mu)\|x_k - x^*\|^2,$$

which is exactly linear convergence of the method with up to $1 - \frac{\mu}{L}$ convergence rate.

Frank-Wolfe Method

Рисунок 11: Marguerite Straus Frank (1927-2024)

Рисунок 12: Philip Wolfe (1927-2016)

Idea

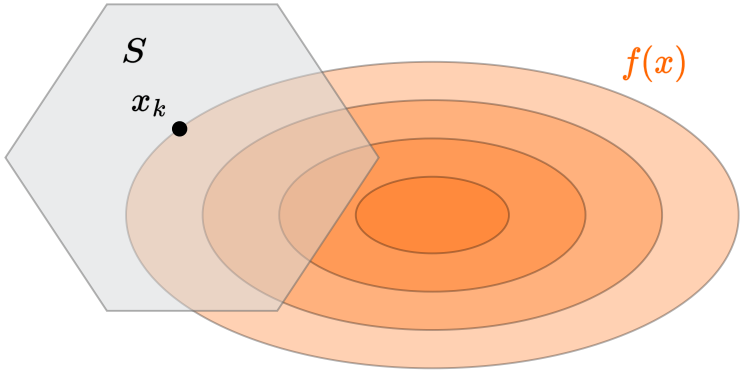

Рисунок 13: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

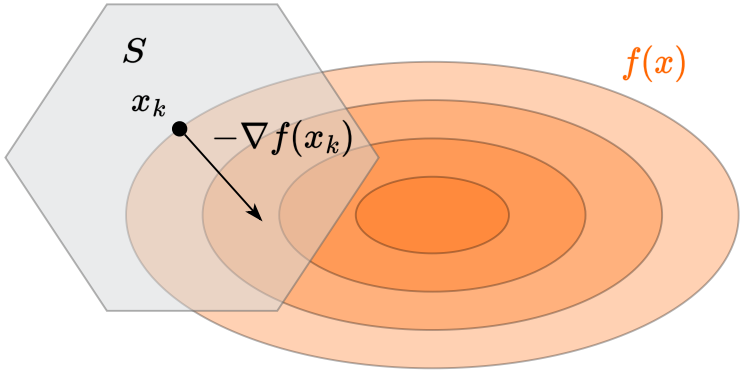

Рисунок 14: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

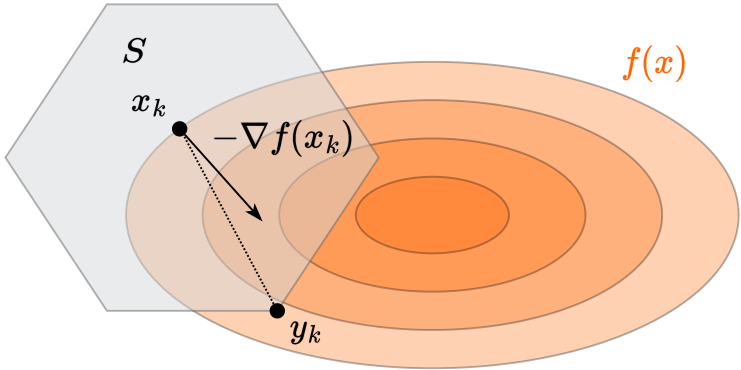

Рисунок 15: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

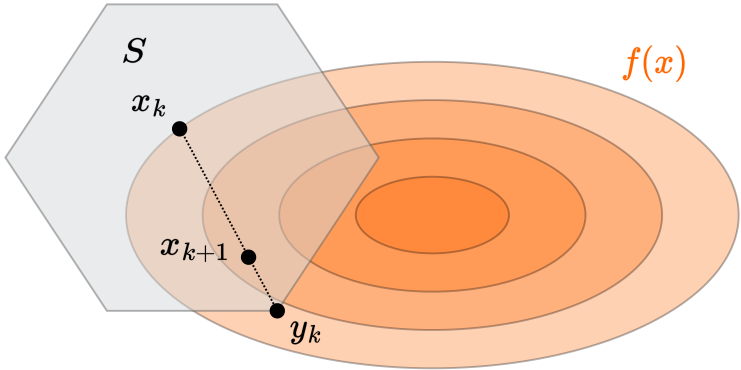

Рисунок 16: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

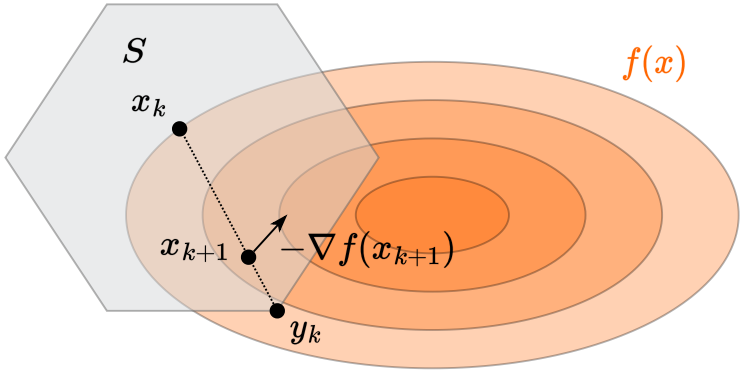

Рисунок 17: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

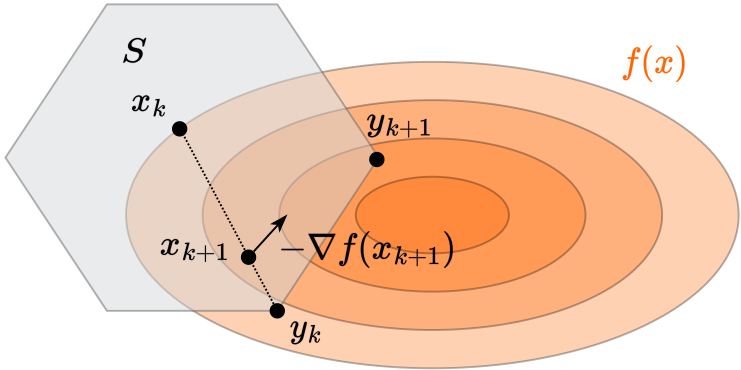

Рисунок 18: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

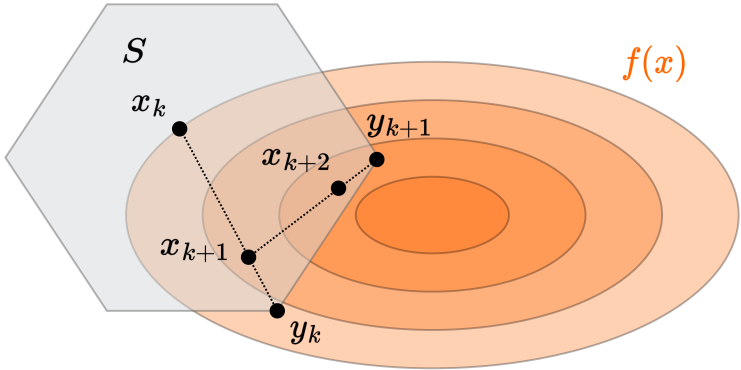

Рисунок 19: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

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

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

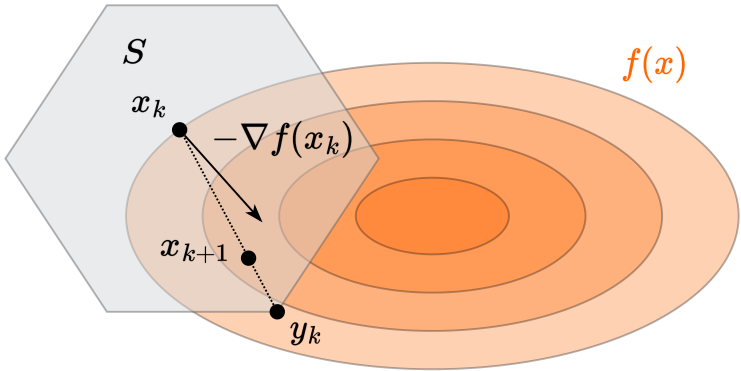

Рисунок 20: Illustration of Frank-Wolfe (conditional gradient) algorithm

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 $x = x^*$:

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

Convergence rate for smooth and convex case

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3. By definition of y_k, we have $\langle \nabla f(x_k), y_k \rangle \leq \langle \nabla f(x_k), x^* \rangle$, thus:

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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:

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

Convergence rate for smooth and convex case

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7. We will prove that $\delta_k \leq \frac{2}{k+1}$ by induction.

which gives us the desired result:

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   - Base: $\delta_2 \leq \frac{1}{2} < \frac{2}{3}$

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   - Assume $\delta_k \leq \frac{2}{k+1}$
   - 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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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

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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

Frank-Wolfe method summary

- Method does not require projections, in some special cases allows to compute iterations in closed form

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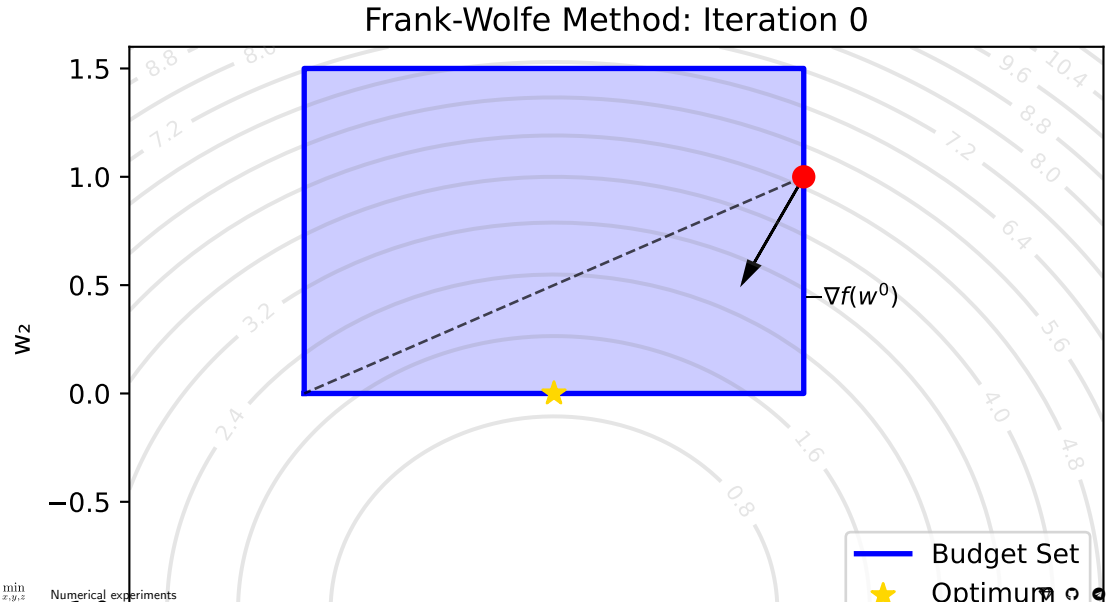
- Recent work showed the extension to non-smooth case (paper) with convergence rate $O\left(\frac{1}{\sqrt{k}}\right)$

Numerical experiments

2d example. Frank-Wolfe method



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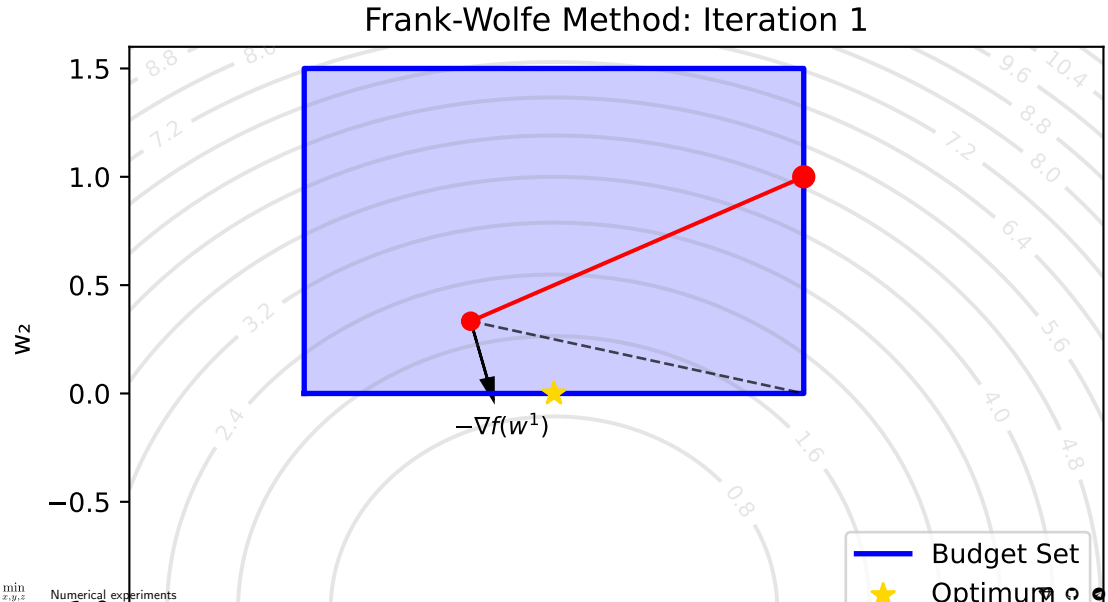

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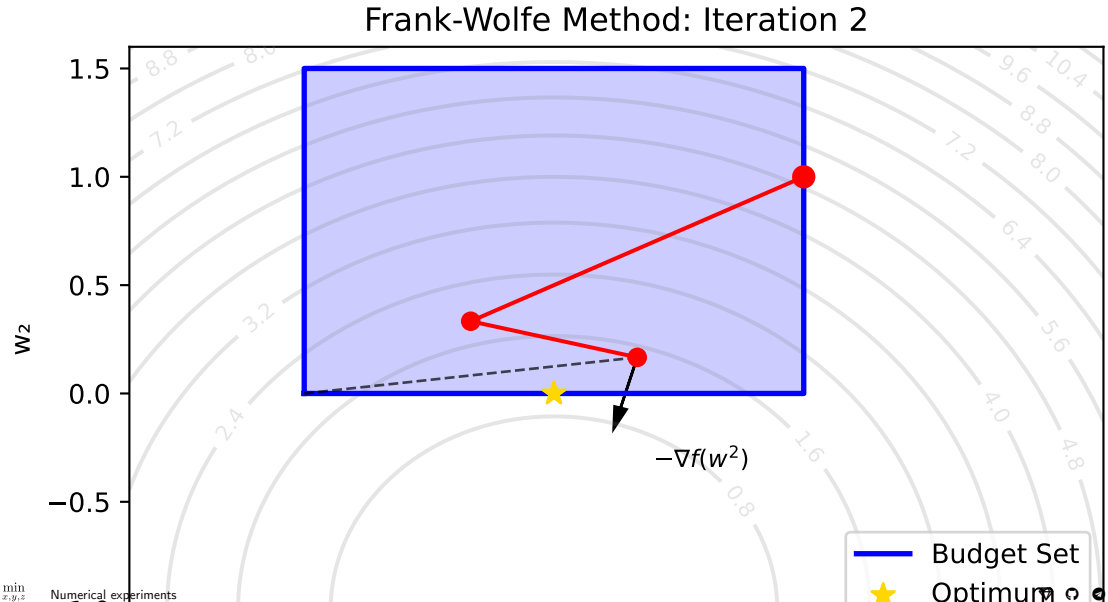

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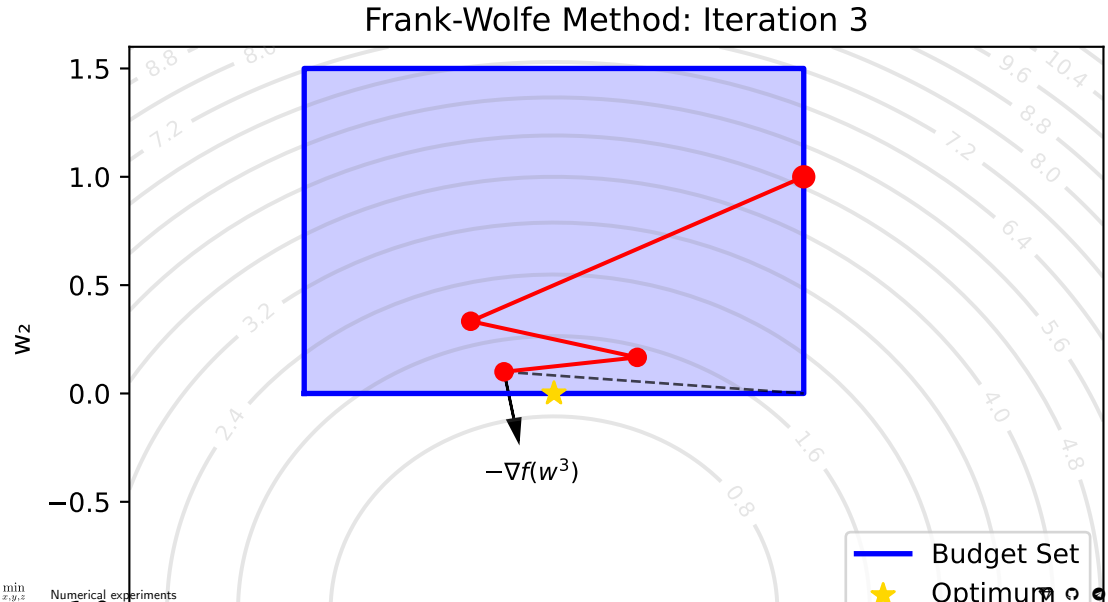

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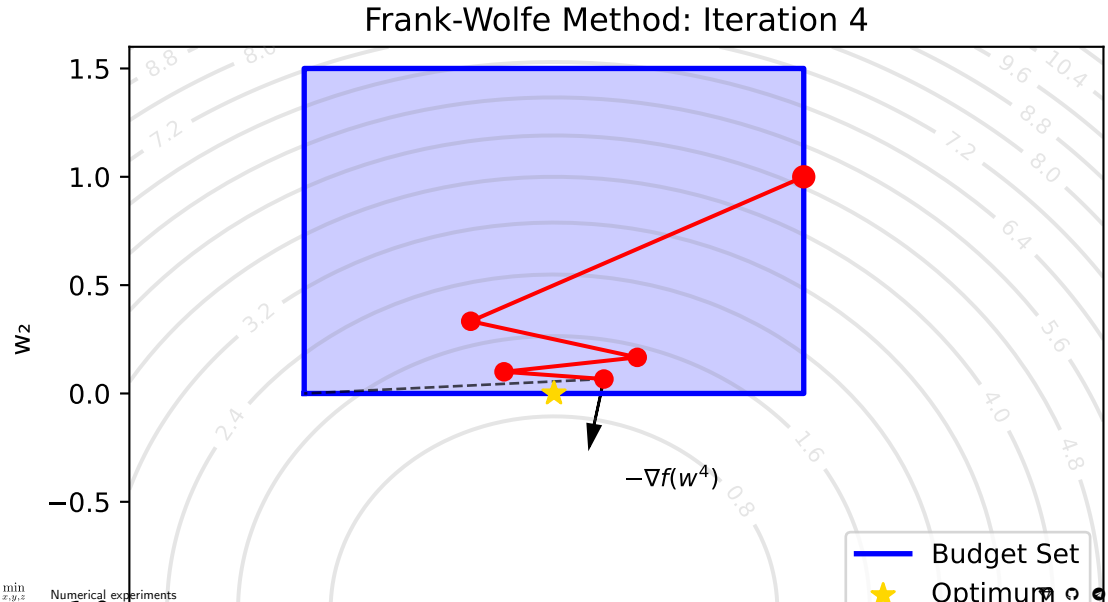

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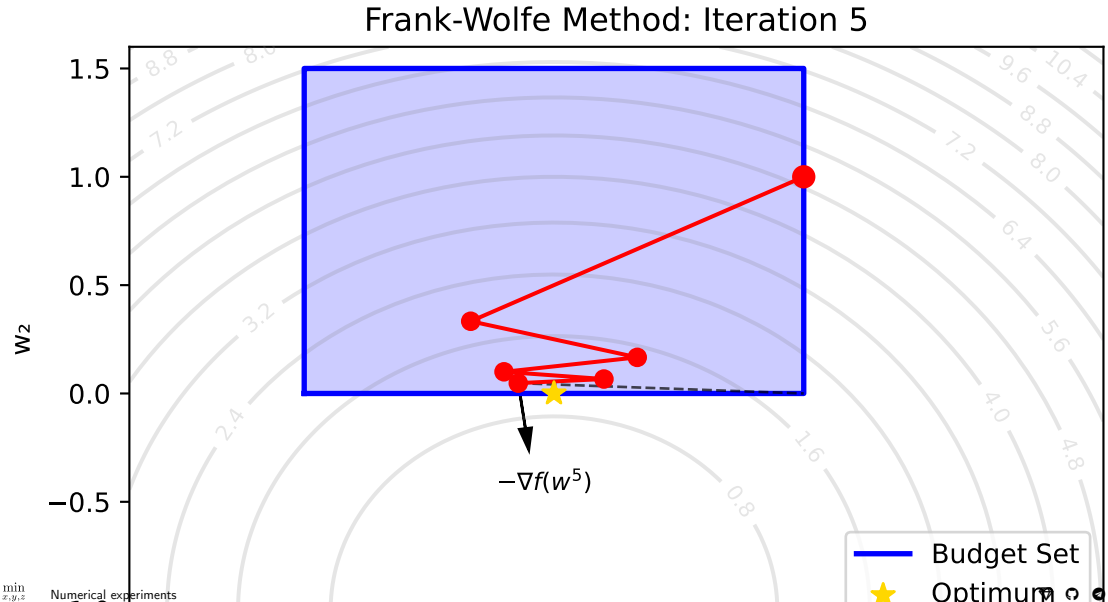

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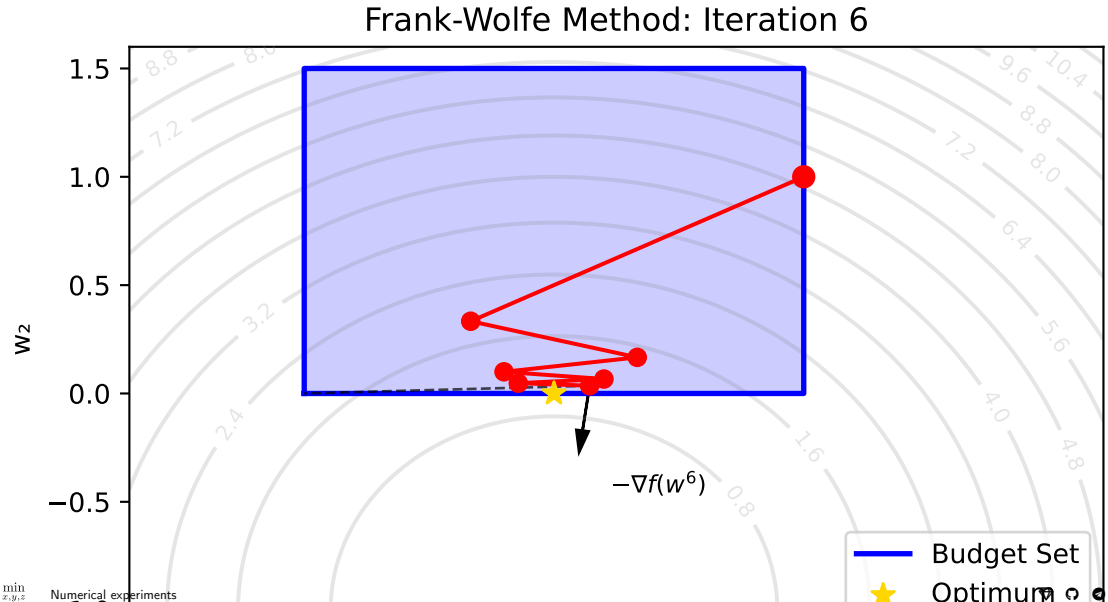

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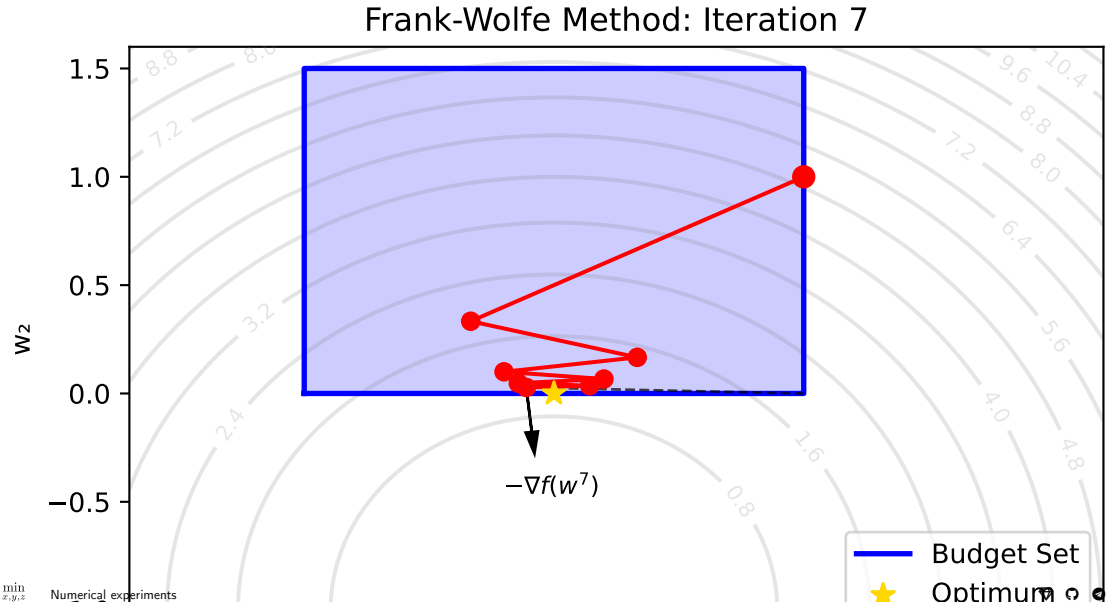
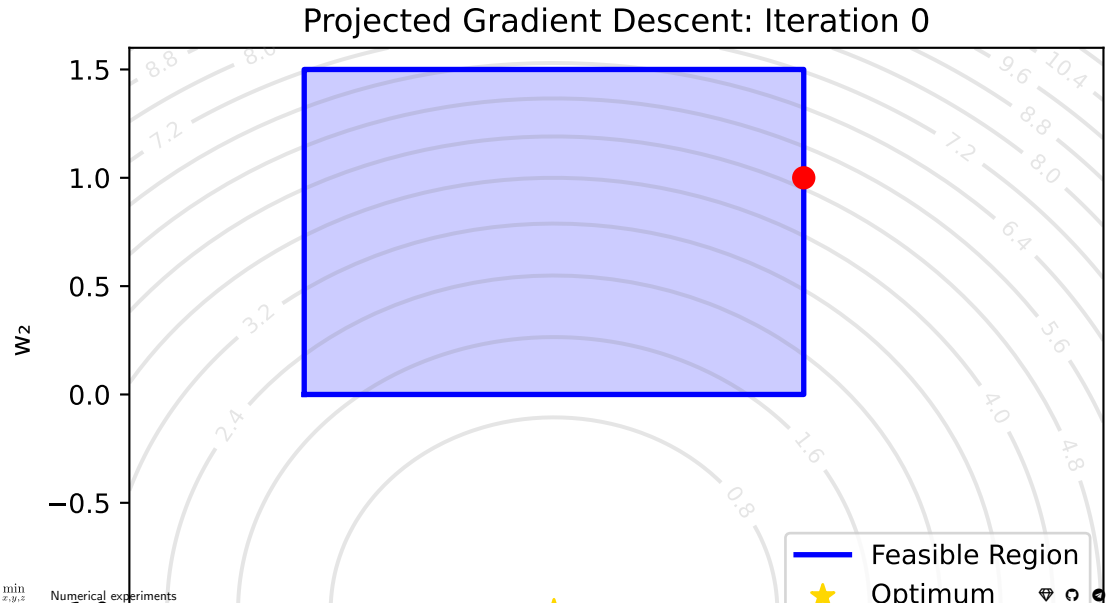


2d example. Projected gradient descent



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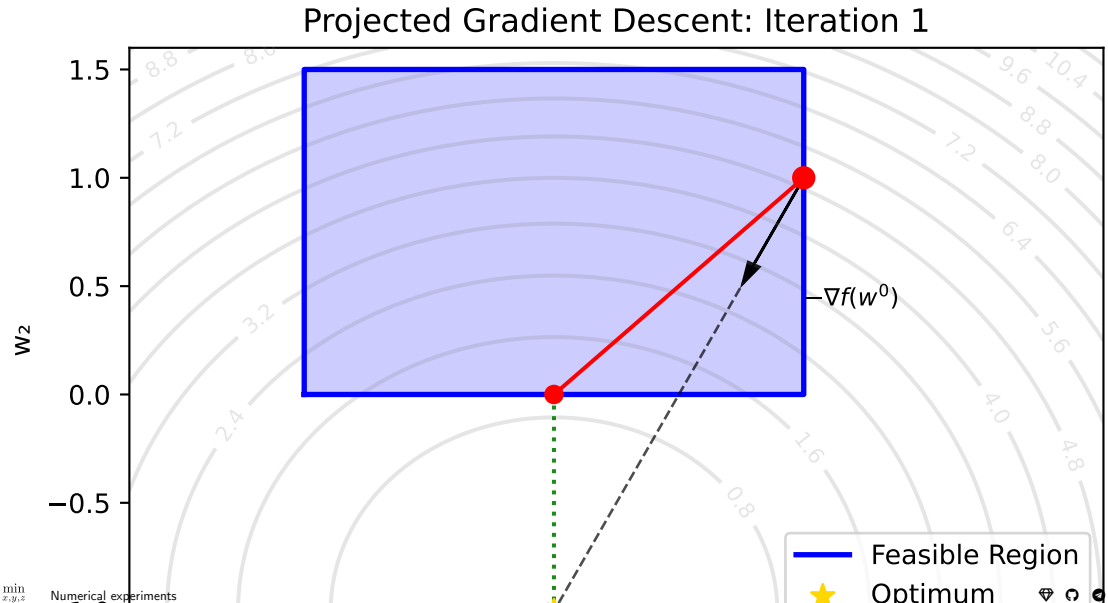

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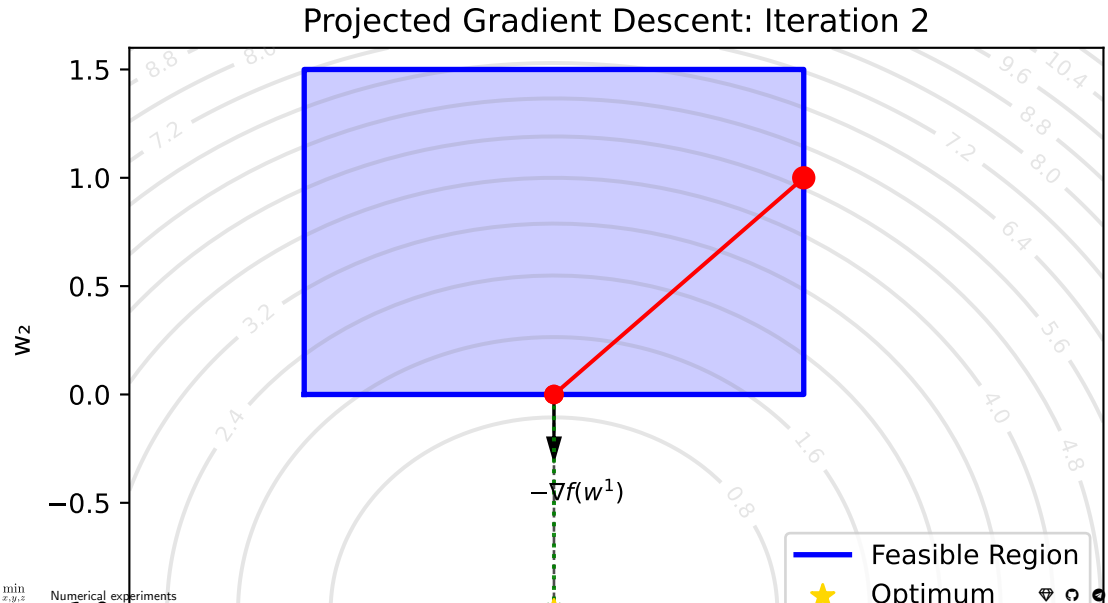


Quadratic function. Box constraints

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

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

The projection is simple:

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

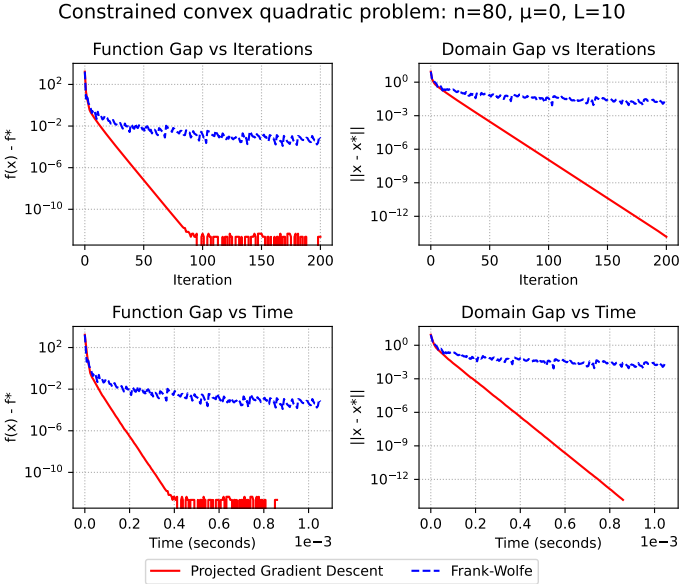
or

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

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

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

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



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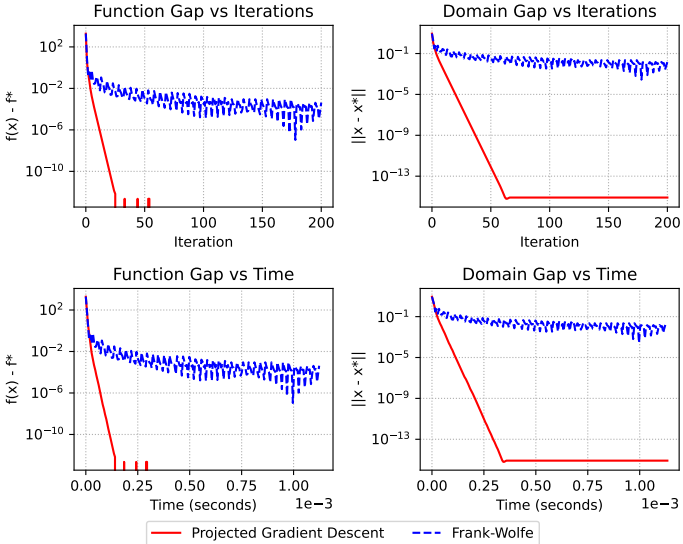
Constrained strongly Convex quadratic problem: n=80, μ=1, L=10



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

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

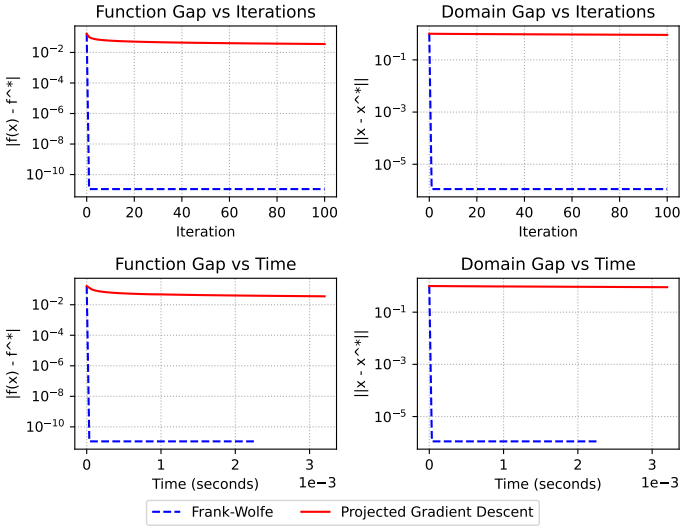
$$A \in \mathbb{R}^{n \times n}, \quad \lambda(A) \in [0; 100].$$

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

$$y = e_j \quad \text{where} \quad j = \underset{i}{\operatorname{argmin}}\, g_i.$$

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



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

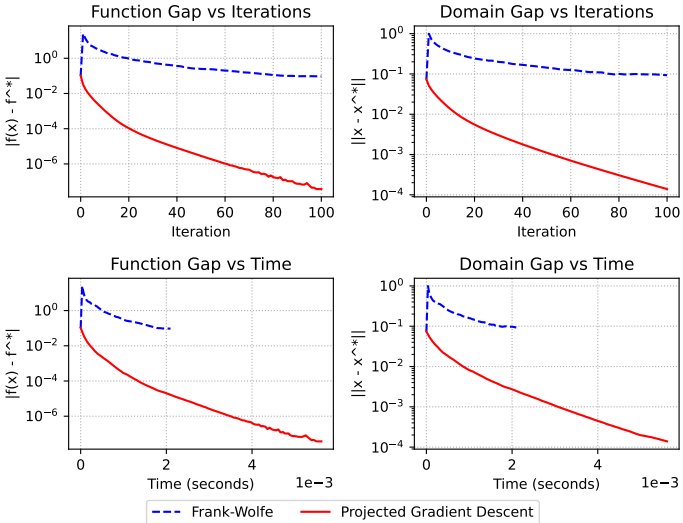
Quadratic function. Simplex constraints

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

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

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

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



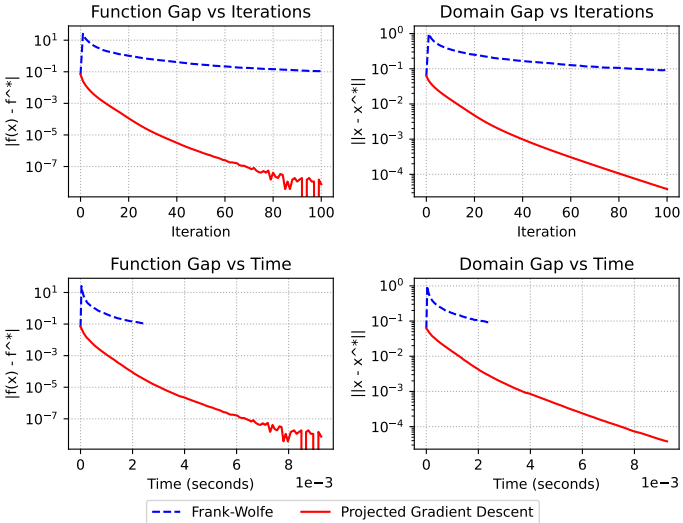
Quadratic function. Simplex constraints

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

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

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

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



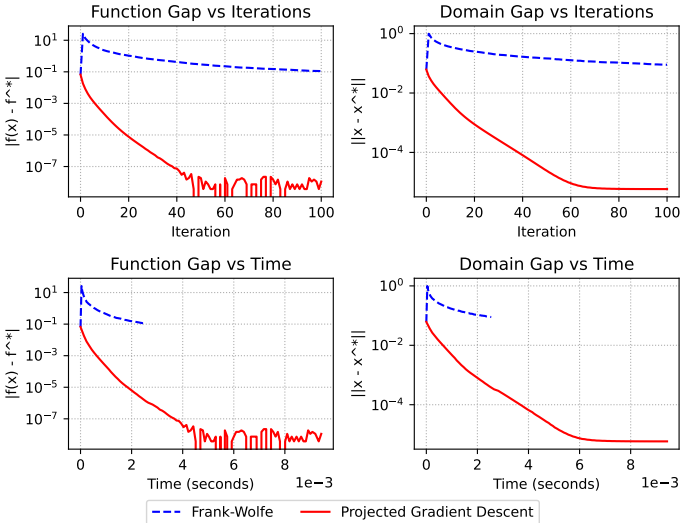
Quadratic function. Simplex constraints

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

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

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.