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

Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University

Constrained optimization

Unconstrained optimization

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- 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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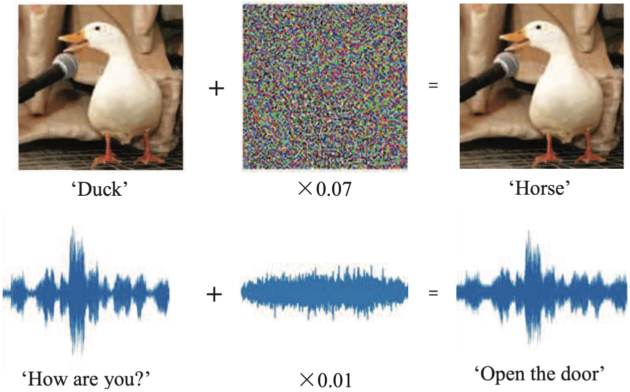
Is it possible to tune GD to fit constrained problem?

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

Example: White-box Adversarial Attacks



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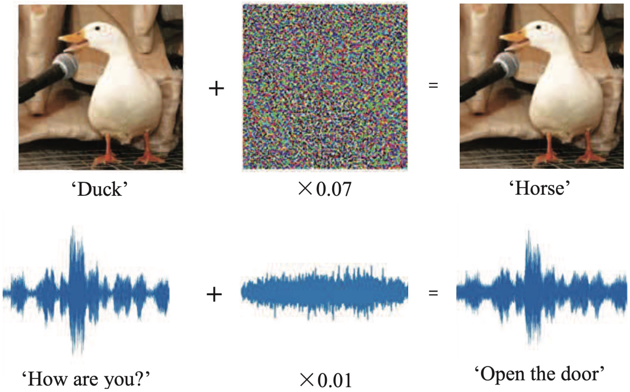

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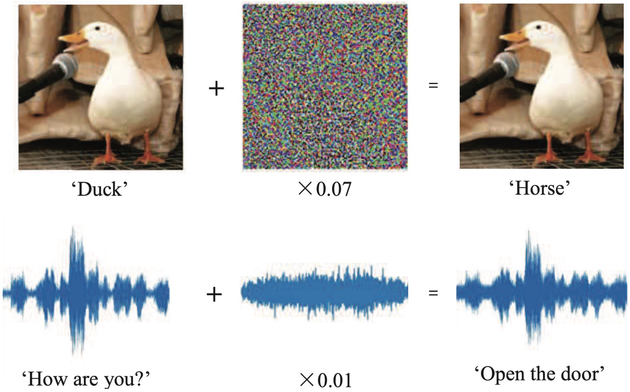

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- Mathematically, a neural network is a function $f(w; x)$
- Typically, input x is given and network weights w optimized
- Could also freeze weights w and optimize x, adversarially!

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

or

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

Idea of Projected Gradient Descent

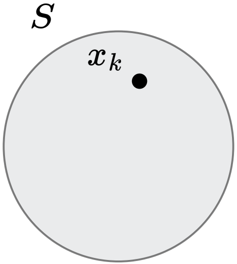

Figure 2: Suppose, we start from a point x_k.

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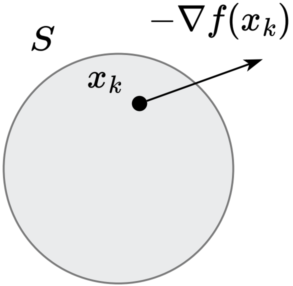

Figure 3: And go in the direction of $-\nabla f(x_k)$.

Idea of Projected Gradient Descent

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

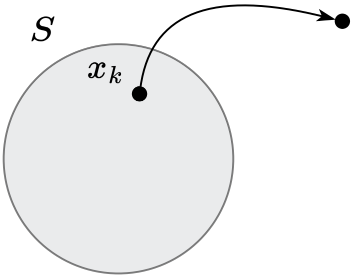

Figure 4: Occasionally, we can end up outside the feasible set.

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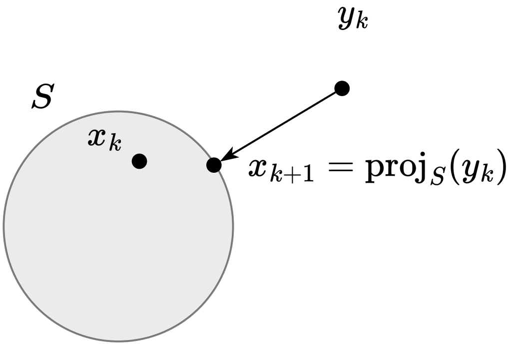

Figure 5: Solve this little problem with projection!

Idea of Projected Gradient Descent

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

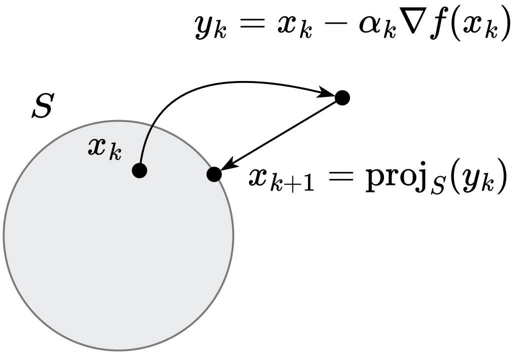

Figure 6: Illustration of Projected Gradient Descent algorithm

Projection

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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- If a point is in set, then its projection is the point itself.

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

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

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

Proof

1. $\text{proj}_S(y)$ is minimizer of differentiable convex function $d(y, S, \|\cdot\|) = \|x - y\|^2$ over S. By first-order characterization of optimality.

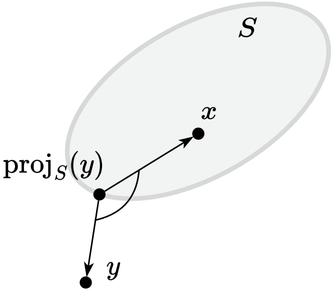

Figure 7: Obtuse or straight angle should be for any point $x \in S$

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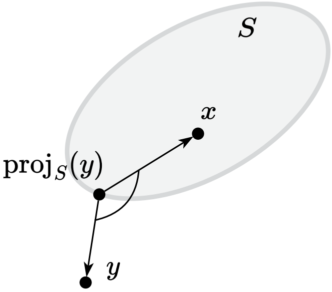

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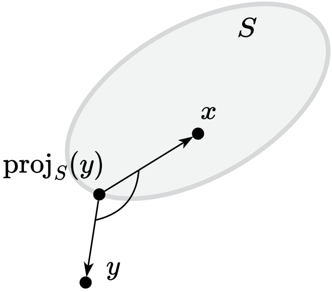

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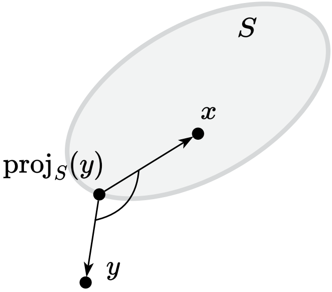

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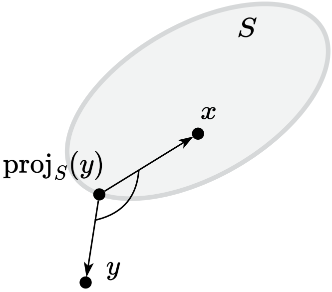

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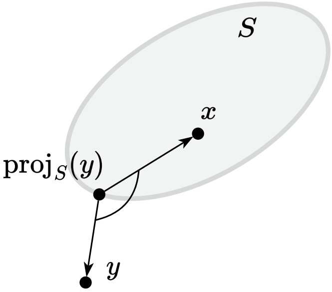

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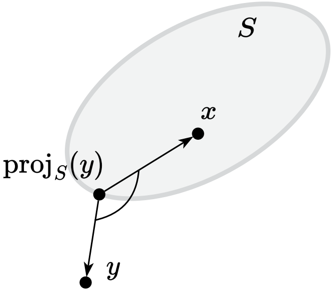

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Projection operator is non-expansive

- 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.

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

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

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Replace x by $\pi(x)$ in Equation 3

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(Equation 4)+(Equation 5) will cancel $\pi(y) - \pi(x)$, not good. So flip the sign of (Equation 5) gives

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

Projection operator is non-expansive

Shorthand notation: let $\pi = \text{proj}$ and $\pi(x)$ denotes $\text{proj}(x)$.

Begins with the variational characterization / obtuse angle inequality

$$\langle y - \pi(y), x - \pi(y) \rangle \leq 0 \quad \forall x \in S. \tag{3}$$

Replace x by $\pi(x)$ in Equation 3

$$\langle y - \pi(y), \pi(x) - \pi(y) \rangle \leq 0. \tag{4}$$

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

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\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}$$

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

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

$$
\frac{R - \|y - x_0\|}{\|y - x_0\|^2} (y - x_0)^T \left((x - x_0) \|y - x_0\| - R (y - x_0) \right) =
$$

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

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

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$$

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

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

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

Example: projection on the ball

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

Build a hypothesis from the figure: $\pi = x_0 + R \cdot \frac{y - x_0}{\|y - x_0\|}$

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

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

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

$$\frac{R - \|y - x_0\|}{\|y - x_0\|^2} (y - x_0)^T \left((x - x_0) \|y - x_0\| - R\left(y - x_0\right) \right) =$$

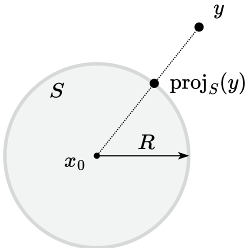
$$\frac{R - \|y - x_0\|}{\|y - x_0\|} \left((y - x_0)^T (x - x_0) - R\|y - x_0\| \right) =$$

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

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

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

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



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:

Example: projection on the halfspace

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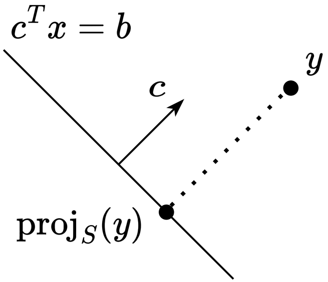

Figure 9: Hyperplane

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:

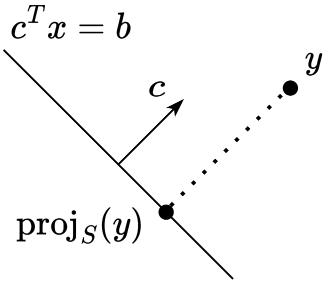

Figure 9: Hyperplane

$$
\begin{aligned}
c^T(y + \alpha c) &= b \\
c^T y + \alpha c^T c &= b \\
c^T y &= b - \alpha c^T c
\end{aligned}
$$

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

$$
\begin{aligned}
(y + \alpha c - y)^T(x - y - \alpha c) &= \\
\alpha c^T(x - y - \alpha c) &= \\
\alpha(c^T x) - \alpha(c^T y) - \alpha^2(c^T c) &= \\
\alpha b - \alpha(b - \alpha c^T c) - \alpha^2 c^T c &= \\
\alpha b - \alpha b + \alpha^2 c^T c - \alpha^2 c^T c &= 0 \geq 0
\end{aligned}
$$

Idea

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

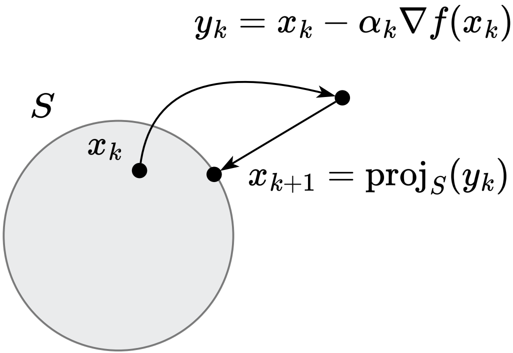

Figure 10: Illustration of Projected Gradient Descent algorithm

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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Proof

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)

Convergence rate for smooth and convex case

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

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

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

Convergence rate for smooth and convex case

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

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

Convergence rate for smooth and convex case

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

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

$$\|x^* - \text{proj}_S(y_k)\|^2 + \|y_k - \text{proj}_S(y_k)\|^2 \leq \|x^* - y_k\|^2$$
$$\|y_k - x^*\|^2 \geq \|x^* - x_{k+1}\|^2 + \|y_k - x_{k+1}\|^2$$

Convergence rate for smooth and convex case

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

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

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

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

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

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 lemma 7:

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

Convergence rate for smooth and convex case

6. Let's show monotonic decrease of the iteration of the method.

Convergence rate for smooth and convex case

6. Let's show monotonic decrease of the iteration of the method.
7. And finalize the convergence bound.

Idea

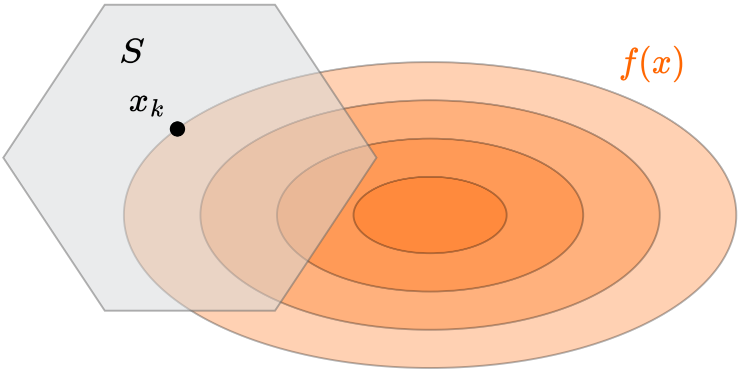

Figure 11: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

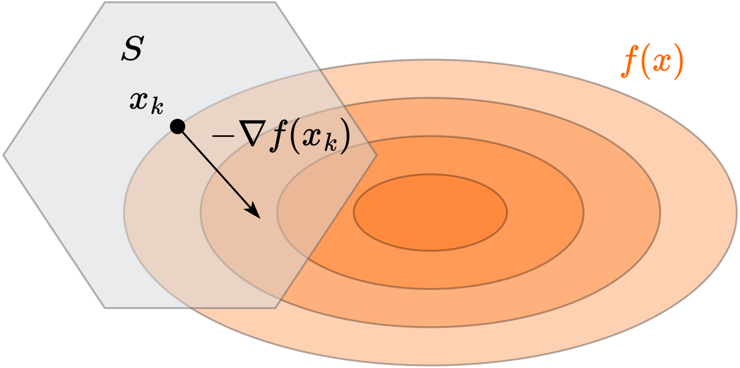

Figure 12: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

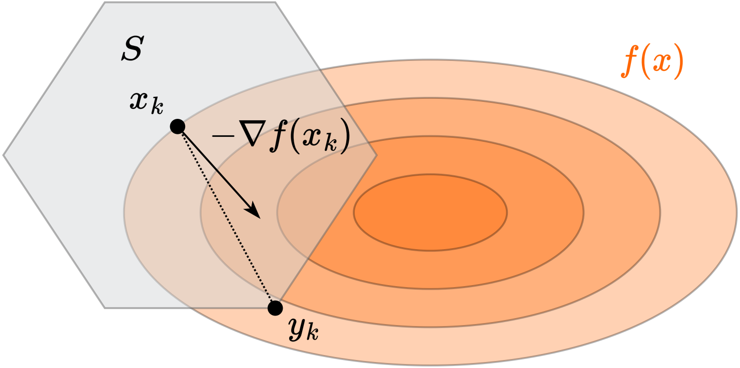

Figure 13: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

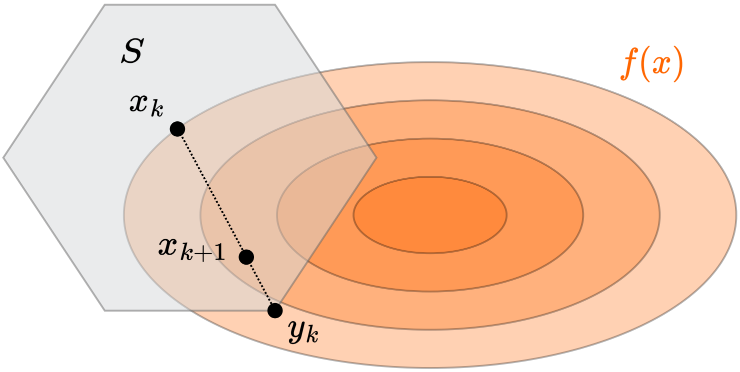

Figure 14: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

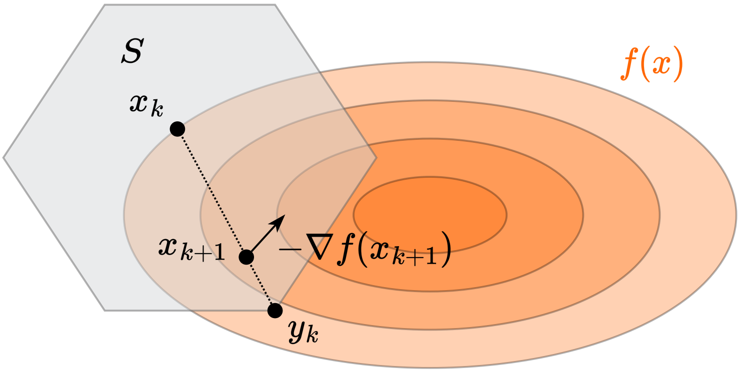

Figure 15: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

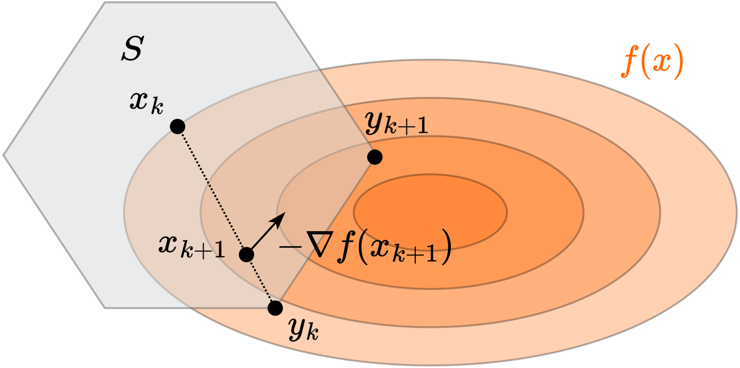

Figure 16: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

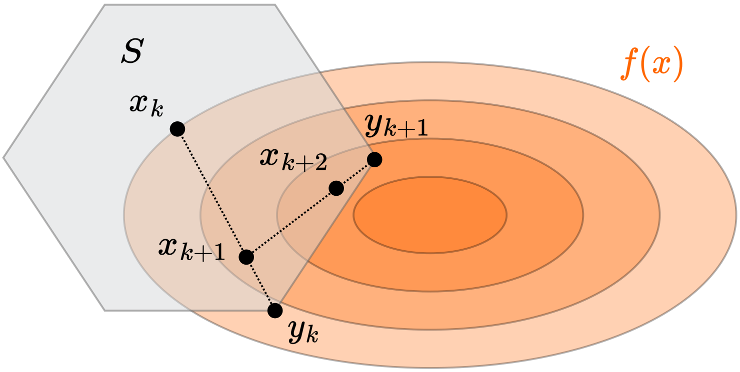

Figure 17: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

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

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

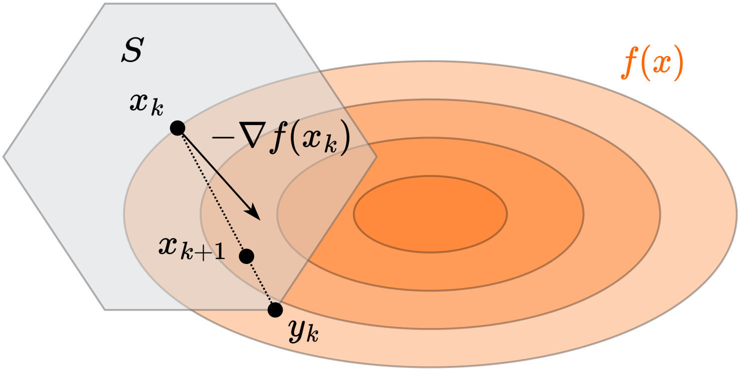

Figure 18: Illustration of Frank-Wolfe (conditional gradient) algorithm

Convergence (1/2)

Consider the problem

$$f(x) \to \min_{x \in S},$$

where f is convex and L-smooth. The Frank-Wolfe method is given by:

$$\begin{cases} x_{k+1} = \gamma_k x_k + (1 - \gamma_k) s_k \\ s_k = \arg\min_{x \in S} f^I_{x_k}(x) = \arg\min_{x \in S} \langle \nabla f(x_k), x \rangle \end{cases},$$

where $f^I_{x_k}(x)$ is the first-order Taylor approximation at the point x_k. For $\gamma_k = \frac{k-1}{k+1}$, it holds that

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

where $R = \max_{x,y \in S} \|x - y\|$. Thus, we have sublinear convergence.

Convergence (2/2)

L-smoothness:

$$f(x) - f(y) - \langle \nabla f(y), x - y \rangle \leqslant \frac{L}{2}\|x - y\|^2, \quad \forall x, y \in S$$

$$f\left(x_{k+1}\right) - f\left(x_k\right) \leqslant \left\langle \nabla f\left(x_k\right), x_{k+1} - x_k \right\rangle + \frac{L}{2}\left\|x_{k+1} - x_k\right\|^2$$

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

Convexity:

$$f(x) - f(y) - \langle \nabla f(y), x - y \rangle \geqslant 0 \quad \forall x, y \in S \Rightarrow \quad x := x^*, y := x_k \Rightarrow \quad \langle \nabla f(x_k), x^* - x_k \rangle \leqslant f(x^*) - f(x_k)$$

$$f\left(x_{k+1}\right) - f\left(x_k\right) \leqslant \left(1 - \gamma_k\right)\left\langle \nabla f\left(x_k\right), x^* - x_k \right\rangle + \frac{L\left(1 - \gamma_k\right)^2}{2} R^2 \leqslant \left(1 - \gamma_k\right)\left(f\left(x^*\right) - f\left(x_k\right)\right) + \left(1 - \gamma_k\right)^2 \frac{LR^2}{2}$$

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

Denote $\delta_k = \frac{f(x_k) - f\left(x^*\right)}{LR^2}$. Then the inequality can be rewritten as

$$\delta_{k+1} \leqslant \gamma_k \delta_k + \frac{\left(1 - \gamma_k\right)^2}{2} = \frac{k-1}{k+1}\delta_k + \frac{2}{(k+1)^2}.$$

Starting from the inequality $\delta_2 \leqslant \frac{1}{2}$, applying induction on k yields the desired result.