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

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

- 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

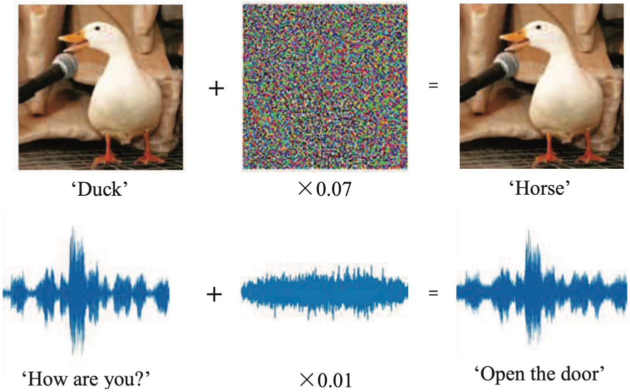

Figure 1: Source

BECA

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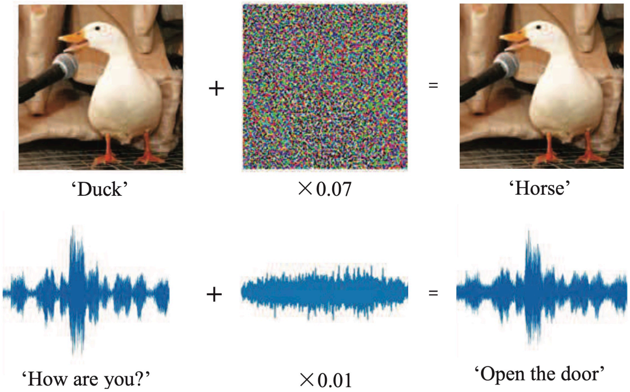

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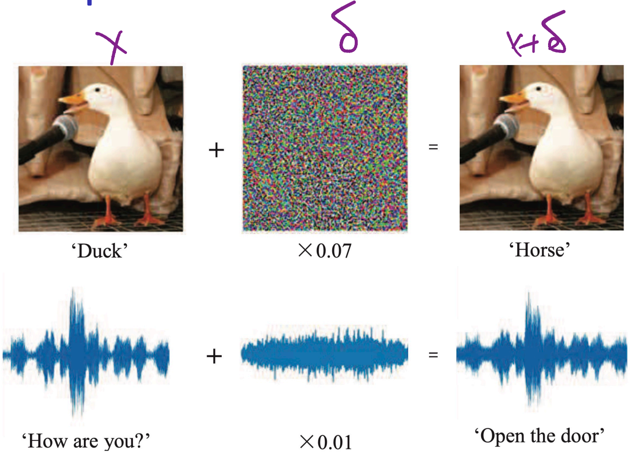

Figure 1: Source

- 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

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

Idea of Projected Gradient Descent

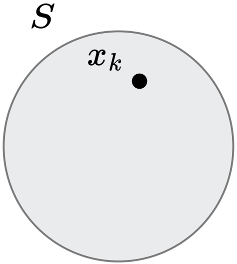

Figure 2: Suppose, we start from a point x_k.

Idea of Projected Gradient Descent

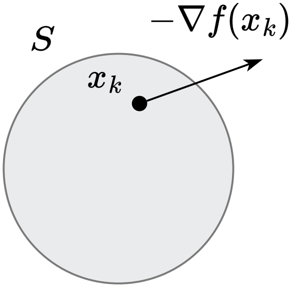

Figure 3: And go in the direction of $-\nabla f(x_k)$.

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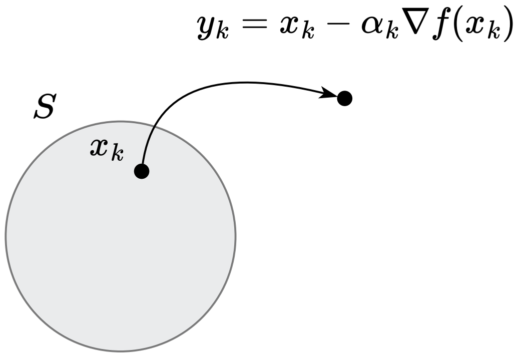

Figure 4: Occasionally, we can end up outside the feasible set.

Idea of Projected Gradient Descent

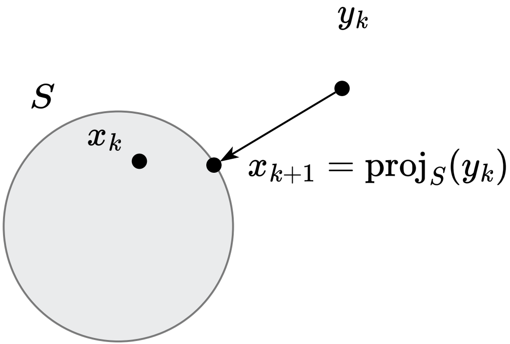

Figure 5: Solve this little problem with projection!

Idea of Projected Gradient Descent

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

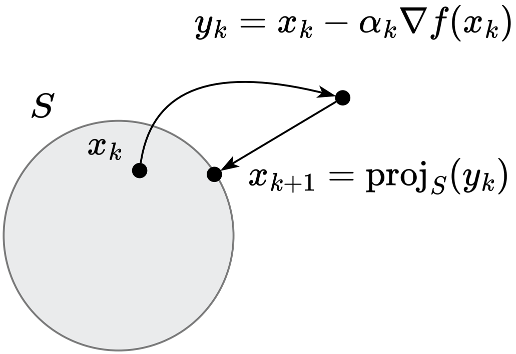

Figure 6: Illustration of Projected Gradient Descent algorithm

Projection

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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MIRROR DESCENT

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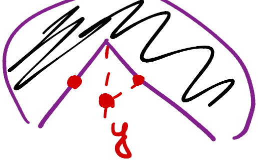

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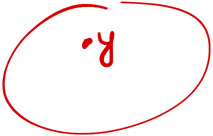

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Projection criterion (Bourbaki-Cheney-Goldstein inequality)

Theorem

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

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

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

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.

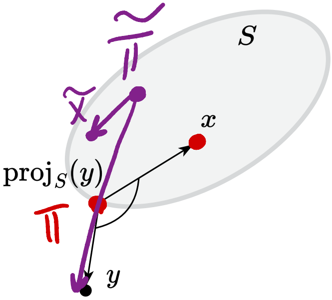

Figure 7: Obtuse or straight angle should be for any point $x \in S$

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проецируемая точка

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Тупоугольность

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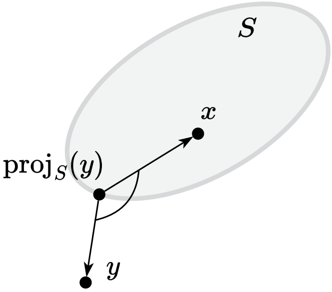

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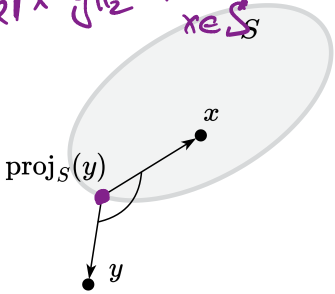

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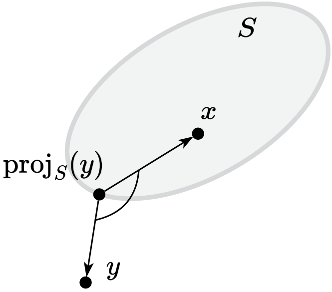

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$\|x-y\|^2 = \|x\|^2 + \|y\|^2 - 2\langle x, y\rangle$

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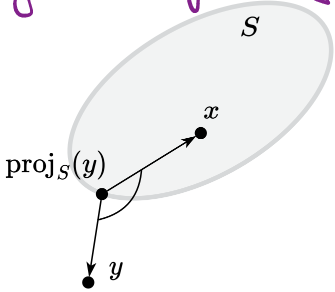
$$\boxed{(y - \text{proj}_S(y))^T (x - \text{proj}_S(y)) \leq 0}$$

2. Use cosine rule $2x^T y = \|x\|^2 + \|y\|^2 - \|x - y\|^2$ with $x = x - \text{proj}_S(y)$ and $y = y - \text{proj}_S(y)$. By the first property of the theorem:



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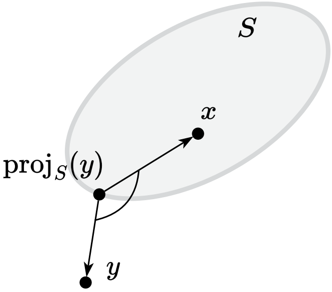

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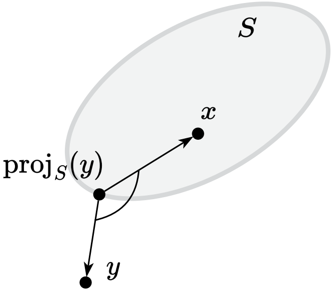

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Projection operator is non-expansive

$\|f(x) - f(y)\| \leq \|x - y\|$

- 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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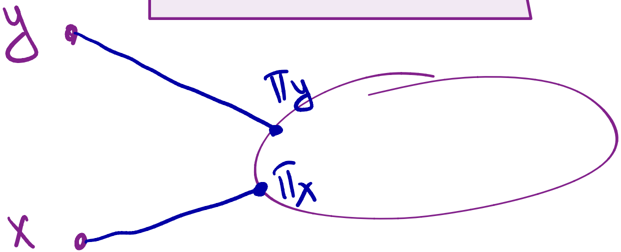
$$\|\text{proj}(x) - \text{proj}(y)\|_2 \leq \|x - y\|_2.$$



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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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Begins with the variational characterization / obtuse angle inequality

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

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

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

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

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Replace y by x and x by $\pi(y)$ 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

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

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$\langle y - \pi(y) + \pi(x) - x, \pi(x) - \pi(y) \rangle \leq 0$ (4)+(6)

$\langle y - x + \pi(x) - \pi(y), \pi(x) - \pi(y) \rangle \leq 0$

$$\langle y - x, \pi(x) - \pi(y) \rangle \leq -\langle \pi(x) - \pi(y), \pi(x) - \pi(y) \rangle$$

$$\langle y - x, \pi(y) - \pi(x) \rangle \geq \|\pi(x) - \pi(y)\|_2^2$$

$$\|(y - x)^\top (\pi(y) - \pi(x))\|_2 \geq \|\pi(x) - \pi(y)\|_2^2$$

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

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

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

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

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

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

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

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

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

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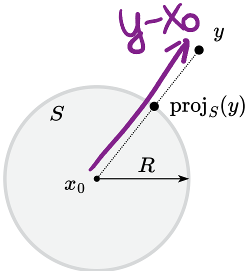
The first factor is negative for point selection y. The second factor is also negative, which follows from the Cauchy-Bunyakovsky inequality:

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

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



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:

Example: projection on the ~~halfspace~~ hyperplane

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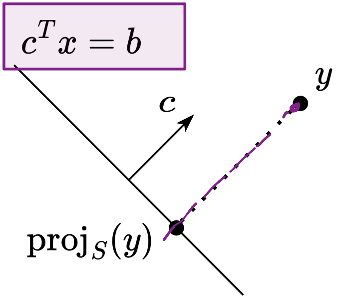

Figure 9: Hyperplane

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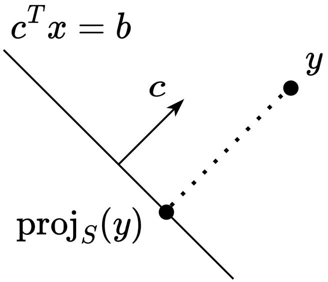


Figure 9: Hyperplane

$$\pi = y + \frac{b - c^T y}{c^T c} c$$

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

$$c^T y + \alpha c^T c = b$$

$$c^T y = b - \alpha c^T c$$

$$\alpha = \frac{b - c^T y}{c^T c}$$

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

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

$$\alpha c^T (x - y - \alpha c) =$$

$$\alpha(c^T x) - \alpha(c^T y) - \alpha^2 (c^T c) =$$

$$\alpha b - \alpha(b - \alpha c^T c) - \alpha^2 c^T c =$$

$$\alpha b - \alpha b + \alpha^2 c^T c - \alpha^2 c^T c = 0 \geq 0$$

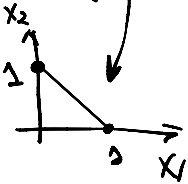
Idea

$$\text{softmax}(x) = \left(\frac{e^{x_i}}{\sum e^{x_i}}\right)$$

$$x_{k+1} = \text{proj}_S \left(x_k - \alpha_k \nabla f(x_k)\right) \quad \Leftrightarrow \quad \begin{array}{l} 1.\; y_k = x_k - \alpha_k \nabla f(x_k) \\ 2.\; x_{k+1} = \text{proj}_S \left(y_k\right) \end{array}$$

вероятный симплекс

$$\begin{cases} 1^T x = 1 \\ x \geq 0 \end{cases}$$



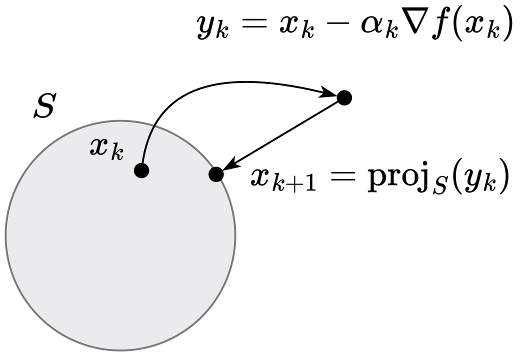


Figure 10: Illustration of Projected Gradient Descent algorithm

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)

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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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$$
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\text{Cosine rule:} \quad & = f(x_k) - \frac{L}{2}\left(\|y_k - x_k\|^2 + \|x_{k+1} - x_k\|^2 - \|y_k - x_{k+1}\|^2\right) + \frac{L}{2}\|x_{k+1} - x_k\|^2
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$$
\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:} & &= 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 \\
& & &= 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 $x = x^*, y = y_k$:

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

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

Convergence rate for smooth and convex case

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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:

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:

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

+ монотонность

$$\Rightarrow f(x_k) - f^* \le \frac{LR^2}{2k}$$

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

PGD $\frac{1}{k}$ $\mu = 0$

лин. $\mu > 0$

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

если не умеем быстро считать проекции

Idea

FRANK-WOLFE

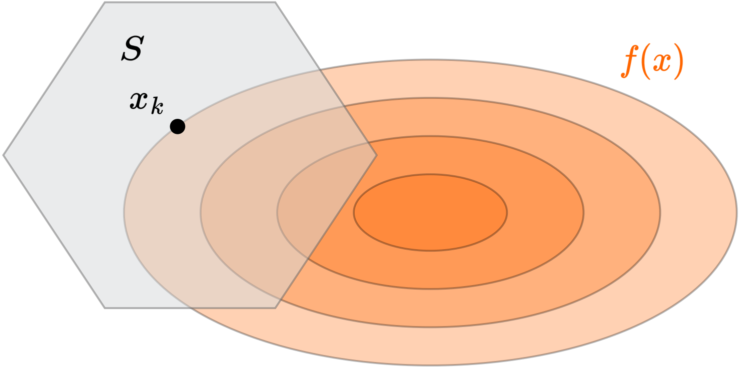

Figure 11: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

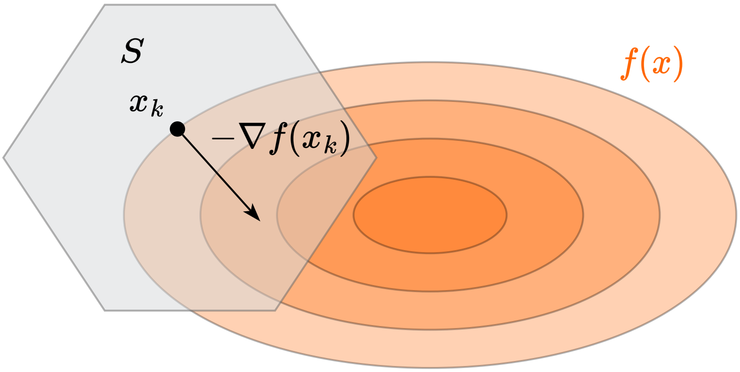

Figure 12: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

Идея: заменить $f(x)$ на $f^I_{x_k}(x)$

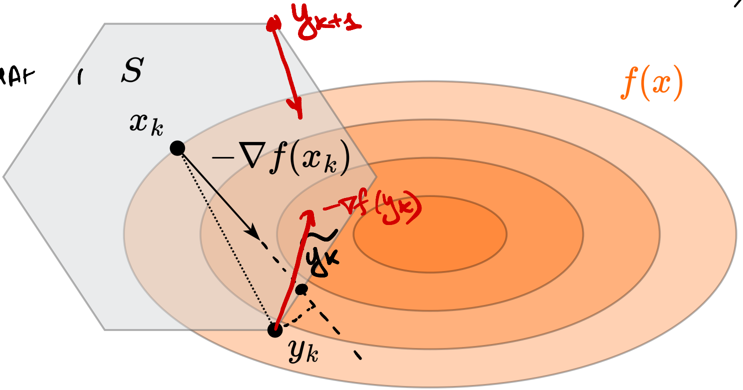

Figure 13: Illustration of Frank-Wolfe (conditional gradient) algorithm

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

Idea

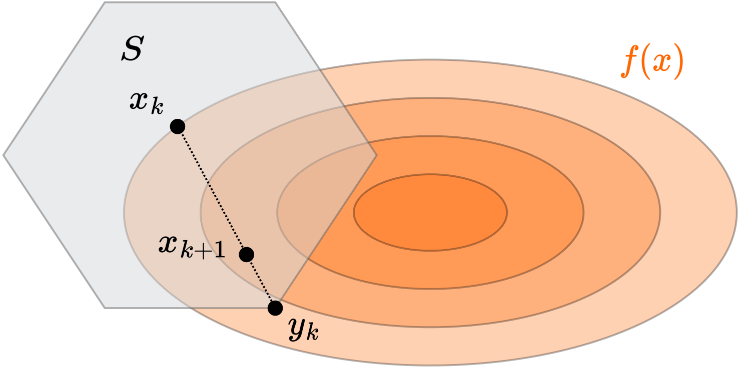

Figure 14: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

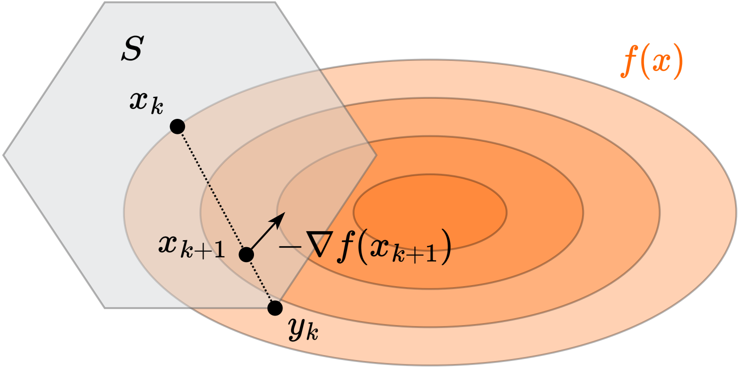

Figure 15: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

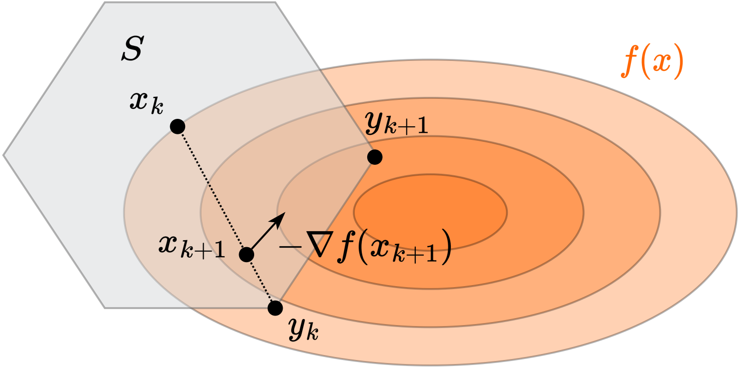

Figure 16: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

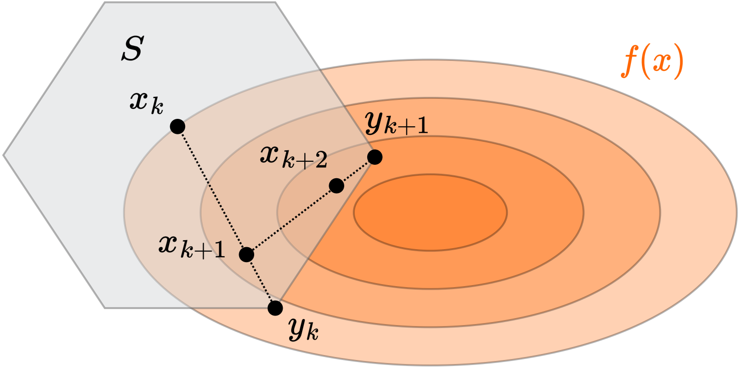

Figure 17: Illustration of Frank-Wolfe (conditional gradient) algorithm

Idea

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

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

$\gamma_k \sim \frac{1}{k}$

γ_k на практике $= const$

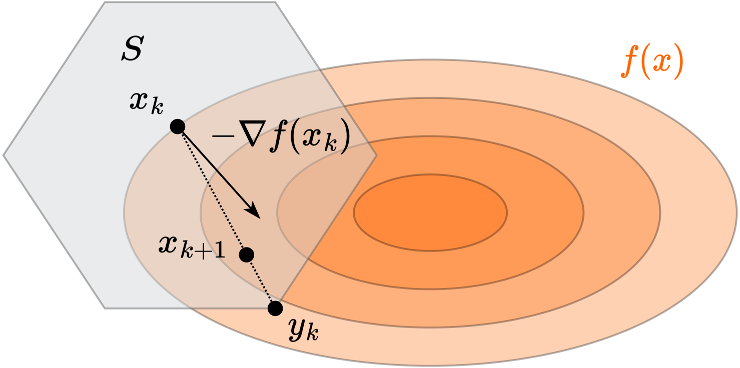

Figure 18: Illustration of Frank-Wolfe (conditional gradient) algorithm

Convergence

Теорема

FW

$$f(x^k) - f^* \le \frac{\max\{2L\,\mathrm{diam}(S), f(x^0) - f^*\}}{k+2}$$

FW

в $\mu = 0$ (выпуклом гладком) случае

в $\mu > 0$

$$\sim \frac{1}{k^2}$$

Comparison to PGD

$$\text{PGD} \quad x_{k+1} = \text{PROJ}\left(x_k - \alpha_k \cdot \nabla f(x_k)\right)$$

$$\sim \quad x_{k+1} = \underset{x \in S}{\operatorname{argmin}} \left(\alpha \langle \nabla f(x_k), x \rangle + \frac{1}{2}\|x - x_k\|^2 \right)$$

$$S = \mathbb{R}^n \Rightarrow \alpha \nabla f(x_k) + x_{k+1} - x_k = 0 \Rightarrow x_{k+1} = x_k - \alpha \nabla f$$

$$S \neq \mathbb{R}^n \Rightarrow$$ MD [illegible]