A Corgi puppy and a yellow rubber duck are positioned inside a wireframe cube. The cube is made of thin, transparent lines forming a 3D geometric shape. The puppy is on the left, looking towards the camera, while the duck is on the right, facing left. The background is a plain, light color.

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

**Daniil Merkulov**

Optimization methods. MIPT

## Conditional methods

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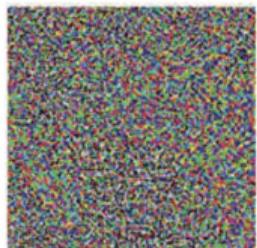
Is it possible to tune GD to fit constrained problem?

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

## Example: White-box Adversarial Attacks



'Duck'



$\times 0.07$



'Horse'



'How are you?'



$\times 0.01$



'Open the door'

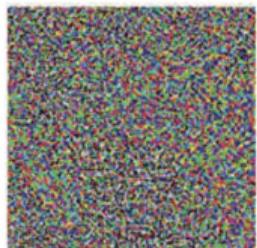
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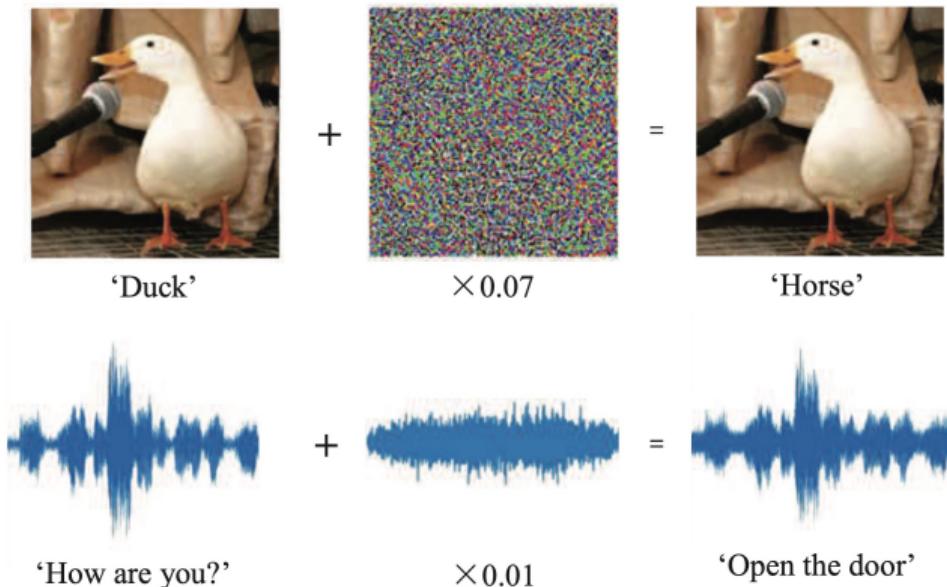


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## Example: White-box Adversarial Attacks



- 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

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

Figure 1: Source

## Idea of Projected Gradient Descent

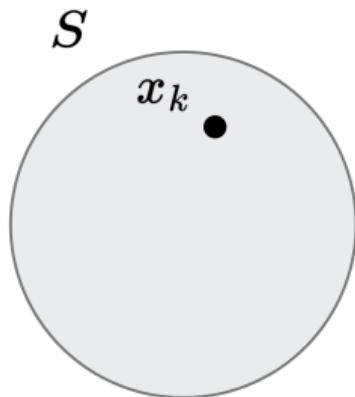


Figure 2: Suppose, we start from a point  $x_k$ .

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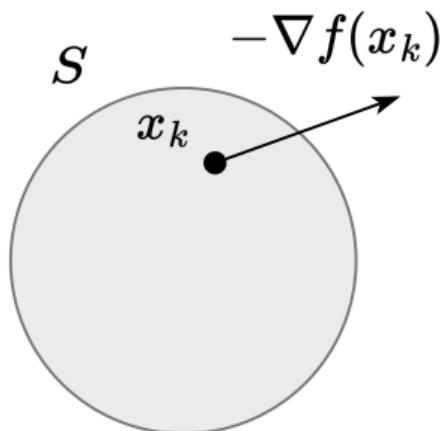


Figure 3: And go in the direction of  $-\nabla f(x_k)$ .

## Idea of Projected Gradient Descent

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

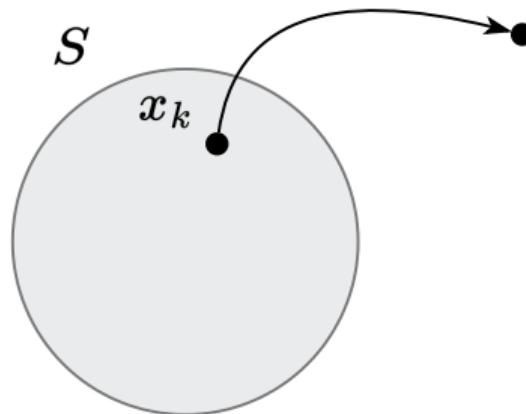


Figure 4: Occasionally, we can end up outside the feasible set.

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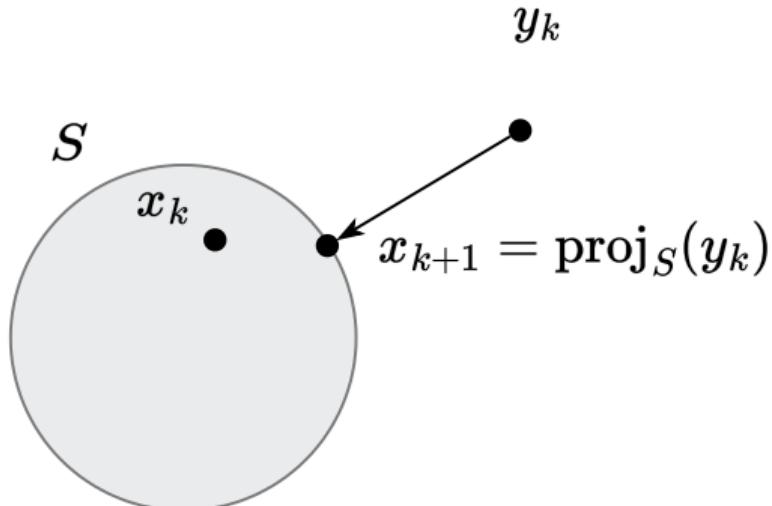


Figure 5: Solve this little problem with projection!

## Idea of Projected Gradient Descent

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

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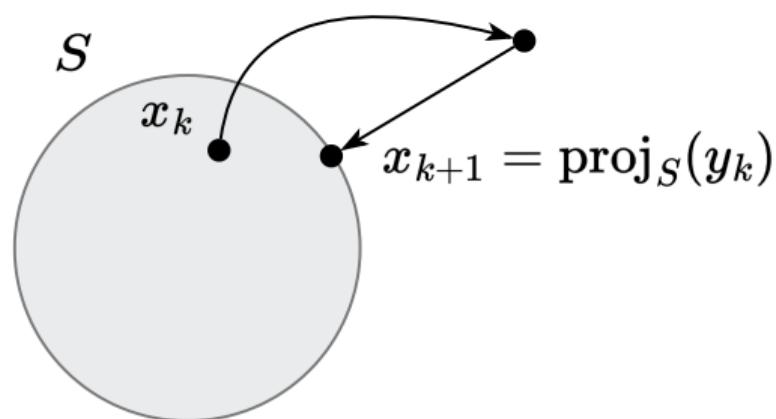


Figure 6: Illustration of Projected Gradient Descent algorithm

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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

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

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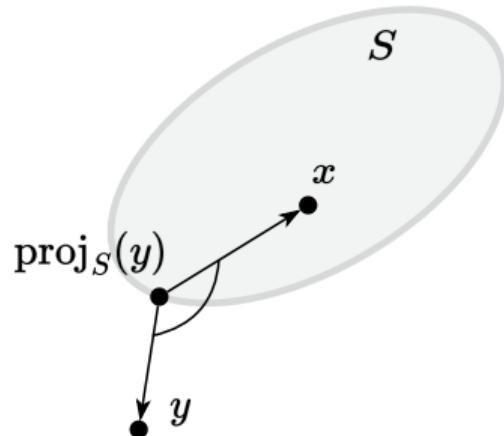


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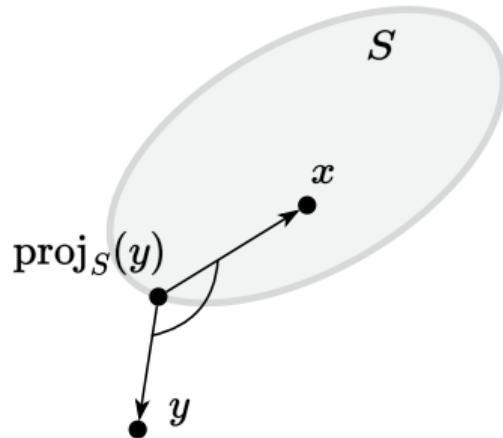


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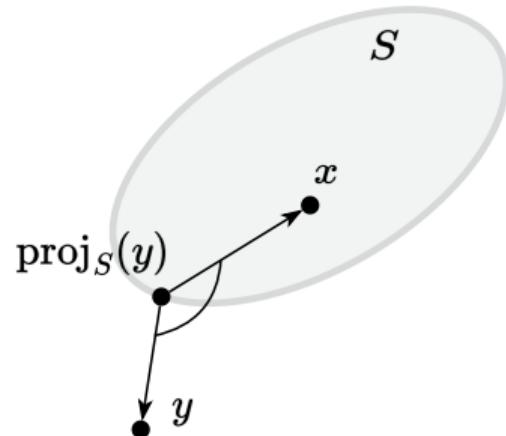


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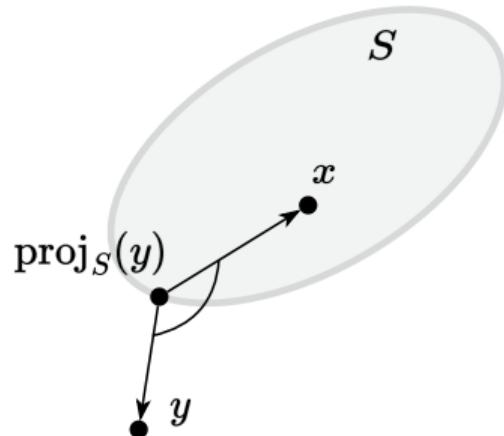


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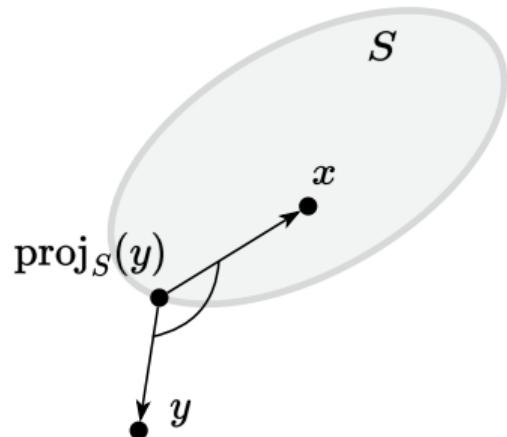


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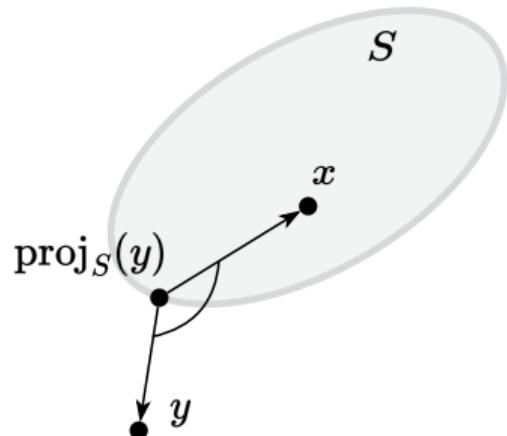


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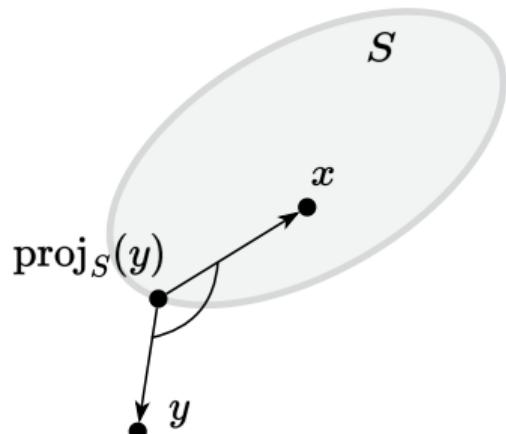


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- Next: variational characterization implies non-expansiveness. i.e.,

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

$$\langle y - \pi(y), \pi(x) - \pi(y) \rangle \leq 0. \quad (4)$$

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Begins with the variational characterization / obtuse angle inequality

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

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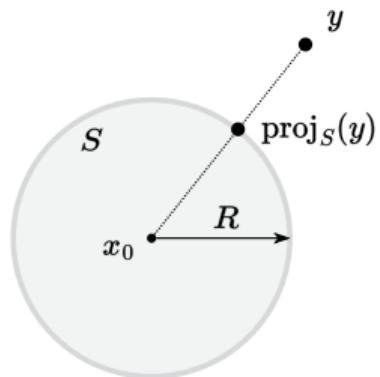
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$$(y - x_0)^T (x - x_0) \leq \|y - x_0\| \|x - x_0\|$$
$$\frac{(y - x_0)^T (x - x_0)}{\|y - x_0\|} - R \leq \frac{\|y - x_0\| \|x - x_0\|}{\|y - x_0\|} - R$$



## 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  $\alpha$  is chosen so that  $\pi \in S$ :  $c^T \pi = b$ , so:

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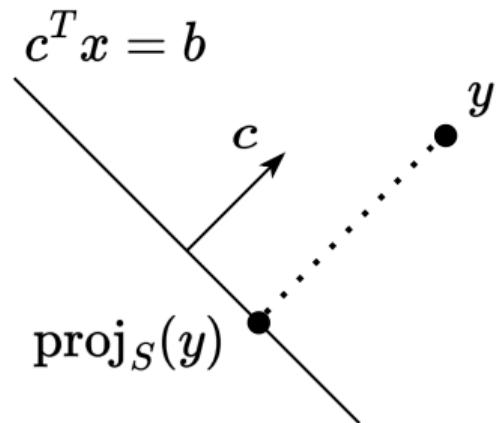


Figure 9: Hyperplane

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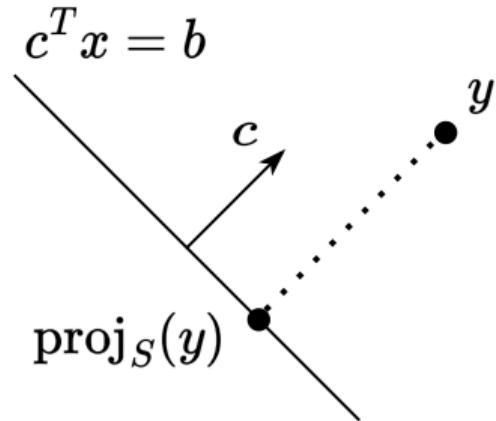


Figure 9: Hyperplane

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

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

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

## Projected Gradient Descent (PGD)

## Idea

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

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

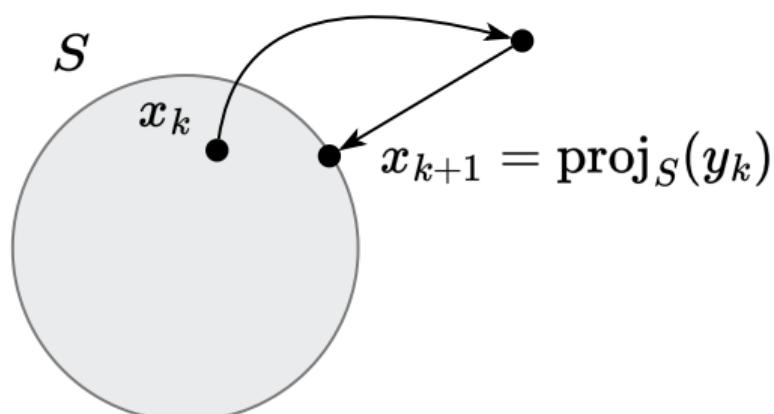


Figure 10: Illustration of Projected Gradient Descent algorithm

## Convergence rate for smooth and convex case

### i Theorem

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  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 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  $2x^T y = \|x\|^2 + \|y\|^2 - \|x - y\|^2$ :

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

## Convergence rate for smooth and convex case

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

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

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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 lemma 7:

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

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

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

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

## Convergence rate for smooth and convex case

- From the sufficient decrease inequality

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

we use the fact that  $x_{k+1} = \text{proj}_S(y_k)$ . 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

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

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.

## Frank-Wolfe Method

## Idea

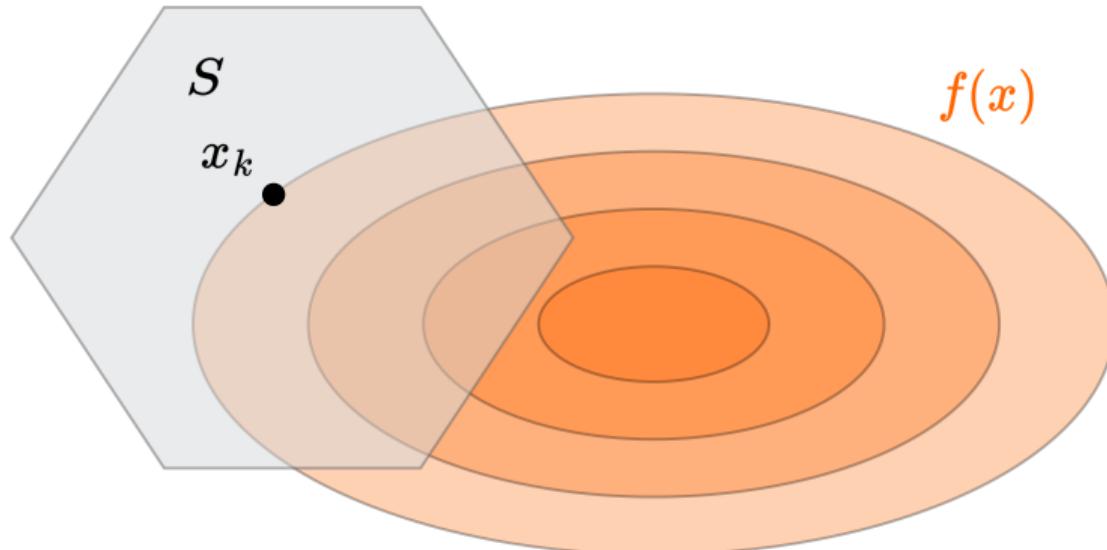


Figure 11: Illustration of Frank-Wolfe (conditional gradient) algorithm

## Idea

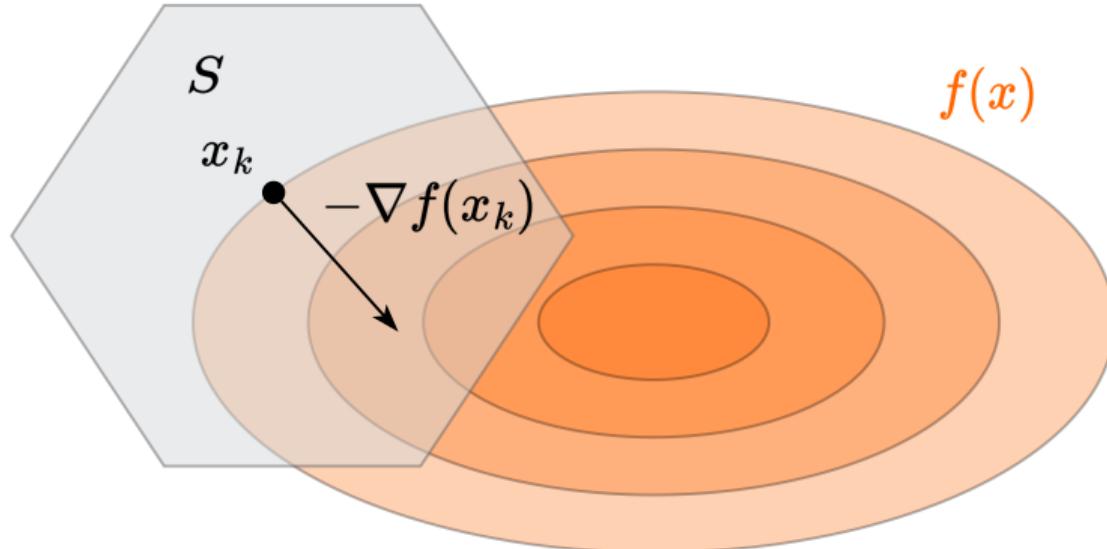


Figure 12: Illustration of Frank-Wolfe (conditional gradient) algorithm

## Idea

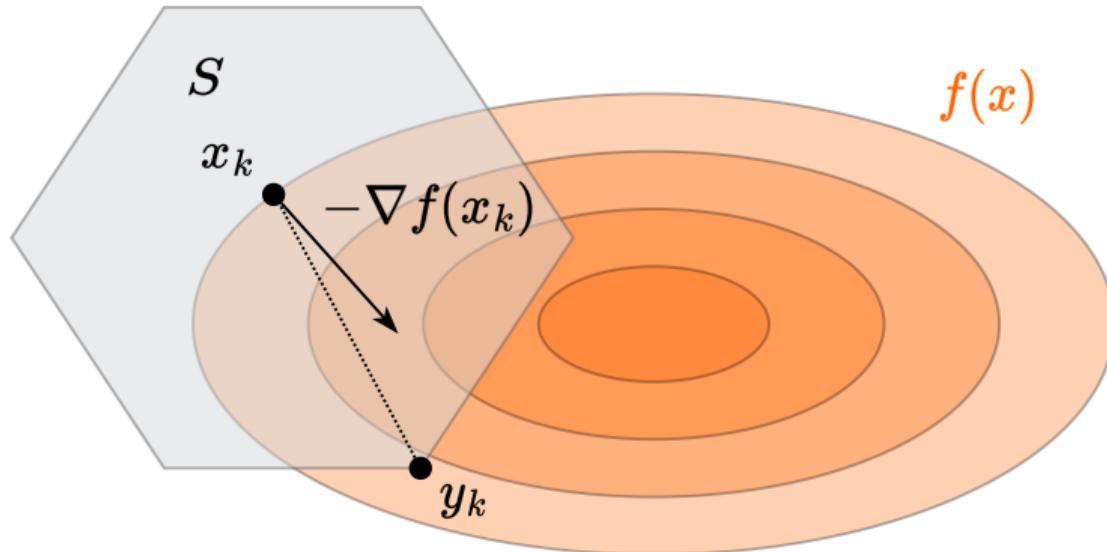


Figure 13: Illustration of Frank-Wolfe (conditional gradient) algorithm

## Idea

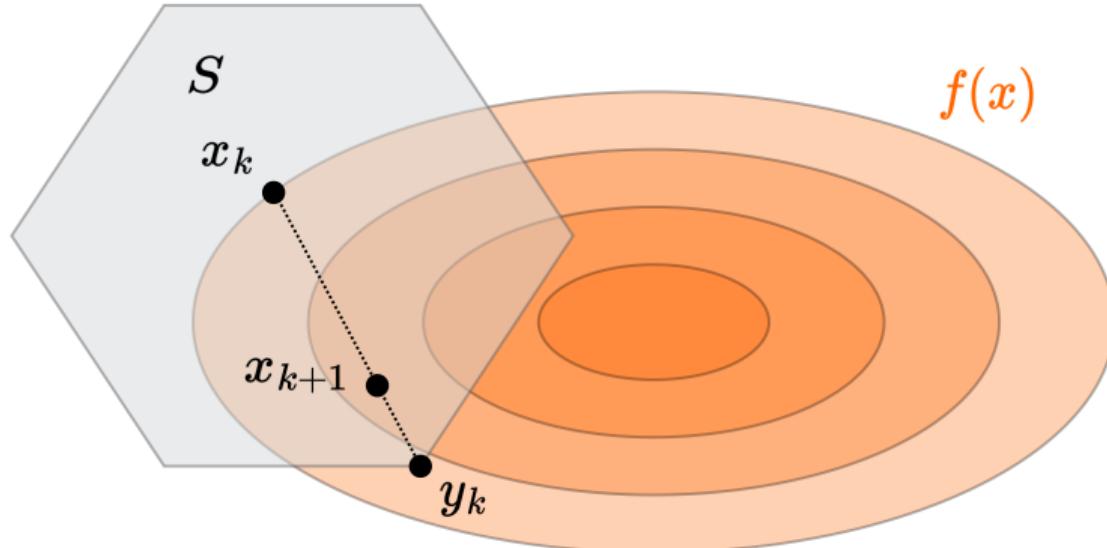


Figure 14: Illustration of Frank-Wolfe (conditional gradient) algorithm

## Idea

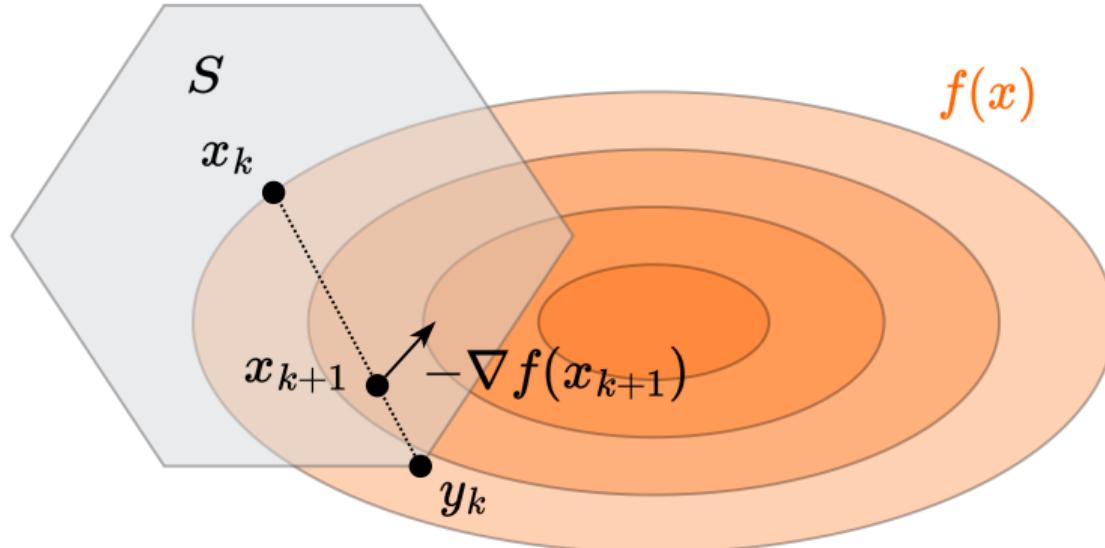


Figure 15: Illustration of Frank-Wolfe (conditional gradient) algorithm

## Idea

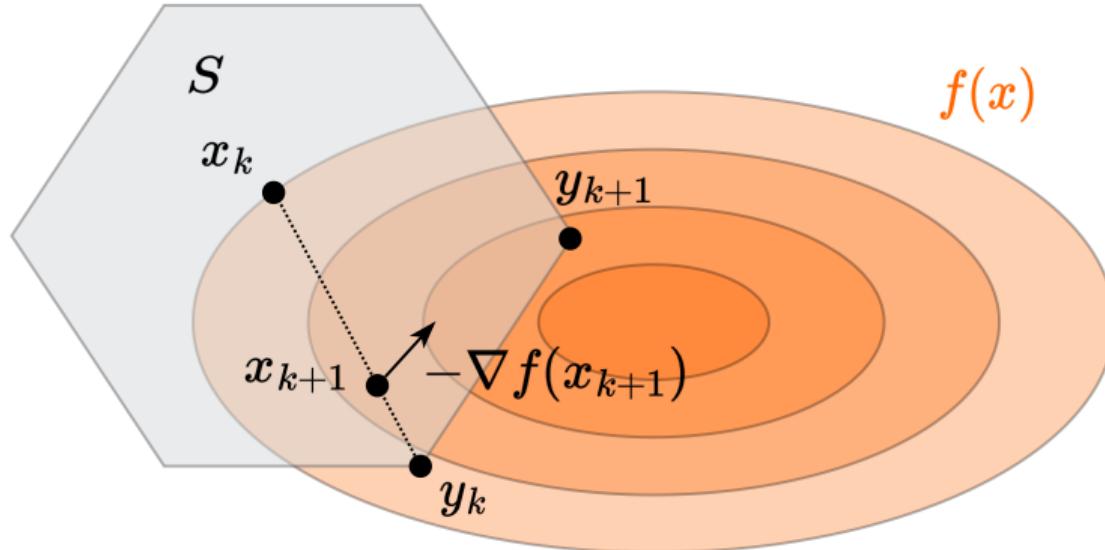


Figure 16: Illustration of Frank-Wolfe (conditional gradient) algorithm

## Idea

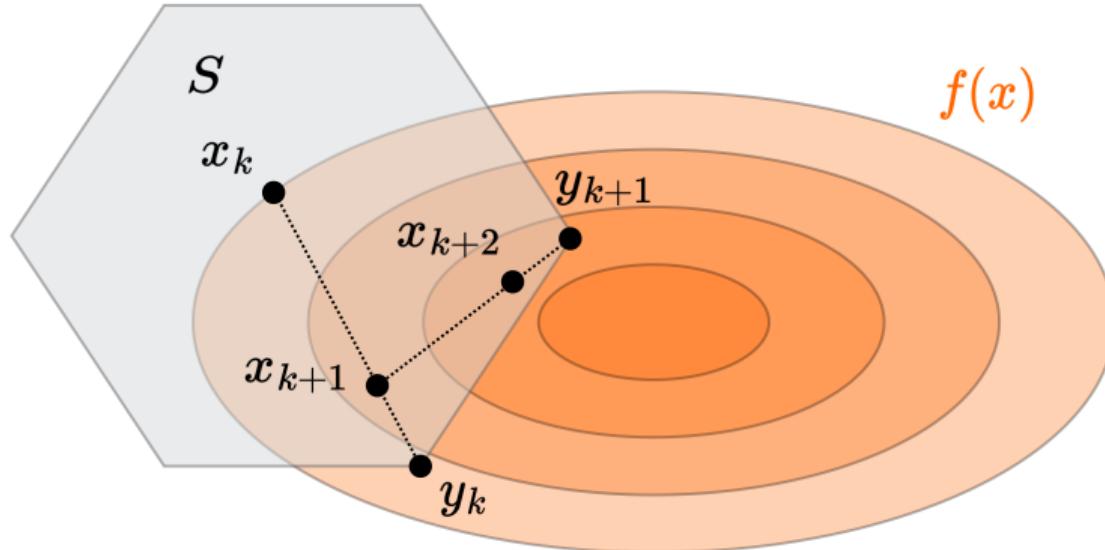


Figure 17: Illustration of Frank-Wolfe (conditional gradient) algorithm

# Idea

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

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

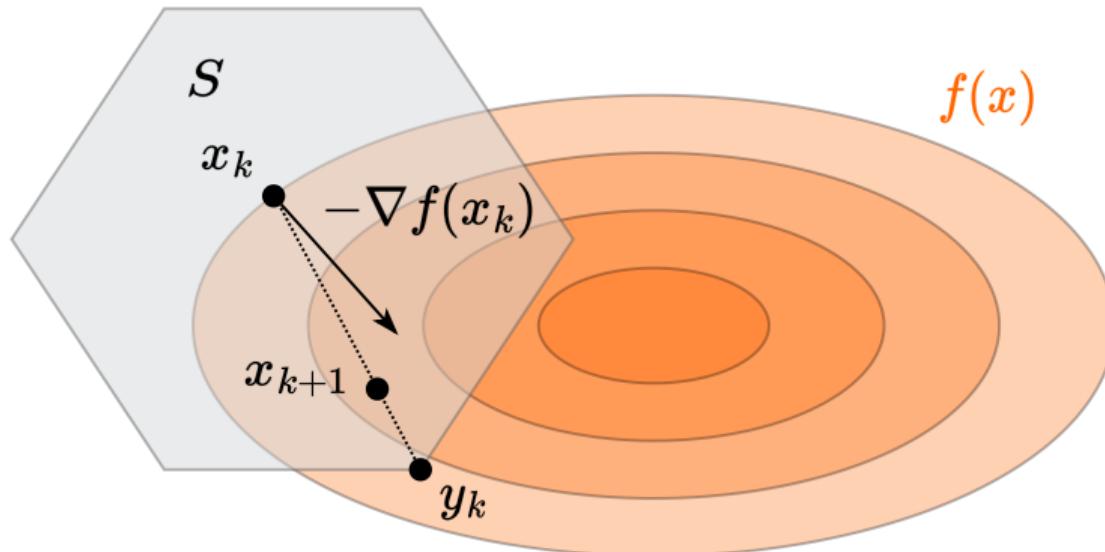


Figure 18: Illustration of Frank-Wolfe (conditional gradient) algorithm

## Convergence rate for smooth and convex case

### i Theorem

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  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  $S$ .

## Convergence rate for smooth and convex case

### i Theorem

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  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  $S$ .

### Proof

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:

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

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

4. Combining the above inequalities:

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

## Convergence rate for smooth and convex case

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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

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

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

7. Starting from  $\delta_2 \leq \frac{1}{2}$  and applying induction on  $k$ , we can show that:

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

which gives us the desired result:

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

## Convergence rate for strongly convex case

### i Theorem

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  be  $\mu$ -strongly 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  $\gamma_k = \frac{2}{k+2}$  achieves the following convergence after iteration  $k > 0$ :

$$f(x_k) - f^* \leq \frac{4LR^2}{(k+2)^2}$$

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

## Convergence rate for strongly convex case

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

### Proof

1. By  $\mu$ -strong convexity of  $f$ , for any  $x, y \in S$ :

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

## Convergence rate for strongly convex case

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

### Proof

1. By  $\mu$ -strong convexity of  $f$ , for any  $x, y \in S$ :

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

2. This gives us a stronger inequality than in the convex case:

$$\langle \nabla f(x_k), x^* - x_k \rangle \leq f(x^*) - f(x_k) - \frac{\mu}{2} \|x^* - x_k\|^2$$

## Convergence rate for strongly convex case

- Following similar steps as in the convex case, but using the stronger inequality:

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

## Convergence rate for strongly convex case

3. Following similar steps as in the convex case, but using the stronger inequality:

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

4. Rearranging terms and using the fact that  $\|x^* - x_k\|^2 \geq 0$ :

$$\begin{aligned} f(x_{k+1}) - f(x^*) &\leq \gamma_k (f(x_k) - f(x^*)) + (1 - \gamma_k)^2 \frac{LR^2}{2} - (1 - \gamma_k) \frac{\mu}{2} \|x^* - x_k\|^2 \\ &\leq \gamma_k (f(x_k) - f(x^*)) + (1 - \gamma_k)^2 \frac{LR^2}{2} \end{aligned}$$

## Convergence rate for strongly convex case

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

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5. With  $\gamma_k = \frac{2}{k+2}$  and denoting  $\delta_k = f(x_k) - f^*$ , we get:

$$\begin{aligned} \delta_{k+1} &\leq \frac{2}{k+2} \delta_k + \frac{LR^2}{2} \left(1 - \frac{2}{k+2}\right)^2 \\ &= \frac{2}{k+2} \delta_k + \frac{LR^2}{2} \frac{(k)^2}{(k+2)^2} \end{aligned}$$

## Convergence rate for strongly convex case

6. It can be shown by induction that:

$$\delta_k \leq \frac{4LR^2}{(k+2)^2}$$

## Convergence rate for strongly convex case

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$$\delta_k \leq \frac{4LR^2}{(k+2)^2}$$

7. This gives us the improved convergence rate of  $\mathcal{O}(\frac{1}{k^2})$  for the strongly convex case, compared to  $\mathcal{O}(\frac{1}{k})$  for the convex case.