

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

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Optimization for ML. Faculty of Computer Science. HSE University



# Constrained optimization

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Is it possible to tune GD to fit constrained problem?

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

## Example: White-box Adversarial Attacks

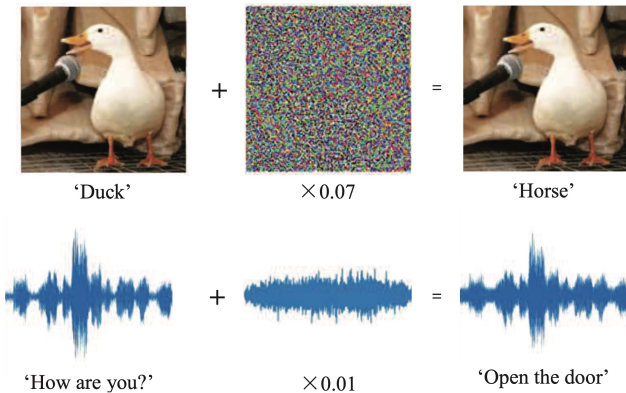


Figure 1: Source

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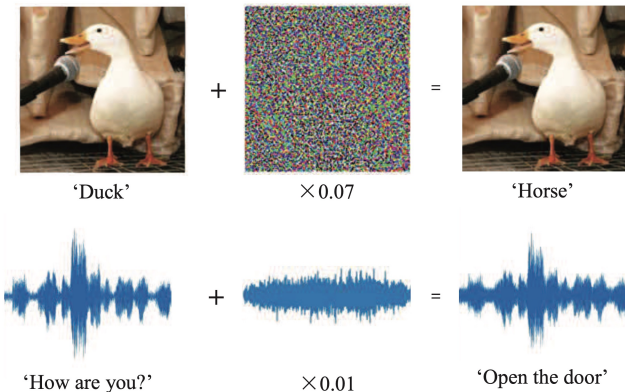


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- Mathematically, a neural network is a function  $f(w; x)$
- Typically, input  $x$  is given and network weights  $w$  optimized
- Could also freeze weights  $w$  and optimize  $x$ , adversarially!

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

or

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

# Idea of Projected Gradient Descent

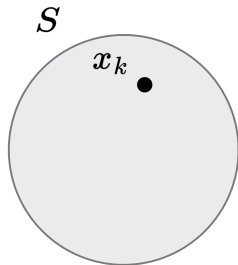


Figure 2: Suppose, we start from a point  $x_k$ .

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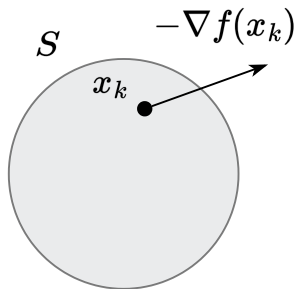


Figure 3: And go in the direction of  $-\nabla f(x_k)$ .

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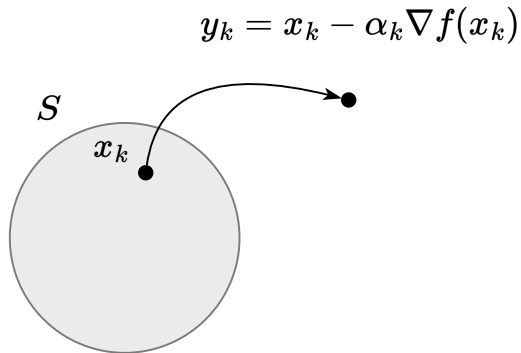


Figure 4: Occasionally, we can end up outside the feasible set.

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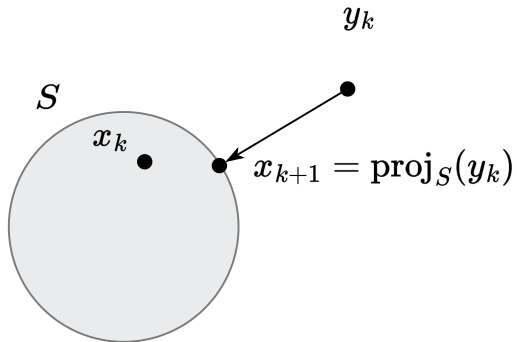


Figure 5: Solve this little problem with projection!



# Idea of Projected Gradient Descent

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

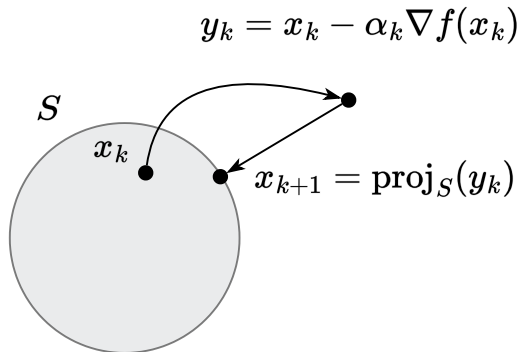


Figure 6: Illustration of Projected Gradient Descent algorithm

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

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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

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

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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.

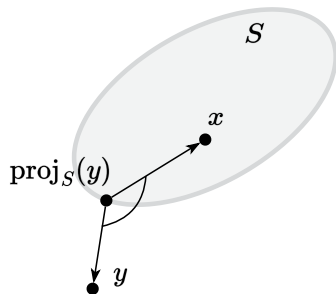


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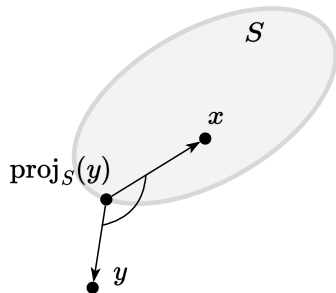


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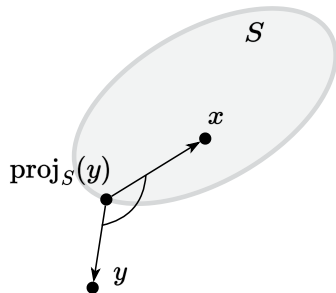


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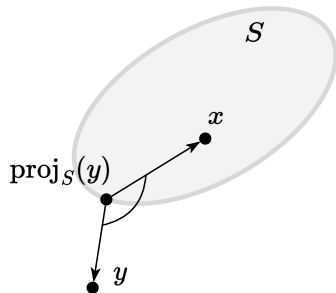


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- Next: variational characterization implies non-expansiveness. i.e.,

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

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

$$\langle \pi(x) - x, \pi(x) - \pi(y) \rangle \leq 0. \quad (6)$$

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

$$\langle x - \pi(x), \pi(y) - \pi(x) \rangle \leq 0. \quad (5)$$

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

$$\langle \pi(x) - x, \pi(x) - \pi(y) \rangle \leq 0. \quad (6)$$

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

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

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

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

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

## 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

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

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

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

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

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

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

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

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

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

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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:

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

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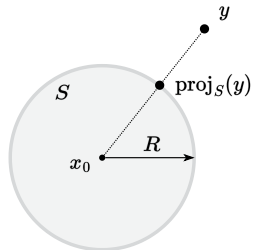
Build a hypothesis from the figure:  $\pi = x_0 + R \cdot \frac{y - x_0}{\|y - x_0\|}$

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



## 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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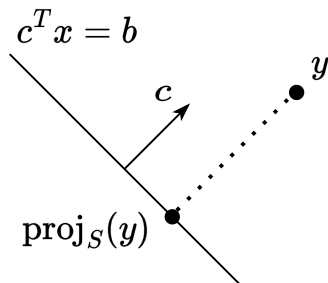


Figure 9: Hyperplane



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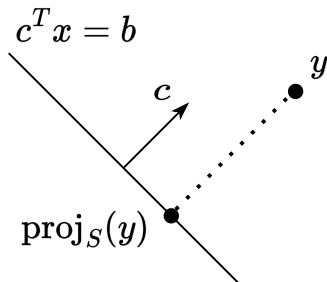


Figure 9: Hyperplane

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

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

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

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

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

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

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

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

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

## Idea

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

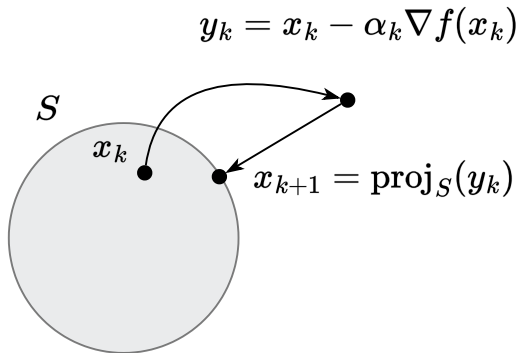


Figure 10: Illustration of Projected Gradient Descent algorithm

## Convergence rate for smooth and convex case

### 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  $2x^T y = \|x\|^2 + \|y\|^2 - \|x - y\|^2$ :

(7)

## Convergence rate for smooth and convex case

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$$\text{Method: } = f(x_k) - L \langle y_k - x_k, x_{k+1} - x_k \rangle + \frac{L}{2} \|x_{k+1} - x_k\|^2$$

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Method: 
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Cosine rule: 
$$= f(x_k) - \frac{L}{2} (\|y_k - x_k\|^2 + \|x_{k+1} - x_k\|^2 - \|y_k - x_{k+1}\|^2) + \frac{L}{2} \|x_{k+1} - x_k\|^2 \quad (7)$$

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



## Convergence rate for smooth and convex case

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

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

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

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

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4. Now, using convexity and previous part:

Convexity:

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

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

# 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

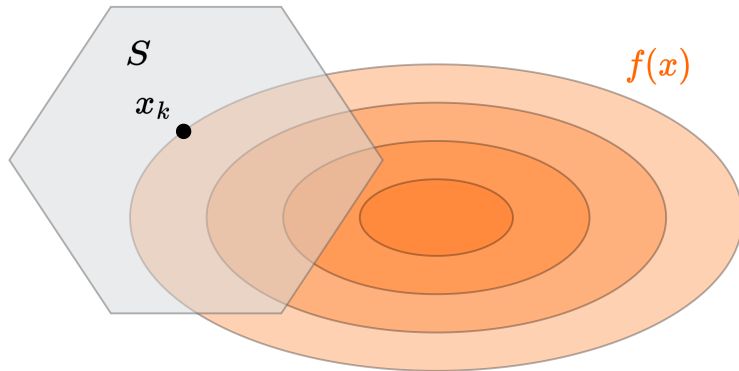


Figure 11: Illustration of Frank-Wolfe (conditional gradient) algorithm

# Idea

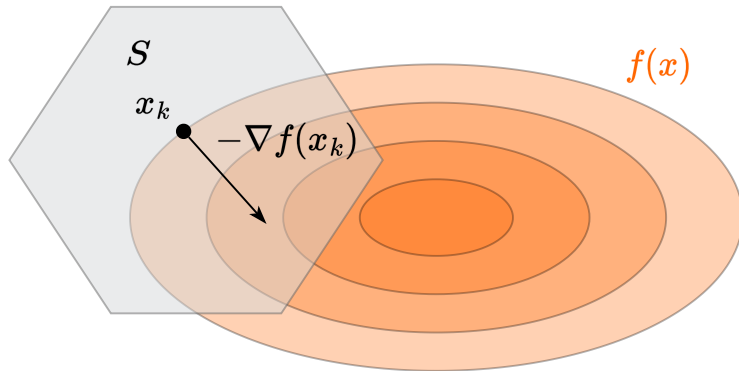


Figure 12: Illustration of Frank-Wolfe (conditional gradient) algorithm



# Idea

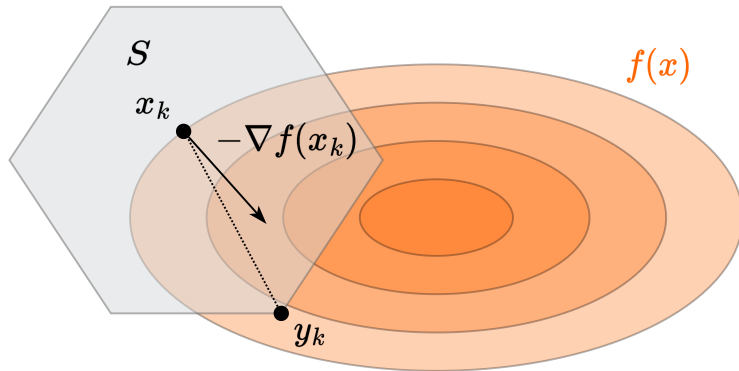


Figure 13: Illustration of Frank-Wolfe (conditional gradient) algorithm

# Idea

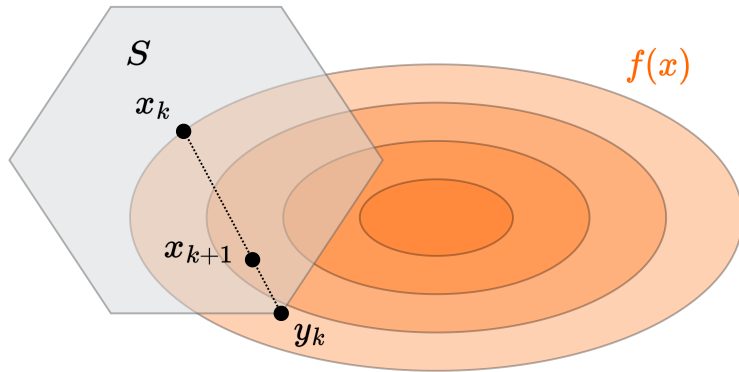


Figure 14: Illustration of Frank-Wolfe (conditional gradient) algorithm

# Idea

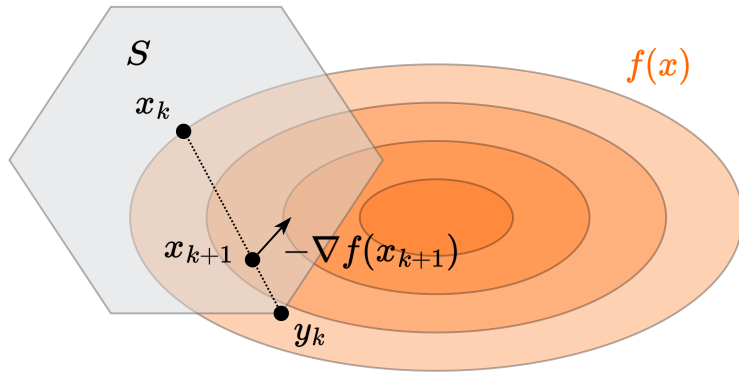


Figure 15: Illustration of Frank-Wolfe (conditional gradient) algorithm

# Idea

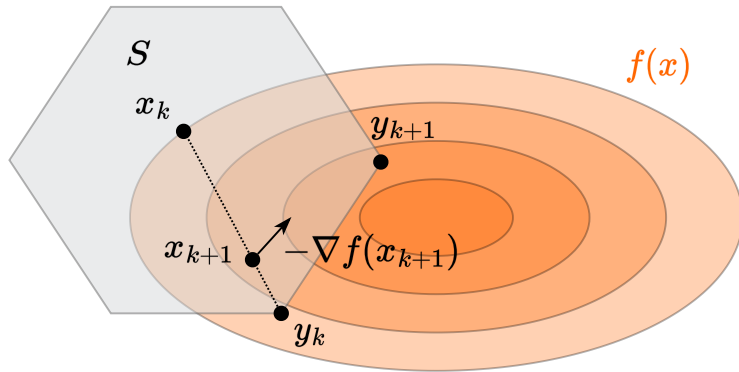


Figure 16: Illustration of Frank-Wolfe (conditional gradient) algorithm

# Idea

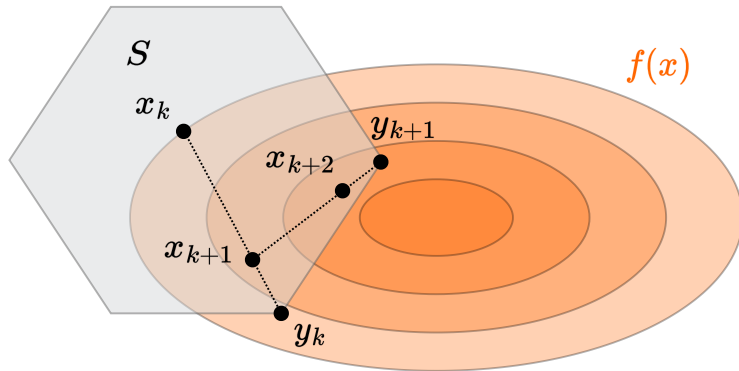


Figure 17: Illustration of Frank-Wolfe (conditional gradient) algorithm

# Idea

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

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



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

# Convergence

# Comparison to PGD