Optimization on "simple" sets. Gradient projection method. Conditional gradient method

Optimization in ML

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Constrained Optimization

Constrained Optimization Problem

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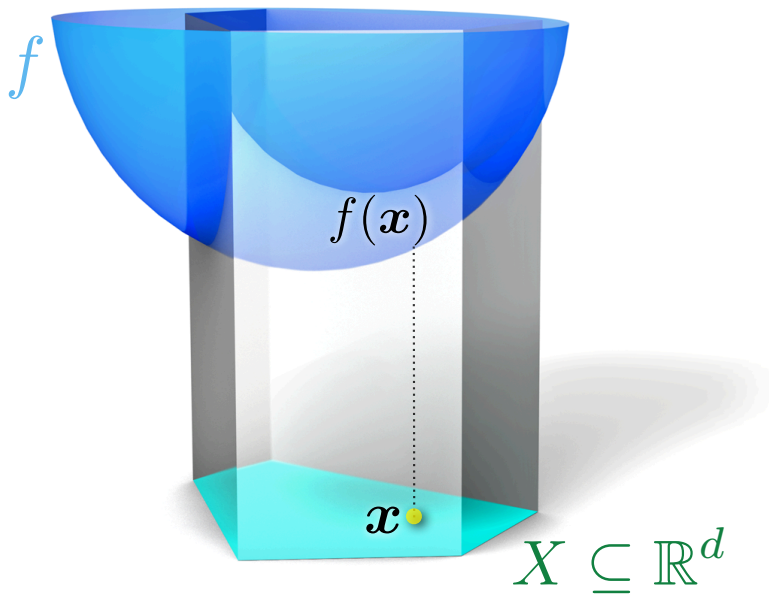

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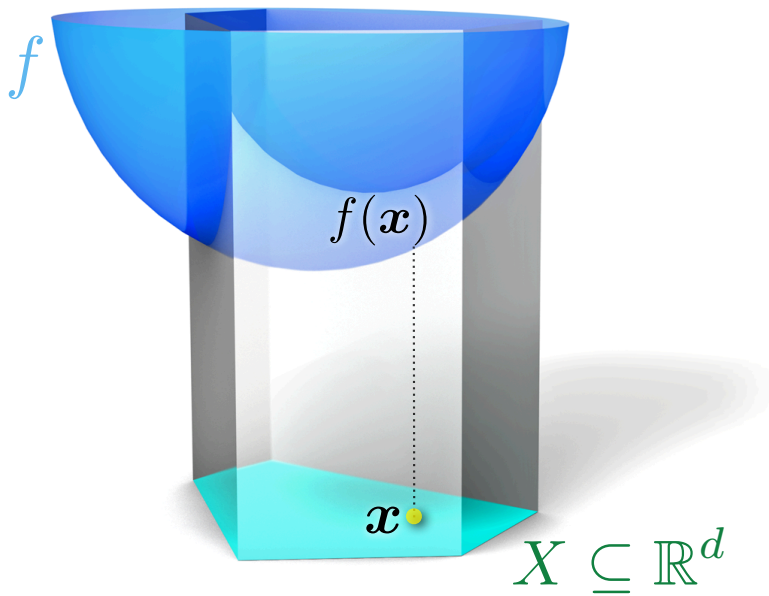

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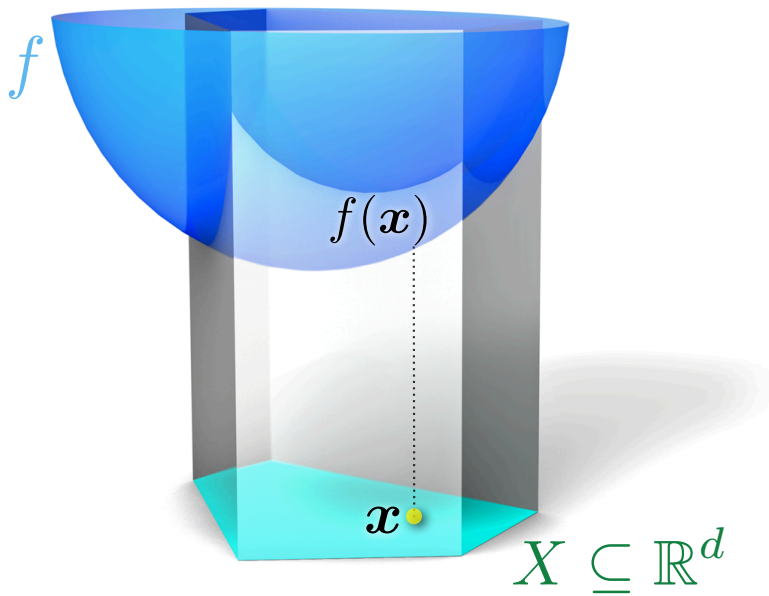

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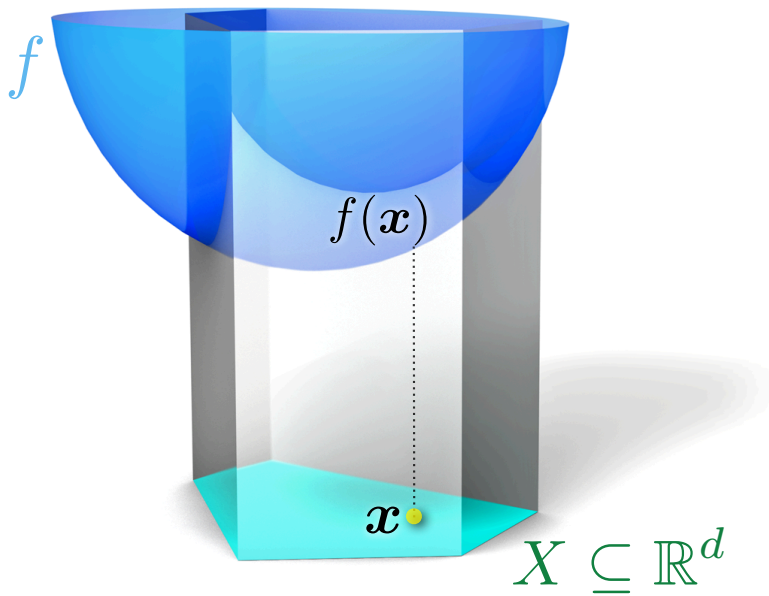

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Question: Why do we need constrains?

Example: PhD's Admission

- Skoltech university is admitting top students to its PhD program, in a competitive application process.
- Applicants are submitting various documents (GPA, TOEFL,...)
- Admission committee would like to compute a (rough) forecast of the applicant's performance in the program, based on the submitted documents.
- Data on the actual performance of students admitted in the past is available.
- In the following (made-up toy) example: consider GPA and TOEFL only...
- ...as predictors for Performance (final score of success obtained in the program).

Example: PhD's Admission

- $0.0 \leq$ GPA ≤ 4.0 (from F to A)
- $0 \leq$ TOEFL
- $1.0 \leq$ Performance ≤ 6.0 (final score of secess)
- Historical data:

GPA	TOEFL	Performance
3.52	100	3.92
3.66	109	4.34
3.76	113	4.80
3.74	100	4.67
3.93	100	5.52
3.88	115	5.44
3.77	115	5.04
3.66	107	4.73
3.87	106	5.03
3.84	107	5.06

PhD's Admission: Linear model

Hypothesis:

$$\text{Performance} \approx w_0 + w_1 \cdot \text{GPA} + w_2 \cdot \text{TOEFL}$$

for weights w_0, w_1, w_2 to be learned.
Approach: Find w_0, w_1, w_2 by minimizing least squares error over the historical data.
Question: what we need to do with data before solving something?

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- Relevant GPA scores span a range of 0.5.
- Relevant TOEFL scores span a range of 20 (from 100 to 120).
- $\Rightarrow$ normalize first so that w_1, w_2 can be compared

General setting

n inputs $x_1, \ldots, x_n$, $x_i \in \mathbb{R}^d$ for all i
d input variables $1, 2, \ldots, d$

- 10 (GPA, TOEFL) pairs, two input variables

n outputs $y_1, \ldots, y_n \in \mathbb{R}$

- 10 Perfomance scores

(x_i, y_i): an observation

- $((3.93, 100), 5.52)$, observation (of a student doing very well)

With weights $w_0, \mathrm{w} = (w_1, \ldots, w_d) \in \mathbb{R}^d$, we plan to minimize the least squares objective

$$f(w_0, \mathrm{w}) = \sum_{i=1}^{n} (w_0 + \mathrm{w}^T x_i - y_i)^2.$$

General setting: centering

Want to assume that

$$\frac{1}{n}\sum_{i=1}^{n} x_i = 0, \quad \frac{1}{n}\sum_{i=1}^{n} y_i = 0.$$

Can be achieved by

- subtracting the mean $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ from every input
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After centering: $w_0^* = 0, \mathrm{w}^*$ is unaffected

$\Rightarrow$ From now on consider function

$$f(\mathrm{w}) = \sum_{i=1}^{n} (\mathrm{w}^T x_i - y_i)^2.$$

General setting: normalization

Want to assume that for all j, the n input values $x_{1j}, \dots x_{nj}$ are on the same scale:

$$\frac{1}{n}\sum_{i=1}^{n} x_{ij}^2 = 1, \quad j = 1, \dots, d.$$

Can be achieved by

- multiplying x_{ij} by $s(j) = \sqrt{n/\sum_{i=1}^{n} x_{ij}^2}$ for all i, j
- in w*, this just multiplies w_j^* by $1/s(j)$

PhD's Admission: Centered and normalized data

x_{i1} (GPA)	x_{i2} (TOEFL)	y_i (Perfomance)
-2.04	-1.28	-0.94
-0.88	0.32	-0.52
-0.05	1.03	-0.05
-0.16	-1.28	-0.18
1.42	-1.28	0.67
1.02	1.39	0.59
0.06	1.39	0.19
-0.88	-0.04	-0.12
0.89	-0.21	0.17
0.62	-0.04	0.21

Least-squares objective:

$$f(w_1, w_2) = \sum_{i=1}^{10} (w_1 x_{i1} + w_2 x_{i2} - y_i)^2.$$

PhD's Admission: Results

Optimal solution: $\mathrm{w}^* = (w_1^*, w_2^*) \approx (0.43, 0.097)$

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Optimal solution: $\mathrm{w}^* = (w_1^*, w_2^*) \approx (0.43, 0.097)$

Under hypothesis (linear model), we expect $y_i \approx y_i^* = 0.43x_{i1} + 0.097x_{i2}$

x_{i1}	x_{i2}	y_i	y_i^*
-2.04	-1.28	-0.94	-1.00
-0.88	0.32	-0.52	-0.35
-0.05	1.03	-0.05	0.08
-0.16	-1.28	-0.18	-0.19
1.42	-1.28	0.67	0.49
1.02	1.39	0.59	0.57
0.06	1.39	0.19	0.16
-0.88	-0.04	-0.12	-0.38
0.62	-0.04	0.21	0.26

Question: what we can say about results? TOEFL has only very small influence ($w_2^* = 0.097$)

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Problems:

- least squares solution is optimized for the training data, not for the future ("overfitting")
- "unimportant" variables should have weight 0, but they typically don't

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Best subset selection: solve least squares subject to an additional constraint that there are at most k nonzero weights. **Question:** easy of not?

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Question: if we have 100 features, how many different subsets (of features) can we have?

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Question: if we have 100 features, how many different subsets (of features) can we have? $2^{100} \approx 1.26 \cdot 10^{30}$.

LASSO: popular approach with some favorable statistical properties

The LASSO: a constrained optimization problem

$$\begin{array}{ll} \text{minimize} & \sum_{i=1}^{n} \|\mathrm{w}^\top x_i - y_i\|^2 \\ \text{subject to} & \|\mathrm{w}\|_1 \leq R, \end{array} \tag{1}$$

where $R \in \mathbb{R}_+$ is some parameter.

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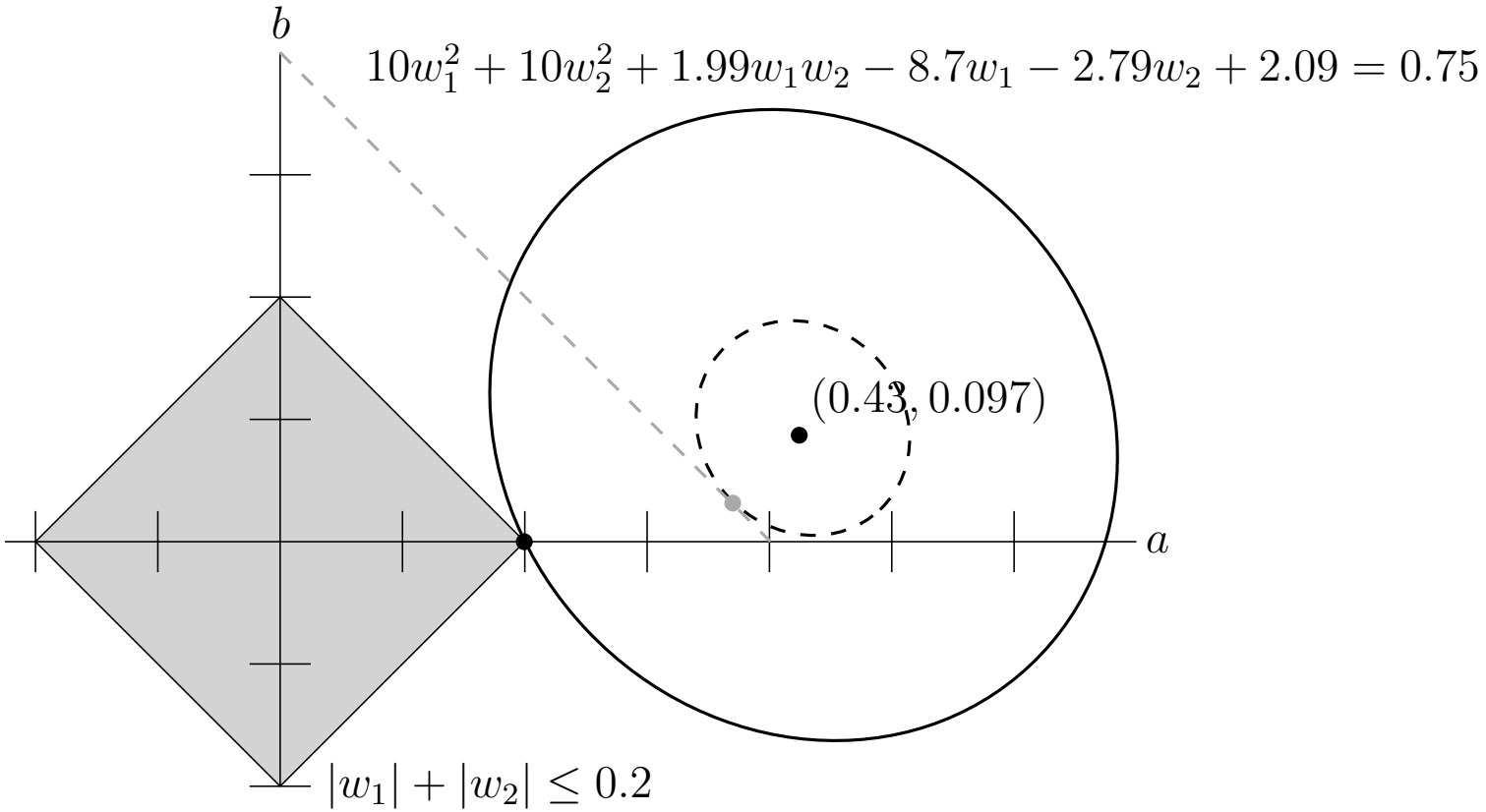
$R \geq 0.6 \Rightarrow \mathrm{w}^* = (w_1^*, w_2^*) = (0.43, 0.097)$

Geometry of the LASSO



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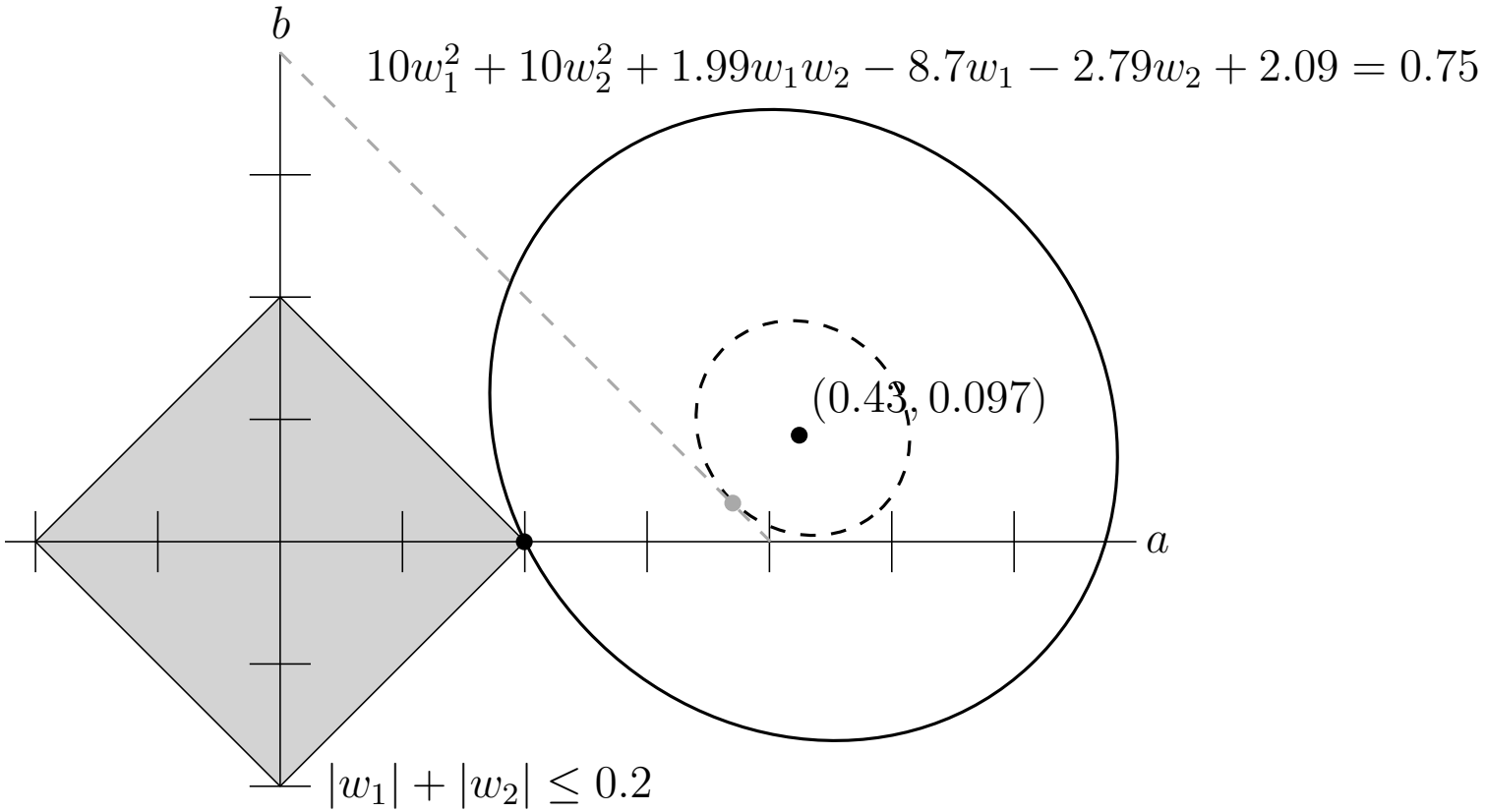
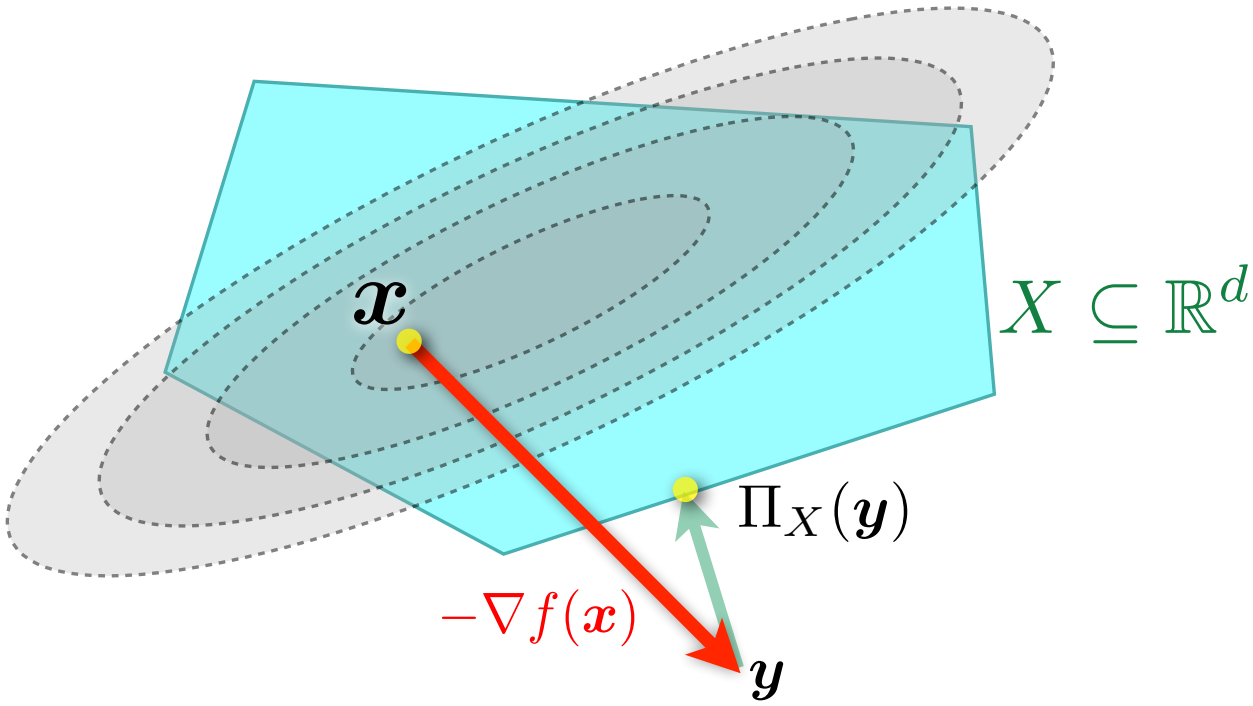


Question: Can we somehow modify gradient method to work with constraints?

Projected Gradient Descent

Idea: project onto X after every step: $\Pi_X(y) := \operatorname{argmin}_{x \in X} \|x - y\|^2$



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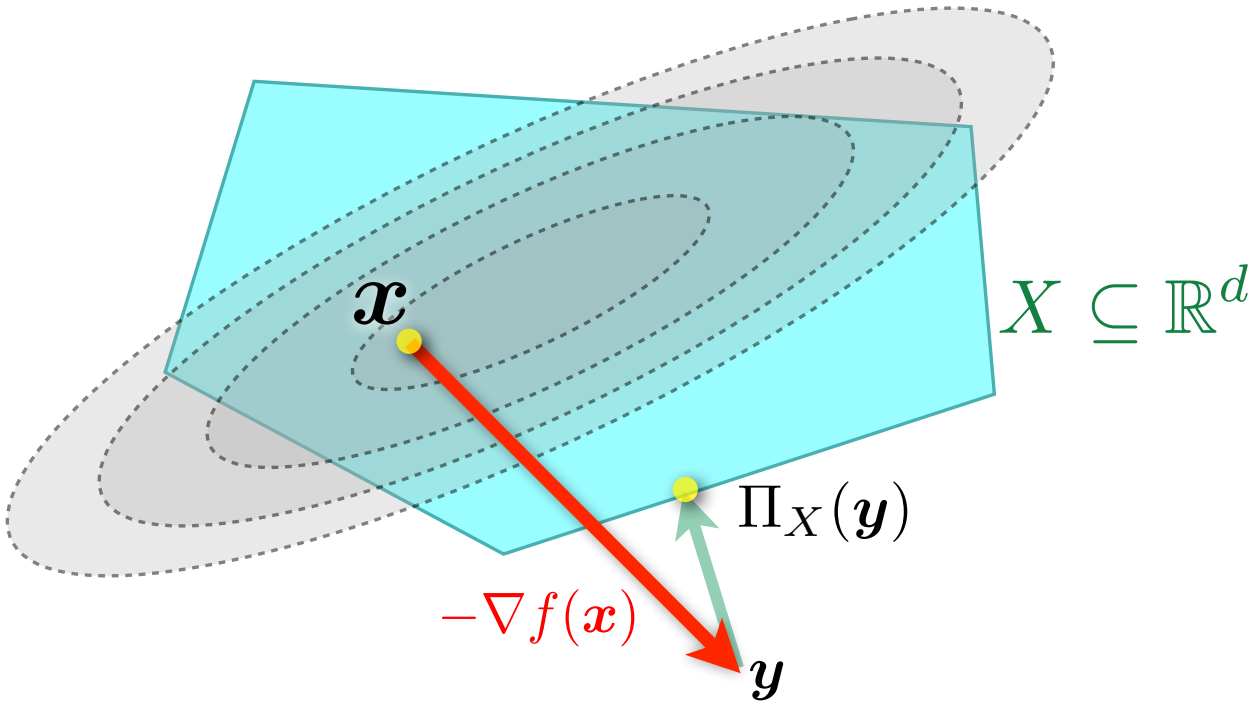

Projected gradient descent: $x_{k+1} := \Pi_X\left[x_k - \gamma \nabla f(x_k)\right]$

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for times $k = 0, 1, \ldots,$ and stepsize $\gamma \geq 0$.

Optimality condition for the problem with constraints

Let there be a convex continuously differentiable on $\mathbb{R}^d$ function $f : \mathbb{R}^d \to \mathbb{R}$ and the convex set $\mathcal{X}$. Then $x^* \in \mathcal{X}$ is a global minimum of f on $\mathcal{X}$ if and only if for all $x \in \mathcal{X}$ the following holds

$$\langle \nabla f(x^*), x - x^* \rangle \geq 0.$$

Proof

- Sufficient condition.

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$$f(x) \geq f(x^*) + \langle \nabla f(x^*), x - x^* \rangle \geq f(x^*).$$

Whence it follows that x^* — the global minimum on $\mathcal{X}$.

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- Necessary condition. Let x^* be a global minimum on $\mathcal{X}$. We prove that $\langle \nabla f(x^*), x - x^* \rangle \geq 0$ for any $x \in \mathcal{X}$. Let us proceed from the contrary, i.e. suppose that there exists $x \in \mathcal{X}$ such that $\langle \nabla f(x^*), x - x^* \rangle < 0$.

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$$x_\lambda = \lambda x + (1 - \lambda)x^*, \text{ where } \lambda \in [0; 1].$$

  Due to the convexity of the set $\mathcal{X}$, the points $x_\lambda \in \mathcal{X}$.

Proof

Let us understand how the function $\phi(\lambda) = f(x_\lambda) = f(\lambda x + (1-\lambda)x^*)$ behaves. In particular, note that

$$\frac{d\phi}{d\lambda} = \frac{d}{d\lambda} f(\lambda x + (1-\lambda)x^*) = \langle \nabla f(x^* + \lambda(x - x^*)), x - x^* \rangle.$$

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Come to the contradiction that x^* — a global minimum on $\mathcal{X}$.

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For a convex set $\mathcal{X}$ and any point, the projection operator exists and takes a singular value.

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Proof: It follows that the projection problem is the minimization of a strongly convex function on a convex set. The solution of such a problem exists and is unique.

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Let $\mathcal{X} \subseteq \mathbb{R}^d$ be a convex set, $x \in \mathcal{X}, y \in \mathbb{R}^d$. Then

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$$\langle \nabla d(\Pi_{\mathcal{X}}(y)), x - \Pi_{\mathcal{X}}(y) \rangle \geq 0 \quad \text{для любой } x \in \mathcal{X}$$

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$$\langle x - \Pi_{\mathcal{X}}(y), y - \Pi_{\mathcal{X}}(y) \rangle \leq 0.$$

Proof: Note that $\Pi_{\mathcal{X}}(y)$ minimizes the differentiable convex function $d(z) = \|z - y\|_2^2$ on the convex set $\mathcal{X}$. **Question:** what then does the optimality condition give us?

$$\langle \nabla d(\Pi_{\mathcal{X}}(y)), x - \Pi_{\mathcal{X}}(y) \rangle \geq 0 \quad \text{для любой } x \in \mathcal{X}$$

Question: what is $\nabla d(z)$?

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Question: what is $\nabla d(z)$? $2(z - y)$. Then

$$2\langle \Pi_{\mathcal{X}}(y) - y, x - \Pi_{\mathcal{X}}(y) \rangle \geq 0 \quad \text{for all } x \in \mathcal{X}.$$

Which is exactly what I needed to prove.

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Non-expansivity property of the projection operator

Let $\mathcal{X} \subseteq \mathbb{R}^d$ be a convex set, $x_1, x_2 \in \mathbb{R}^d$. Then

$$\|\Pi_{\mathcal{X}}(x_1) - \Pi_{\mathcal{X}}(x_2)\|_2 \leq \|x_1 - x_2\|_2.$$

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The same:

$$\langle x_2 - \Pi_{\mathcal{X}}(x_2), \Pi_{\mathcal{X}}(x_1) - \Pi_{\mathcal{X}}(x_2)\rangle \leq 0$$

Properties of the projection operator

Sum it up

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CBS gives the result we want

$$\|\Pi_{\mathcal{X}}(x_2) - \Pi_{\mathcal{X}}(x_1)\|_2^2 \leq \|\Pi_{\mathcal{X}}(x_2) - \Pi_{\mathcal{X}}(x_1)\| \cdot \|x_2 - x_1\|$$

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For x^* – the solution of the conditional problem of minimization of a convex continuously differentiable function f on the convex set $\mathcal{X}$ it is true that

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Proofs of convergence

- We're still considering it:

$$\|x^{k+1} - x^*\|_2^2 = \|\Pi_{\mathcal{X}}\left[x^k - \gamma_k \nabla f(x^k)\right] - x^*\|_2^2$$

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- Now the third property

$$\begin{aligned}\|x^{k+1} - x^*\|_2^2 \leq& \|x^k - \gamma_k \nabla f(x^k) - x^* + \gamma_k \nabla f(x^*)\|_2^2 \\ =& \|x^k - x^*\|_2^2 - 2\gamma_k \langle \nabla f(x^k) - \nabla f(x^*), x^k - x^* \rangle \\ &+ \gamma_k^2 \|\nabla f(x^k) - \nabla f(x^*)\|_2^2\end{aligned}$$

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- Let us introduce the following object the Bragman divergence generated by the convex function f:

$$V_f(x, y) = f(x) - f(y) - \langle \nabla f(y), x - y \rangle \geq 0.$$

Question: why is divergence always positive?

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$$V_f(x, y) = f(x) - f(y) - \langle \nabla f(y), x - y \rangle \geq 0.$$

Question: why is divergence always positive? Because of the convexity of f.

Proof of convergence

- Let us take advantage of the strong convexity and smoothness as before:

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

- Further as before, due to the non-negativity of the Bragman divergence.

Convergence

- The gradient descent method with projection for a L-smooth and (μ-strongly) convex target function has the same convergence as the gradient descent method for a similar unconditional optimization problem.
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- The gradient descent method with projection for a L-smooth and (μ-strongly) convex target function has the same convergence as the gradient descent method for a similar unconditional optimization problem.
- It turns out that the iterative and oracle complexities of these methods coincide.
- One problem remains — projection is an additional optimization problem that needs to be solved.

Projecting is additional problem

- The projection has analytical solution for ℓ_2-ball with radius $R > 0$:

$$X = B_2(R) = \left\{ x \in \mathbb{R}^d \mid \|x\|_2^2 = \sum_{i=1}^{d} x_i^2 \leq R \right\}$$

$$\Pi_X(x) = \max\left\{1, \frac{R}{\|x\|_2}\right\} x$$

- For other quite simple sets we need to run additional optimization algorithms. For example, for $B_1(R)$ $\left(\left\{ x \in \mathbb{R}^d \mid \|x\|_1 = \sum_{i=1}^{d} |x_i| \leq R \right\}\right)$ the projection can be computed in time $\mathcal{O}(d \log d)$.

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- The next approach can help.

Linear minimization

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$$\min_{s \in X} \langle s, g \rangle$$

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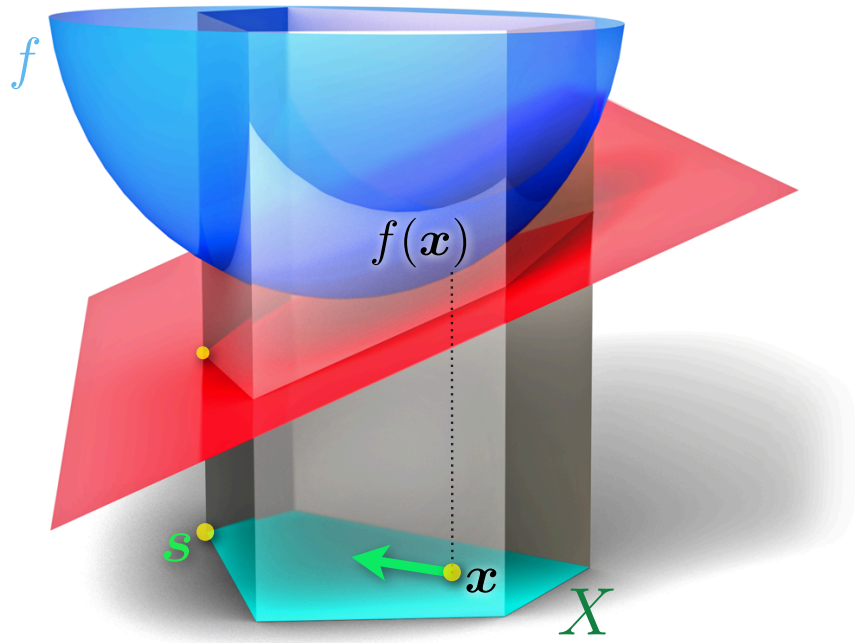
Examples	Solution of LM
ℓ_1-ball	$-\text{sign}(g_i)e_i$ with $\text{argmax}_i \lvert g_i \rvert$
Simplex	e_i with $\text{argmin}_i g_i$
ℓ_∞-ball	$-\sum_{i=1}^{d} \text{sign}(g_i)e_i$

Frank-Wolfe Algorithm

Frank-Wolfe Algorithm:

$$\begin{aligned} s &:= \text{LMO}(\nabla f(x_k)), \\ x_{k+1} &:= (1-\gamma)x_k + \gamma s, \end{aligned}$$

for timesteps $k = 0, 1, \ldots,$ and stepsize $\gamma := \frac{2}{k+2}$.



Linear Minimization Oracle:

$$\text{LMO}(g) := \operatorname*{argmin}_{s \in X} \langle s, g \rangle$$

Properties

- Aways feasible: $x_0, x_1, \ldots, x_k \in X$.
  x_{k+1} is on line segment $[s, x_k]$, for $\gamma \in [0, 1]$.
- Reduces non-linear to linear optimization
- Projection-free
- Sparse iterates (in terms of corners s used)

Invented and analyzed 1956 by Marguerite Frank and Philip Wolfe.
Check **Marguerite Frank - Honorary Discussion Panel @ NeurIPS 2013 workshop**
`https://www.youtube.com/watch?v=24e08AX9Eww`

Convergence in $\mathcal{O}(1/\varepsilon)$ steps

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and smooth with parameter L, and $x_0 \in X$. Then choosing any of the above stepsizes, the Frank-Wolfe algorithm yields

$$f(x_K) - f(x^*) \leq \frac{\max\{2L\,\mathrm{diam}(X)^2, f(x_0) - f(x^*)\}}{K+1}$$

Where $\mathrm{diam}(X) := \max_{x,y \in X} \|x - y\|$ is the diameter of X.

Proof of Convergence in $\mathcal{O}(1/\varepsilon)$ steps

- L -smoothness gives

$$\begin{aligned} f(x_{k+1}) =& f(x_k + \gamma_k(s - x_k)) \\ \leq& f(x_k) + \gamma_k \langle s - x_k, \nabla f(x_k) \rangle + \frac{\gamma_k^2}{2} L \|s - x_k\|^2 \\ \leq& f(x_k) + \gamma_k \langle s - x_k, \nabla f(x_k) \rangle + \frac{\gamma_k^2}{2} L \operatorname{diam}(X)^2. \end{aligned}$$

- By LMO property and convexity gives

$$\begin{aligned} f(x_{k+1}) - f(x^*) \leq& f(x_k) - f(x^*) + \gamma_k \langle x^* - x_k, \nabla f(x_k) \rangle + \frac{\gamma_k^2}{2} L \operatorname{diam}(X)^2 \\ =& f(x_k) - f(x^*) - \gamma_k (f(x_k) - f(x^*)) + \frac{\gamma_k^2}{2} L \operatorname{diam}(X)^2 \\ =& (1 - \gamma_k)(f(x_k) - f(x^*)) + \gamma_k^2 C. \end{aligned}$$

Here $C = \frac{L \operatorname{diam}(X)^2}{2}$.

The induction step

We will now use induction over k to prove our claimed bound, i.e.

$$f(x_k) - f(x^*) \leq \frac{\max\{4C; f(x_0) - f(x^*)\}}{k+2} \quad k = 0, 1, \ldots$$

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The base-case $k = 0$ follows automatically.
Now considering $k \geq 1$,

$$\begin{aligned} f(x_{k+1}) - f(x^*) \leq & \quad (1 - \gamma_k)(f(x_k) - f(x^*)) + {\gamma_t}^2 C \\ = & \quad \left(1 - \frac{2}{k+2}\right)(f(x_k) - f(x^*)) + \left(\frac{2}{k+2}\right)^2 C \\ \leq & \quad \left(1 - \frac{2}{k+2}\right) \frac{\max\{4C; f(x_0) - f(x^*)\}}{k+2} + \left(\frac{2}{k+2}\right)^2 C \ , \end{aligned}$$

where in the last inequality we have used the induction hypothesis of induction.

The induction step

Simply rearranging the terms gives

$$\begin{aligned} f(x_{k+1}) - f(x^*) &\leq \frac{\max\{4C; f(x_0) - f(x^*)\}}{k+2}\left(1 - \tfrac{2}{k+2} + \tfrac{1}{k+2}\right) \\ &= \frac{\max\{4C; f(x_0) - f(x^*)\}}{k+2}\left(1 - \tfrac{1}{k+2}\right) \\ &= \frac{\max\{4C; f(x_0) - f(x^*)\}}{k+2}\,\frac{k+2-1}{k+2} \\ &\leq \frac{\max\{4C; f(x_0) - f(x^*)\}}{k+2}\,\frac{k+2}{k+3} \\ &= \frac{\max\{4C; f(x_0) - f(x^*)\}}{k+3}, \end{aligned}$$

which is our claimed bound for $k \geq 1$.

Convergence

Convergence theorem of the Frank-Wolfe method

Let a continuously differentiable convex L-smooth function $f : \mathbb{R}^d \to \mathbb{R}$ be given, then the following convergence estimate is valid for the Frank-Wolfe method

$$f(x^K) - f(x^*) \leq \frac{\max\{2L \operatorname{diam}(\mathcal{X})^2, f(x^0) - f(x^*)\}}{K + 2}$$

where $\operatorname{diam}(\mathcal{X}) := \max_{x,y \in \mathcal{X}} \|x - y\|$ – set $\mathcal{X}$ diameter.

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Convergence

- The $1/K$ sublinear convergence is the same as that of gradient descent for a convex L-smooth function.
- The problem that for a strongly convex target function, linear convergence will not appear in the general case. It is related to linear minimization.