

Optimization for Machine Learning

CS-439

Lecture 9: Frank-Wolfe algorithm

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EPFL – github.com/epfml/0ptML_course

May 6, 2022

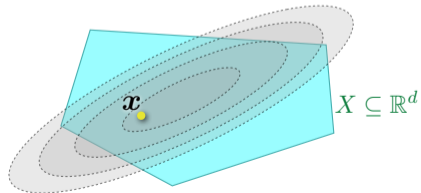
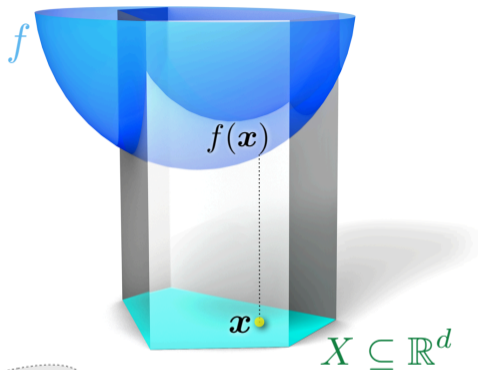
Chapter 9

Frank-Wolfe

Constrained Optimization

Constrained Optimization Problem

$$\begin{array}{ll} \text{minimize} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in X \end{array}$$



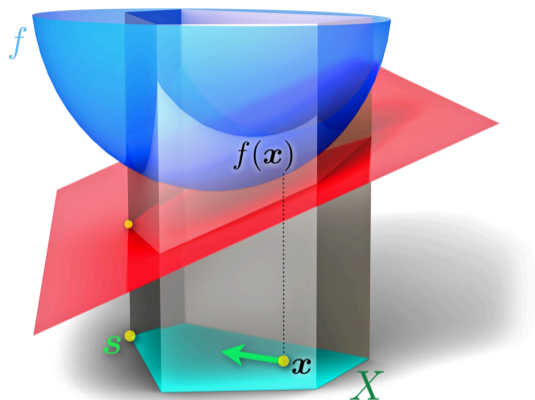
Frank-Wolfe Algorithm

Frank-Wolfe Algorithm:

$$\mathbf{s} := \text{LMO}(\nabla f(\mathbf{x}_t)),$$

$$\mathbf{x}_{t+1} := (1 - \gamma)\mathbf{x}_t + \gamma\mathbf{s},$$

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



Linear Minimization Oracle:

$$\text{LMO}(\mathbf{g}) := \underset{\mathbf{s} \in X}{\text{argmin}} \langle \mathbf{s}, \mathbf{g} \rangle$$

Properties

- ▶ **Always feasible:** $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_t \in X$.
 \mathbf{x}_{t+1} is on line segment $[\mathbf{s}, \mathbf{x}_t]$, for $\gamma \in [0, 1]$.
- ▶ **Reduces** non-linear to linear optimization
- ▶ **Projection-free**
- ▶ **Sparse iterates** (in terms of corners \mathbf{s} used)

Invented and analyzed 1956 by Marguerite Frank and Philip Wolfe.

Example

Lasso Regression

$$\min_{\mathbf{x}} \|\mathbf{Ax} - \mathbf{b}\|^2 \quad \text{s.t.} \quad \|\mathbf{x}\|_1 \leq 1$$

L1-ball is the convex hull of the unit basis vectors:

$$X = \{\mathbf{x} \mid \|\mathbf{x}\|_1 \leq 1\} = \text{conv}(\{\pm \mathbf{e}_1, \dots, \pm \mathbf{e}_n\}).$$

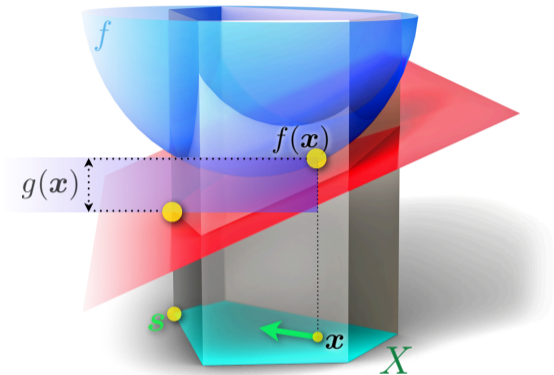
- ▶ $\nabla f(\mathbf{x}) = \mathbf{g} := \mathbf{A}^\top (\mathbf{Ax} - \mathbf{b})$
- ▶ $\text{LMO}(\mathbf{g}) = -\text{sign}(g_i) \mathbf{e}_i$ with $i := \underset{i \in [n]}{\text{argmax}} |g_i|$

simpler than projection onto L1-ball !

Duality Gap

Duality Gap

$$g(\mathbf{x}) := \langle \mathbf{x} - \mathbf{s}, \nabla f(\mathbf{x}) \rangle$$



Certificate for optimization quality:

$$\begin{aligned} g(\mathbf{x}) &= \max_{\mathbf{s} \in X} \langle \mathbf{x} - \mathbf{s}, \nabla f(\mathbf{x}) \rangle \\ &\geq \langle \mathbf{x} - \mathbf{x}^*, \nabla f(\mathbf{x}) \rangle \\ &\geq f(\mathbf{x}) - f(\mathbf{x}^*) \end{aligned}$$

Stepsize variants

$$\gamma_t := \frac{2}{t+2},$$

$$\gamma_t := \operatorname{argmin}_{\gamma \in [0,1]} f((1-\gamma)\mathbf{x}_t + \gamma\mathbf{s}), \quad (\text{line-search})$$

$$\gamma_t := \min \left\{ \frac{g(\mathbf{x}_t)}{L \|\mathbf{s} - \mathbf{x}_t\|^2}, 1 \right\}, \quad (\text{gap-based})$$

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

Theorem

Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be convex and *smooth* with parameter L , and $\mathbf{x}_0 \in X$. Then choosing any of the above stepsizes, the Frank-Wolfe algorithm yields

$$f(\mathbf{x}_T) - f(\mathbf{x}^*) \leq \frac{2L \operatorname{diam}(X)^2}{T + 1}$$

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

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

Lemma

For a step $\mathbf{x}_{t+1} := \mathbf{x}_t + \gamma(\mathbf{s} - \mathbf{x}_t)$ with arbitrary step-size $\gamma \in [0, 1]$, it holds that

$$f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \gamma g(\mathbf{x}_t) + \frac{\gamma^2}{2} L \operatorname{diam}(X)^2 ,$$

if $\mathbf{s} = \operatorname{LMO}(\nabla f(\mathbf{x}_t))$.

Proof.

We write $\mathbf{x} := \mathbf{x}_t$, $\mathbf{y} := \mathbf{x}_{t+1} = \mathbf{x} + \gamma(\mathbf{s} - \mathbf{x})$. From the definition of smoothness of f , we have

$$\begin{aligned} f(\mathbf{y}) &= f(\mathbf{x} + \gamma(\mathbf{s} - \mathbf{x})) \\ &\leq f(\mathbf{x}) + \gamma \langle \mathbf{s} - \mathbf{x}, \nabla f(\mathbf{x}) \rangle + \frac{\gamma^2}{2} L \operatorname{diam}(X)^2 . \end{aligned}$$

The lemma follows by definition of the duality gap. □

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

From the Lemma we know that for every step of FW, it holds that

$$f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \gamma g(\mathbf{x}_t) + \gamma^2 C,$$

if we chose $\gamma := \frac{2}{t+2}$ and write $C := \frac{1}{2}L \text{diam}(X)^2$. This bound holds also for all mentioned line-search variants (*different LHS, same RHS*).

Writing $h(\mathbf{x}) := f(\mathbf{x}) - f(\mathbf{x}^*)$ for the (unknown) objective error at any point \mathbf{x} , this implies that

$$\begin{aligned} h(\mathbf{x}_{t+1}) &\leq h(\mathbf{x}_t) - \gamma g(\mathbf{x}_t) + \gamma^2 C \\ &\leq h(\mathbf{x}_t) - \gamma h(\mathbf{x}_t) + \gamma^2 C \\ &= (1 - \gamma)h(\mathbf{x}_t) + \gamma^2 C, \end{aligned}$$

by the certificate property $h(\mathbf{x}) \leq g(\mathbf{x})$ of the duality gap.

The theorem then follows by induction (Exercise 1 of Lab 9). □

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

Affine Invariance

Curvature Constant

$$C_f := \sup_{\substack{\mathbf{x}, \mathbf{s} \in X, \gamma \in [0,1] \\ \mathbf{y} = \mathbf{x} + \gamma(\mathbf{s} - \mathbf{x})}} \frac{1}{\gamma^2} (f(\mathbf{y}) - f(\mathbf{x}) - \langle \mathbf{y} - \mathbf{x}, \nabla f(\mathbf{x}) \rangle)$$

Algorithm is invariant to scaling (affine transformations) of the input problem.

So is C_f .

(same as Newton, but here for **constrained** problems)

$$C_f \leq \frac{L}{2} \text{diam}(X)^2 \quad \text{for any norm!}$$

All proofs hold for C_f , instead of picking a particular $L \text{diam}(X)^2$.

Convergence in Duality Gap

Theorem

Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be convex and *smooth* with parameter L , and $\mathbf{x}_0 \in X$, $T \geq 2$. Then choosing any of the above stepsizes, the Frank-Wolfe algorithm yields a t , $1 \leq t \leq T$ s.t.

$$g(\mathbf{x}_t) \leq \frac{27/2 C_f}{T + 1}$$

Proof.

Idea: not all gaps can be small (use Lemma again).



Proof (I)

Proof (II)

Proof (III)

Extensions and Use Cases

Extensions:

- ▶ **Approximate** LMO (of additive or multiplicative accuracy)
- ▶ **Randomized** LMO
- ▶ unconstrained problems (Matching Pursuit variants)

Use cases:

Whenever projection is more costly than solving a linear problem

- ▶ **Lasso** and other L1-constrained problems
- ▶ **Matrix Completion**: scalable algorithm
- ▶ Relaxation of **combinatorial problems**
(e.g. matchings, network flows etc)

Applications

recall: $\text{LMO}(\mathbf{g}) := \underset{\mathbf{s} \in X}{\text{argmin}} \langle \mathbf{s}, \mathbf{g} \rangle$

$$X := \text{conv}(\mathcal{A})$$

| Examples | \mathcal{A} | $ \mathcal{A} $ | d | LMO (\mathbf{g}) |
|--------------|---|-----------------|----------|--|
| L1-ball | $\{\pm \mathbf{e}_i\}$ | $2d$ | d | $\pm \mathbf{e}_i$ with $\text{argmax}_i g_i $ |
| Simplex | $\{\mathbf{e}_i\}$ | d | d | \mathbf{e}_i with $\text{argmin}_i g_i$ |
| Norms | $\{\mathbf{x}, \ \mathbf{x}\ \leq 1\}$ | ∞ | d | $\text{argmin}_{\mathbf{s}, \ \mathbf{s}\ \leq 1} \langle \mathbf{s}, \mathbf{g} \rangle$ |
| Nuclear norm | $\{Y, \ Y\ _* \leq 1\}$ | ∞ | d^2 | .. |
| Wavelets | .. | ∞ | ∞ | .. |