Optimization for Machine Learning CS-439

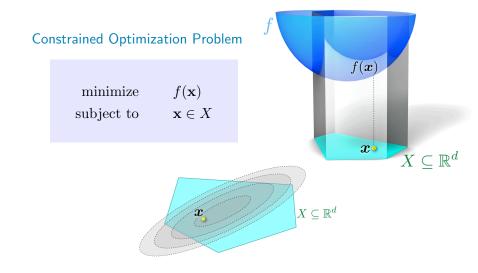
Lecture 8: Frank-Wolfe

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EPFL - github.com/epfml/OptML_course

April 27, 2018

Constrained Optimization



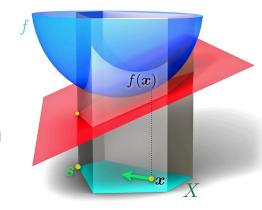
Frank-Wolfe Algorithm

Frank-Wolfe Algorithm:

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

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

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



Linear Minimization Oracle:

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

Properties

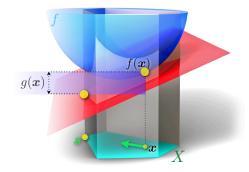
- Aways feasible: $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_t \in X$. \mathbf{x}_{t+1} is on line segment $[\mathbf{s}, \mathbf{x}_t]$, for $\gamma \in [0, 1]$.
- ▶ Reduces non-linear to linear optimization
- ► Projection-free
- Sparse iterates (in terms of corners s used)

Invented and analyzed 1956 by Marguerite Frank, and Philip Wolfe.

Duality Gap

Duality Gap

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



Certificate for optimization quality:

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

$$\geq \langle \mathbf{x} - \mathbf{x}^*, \nabla f(\mathbf{x}) \rangle$$

$$\geq f(\mathbf{x}) - f(\mathbf{x}^*)$$

Stepsize variants

$$\begin{array}{ll} \gamma_t &:=& \frac{2}{t+2}, \\ \gamma_t &:=& \operatornamewithlimits{argmin}_{\gamma \in [0,1]} f \big((1-\gamma) \mathbf{x}_t + \gamma \mathbf{s} \big), \\ \gamma_t &:=& \min \Big\{ \frac{g(\mathbf{x}_t)}{L \, \|\mathbf{s} - \mathbf{x}_t\|^2}, 1 \Big\}, \end{array} \qquad \text{(gap-based)}$$

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

Theorem

Let $f: \mathbb{R}^d \to \mathbb{R}$ 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

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

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

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

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

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

$$f(\mathbf{y}) = f(\mathbf{x} + \gamma(\mathbf{s} - \mathbf{x}))$$

$$\leq f(\mathbf{x}) + \gamma(\mathbf{s} - \mathbf{x}, \nabla f(\mathbf{x})) + \frac{\gamma^2}{2} L \operatorname{diam}(X)^2.$$

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 $C := \frac{1}{2} L \operatorname{diam}(X)^2$. This bound holds also for all mentioned line-search variants (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

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

$$\leq h(\mathbf{x}_t) - \gamma h(\mathbf{x}_t) + \gamma^2 C$$

$$= (1 - \gamma)h(\mathbf{x}_t) + \gamma^2 C,$$

where we have used the certificate property $h(\mathbf{x}) \leq g(\mathbf{x})$ of the duality gap.

The theorem then follows by induction (Exercise 1 of Lab 8).

Affine Invariance

Curvature Constant

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

Algorithm is invariant to scaling of the input problem.

So is C_f .

(same as Newton, but here for constrained problems)

$$C_f \le L \operatorname{diam}(X)^2$$
 for any norm!

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

Convergence in duality gap

Theorem

Let $f: \mathbb{R}^d \to \mathbb{R}$ 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.

$$g(\mathbf{x}_t) \le \frac{27/4 \, C_f}{T+1}$$

Proof.

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

Extensions and Use Cases

Extensions:

- ► Approximate LMO (of additive of 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

$$\mathsf{recall} \colon \operatorname{LMO}(\mathbf{g}) := \operatornamewithlimits{argmin}_{\mathbf{s} \in X} \langle \mathbf{s}, \mathbf{g} \rangle$$

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

Examples	\mathcal{A}	$ \mathcal{A} $	d	LMO (d = -g)
L1-ball	$\{\pm \mathbf{e}_i\}$	2d	d	$\pm \mathbf{e}_i$ with $\operatorname{argmax}_i d_i $
Simplex	$\{\mathbf e_i\}$	d	d	\mathbf{e}_i with $\operatorname{argmax}_i d_i$
Norms	$\left\{\mathbf{x}, \ \mathbf{x}\ \le 1\right\}$	∞	d	$\operatorname{argmax} \langle \mathbf{s}, \mathbf{d} \rangle$
			_	$\mathbf{s}, \ \mathbf{s}\ \leq 1$
Nuclear norm	$ \{Y, Y _* \le 1\}$	∞	d^2	
Wavelets		∞	∞	