Optimization for Machine Learning CS-439

Lecture 9: Frank-Wolfe algorithm

Martin Jaggi

EPFL - github.com/epfml/0ptML_course May 3, 2024

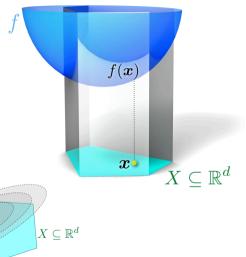
Chapter 9

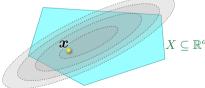
Frank-Wolfe

Constrained Optimization

Constrained Optimization Problem

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





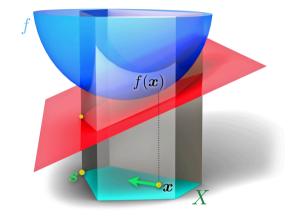
Frank-Wolfe Algorithm

Frank-Wolfe Algorithm:

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

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

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

- 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 s used)

Invented and analyzed 1956 by Marguerite Frank and Philip Wolfe.

Example

Lasso Regression

$$\min_{\mathbf{x}} \|A\mathbf{x} - \mathbf{b}\|^2 \quad s.t. \quad \|\mathbf{x}\|_1 \le 1$$

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

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

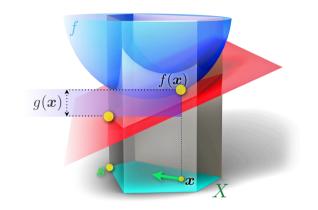
- $\triangleright \nabla f(\mathbf{x}) = \mathbf{g} := A^{\top} (A\mathbf{x} \mathbf{b})$
- ► LMO(g) = $-\text{sign}(g_i)\mathbf{e}_i$ with $i := \underset{i \in [n]}{\operatorname{argmax}} |g_i|$

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:

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

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

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

Stepsize variants

$$egin{array}{lll} \gamma_t &:=& rac{2}{t+2}, \ \gamma_t &:=& rgmin_{\gamma \in [0,1]} fig((1-\gamma)\mathbf{x}_t + \gamma \mathbf{s}ig), & ext{(line-search)} \ \gamma_t &:=& \min\Big\{rac{g(\mathbf{x}_t)}{L\,\|\mathbf{s} - \mathbf{x}_t\|^2}, 1\Big\}, & ext{(gap-based)} \end{array}$$

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 $diam(X) := \max_{\mathbf{x}, \mathbf{y} \in X} \|\mathbf{x} - \mathbf{y}\|$ 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 $f(\mathbf{v}) = f(\mathbf{x} + \gamma(\mathbf{s} - \mathbf{x}))$ $< f(\mathbf{x}) + \gamma \langle \mathbf{s} - \mathbf{x}, \nabla f(\mathbf{x}) \rangle + \frac{\gamma^2}{2} L \operatorname{diam}(X)^2$.

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

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

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 (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

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

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

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

by the certificate property $h(\mathbf{x}) \leq g(\mathbf{x})$ of the duality gap. The theorem then follows by induction (Lab 9, Exercise 1).

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

Affine Invariance

Curvature Constant

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

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

So is C_f .

(same as Newton, but here for constrained problems)

$$C_f \leq \frac{L}{2} \operatorname{diam}(X)^2$$
 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 $f: \mathbb{R}^d \to \mathbb{R}$ and X be convex with $C_{(f,X)} < \infty$, 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.

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

Proof.

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

Proof (I)

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

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

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

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