Optimization for Machine Learning
CS-439

Lecture 8: Frank-Wolfe algorithm

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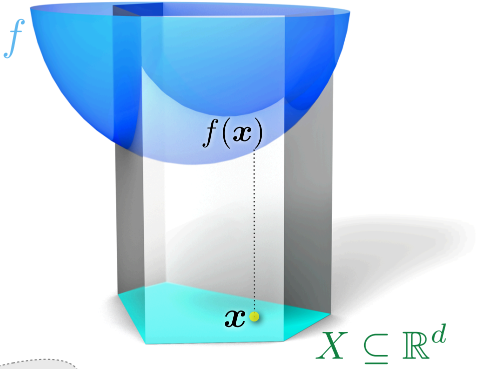
Chapter 9

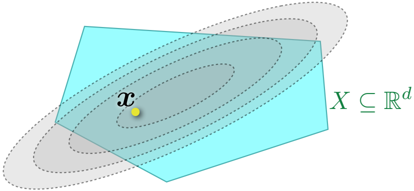
Frank-Wolfe

Constrained Optimization



Constrained Optimization Problem

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

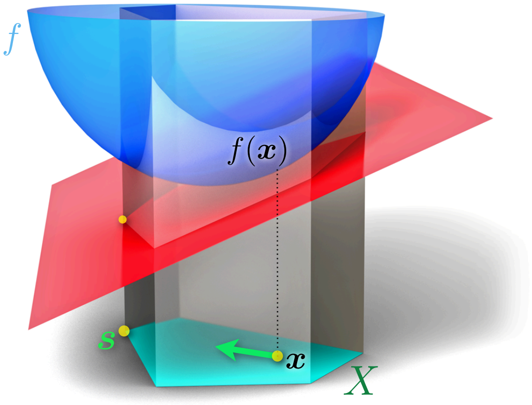


Frank-Wolfe Algorithm

Frank-Wolfe Algorithm:

$$\begin{aligned} \mathbf{s} &:= \mathrm{LMO}(\nabla f(\mathbf{x}_t)), \\ \mathbf{x}_{t+1} &:= (1-\gamma)\mathbf{x}_t + \gamma \mathbf{s}, \end{aligned}$$

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



Linear Minimization Oracle:

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

Properties

- Aways feasible: $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_t \in X$.
  $\mathbf{x}_{t+1}$ 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

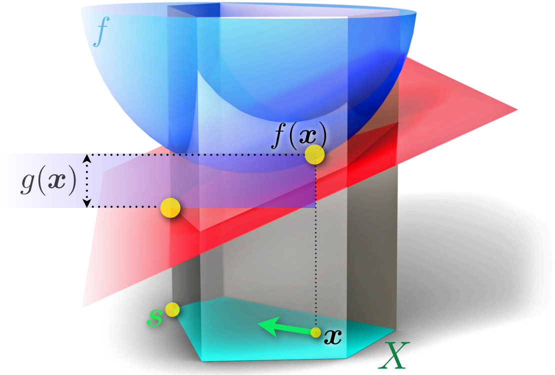
$$\min_{\mathbf{x}} \|A\mathbf{x} - \mathbf{b}\|^2 \ \ s.t. \ \ \|\mathbf{x}\|_1 \leq 1$$

L1-ball is the convex hull of the unit basis vectors:
$X = \{\mathbf{x} \mid \|\mathbf{x}\|_1 \leq 1\} = \mathrm{conv}(\{\pm\mathbf{e}_1, \ldots, \pm\mathbf{e}_n\})$.

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

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:

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

Stepsize variants

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

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

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

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

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

Where $\mathrm{diam}(X) := \max_{\mathbf{x},\mathbf{y}\in X} \|\mathbf{x} - \mathbf{y}\|$ 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*

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

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

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

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

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

Writing $h(\mathbf{x}) := f(\mathbf{x}) - f(\mathbf{x}^\star)$ 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

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

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

So is C_f.

(same as Newton, but here for constrained problems)

$$C_f \leq L\,\mathrm{diam}(X)^2 \qquad \text{for any norm!}$$

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

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.

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

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 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

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

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

Examples	$\mathcal{A}$	$\lvert\mathcal{A}\rvert$	d	$\mathrm{LMO}\ (\mathbf{g})$
L1-ball	$\{\pm \mathbf{e}_i\}$	$2d$	d	$\pm \mathbf{e}_i$ with $\operatorname{argmax}_i \lvert g_i \rvert$
Simplex	$\{\mathbf{e}_i\}$	d	d	$\mathbf{e}_i$ with $\operatorname{argmin}_i g_i$
Norms	$\{\mathbf{x}, \lVert\mathbf{x}\rVert \leq 1\}$	∞	d	$\underset{\mathbf{s}, \lVert\mathbf{s}\rVert \leq 1}{\operatorname{argmin}} \langle \mathbf{s}, \mathbf{g} \rangle$
Nuclear norm	$\{Y, \lVert Y\rVert_* \leq 1\}$	∞	d^2	..
Wavelets	..	∞	∞	..