Conditional Gradient (Frank-Wolfe) Method

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Last time: ADMM

Consider a problem of the form:

$$\min_{x,z} \; f(x) + g(z) \;\; \text{subject to} \;\; Ax + Bz = c.$$

Augmented Lagrangian (for some $\rho > 0$)

$$L_\rho(x, z, u) = f(x) + g(z) + u^T(Ax + Bz - c) + \frac{\rho}{2}\|Ax + Bz - c\|_2^2$$

ADMM: for $k = 1, 2, 3, \ldots$

$$\begin{aligned} x^{(k)} &= \operatorname*{argmin}_x \; L_\rho(x, z^{(k-1)}, u^{(k-1)}) \\ z^{(k)} &= \operatorname*{argmin}_z \; L_\rho(x^{(k)}, z, u^{(k-1)}) \\ u^{(k)} &= u^{(k-1)} + \rho(Ax^{(k)} + Bz^{(k)} - c) \end{aligned}$$

ADMM in scaled form

Replace the dual variable u by a scaled variable $w = u/\rho$.

In this parametrization, the ADMM steps are:

$$\begin{aligned} x^{(k)} &= \underset{x}{\operatorname{argmin}} \; f(x) + \frac{\rho}{2}\|Ax + Bz^{(k-1)} - c + w^{(k-1)}\|_2^2 \\ z^{(k)} &= \underset{z}{\operatorname{argmin}} \; g(z) + \frac{\rho}{2}\|Ax^{(k)} + Bz - c + w^{(k-1)}\|_2^2 \\ w^{(k)} &= w^{(k-1)} + Ax^{(k)} + Bz^{(k)} - c \end{aligned}$$

Outline

Today:

- Conditional gradient method
- Convergence analysis
- Properties and variants

Consider the constrained problem

$$\min_x \ f(x) \ \text{ subject to } \ x \in C$$

where f is convex and smooth, and C is convex.
Recall projected gradient descent: choose an initial $x^{(0)}$, and for $k = 1, 2, 3, \ldots$

$$x^{(k)} = P_C\big(x^{(k-1)} - t_k \nabla f(x^{(k-1)})\big)$$

where P_C is the projection operator onto the set C

This was a special case of proximal gradient descent, motivated by a local quadratic expansion of f:

$$x^{(k)} = P_C\left(\underset{y}{\operatorname{argmin}} \ \nabla f(x^{(k-1)})^T(y - x^{(k-1)}) + \frac{1}{2t}\|y - x^{(k-1)}\|_2^2\right)$$

Conditional gradient (Frank-Wolfe) method

Choose an initial $x^{(0)} \in C$ and for $k = 1, 2, 3, \ldots$

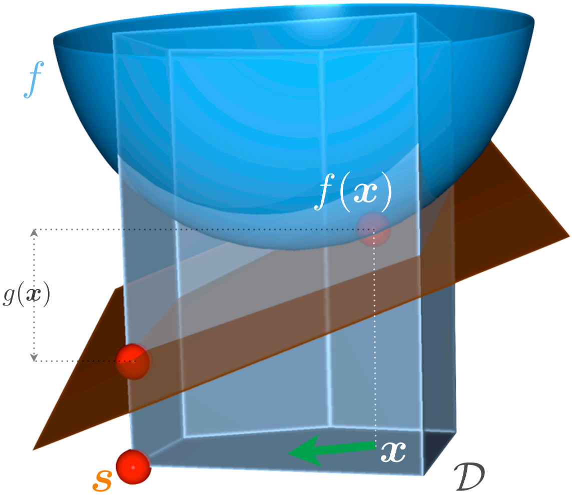
$$s^{(k-1)} \in \underset{s \in C}{\operatorname{argmin}} \; \nabla f(x^{(k-1)})^T s$$
$$x^{(k)} = (1 - \gamma_k) x^{(k-1)} + \gamma_k s^{(k-1)}$$

Note that there is no projection; update is solved directly over the constraint set C

The default choice for step sizes is $\gamma_k = 2/(k+1)$, $k = 1, 2, 3, \ldots$. For any choice $0 \leq \gamma_k \leq 1$, we see that $x^{(k)} \in C$ by convexity. Can also think of the update as

$$x^{(k)} = x^{(k-1)} + \gamma_k (s^{(k-1)} - x^{(k-1)})$$

i.e., we are moving less and less in the direction of the linearization minimizer as the algorithm proceeds



(From Jaggi 2011)

Norm constraints

What happens when $C = \{x : \|x\| \leq t\}$ for a norm $\|\cdot\|$? Then

$$\begin{aligned} s &\in \operatorname*{argmin}_{\|s\|\leq t} \; \nabla f(x^{(k-1)})^T s \\ &= -t \cdot \left(\operatorname*{argmax}_{\|s\|\leq 1} \; \nabla f(x^{(k-1)})^T s \right) \\ &= -t \cdot \partial \|\nabla f(x^{(k-1)})\|_* \end{aligned}$$

where $\|\cdot\|_*$ is the corresponding dual norm. In other words, if we know how to compute subgradients of the dual norm, then we can easily perform Frank-Wolfe steps

A key to Frank-Wolfe: this can often be simpler or cheaper than projection onto $C = \{x : \|x\| \leq t\}$. Also often simpler or cheaper than the prox operator for $\|\cdot\|$

Example: ℓ_1 regularization

For the ℓ_1-regularized problem

$$\min_x \; f(x) \;\; \text{subject to} \;\; \|x\|_1 \le t$$

we have $s^{(k-1)} \in -t\partial\|\nabla f(x^{(k-1)})\|_\infty$. Frank-Wolfe update is thus

$$i_{k-1} \in \operatorname*{argmax}_{i=1,\ldots p} \left|\nabla_i f(x^{(k-1)})\right|$$
$$x^{(k)} = (1-\gamma_k)x^{(k-1)} - \gamma_k t \cdot \text{sign}\big(\nabla_{i_{k-1}} f(x^{(k-1)})\big) \cdot e_{i_{k-1}}$$

This is a kind of *coordinate descent.* (More on coordinate descent later.)

Note: this is a lot simpler than projection onto the ℓ_1 ball, though both require $O(n)$ operations

Example: ℓ_p regularization

For the ℓ_p-regularized problem

$$\min_x \; f(x) \;\; \text{subject to} \;\; \|x\|_p \leq t$$

for $1 \leq p \leq \infty$, we have $s^{(k-1)} \in -t\partial \|\nabla f(x^{(k-1)})\|_q$, where p, q are dual, i.e., $1/p + 1/q = 1$. Claim: can choose

$$s_i^{(k-1)} = -\alpha \cdot \text{sign}\big(\nabla f_i(x^{(k-1)})\big) \cdot \big|\nabla f_i(x^{(k-1)})\big|^{p/q}, \quad i = 1, \ldots n$$

where α is a constant such that $\|s^{(k-1)}\|_q = t$ (check this), and then Frank-Wolfe updates are as usual

Note: this is a lot simpler than projection onto the ℓ_p ball, for general p. Aside from special cases ($p = 1, 2, \infty$), these projections cannot be directly computed (must be treated as an optimization)

Example: trace norm regularization

For the trace-regularized problem

$$\min_X \; f(X) \;\; \text{subject to} \;\; \|X\|_{\text{tr}} \le t$$

we have $S^{(k-1)} \in -t\|\nabla f(X^{(k-1)})\|_{\text{op}}$. Claim: can choose

$$S^{(k-1)} = -t \cdot uv^T$$

where u, v are leading left, right singular vectors of $\nabla f(X^{(k-1)})$ (check this), and then Frank-Wolfe updates are as usual

Note: this is a lot simpler and more efficient than projection onto the trace norm ball, which requires a singular value decomposition.

Constrained and Lagrange forms

Recall that solution of the constrained problem

$$\min_x \; f(x) \;\; \text{subject to} \;\; \|x\| \leq t$$

are equivalent to those of the Lagrange problem

$$\min_x \; f(x) + \lambda\|x\|$$

as we let the tuning parameters t and λ vary over $[0, \infty]$.

We should also compare the Frank-Wolfe updates under $\|\cdot\|$ to the proximal operator of $\|\cdot\|$

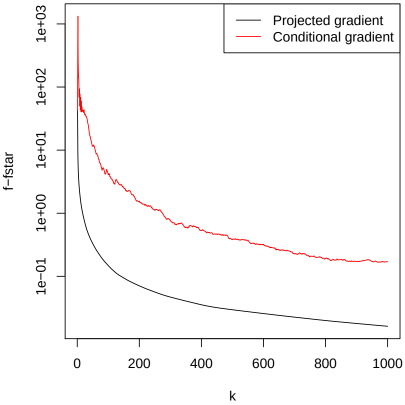
- ℓ_1 norm: Frank-Wolfe update scans for maximum of gradient; proximal operator soft-thresholds the gradient step; both use $O(n)$ flops

- ℓ_p norm: Frank-Wolfe update raises each entry of gradient to power and sums, in $O(n)$ flops; proximal operator not generally directly computable

- Trace norm: Frank-Wolfe update computes top left and right singular vectors of gradient; proximal operator soft-thresholds the gradient step, requiring a singular value decomposition

Many other regularizers yield efficient Frank-Wolfe updates, e.g., special polyhedra or cone constraints, sum-of-norms (group-based) regularization, atomic norms. See Jaggi (2011)

Comparing projected and conditional gradient for constrained lasso problem, with $n = 100$, $p = 500$:



We will see that Frank-Wolfe methods match convergence rates of known first-order methods; but in practice they can be slower to converge to high accuracy (note: fixed step sizes here, line search would probably improve convergence)

Duality gap

Frank-Wolfe iterations admit a very natural duality gap (truly, a suboptimality gap):

$$\max_{s \in C} \; \nabla f(x^{(k-1)})^T (x^{(k-1)} - s)$$

This is an upper bound on $f(x^{(k-1)}) - f^\star$

Proof: by the first-order condition for convexity

$$f(s) \geq f(x^{(k-1)}) + \nabla f(x^{(k-1)})^T (s - x^{(k-1)})$$

Minimizing both sides over all $s \in C$ yields

$$f^\star \geq f(x^{(k-1)}) + \min_{s \in C} \; \nabla f(x^{(k-1)})^T (s - x^{(k-1)})$$

Rearranged, this gives the duality gap above

Note that

$$\max_{s \in C} \nabla f(x^{(k-1)})^T (x^{(k-1)} - s) = \nabla f(x^{(k-1)})^T (x^{(k-1)} - s^{(k-1)})$$

so this quantity comes directly from the Frank-Wolfe update. Why do we call it "duality gap"? Rewrite original problem as

$$\min_x f(x) + I_C(x)$$

where I_C is the indicator function of C. The dual problem is

$$\max_u -f^*(u) - I_C^*(-u)$$

where I_C^* is the support function of C. Duality gap at x, u is

$$f(x) + f^*(u) + I_C^*(-u) \geq x^T u + I_C^*(-u)$$

Evaluated at $x = x^{(k-1)}$, $u = \nabla f(x^{(k-1)})$, this gives claimed gap

Convergence analysis

Following Jaggi (2011), define the curvature constant of f over C:

$$M = \max_{\substack{x,s,y \in C \\ y=(1-\gamma)x+\gamma s}} \frac{2}{\gamma^2}\Big(f(y) - f(x) - \nabla f(x)^T(y-x)\Big)$$

(Above we restrict $\gamma \in [0,1]$.) Note that $M = 0$ when f is linear. The quantity $f(y) - f(x) - \nabla f(x)^T(y-x)$ is called the Bregman divergence defined by f

Theorem: Conditional gradient method using fixed step sizes $\gamma_k = 2/(k+1)$, $k = 1, 2, 3, \ldots$ satisfies

$$f(x^{(k)}) - f^\star \le \frac{2M}{k+2}$$

Number of iterations needed to have $f(x^{(k)}) - f^\star \le \epsilon$ is $O(1/\epsilon)$

This matches the known rate for projected gradient descent when ∇f is Lipschitz, but how do the assumptions compare?. In fact, if ∇f is Lipschitz with constant L then $M \le \mathrm{diam}^2(C) \cdot L$, where

$$\mathrm{diam}(C) = \max_{x,s \in C} \|x - s\|_2$$

To see this, recall that ∇f Lipschitz with constant L means

$$f(y) - f(x) - \nabla f(x)^T (y - x) \le \frac{L}{2} \|y - x\|_2^2$$

Maximizing over all $y = (1 - \gamma)x + \gamma s$, and multiplying by $2/\gamma^2$,

$$M \le \max_{\substack{x,s,y \in C \\ y = (1-\gamma)x + \gamma s}} \frac{2}{\gamma^2} \cdot \frac{L}{2} \|y - x\|_2^2 = \max_{x,s \in C} L \|x - s\|_2^2$$

and the bound follows. Essentially, assuming a bounded curvature is no stronger than what we assumed for proximal gradient

Basic inequality

The key inequality used to prove the Frank-Wolfe convergence rate is:

$$f(x^{(k)}) \leq f(x^{(k-1)}) - \gamma_k g(x^{(k-1)}) + \frac{\gamma_k^2}{2} M$$

Here $g(x) = \max_{s \in C} \nabla f(x)^T (x - s)$ is the duality gap discussed earlier. The rate follows from this inequality, using induction

Proof: write $x^+ = x^{(k)}$, $x = x^{(k-1)}$, $s = s^{(k-1)}$, $\gamma = \gamma_k$. Then

$$\begin{aligned} f(x^+) &= f\big(x + \gamma(s - x)\big) \\ &\leq f(x) + \gamma \nabla f(x)^T (s - x) + \frac{\gamma^2}{2} M \\ &= f(x) - \gamma g(x) + \frac{\gamma^2}{2} M \end{aligned}$$

Second line used definition of M, and third line the definition of g

Affine invariance

Important property of Frank-Wolfe: its updates are affine invariant. Given nonsingular $A : \mathbb{R}^n \to \mathbb{R}^n$, define $x = Ax'$, $h(x') = f(Ax')$. Then Frank-Wolfe on $h(x')$ proceeds as

$$s' = \underset{z \in A^{-1}C}{\operatorname{argmin}} \; \nabla h(x')^T z$$
$$(x')^+ = (1 - \gamma)x' + \gamma s'$$

Multiplying by A reveals precisely the same Frank-Wolfe update as would be performed on $f(x)$. Even convergence analysis is affine invariant. Note that the curvature constant M of h is

$$M = \max_{\substack{x', s', y' \in A^{-1}C \\ y' = (1-\gamma)x' + \gamma s'}} \; \frac{2}{\gamma^2} \Big(h(y') - h(x') - \nabla h(x')^T (y' - x') \Big)$$

matching that of f, because $\nabla h(x')^T (y' - x') = \nabla f(x)^T (y - x)$

Inexact updates

Jaggi (2011) also analyzes inexact Frank-Wolfe updates. That is, suppose we choose $s^{(k-1)}$ so that

$$\nabla f(x^{(k-1)})^T s^{(k-1)} \leq \min_{s \in C} \; \nabla f(x^{(k-1)})^T s + \frac{M\gamma_k}{2} \cdot \delta$$

where $\delta \geq 0$ is our inaccuracy parameter. Then we basically attain the same rate

Theorem: Conditional gradient method using fixed step sizes $\gamma_k = 2/(k+1)$, $k = 1, 2, 3, \ldots$, and inaccuracy parameter $\delta \geq 0$, satisfies

$$f(x^{(k)}) - f^\star \leq \frac{2M}{k+2}(1+\delta)$$

Note: the optimization error at step k is $\frac{M\gamma_k}{2} \cdot \delta$. Since $\gamma_k \to 0$, we require the errors to vanish

Some variants

Some variants of the conditional gradient method:

- Line search: instead of fixing $\gamma_k = 2/(k+1)$, $k = 1, 2, 3, \ldots$, use exact line search for the step sizes

$$\gamma_k = \underset{\gamma \in [0,1]}{\operatorname{argmin}} \ f\big(x^{(k-1)} + \gamma(s^{(k-1)} - x^{(k-1)})\big)$$

  at each $k = 1, 2, 3, \ldots$. Or, we could use backtracking

- Fully corrective: directly update according to

$$x^{(k)} = \underset{y}{\operatorname{argmin}} \ f(y) \ \text{ subject to } \ y \in \operatorname{conv}\{x^{(0)}, s^{(0)}, \ldots s^{(k-1)}\}$$

  Can make much better progress, but is also quite a bit harder

Another variant: away steps

Suppose $C = \text{conv}(A)$ for a set of atoms A.

Keep explicit description of $x \in C$ as a convex combination of elements in A

$$x = \sum_{a \in A} \lambda_a(x) a$$

Conditional gradient with away steps:

1. choose $x^{(0)} = a^{(0)} \in A$
2. for $k = 1, 2, 3, \ldots$

$$s^{(k-1)} \in \underset{a \in A}{\text{argmin}} \ \nabla f(x^{(k-1)})^T a,$$

$$a^{(k-1)} \in \underset{\substack{a \in A \\ \lambda_a(x^{(k-1)}) > 0}}{\text{argmax}} \ \nabla f(x^{(k-1)})^T a$$

choose $v = s^{(k-1)} - x^{(k-1)}$ or $v = x^{(k-1)} - a^{(k-1)}$

$$x^{(k)} = x^{(k-1)} + \gamma_k v$$

end for

Linear convergence

Consider the unconstrained problem

$$\min_x \ f(x) \ \text{ subject to } \ x \in \mathbb{R}^n$$

where f is μ-strongly convex and ∇f is L-Lipschitz.

For $t_k = 1/L$ gradient descent iterates $x^{(k+1)} = x^{(k)} - t_k \nabla f(x^{(k)})$ satisfy

$$f(x^{(k)}) - f^\star \leq \left(1 - \frac{\mu}{L}\right)^k (f(x^{(0)}) - f^\star)$$

Linear convergence

Consider the constrained problem

$$\min_x \; f(x) \;\; \text{subject to} \;\; x \in \mathsf{conv}(A) \subseteq \mathbb{R}^n$$

Theorem (Lacoste-Julien & Jaggi 2013)

Assume f is μ-strongly convex, ∇f is L-Lipschitz, and $A \subseteq \mathbb{R}^n$ finite.

For suitable γ_k the iterates generated by the conditional gradient algorithm with away steps satisfy

$$f(x^{(k)}) - f^\star \le (1-r)^{k/2}(f(x^{(0)}) - f^\star) \;\; \textit{for} \;\; r = \frac{\mu}{L} \cdot \frac{\Phi(A)^2}{4\mathsf{diam}(A)^2}.$$

Peña & Rodríguez (2016):

$$\Phi(A) = \min_{F \in \mathsf{faces}(\mathsf{conv}(A))} \mathsf{dist}(F, \mathsf{conv}(A \setminus F)).$$

Path following

Given the norm constrained problem

$$\min_x \ f(x) \ \text{ subject to } \ \|x\| \le t$$

the Frank-Wolfe algorithm can be used for path following, i.e., can produce an (approximate) solution path $\hat{x}(t)$, $t \ge 0$. Beginning at $t_0 = 0$ and $x^\star(0) = 0$, we fix parameters $\epsilon, m > 0$, then repeat for $k = 1, 2, 3, \ldots$:

- Calculate

$$t_k = t_{k-1} + \frac{(1 - 1/m)\epsilon}{\|\nabla f(\hat{x}(t_{k-1}))\|_*}$$

  and set $\hat{x}(t) = \hat{x}(t_{k-1})$ for all $t \in (t_{k-1}, t_k)$
- Compute $\hat{x}(t_k)$ by running Frank-Wolfe at $t = t_k$, terminating when the duality gap is $\le \epsilon/m$

This is a simplification of the strategy given in Giesen et al. (2012)

With this path following strategy, we are guaranteed that

$$f(\hat{x}(t)) - f(x^\star(t)) \leq \epsilon \quad \text{for all } t \text{ visited}$$

i.e., we produce a (piecewise-constant) path with suboptimality gap uniformly bounded by ϵ, over all t

To see this, it helps to rewrite the Frank-Wolfe duality gap as

$$g_t(x) = \max_{\|s\| \leq 1} \nabla f(x)^T (x - s) = \nabla f(x)^T x + t \|\nabla f(x)\|_*$$

This is a linear function of t. Hence if $g_t(x) \leq \epsilon/m$, then we can increase t until $t^+ = t + (1 - 1/m)\epsilon/\|\nabla f(x)\|_*$, because at this value

$$g_{t^+}(x) = \nabla f(x)^T x + t\|\nabla f(x)\|_* + \epsilon - \epsilon/m \leq \epsilon$$

i.e., the duality gap remains $\leq \epsilon$ for the same x, between t and t^+

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