Conditional Gradient (Frank-Wolfe) Method

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Last time: coordinate descent

For the problem

$$\min_{x} g(x) + \sum_{i=1}^{n} h_i(x_i)$$

with g convex and smooth and each h_i convex, can use coordinate descent, which begins with an initial points $x^{(0)}$ and repeats:

$$x_1^{(k)} \in \underset{x_1}{\operatorname{argmin}} f(x_1, x_2^{(k-1)}, x_3^{(k-1)}, \dots, x_n^{(k-1)})$$
$$x_2^{(k)} \in \underset{x_2}{\operatorname{argmin}} f(x_1^{(k)}, x_2, x_3^{(k-1)}, \dots, x_n^{(k-1)})$$
$$\dots$$

$$x_n^{(k)} \in \operatorname*{argmin}_{x_2} f(x_1^{(k)}, x_2^{(k)}, x_3^{(k)}, \dots x_n)$$

for $k=1,2,3,\ldots$. The above minimizations can also be replaced by proximal gradient steps

Strengths:

- Relatively simple and can be surprisingly efficient and scalable when updates are implemented carefully
- When combined with a pathwise approach, and when utilizing active set tricks, takes advantage of low-dimensional structure inherent in a problem

Weaknesses/unknowns:

- Not always applicable, when nonsmooth parts do not separate
- Not generically parallelizable, as updates are "one-at-a-time"
- Precise rates for cyclic coordinate descent not well-understood (especially for exact coordinatewise minimization)

Conditional gradient method

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 chooses an initial $x^{(0)}$, repeats for k = 1, 2, 3, ...

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

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:

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

The conditional gradient method, also known as the Frank-Wolfe method, uses a local linear expansion of f:

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

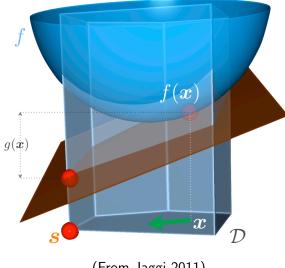
 $x^{(k)} = (1 - \gamma_k) x^{(k-1)} + \gamma_k s^{(k-1)}$

Note that there is no projection; update is solved directly over the constraint set ${\cal C}$

The default choice for step sizes is $\gamma_k = 2/(k+1)$, k = 1, 2, 3, ...For any choice $0 \le \gamma_k \le 1$, 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

$$s \in \underset{\|s\| \le t}{\operatorname{argmin}} \nabla f(x^{(k-1)})^T s$$
$$= -t \cdot \left(\underset{\|s\| \le 1}{\operatorname{argmax}} \nabla f(x^{(k-1)})^T s \right)$$
$$= -t \cdot \partial \|\nabla f(x^{(k-1)})\|_*$$

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 $C = \{x : ||x|| \le t\}$. Also often simpler or cheaper than the prox operator for $|| \cdot ||$

Outline

Today:

- Examples
- Convergence analysis
- Properties and variants
- Path following

Example: ℓ_1 regularization

For the $\ell_1\text{-regularized}$ problem

$$\begin{split} \min_{x} f(x) & \text{subject to} \quad \|x\|_{1} \leq t \\ \text{we have } s^{(k-1)} \in -t\partial \|\nabla f(x^{(k-1)})\|_{\infty}. & \text{Frank-Wolfe update is thus} \\ & i_{k-1} \in \operatorname*{argmax}_{i=1,\dots,p} \ \left|\nabla_{i}f(x^{(k-1)})\right| \\ & x^{(k)} = (1-\gamma_{k})x^{(k-1)} - \gamma_{k}t \cdot \operatorname{sign}\left(\nabla_{i_{k-1}}f(x^{(k-1)})\right) \cdot e_{i_{k-1}} \end{split}$$

Like greedy coordinate descent!

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

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

for $1 \le p \le \infty$, 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

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

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 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

$$\min_{X} f(X) \text{ subject to } \|X\|_{\mathrm{tr}} \leq t$$

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

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

are equivalent to those of the Lagrange problem

 $\min_{x} f(x) + \lambda \|x\|$

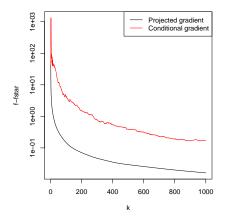
as we let the tuning parameters t and λ vary over $[0, \infty]$. Typically in statistics and ML problems, we would just solve whichever form is easiest, over wide range of parameter values

So 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 computes 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

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

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

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

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

$$f(x) + f^*(u) + I^*_C(-u) \ge x^T u + I^*_C(-u)$$

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 $\kappa = 0$ 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

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

Hence the number of iterations needed to achieve $f(x^{(k)}) - f^\star \leq \epsilon$ 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 $M \leq \text{diam}^2(C) \cdot L$, where

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

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:

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

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

$$f(x^{+}) = f\left(x + \gamma(s - x)\right)$$

$$\leq f(x) + \gamma \nabla f(x)^{T}(s - x) + \frac{\gamma^{2}}{2}M$$

$$= f(x) - \gamma g(x) + \frac{\gamma^{2}}{2}M$$

Second line used definition of $M_{\rm J}$ 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 $f(\boldsymbol{x})$

In fact, even the convergence analysis is affine invariant. Note that the curvature constant ${\cal M}$ 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

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

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 $\delta \ge 0$, satisfies

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

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

Two variants

Two important 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

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

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

• Fully corrective: directly update according to

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

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

Both variants have the same ${\cal O}(1/\epsilon)$ complexity, measured by the number of iterations

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 $x^*(0) = 0$, 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 $\leq \epsilon/m$

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

With this path following strategy, we are guaranteed that

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

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

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

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

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

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