

Frank-Wolfe Method

Ryan Tibshirani
Convex Optimization 10-725

Last time: ADMM

For the problem

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

we form **augmented Lagrangian** (scaled form):

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

Alternating direction method of multipliers or **ADMM**:

$$x^{(k)} = \underset{x}{\operatorname{argmin}} L_\rho(x, z^{(k-1)}, w^{(k-1)})$$

$$z^{(k)} = \underset{z}{\operatorname{argmin}} L_\rho(x^{(k)}, z, w^{(k-1)})$$

$$w^{(k)} = w^{(k-1)} + Ax^{(k)} + Bz^{(k)} - c$$

Converges like a first-order method. Very flexible framework

Projected gradient descent

Consider constrained problem

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

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

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

where P_C is the projection operator onto the set C . Special case of proximal gradient, motivated by local quadratic expansion of f :

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

Motivation for today: **projections are not always easy!**

Frank-Wolfe method

The **Frank-Wolfe method**, also called conditional gradient method, uses a local linear expansion of f :

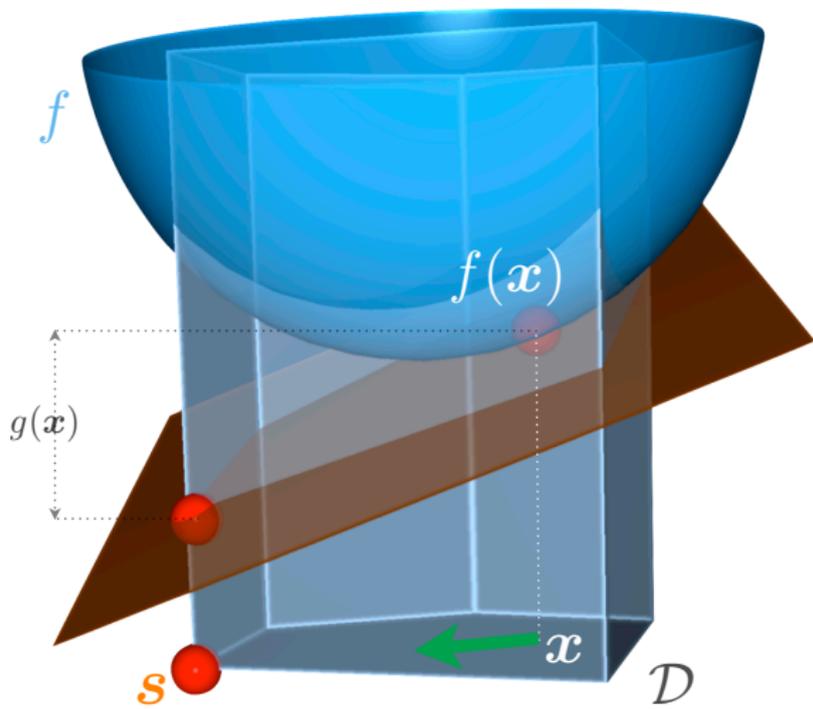
$$s^{(k-1)} \in \operatorname{argmin}_{s \in C} \nabla f(x^{(k-1)})^T s$$
$$x^{(k)} = (1 - \gamma_k)x^{(k-1)} + \gamma_k s^{(k-1)}$$

Note that there is **no projection**; update is solved directly over C

Default step sizes: $\gamma_k = 2/(k + 1)$, $k = 1, 2, 3, \dots$. Note for any $0 \leq \gamma_k \leq 1$, we have $x^{(k)} \in C$ by convexity. Can rewrite 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 $\|\cdot\|_*$ denotes the corresponding dual norm. That is, 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 $C = \{x : \|x\| \leq t\}$

Outline

Today:

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

Example: ℓ_1 regularization

For the ℓ_1 -regularized problem

$$\min_x f(x) \quad \text{subject to} \quad \|x\|_1 \leq t$$

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

$$i_{k-1} \in \operatorname{argmax}_{i=1,\dots,p} |\nabla_i f(x^{(k-1)})|$$

$$x^{(k)} = (1 - \gamma_k)x^{(k-1)} - \gamma_k t \cdot \operatorname{sign}(\nabla_{i_{k-1}} f(x^{(k-1)})) \cdot e_{i_{k-1}}$$

Like greedy coordinate descent! (But with diminishing steps)

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

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

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

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

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

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

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

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

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

Note: this is substantially simpler and cheaper than **projection onto the trace norm ball**, which requires a singular value decomposition!

Constrained and Lagrange forms

Recall that solution of the **constrained** problem

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

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 $[0, \infty]$. Typically in statistics and ML problems, we would just solve **whichever form is easiest**, over wide range of parameter values, then use CV

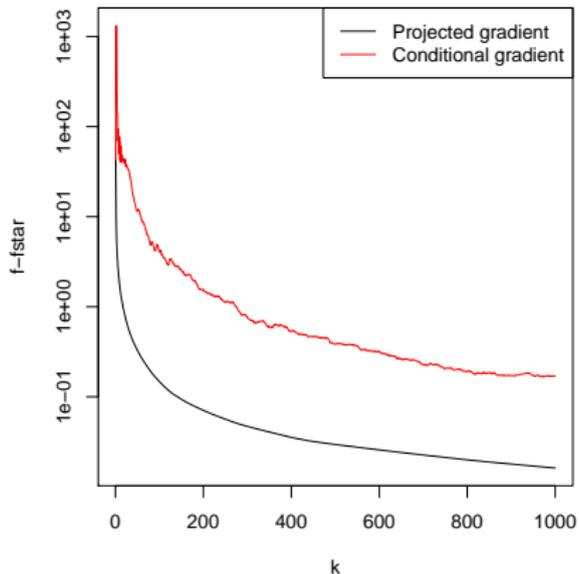
So we should also compare the Frank-Wolfe updates under $\|\cdot\|$ to the proximal operator of $\|\cdot\|$

- 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

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

Example: lasso comparison

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



Note: FW uses standard step sizes, line search would probably help

Duality gap

Frank-Wolfe iterations admit a very natural **duality gap**:

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

Claim: this upper bounds on $f(x^{(k)}) - f^*$

Proof: by the first-order condition for convexity

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

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

$$\begin{aligned} f^* &\geq f(x^{(k)}) + \min_{s \in C} \nabla f(x^{(k)})^T (s - x^{(k)}) \\ &= f(x^{(k)}) + \nabla f(x^{(k)})^T (s^{(k)} - x^{(k)}) \end{aligned}$$

Rearranged, this gives the duality gap above

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 $x = x^{(k)}$, $u = \nabla f(x^{(k)})$, this gives

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

which is our gap

Convergence analysis

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

$$M = \max_{\substack{\gamma \in [0,1] \\ x, s, y \in C \\ y = (1-\gamma)x + \gamma s}} \frac{2}{\gamma^2} \left(f(y) - f(x) - \nabla f(x)^T (y - x) \right)$$

Note that $M = 0$ for linear f , and $f(y) - f(x) - \nabla f(x)^T (y - x)$ is called the **Bregman divergence**, defined by f

Theorem: The Frank-Wolfe method using standard step sizes $\gamma_k = 2/(k + 1)$, $k = 1, 2, 3, \dots$ satisfies

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

Thus number of iterations needed for $f(x^{(k)}) - f^* \leq \epsilon$ is $O(1/\epsilon)$

This matches the sublinear rate for projected gradient descent for Lipschitz ∇f , but how do the assumptions compare?

For Lipschitz ∇f with constant L , recall

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

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

$$\begin{aligned} M &\leq \max_{\substack{\gamma \in [0,1] \\ x, s, y \in C \\ y = (1-\gamma)x + \gamma s}} \frac{2}{\gamma^2} \cdot \frac{L}{2} \|y - x\|_2^2 \\ &= \max_{x, s \in C} L \|x - s\|_2^2 = L \cdot \text{diam}^2(C) \end{aligned}$$

Hence assuming a bounded curvature is **basically no stronger** than what we assumed for projected gradient

Basic inequality

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

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

Here $g(x) = \max_{s \in C} \nabla f(x)^T (x - s)$ is duality gap defined earlier

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

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

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

The proof of the convergence result is now straightforward. Denote by $h(x) = f(x) - f^*$ the suboptimality gap at x . Basic inequality:

$$\begin{aligned}h(x^{(k)}) &\leq h(x^{(k-1)}) - \gamma_k g(x^{(k-1)}) + \frac{\gamma_k^2}{2} M \\&\leq h(x^{(k-1)}) - \gamma_k h(x^{(k-1)}) + \frac{\gamma_k^2}{2} M \\&= (1 - \gamma_k) h(x^{(k-1)}) + \frac{\gamma_k^2}{2} M\end{aligned}$$

where in the second line we used $g(x^{(k-1)}) \geq h(x^{(k-1)})$

To get the desired result we use induction:

$$h(x^{(k)}) \leq \left(1 - \frac{2}{k+1}\right) \frac{2M}{k+1} + \left(\frac{2}{k+1}\right)^2 \frac{M}{2} \leq \frac{2M}{k+2}$$

Affine invariance

Frank-Wolfe updates are **affine invariant**: for nonsingular matrix A , define $x = Ax'$, $F(x') = f(Ax')$, consider Frank-Wolfe on F :

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

Multiplying by A produces same Frank-Wolfe update as that from f . Convergence analysis is also affine invariant: curvature constant

$$M = \max_{\substack{\gamma \in [0,1] \\ x', s', y' \in A^{-1}C \\ y' = (1-\gamma)x' + \gamma s'}} \frac{2}{\gamma^2} \left(F(y') - F(x') - \nabla F(x')^T (y' - x') \right)$$

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

Inexact updates

Jaggi (2011) also analyzes **inexact Frank-Wolfe updates**: 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: Frank-Wolfe using step sizes $\gamma_k = 2/(k+1)$, $k = 1, 2, 3, \dots$, and inaccuracy parameter $\delta \geq 0$, satisfies

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

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

Two variants

Two important variants of Frank-Wolfe:

- **Line search**: instead of using standard step sizes, use

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

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

- **Fully corrective**: directly update according to

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

Both variants lead to the same $O(1/\epsilon)$ iteration complexity

Another popular variant: **away steps**, which get linear convergence under strong convexity

Path following

Given the norm constrained problem

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

Frank-Wolfe can be used for **path following**, i.e., we can produce an approximate solution path $\hat{x}(t)$ that is ϵ -suboptimal for every $t \geq 0$

Let $t_0 = 0$ and $x^*(0) = 0$, fix $m > 0$, repeat for $k = 1, 2, 3, \dots$:

- 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 from Giesen et al., 2012)

Claim: this produces (piecewise-constant) path with

$$f(\hat{x}(t)) - f(x^*(t)) \leq \epsilon \quad \text{for all } t \geq 0$$

Proof: 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

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

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

References

- K. Clarkson (2010), “Coresets, sparse greedy approximation, and the Frank-Wolfe algorithm”
- J. Giesen and M. Jaggi and S. Laue, S. (2012), “Approximating parametrized convex optimization problems”
- M. Jaggi (2011), “Sparse convex optimization methods for machine learning”
- M. Jaggi (2011), “Revisiting Frank-Wolfe: projection-free sparse convex optimization”
- M. Frank and P. Wolfe (2011), “An algorithm for quadratic programming”
- R. J. Tibshirani (2015), “A general framework for fast stagewise algorithms”