CS6301: Optimization in Machine Learning

Lecture 13: Conditional Gradient Descent

Rishabh Iyer

Department of Computer Science
University of Texas, Dallas
https://sites.google.com/view/cs-6301-optml/home

March 4th, 2020

Summary So Far

- Unconstrained First Order:
  - Basic Gradient Descent
  - Accelerated Gradient Descent
  - Proximal Gradient Descent (Special case of smooth + simple)
- Second Order/Quasi newton
  - Newton
  - SR1/BFGS/DFP
  - LBFGS
  - Conjugate Gradient
  - Barzelia Borwein GD
- Constrained Minimization
  - Projected Gradient Descent

Outline

- Recall Projected Gradient
- Conditional Gradient as an Alternative
- Examples of Conditional Gradient Methods

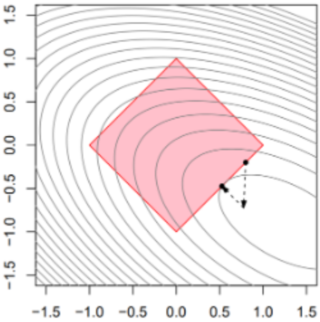
Recall: Proximal Gradient Descent

- Consider the optimization problem $\min_x [f(x) + h(x)]$ where h is a non-differentiable function.
- Define $\text{prox}_{th}(x) = \text{argmin}_z \frac{1}{2t} ||x - z||^2 + h(z)$
- Proximal update:

$$x_{t+1} = \text{prox}_{\gamma h}(x_t - \gamma \nabla f(x_t))$$

Recall: Projected Gradient Descent

- Consider the Problem of Constrained Convex Minimization: $\min_{x \in \mathcal{C}} f(x)$
- A simple modification of the gradient descent procedure is:
  1. At every iteration t: (Gradient Step): Compute $y_{t+1} = x_t - \alpha \nabla f(x_t)$
  2. (Projection step) $x_{t+1} = P_{\mathcal{C}}(y_{t+1})$
- Key here is the Projection step. Define $P_{\mathcal{C}}(x) = \text{argmin}_{y \in \mathcal{C}} \frac{1}{2}||x - y||^2$



Projected Gradient Descent and Proximal Gradient Descent

- There is a close connection between Proximal and Projected Gradient Descent.
- Define $h(x) = I(x \in \mathcal{C})$ where $I(.)$ is the Indicator function.
- Its easy to see that the $\text{prox}_h(x) = P_{\mathcal{C}}(x)$, i.e. the Prox operator is exactly the same as a projection operator.
- As a result, projected gradient descent becomes a special case of proximal gradient descent.
- Theoretical results of Proj. GD: All results for standard Gradient descent carry over to the projected case as long as the projection operator is easy to compute!

Algorithm: Projected Gradient Descent

Find a starting point $\mathbf{x}_p^0 \in \mathcal{C}$.
Set $k = 1$
repeat

1. Choose a step size $t^k \propto 1/\sqrt{k}$.
2. Set $\mathbf{x}_u^k = \mathbf{x}_p^{k-1} - t^k \nabla f(\mathbf{x}_p^{k-1})$.
3. Set $\mathbf{x}_p^k = \underset{\mathbf{z} \in \mathcal{C}}{\operatorname{argmin}} ||\mathbf{x}_u^k - \mathbf{z}||_2^2$.
4. Set $k = k + 1$.

until stopping criterion (such as $||\mathbf{x}_p^k - \mathbf{x}_p^{k-1}|| \leq \epsilon$ or $f(\mathbf{x}_p^k) > f(\mathbf{x}_p^{k-1})$) is satisfied[1]

Figure 1: The projected gradient descent algorithm.

[1] Better criteria can be found using Lagrange duality theory, etc.

Convergence Results for Projected Gradient Descent

- Lipschitz continuous functions PGD: R^2B^2/ϵ^2 iterations*
- Lipschitz continuous functions + Strongly Convex PGD: $2B^2/\epsilon - 1$ iterations*
- Smooth Functions PGD: $\frac{R^2L}{\epsilon}$ iterations.
- Smooth Functions Nesterov's PGD: $\sqrt{\frac{2LR^2}{\epsilon}}$ iterations*
- Smooth + Strongly Convex PGD: With $\gamma = 1/L$, achieve an ϵ-approximate solution in $\frac{L}{\mu}\log(\frac{R^2L}{2\epsilon})$ iterations.
- Smooth + Strongly Convex Nesterov's PGD: With $\gamma = 1/L$, achieve an ϵ-approximate solution in $\sqrt{\frac{L}{\mu}}\log(\frac{R^2L}{2\epsilon})$ iterations*.
- **Key Requirement for Projected Gradient to Work:** Projection must be easy (closed form obtainable) for the constraint.

UT DALLAS

Computing the Projection Operator

- Lets assume for simplicity that $\mathcal{C} = \{x | f(x) \leq c\}$
- Computing the projection step involves solving: $\min_z \{\frac{1}{2}||z - x||^2$, such that $f(z) \leq c\}$.
- Use the idea of Lagrange multipliers!
- Define $g(z, \lambda) = \frac{1}{2}||z - x||^2 + \lambda(f(z) - c)$.
- Optimality conditions are: $\nabla_z g = 0$ and $\nabla_\lambda g = 0$!
- There are two options. Either $x \in \mathcal{C}$, in which case the constraints are not active, or x is outside $\mathcal{C}$ in which case we need $\nabla_z g = 0$ and $\nabla_\lambda g = 0$.
- The second case implies: $f(z) = c$ and $z - x + \lambda \nabla f(z) = 0$. If both these can be solved in closed form, we are done!

Easy to Project Sets $\mathcal{C}$ (with closed form solutions)

- Solution set of a linear system $\mathcal{C} = \{\mathbf{x} \in \Re^n : A^T\mathbf{x} = \mathbf{b}\}$
- Affine images $\mathcal{C} = \{A\mathbf{x} + \mathbf{b} : \mathbf{x} \in \Re^n\}$
- Nonnegative orthant $\mathcal{C} = \{\mathbf{x} \in \Re^n : \mathbf{x} \succeq 0\}$. It may be hard to project on arbitrary polyhedron.
- Norm balls $\mathcal{C} = \{\mathbf{x} \in \Re^n : \|\mathbf{x}\|_p \leq 1\}$, for $p = 1, 2, \infty$

Table of Orthogonal Projections: See https://archive.siam.org/books/mo25/mo25_ch6.pdf

$$P_C(\mathbf{z}) = prox_{I_C}(\mathbf{z}) = \operatorname*{argmin}_{\mathbf{x}} \frac{1}{2t}||\mathbf{x}-\mathbf{z}||^2 + I_C(\mathbf{x}) = \operatorname*{argmin}_{\mathbf{x}\in C} \frac{1}{2t}||\mathbf{x}-\mathbf{z}||^2$$

Set $C =$	For $t=1$, $P_C(\mathbf{z}) =$	Assumptions
$\Re^n_+$	$[\mathbf{z}]_+$	
$\mathrm{Box}[\mathbf{l},\mathbf{u}]$	$P_C(\mathbf{z})_i = min\{max\{z_i, l_i\}, u_i\}$	$l_i \le u_i$
$\mathrm{Ball}[\mathbf{c}, r]$	$\mathbf{c} + \frac{r}{max\{\Vert\mathbf{z}-\mathbf{c}\Vert_2, r\}}(\mathbf{z}-\mathbf{c})$	$\Vert.\Vert_2$ ball, centre $\mathbf{c} \in \Re^n$ & radius $r > 0$
$\{\mathbf{x} \mid A\mathbf{x} = \mathbf{b}\}$	$\mathbf{z} - A^T(AA^T)^{-1}(A\mathbf{z}-\mathbf{b})$	$A \in \Re^{m\times n}$, $\mathbf{b} \in \Re^m$, A is full row rank
$\{\mathbf{x} \mid \mathbf{a}^T\mathbf{x} \le b\}$	$\mathbf{z} - \frac{[\mathbf{a}^T\mathbf{z}-b]_+}{\Vert\mathbf{a}\Vert^2}a$	$0 \ne \mathbf{a} \in \Re^n$ $b \in \Re$
Δ_n	$[\mathbf{z}-\mu^*\mathbf{e}]_+$ where $\mu^* \in \Re$ satisfies $\mathbf{e}^T[\mathbf{z}-\mu^*\mathbf{e}]_+ = 1$	
$H_{\mathbf{a},b} \cap \mathrm{Box}[\mathbf{l},\mathbf{u}]$	$P_{\mathrm{Box}[\mathbf{l},\mathbf{u}]}(\mathbf{z}-\mu^*\mathbf{a})$ where $\mu^* \in \Re$ satisfies $\mathbf{a}^T P_{\mathrm{Box}[\mathbf{l},\mathbf{u}]}(\mathbf{z}-\mu^*\mathbf{a}) = b$	$0 \ne \mathbf{a} \in \Re^n$ $b \in \Re$
$H^-{}_{\mathbf{a},b} \cap \mathrm{Box}[\mathbf{l},\mathbf{u}]$	$P_{\mathrm{Box}[\mathbf{l},\mathbf{u}]}(\mathbf{z})$ $\quad \mathbf{a}^T P_{\mathrm{Box}[\mathbf{l},\mathbf{u}]}(\mathbf{z}) \le b$ $P_{\mathrm{Box}[\mathbf{l},\mathbf{u}]}(\mathbf{z}-\lambda^*\mathbf{a})$ $\quad \mathbf{a}^T P_{\mathrm{Box}[\mathbf{l},\mathbf{u}]}(\mathbf{z}) > b$ where $\lambda^* \in \Re$ satisfies $\mathbf{a}^T P_{\mathrm{Box}[\mathbf{l},\mathbf{u}]}(\mathbf{z}-\lambda^*\mathbf{a}) = b$ & $\lambda^* > 0$	$0 \ne \mathbf{a} \in \Re^n$ $b \in \Re$
$B_{\Vert\cdot\Vert_1}[0,\alpha]$	$\mathbf{z}$ $\quad \Vert z\Vert_1 \le \alpha$ $[\mathbf{z}-\lambda^*\mathbf{e}]_+ \odot sign(\mathbf{z})$ $\quad \Vert z\Vert_1 > \alpha$ where $\lambda^* > 0$, & $[\mathbf{z}-\lambda^*\mathbf{e}]_+ \odot sign(\mathbf{z}) = \alpha$	$\alpha > 0$

Computing the Projection Operator

- Note that the Projected gradient descent can be seen as optimizing the local quadratic expansion of f:

$$x_{k+1} = P_{\mathcal{C}}(\text{argmin}_y[f(x_k) + \nabla f(x_k)^T(y - x_k) + \frac{1}{2\alpha_k}||y - x_k||^2])$$
$$= P_{\mathcal{C}}(\text{argmin}_y||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

Computing the Projection Operator

- Note that the Projected gradient descent can be seen as optimizing the local quadratic expansion of f:

$$\begin{aligned} x_{k+1} &= P_{\mathcal{C}}(\text{argmin}_y[f(x_k) + \nabla f(x_k)^T(y - x_k) + \frac{1}{2\alpha_k}||y - x_k||^2]) \\ &= P_{\mathcal{C}}(\text{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2) \end{aligned}$$

- This involves optimizing a quadratic function over the constraints, which is easy for only a smaller class of constraints.

Computing the Projection Operator

- Note that the Projected gradient descent can be seen as optimizing the local quadratic expansion of f:

$$x_{k+1} = P_{\mathcal{C}}(\operatorname{argmin}_y [f(x_k) + \nabla f(x_k)^T (y - x_k) + \frac{1}{2\alpha_k} ||y - x_k||^2])$$
$$= P_{\mathcal{C}}(\operatorname{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- This involves optimizing a quadratic function over the constraints, which is easy for only a smaller class of constraints.
- For example, the Projection operator can only be computed for L_p norms with $p = 1, 2, \infty$ and not for other values of p.

Computing the Projection Operator

- Note that the Projected gradient descent can be seen as optimizing the local quadratic expansion of f:

$$x_{k+1} = P_{\mathcal{C}}(\text{argmin}_y[f(x_k) + \nabla f(x_k)^T(y - x_k) + \frac{1}{2\alpha_k}||y - x_k||^2])$$
$$= P_{\mathcal{C}}(\text{argmin}_y||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- This involves optimizing a quadratic function over the constraints, which is easy for only a smaller class of constraints.
- For example, the Projection operator can only be computed for L_p norms with $p = 1, 2, \infty$ and not for other values of p.
- Similarly, projection is not easy on Polyhedral constraints (like the submodular polyhedron, combinatorial constraints like paths, cuts, ...)

Pros and Cons of Projected Gradient Descent

- Projected Gradient Descent:

$$x_{k+1} = P_{\mathcal{C}}(\text{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

Pros and Cons of Projected Gradient Descent

- Projected Gradient Descent:

$$x_{k+1} = P_{\mathcal{C}}(\operatorname{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- Pros:

Pros and Cons of Projected Gradient Descent

- Projected Gradient Descent:

$$x_{k+1} = P_{\mathcal{C}}(\text{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- Pros:
  - Computing Projection operator easy in some cases: L2 Ball, convex cone, halfspaces, box, simplex

Pros and Cons of Projected Gradient Descent

- Projected Gradient Descent:

$$x_{k+1} = P_{\mathcal{C}}(\text{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- Pros:
  - Computing Projection operator easy in some cases: L2 Ball, convex cone, halfspaces, box, simplex
  - Enjoys the same convergence rates as the unconstrained case

Pros and Cons of Projected Gradient Descent

- Projected Gradient Descent:

$$x_{k+1} = P_{\mathcal{C}}(\text{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- Pros:
  - Computing Projection operator easy in some cases: L2 Ball, convex cone, halfspaces, box, simplex
  - Enjoys the same convergence rates as the unconstrained case
- Cons:

Pros and Cons of Projected Gradient Descent

- Projected Gradient Descent:

$$x_{k+1} = P_{\mathcal{C}}(\text{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- Pros:
  - Computing Projection operator easy in some cases: L2 Ball, convex cone, halfspaces, box, simplex
  - Enjoys the same convergence rates as the unconstrained case
- Cons:
  - For high dimensional problems, projection can be expensive: $O(n)$ for Simplex, $O(nm^2)$ for nuclear norms, and involves a QP for general polyhedrons

Pros and Cons of Projected Gradient Descent

- Projected Gradient Descent:

$$x_{k+1} = P_{\mathcal{C}}(\mathrm{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- Pros:
  - Computing Projection operator easy in some cases: L2 Ball, convex cone, halfspaces, box, simplex
  - Enjoys the same convergence rates as the unconstrained case
- Cons:
  - For high dimensional problems, projection can be expensive: $O(n)$ for Simplex, $O(nm^2)$ for nuclear norms, and involves a QP for general polyhedrons
  - Full Gradient Descent may destroy certain desirable structure like sparsity

Pros and Cons of Projected Gradient Descent

- Projected Gradient Descent:

$$x_{k+1} = P_{\mathcal{C}}(\text{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- Pros:
  - Computing Projection operator easy in some cases: L2 Ball, convex cone, halfspaces, box, simplex
  - Enjoys the same convergence rates as the unconstrained case
- Cons:
  - For high dimensional problems, projection can be expensive: $O(n)$ for Simplex, $O(nm^2)$ for nuclear norms, and involves a QP for general polyhedrons
  - Full Gradient Descent may destroy certain desirable structure like sparsity
- On the other hand, optimizing a linear function over constraints are much easier.

Pros and Cons of Projected Gradient Descent

- Projected Gradient Descent:

$$x_{k+1} = P_{\mathcal{C}}(\text{argmin}_y ||y - (x_k - \alpha_k \nabla f(x_k))||^2)$$

- Pros:
  - Computing Projection operator easy in some cases: L2 Ball, convex cone, halfspaces, box, simplex
  - Enjoys the same convergence rates as the unconstrained case
- Cons:
  - For high dimensional problems, projection can be expensive: $O(n)$ for Simplex, $O(nm^2)$ for nuclear norms, and involves a QP for general polyhedrons
  - Full Gradient Descent may destroy certain desirable structure like sparsity
- On the other hand, optimizing a linear function over constraints are much easier.
- Can we come up with an algorithm that only needs to optimize a linear function over constraints?

Conditional Gradient Descent

- Conditional Gradient Descent, also known as Frank Wolfe Method uses a local linear expansion of f:

$$s_k = \text{argmin}_{s \in \mathcal{C}} \nabla f(x_k)^T s \tag{1}$$

$$x_{k+1} = (1 - \gamma_k) x_k + \gamma_k s_k \tag{2}$$

Conditional Gradient Descent

- Conditional Gradient Descent, also known as Frank Wolfe Method uses a local linear expansion of f:

$$s_k = \text{argmin}_{s \in \mathcal{C}} \nabla f(x_k)^T s \tag{1}$$
$$x_{k+1} = (1 - \gamma_k) x_k + \gamma_k s_k \tag{2}$$

- Most critically, there is **no projection**! Just involves solving a linear program over $\mathcal{C}$

Conditional Gradient Descent

- Conditional Gradient Descent, also known as Frank Wolfe Method uses a local linear expansion of f:

$$s_k = \text{argmin}_{s \in \mathcal{C}} \nabla f(x_k)^T s \tag{1}$$
$$x_{k+1} = (1 - \gamma_k) x_k + \gamma_k s_k \tag{2}$$

- Most critically, there is **no projection**! Just involves solving a linear program over $\mathcal{C}$
- Default choice of step sizes is $\gamma_k = 2/(k+1), k = 1, 2, \cdots,$

Conditional Gradient Descent

- Conditional Gradient Descent, also known as Frank Wolfe Method uses a local linear expansion of f:

$$s_k = \text{argmin}_{s \in \mathcal{C}} \nabla f(x_k)^T s \quad (1)$$
$$x_{k+1} = (1 - \gamma_k) x_k + \gamma_k s_k \quad (2)$$

- Most critically, there is **no projection**! Just involves solving a linear program over $\mathcal{C}$
- Default choice of step sizes is $\gamma_k = 2/(k+1), k = 1, 2, \cdots,$
- Since $x_k, s_k \in \mathcal{C}$, it implies that $x_{k+1} \in \mathcal{C}$

Conditional Gradient Descent

- Conditional Gradient Descent, also known as Frank Wolfe Method uses a local linear expansion of f:

$$s_k = \text{argmin}_{s \in \mathcal{C}} \nabla f(x_k)^T s \quad (1)$$
$$x_{k+1} = (1 - \gamma_k) x_k + \gamma_k s_k \quad (2)$$

- Most critically, there is **no projection**! Just involves solving a linear program over $\mathcal{C}$
- Default choice of step sizes is $\gamma_k = 2/(k+1), k = 1, 2, \cdots,$
- Since $x_k, s_k \in \mathcal{C}$, it implies that $x_{k+1} \in \mathcal{C}$
- We are moving less and less in the direction of the linearization as the algorithm proceeds!

Example: Norm Constraints

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

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

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 $\|\cdot\|$

Aside Dual Norms

- Define $f(x) = ||x||$ as a norm
- The dual norm $||x||_*$ is defined as:

$$||x||_* = \max_{||z|| \leq 1} z^T x$$

- Examples: Consider p-norm
- The dual norm of a p-norm $f(x) = ||x||_p$ is a q-norm such that $1/p + 1/q = 1$
- Dual of the 1-norm is the ∞-norm, Dual of the 2-norm is itself!
- Also,

$$\partial||x||_* = \text{argmax}_{||Z|| \leq 1} z^T x$$

Example: L_1 Norm Constraints

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

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

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 Norm Constraints

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

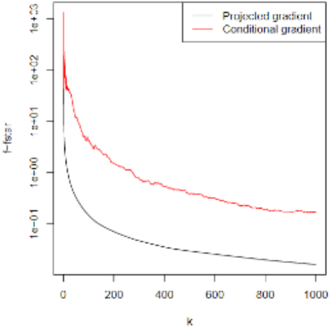
$$s_i^{(k-1)} = -\alpha \cdot \text{sign}\big(\nabla f_i(x^{(k-1)})\big) \cdot \big|\nabla f_i(x^{(k-1)})\big|^{p/q}, \quad i = 1, \ldots n$$

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 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)

Empirically: Projected vs Conditional Gradient Descent

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

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

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

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

Rearranged, this gives the duality gap above

Convergence Results

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 $f(x^{(k)}) - f^\star \le \epsilon$ is $O(1/\epsilon)$

Convergence Results

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 $M \leq \mathrm{diam}^2(C) \cdot L$, where

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

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

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

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

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

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

ALLAS

Step Size Variants

- Convergence analysis:
$$\gamma_k = 2/(k+1)$$
- Line Search:
$$\gamma_k = \text{argmin}_{\gamma \in [0,1]} f((1-\gamma)x_k + \gamma s_k)$$
(Can also be done using backtracking line search)
- Gap based:
$$\gamma_k = \min\left(\frac{f(x_k)}{L||s_k - x_k||^2}, 1\right)$$
(L is the Lipschitz constant of f)

Frank Wolfe Algorithm

$$
\begin{aligned}
&\textbf{Input} : \text{initial guess } \boldsymbol{x}_0, \text{ tolerance } \delta > 0 \\
&\textbf{For } t = 0, 1, \ldots \textbf{ do} && (2)\\
&\quad \boldsymbol{s}_t \in \arg\max_{\boldsymbol{s} \in \mathcal{D}} \langle -\nabla f(\boldsymbol{x}_t), \boldsymbol{s} \rangle && (3)\\
&\quad \boldsymbol{d}_t = \boldsymbol{s}_t - \boldsymbol{x}_t && (4)\\
&\quad g_t = -\langle \nabla f(\boldsymbol{x}_t), \boldsymbol{d}_t \rangle && (5)\\
&\quad \textbf{If } g_t < \delta : && (6)\\
&\qquad // \text{ exit if gap is below tolerance} \\
&\qquad \textbf{return } \boldsymbol{x}_t && (7)\\
&\quad \textbf{Variant 1} : \text{set step size as} \\
&\qquad \gamma_t = \min\left\{ \frac{g_t}{L\|\boldsymbol{d}_t\|^2}, 1 \right\} && (8)\\
&\quad \textbf{Variant 2} : \text{set step size by line search} \\
&\qquad \gamma_t = \arg\min_{\gamma \in [0,1]} f(\boldsymbol{x}_t + \gamma \boldsymbol{d}_t) && (9)\\
&\quad \boldsymbol{x}_{t+1} = \boldsymbol{x}_t + \gamma_t \boldsymbol{d}_t \ . && (10)\\
&\textbf{end For loop} && (11)\\
&\textbf{return } \boldsymbol{x}_t && (12)
\end{aligned}
$$

Convergence for Non Convex Objectives

- Define $g_k = \max_{s \in \mathcal{C}} \langle s - x_k, -\nabla f(x_k) \rangle$
- Then a point x_k is a stationary point for constrained optimization if and only if $g_k = 0$.
- Then (Simon Lacoste-Julien, 2017: Convergence rates of Frank Wolfe for Non-Convex Objectives) shoed that:

$$\min_{0 \leq i \leq t} g_i \leq \frac{\max(2h_0, L\text{diam}(\mathcal{C})^2)}{\sqrt{t+1}}$$

  where $h_0 = f(x_0) - \min_{x \in \mathcal{C}} f(x)$ is the initial global suboptimality.
- Similar result also holds for projected gradient descent.

More Results and Additional Reading

- Lower Bound: Conditional Gradient Analysis is tight. For any $x_0 \in \mathbb{R}^d$ and for $1 \leq k \leq d/2 - 1$, there exists a L smooth convex function and convex set $\mathcal{C}$ with diameter D s.t. for any algorithm of f that computes local gradients of f and does a linear minimization over $\mathcal{C}$, we have $f(x_k) - f_* \geq \frac{LD^2}{8(k+1)}, \forall k \geq 1$
- Additionally, Linear Convergence, i.e. $O(\log 1/\epsilon)$ can be shown under certain cases (domain is given by a polyhedron or optimum lies in the interior)

BS16 A. Beck and S. Shtern, "Linearly convergent away-step conditional gradient for non-strongly convex functions," Mathematical Programming, 1–27, 2016.

LJ15 S. Lacoste-Julien and M. Jaggi, "On the Global Linear Convergence of Frank-Wolfe Optimization Variants," NIPS, 2015.

Projected Gradient vs Conditional Gradient: Takeaways

- Projected Gradient Descent requires optimizing a quadratic function over the constraints

Projected Gradient vs Conditional Gradient: Takeaways

- Projected Gradient Descent requires optimizing a quadratic function over the constraints
- While it is easy for a few constraints, several common constraints do not admit easy projection operators

Projected Gradient vs Conditional Gradient: Takeaways

- Projected Gradient Descent requires optimizing a quadratic function over the constraints
- While it is easy for a few constraints, several common constraints do not admit easy projection operators
- Conditional Gradient Descent requires solving a linear program over constraints

Projected Gradient vs Conditional Gradient: Takeaways

- Projected Gradient Descent requires optimizing a quadratic function over the constraints
- While it is easy for a few constraints, several common constraints do not admit easy projection operators
- Conditional Gradient Descent requires solving a linear program over constraints
- This is easy for a large class of constraints (e.g. combinatorial constraints, polyhedral constraints etc.)

Projected Gradient vs Conditional Gradient: Takeaways

- Projected Gradient Descent requires optimizing a quadratic function over the constraints
- While it is easy for a few constraints, several common constraints do not admit easy projection operators
- Conditional Gradient Descent requires solving a linear program over constraints
- This is easy for a large class of constraints (e.g. combinatorial constraints, polyhedral constraints etc.)
- In contrast, conditional gradient can be slower in terms of convergence

Projected Gradient vs Conditional Gradient: Takeaways

- Projected Gradient Descent requires optimizing a quadratic function over the constraints
- While it is easy for a few constraints, several common constraints do not admit easy projection operators
- Conditional Gradient Descent requires solving a linear program over constraints
- This is easy for a large class of constraints (e.g. combinatorial constraints, polyhedral constraints etc.)
- In contrast, conditional gradient can be slower in terms of convergence
- Takeaways: If projection is easy, use projected gradient descent. Else, conditional gradient is the go to algorithm!