CS794/CO673: Optimization for Data Science

Lec 06: Conditional Gradient

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Problem

Constrained smooth minimization:

$$f_\star = \inf_{\mathbf{w} \in C} \; f(\mathbf{w})$$

- f: smooth and possibly nonconvex
- C: (closed) bounded and convex
- Minimizer may or may not be attained
- Maximization is just negation
- Projection P_C is expensive to compute

Alice	1			4		
Bob		2	5			
Carol			4	5		
Dave	5				4	
⋮						

Matrix Completion

$$\min_{X:\mathrm{rank}(X)\le k} \sum_{(i,j)\in\mathcal{O}} (A_{ij} - X_{ij})^2,$$

- rank is nonconvex (in fact, discrete valued)

$$\min_{X:\|X\|_{\mathrm{tr}}\le\lambda} \sum_{(i,j)\in\mathcal{O}} (A_{ij} - X_{ij})^2,$$

- $\|\cdot\|_{\mathrm{tr}}$: trace norm, sum of singular values
- Let $X = U\Sigma V^\top$ be its singular value decomposion. Then,

$$\mathrm{P}_{\|\cdot\|_{\mathrm{tr}}}(X) = U\,\mathrm{diag}(\boldsymbol{\gamma})V^\top, \quad \text{where} \quad \boldsymbol{\gamma} = \mathrm{P}_{\|\cdot\|_1}(\boldsymbol{\sigma})$$

- Expensive operation: $O(nm^2)$

Sparsity

$$\min_{\mathbf{w}} \underbrace{\frac{1}{n}\|\mathbf{wX} - \mathbf{y}\|_2^2}_{\ell} + \underbrace{\lambda \cdot \|\mathbf{w}\|_0}_{r}$$

- Balancing square error with sparsity
- ℓ is convex and L-smooth, r is nonsmooth and nonconvex

$$\min_{\mathbf{w}} \underbrace{\frac{1}{n}\|\mathbf{wX} - \mathbf{y}\|_2^2}_{\ell} + \underbrace{\lambda \cdot \|\mathbf{w}\|_1}_{r}$$

- Convex relaxation: r is now convex but remains nonsmooth (crucial)

R. Tibshirani (1996). "Regression Shrinkage and Selection via the Lasso". *Journal of the Royal Statistical Society: Series B*, vol. 58, no. 1, pp. 267–288.

Indicator and Support

Recall that the indicator function of a set C is:

$$\iota_C(\mathbf{w}) = \begin{cases} 0, & \text{if } \mathbf{w} \in C \\ \infty, & \text{otherwise} \end{cases}$$

The support function of a set C is:

$$\sigma_C(\mathbf{w}^*) = \max_{\mathbf{w} \in C} \langle \mathbf{w}, \mathbf{w}^* \rangle = \max_{\mathbf{w}} \langle \mathbf{w}, \mathbf{w}^* \rangle - \iota_C(\mathbf{w})$$

- Always (closed) convex and positive homogeneous
- Any norm is a support function of the unit ball of its dual
- The subdifferential $\partial \sigma_C$ will play a crucial role

From Linear to Quadratic

- Suppose we have an algorithm to solve a linear program:

$$\min_{\mathbf{w} \geq \mathbf{0}} \langle \mathbf{w}, \mathbf{c} \rangle \quad \text{s.t.} \quad A\mathbf{w} = \mathbf{b}$$

- How do we solve a quadratic program?

$$\min_{\mathbf{w} \geq \mathbf{0}} \langle \mathbf{w}, A\mathbf{w} \rangle + \langle \mathbf{w}, \mathbf{c} \rangle \quad \text{s.t.} \quad A\mathbf{w} = \mathbf{b}$$

- The power of reduction: try to reduce quadratic to linear!

Algorithm 1: Conditional gradient (condgrad)

Input: $\mathbf{w}_0 \in C$

1 **for** $t = 0, 1, \ldots$ **do**

2 $\quad \mathbf{z}_t \leftarrow \operatorname*{argmax}_{\mathbf{z} \in C} \langle \mathbf{z}; -\nabla f(\mathbf{w}_t) \rangle$ // polar operator

3 $\quad$ choose step size $\eta_t \in [0, 1]$

4 $\quad \mathbf{w}_{t+1} \leftarrow (1 - \eta_t)\mathbf{w}_t + \eta_t \mathbf{z}_t$ // convex combination

- The only nontrivial step in Line 2 has a linear objective
- It is in fact $\partial \sigma_C(-\mathbf{g})$ where $\mathbf{g} = \nabla f(\mathbf{w}_t)$
- We find a point in C that "correlates" the most with $-\nabla f(\mathbf{w}_t)$
- No projection to C needed: Line 4 remains in C

M. Frank and P. Wolfe (1956). "An Algorithm for Quadratic Programming". *Naval Research Logistics Quarterly*, vol. 3, no. 1-2, pp. 95–110; V. F. Dem'yanov and A. M. Rubinov (1967). "The Minimization of a Smooth Convex Functional on a Convex Set". *SIAM Journal on Control*, vol. 5, no. 2, pp. 280–294. [English translation of paper in *Vestnik Leningradskogo Universitera, Seriya Matematiki, Mekhaniki i Astronomii* vol. 19, pp. 7–17, 1964].

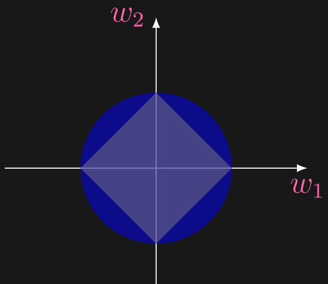
Definition: Extreme point

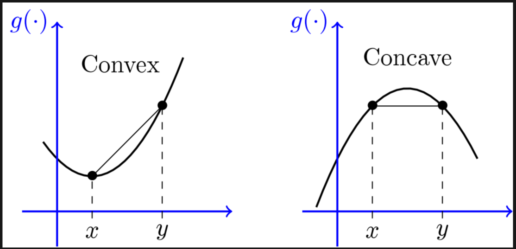
$\mathbf{w} \in C$ is an extreme point (of C) if it does not lie on the line segment of any two points in C. In other words, if $\mathbf{w} \in [\mathbf{w}_1, \mathbf{w}_2], \mathbf{w}_1, \mathbf{w}_2 \in C$ then $\mathbf{w} = \mathbf{w}_1 = \mathbf{w}_2$.

- For a convex set C, $\mathbf{w} \in C$ is an extreme point iff $C \setminus \{\mathbf{w}\}$ remains convex.

Theorem: Convex maximizer is at the boundary

The maximizer of a convex f over C can always be chosen from the extreme points.

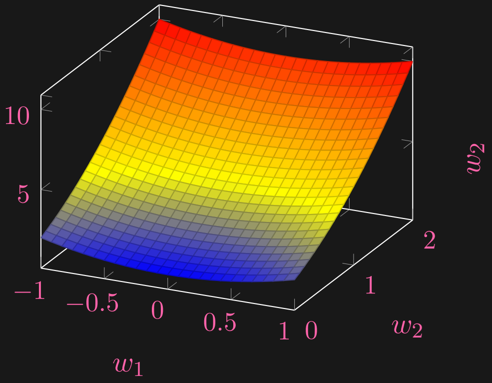


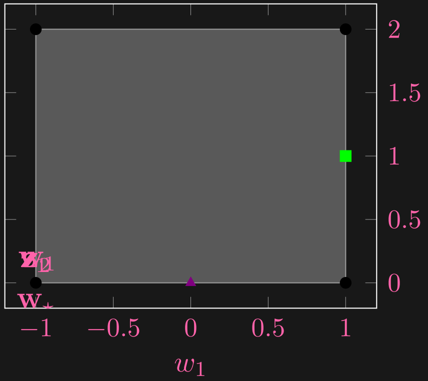


Consider the following simple problem:

$$\min_{\mathbf{w}\in C} \; w_1^2 + (w_2+1)^2 \quad \text{and} \quad C := \{\mathbf{w} : w_1 \in [-1,1], w_2 \in [0,2]\}.$$

The global minimizer is clearly at $\mathbf{w}_\star = (0,0)$, as shown below.





Let us see how the conditional gradient works on this toy problem:

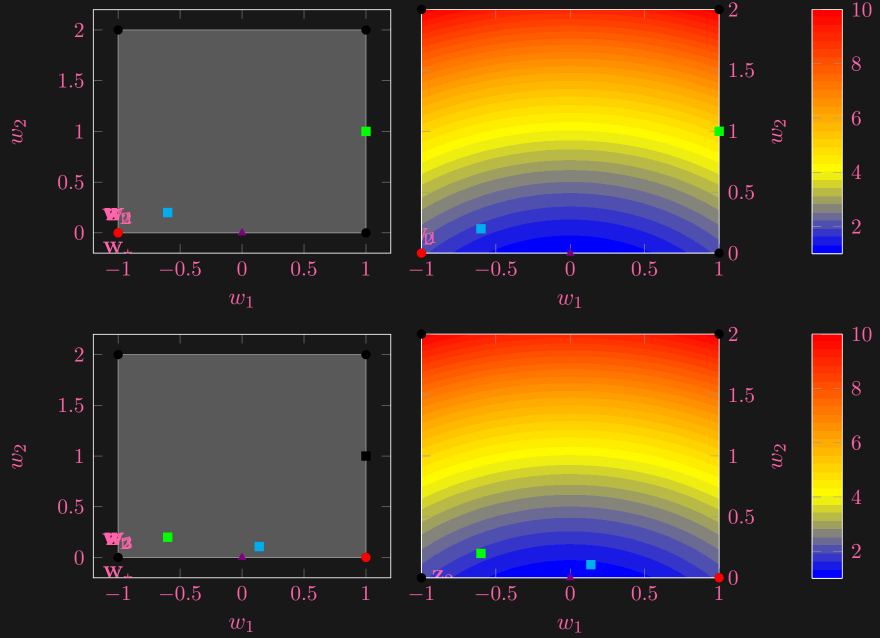
- We first identify the four extreme points of C as

$$\mathbf{z}_1 = (-1, 0), \quad \mathbf{z}_2 = (1, 0), \quad \mathbf{z}_3 = (1, 2), \quad \mathbf{z}_4 = (-1, 2).$$

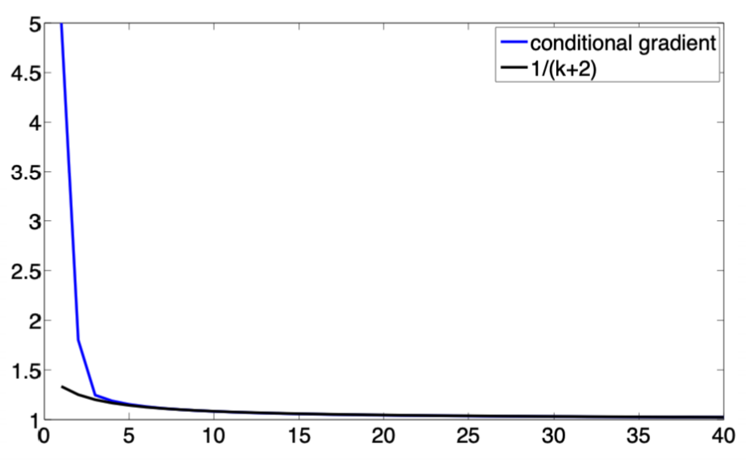
- Start with say $\mathbf{w}_1 = (1, 1)$, we compute the gradient $\nabla f(\mathbf{w}_1) = (2, 4)$.
- We pick the extreme point $\mathbf{z}$ that maximizes $\langle \mathbf{z}; -\nabla f(\mathbf{w}_1) \rangle$. Clearly, $\mathbf{z}_1$ wins.
- Next, we find $\eta > 0$ to minimize $f((1-\eta)\mathbf{w}_1 + \eta \mathbf{z}_1)$ by setting its derivative w.r.t. η to 0 :

$$\eta_1 = \eta = \frac{\langle \mathbf{w} + (0, 1), \mathbf{w} - \mathbf{z} \rangle}{\|\mathbf{w} - \mathbf{z}\|_2^2} = \frac{4}{5}.$$

- Lastly, we compute $\mathbf{w}_2 = (1 - \eta_1)\mathbf{w}_1 + \eta_1 \mathbf{z}_1 = (-\frac{3}{5}, \frac{1}{5})$, and the process repeats.


w_1
w_2
−1 −0.5 0 0.5 1
0 0.5 1 1.5 2
2 4 6 8 10

Convergence rate closely follows $\Theta(1/t)$, while projected gradient converges in 2 iterations on this example!



Sparsity

Let $C := \{\mathbf{w} : \|\mathbf{w}\|_1 \leq \lambda\}$, whose polar operator reduces to

$$\mathbf{z}_t = \operatorname*{argmax}_{\|\mathbf{z}\|_1 \leq \lambda} \langle \mathbf{z}; -\nabla f(\mathbf{w}_t) \rangle \ni -\lambda \mathbf{e}_i, \quad \text{where} \quad \langle \mathbf{e}_i; \nabla_i f(\mathbf{w}_t) \rangle = \max_j |\nabla_j f(\mathbf{w}_t)|.$$

- May choose $\mathbf{e}_i$ to be the i-th standard basis (i.e. 1 at the i-th entry and 0 elsewhere)
- After t steps, the iterate $\mathbf{w}_t$ has (added) at most t nonzeros! In comparison, after even a single iteration, projected gradient can result in a fully dense iterate!
- The resulting coordinate-wise update is a bit wasteful though: we compute the entire gradient ∇f only to find its minimum index and throw out everything else...

Sparsity in Rank

- For the matrix setting:

$$Z_t = \underset{\|Z\|_{\mathrm{tr}} \le \lambda}{\operatorname{argmax}} \; \langle Z; -\nabla f(W_t) \rangle = -\lambda \mathbf{u}\mathbf{v}^\top, \quad \text{where} \quad \mathbf{u}^\top \nabla f(W_t) \mathbf{v} = \|\nabla f(W_t)\|_{\mathrm{sp}}$$

- After t steps, the iterate W_t has (added) rank at most t
- Computing the spectral norm, i.e. the largest singular value, costs $O(mn)$, an order of magnitude cheaper than projection
- Same for tensors

Theorem: convergence of conditional gradient

Suppose f is convex and L-smooth, and C is compact convex with bounded diameter ρ. Then, conditional gradient satisfies:

$$f(\mathbf{w}_{t+1}) \le f(\mathbf{w}) + \pi_t(1-\eta_0)(f(\mathbf{w}_0) - f(\mathbf{w})) + \frac{\mathsf{L}\rho^2}{2}\sum_{s=0}^{t}\frac{\pi_t}{\pi_s}\eta_s^2,$$

where $\pi_t := \prod_{s=1}^{t}(1-\eta_s)$ with $\pi_0 := 1$.

- Setting $\eta_t = \frac{2}{t+2}$, we have $\eta_0 = 1$, $\pi_t = \frac{2}{(t+1)(t+2)}$ and

$$f(\mathbf{w}_t) - f(\mathbf{w}) \le \langle \mathbf{w}_t - \mathbf{z}_t; \nabla f(\mathbf{w}_t)\rangle \le \frac{2\mathsf{L}\rho^2}{t+3},$$

where the initializer $\mathbf{w}_0$, surprisingly, does not play any role.

The Proof

$$
\begin{aligned}
f(\mathbf{w}_{t+1}) - f(\mathbf{w}) &= f((1-\eta_t)\mathbf{w}_t + \eta_t \mathbf{z}_t) - f(\mathbf{w}) \\
\text{(L-smoothness)} \quad &\leq f(\mathbf{w}_t) - f(\mathbf{w}) + \eta_t \langle \mathbf{z}_t - \mathbf{w}_t; \nabla f(\mathbf{w}_t) \rangle + \frac{\eta_t^2}{2} \mathsf{L} \underbrace{\|\mathbf{w}_t - \mathbf{z}_t\|^2}_{\leq \rho^2} \\
\text{(optimality of } \mathbf{z}_t\text{)} \quad &\leq f(\mathbf{w}_t) - f(\mathbf{w}) + \eta_t \langle \mathbf{w} - \mathbf{w}_t; \nabla f(\mathbf{w}_t) \rangle + \frac{\eta_t^2}{2} \mathsf{L} \rho^2 \\
\text{(convexity of } f\text{)} \quad &\leq (1-\eta_t)(f(\mathbf{w}_t) - f(\mathbf{w})) + \frac{\eta_t^2}{2} \mathsf{L} \rho^2
\end{aligned}
$$

Telescoping and collecting the terms we arrive at the claim

Disccussions

- The rate $O(\frac{1}{t})$ is tight and cannot be improved (disappointing)
- Polar operator can be solved approximately
  - additive error: $\langle \mathbf{z}_t, -\mathbf{g}_t \rangle \leq \max_{\mathbf{w} \in C} \langle \mathbf{w}, -\mathbf{g}_t \rangle - \epsilon_t$
  - multiplicative error: $\langle \mathbf{z}_t, -\mathbf{g}_t \rangle \leq \frac{1}{\alpha_t} \cdot \max_{\mathbf{w} \in C} \langle \mathbf{w}, -\mathbf{g}_t \rangle$
- Choices of the step size η_t
  - Open-loop rule: $\eta_t = \frac{2}{t+2}$, or more generally $\eta_t = \Theta(1/t)$.
  - Cauchy's rule: $\eta_t \in \operatorname*{argmin}_{0 \leq \eta \leq 1} f((1-\eta)\mathbf{w}_t + \eta \mathbf{z}_t)$.
  - Quadratic rule:

    $$\eta_t = \operatorname*{argmin}_{0 \leq \eta \leq 1} f(\mathbf{w}_t) + \eta_t \langle \mathbf{z}_t - \mathbf{w}_t; \nabla f(\mathbf{w}_t) \rangle + \frac{\mathsf{L}^2 \eta_t^2 \|\mathbf{w}_t - \mathbf{z}_t\|^2}{2} = \left[\frac{\langle \mathbf{w}_t - \mathbf{z}_t; \nabla f(\mathbf{w}_t) \rangle}{\mathsf{L}^2 \|\mathbf{w}_t - \mathbf{z}_t\|^2} \right]_0^1.$$
- Possible to accelerate

Extension to Composite

$$\min_{\mathbf{w}} \; f(\mathbf{w}), \quad \text{where} \quad \ell(\mathbf{w}) + r(\mathbf{w})$$

Algorithm 2: Generalized conditional gradient (GCG)

Input: $\mathbf{w}_0 \in C$, functions ℓ and r

for $t = 0, 1, \ldots$ **do**

- $\mathbf{z}_t \leftarrow \operatorname*{argmin}_{\mathbf{z}} \langle \mathbf{z}; \nabla \ell(\mathbf{w}_t) \rangle + r(\mathbf{w})$ `// conjugate of r`
- choose step size $\eta_t \in [0, 1]$
- $\mathbf{w}_{t+1} \leftarrow (1 - \eta_t)\mathbf{w}_t + \eta_t \mathbf{z}_t$ `// convex combination`

T. Bonesky et al. (2007). "A Generalized Conditional Gradient Method for Nonlinear Operator Equations with Sparsity Constraints". *Inverse Problems*, vol. 23, no. 5, pp. 2041–2058; K. Bredies et al. (2009). "A Generalized Conditional Gradient Method and its Connection to an Iterative Shrinkage Method". *Computational Optimization and Applications*, vol. 42, pp. 173–193; Y. Yu et al. (2017). "Generalized Conditional Gradient for Structured Sparse Estimation". *Journal of Machine Learning Research*, vol. 18, pp. 1–46.

Totally Corrective

- Inspecting the conditional gradient algorithm we realize that

$$\mathbf{w}_{t+1} \in \operatorname{conv}\{\mathbf{w}_0, \mathbf{z}_1, \ldots, \mathbf{z}_t\},$$

  where the extreme points $\mathbf{z}_k$ are repeatedly identified and averaged.

- One immediate, natural idea is to replace the next iterate $\mathbf{w}_{t+1}$ as the best approximation in the entire convex hull:

$$\mathbf{w}_{t+1} = \operatorname*{argmin}_{\mathbf{w} \in \operatorname{conv}\{\mathbf{w}_0, \mathbf{z}_1, \ldots, \mathbf{z}_t\}} f(\mathbf{w}).$$

- Potentially much faster, but more expensive in each step
- Can restrict memory size, even to 2

G. Meyer (1974). "Accelerated Frank–Wolfe Algorithms". *SIAM Journal on Control*, vol. 12, no. 4, pp. 655–655; C. A. Holloway (1974). "An extension of the Frank and Wolfe method of feasible directions". *Mathematical Programming*, vol. 6, pp. 14–27.