

Chapter 5: First order methods

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Statistics and optimization in high dimensions
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$\mathbb{X} \in \mathbb{R}^{n \times d}$, $Y \in \mathbb{R}^n$ (random).

$$\hat{\theta} \in \arg \min_{\theta \in \mathbb{R}^d} \|\mathbb{X}\theta - Y\|_2^2$$

$$\hat{\theta} \in \arg \min_{\theta \in \mathbb{R}^d} \|\mathbb{X}\theta - Y\|_2^2, \quad \text{s.t.} \quad \|\theta\|_1 \leq 1$$

$$\hat{\theta} \in \arg \min_{\theta \in \mathbb{R}^d} \|\mathbb{X}\theta - Y\|_2^2, \quad \text{s.t.} \quad \|\theta\|_0 \leq k$$

$$\hat{\theta} \in \arg \min_{\theta \in \mathbb{R}^d} \|\mathbb{X}\theta - Y\|_2^2 + \lambda \|\theta\|_0$$

$$\hat{\theta} \in \arg \min_{\theta \in \mathbb{R}^d} \|\mathbb{X}\theta - Y\|_2^2 + \lambda \|\theta\|_1$$

$$\hat{\theta} \in \arg \min_{\theta \in \mathbb{R}^d} \|\theta\|_1, \quad \text{s.t.} \quad \mathbb{X}\theta = Y.$$

- The first one can be computed in $O(n^2d)$ operations.
- How about the other ones?
- How to deal with large values of n and d .

- $\|\cdot\|_0$: hard to handle computationally.
- ℓ_1 norm estimators are solutions to conic programs.
- General purpose solvers (interior point methods).
- Iterative methods: at least d^3 per iteration.

Plan for today: if one cannot afford d^3 . Introduction to first order methods and nonsmooth analysis.

- Analysis of gradient descent algorithm.
- Introduction to the notion of subgradient.
- Algorithm for nonsmooth optimization: subgradient and proximal gradient.
- Acceleration.

Sources are diverse, see the lecture notes.

Plan

1. Gradient descent algorithm
2. Nonsmooth analysis
3. Subgradient descent
4. Composite optimization
5. Lower bounds and acceleration

Proposition

Let $f: \mathbb{R}^p \mapsto \mathbb{R}$ be twice differentiable with compact sublevel sets. Consider the differential equation, for $x_0 \in \mathbb{R}^p$,

$$\dot{x}(t) = -\nabla f(x(t)) \quad (1)$$

$$x(0) = x_0. \quad (2)$$

Then, there exists a solution to the initial value problem defined for all $t > 0$.

- $\int_0^{+\infty} \|\nabla f(x(t))\|_2^2 dt < +\infty$ and $\lim_{t \rightarrow \infty} \|\nabla f(x(t))\| = 0$.
- Any accumulation point \bar{x} of the trajectory satisfies $\nabla f(\bar{x}) = 0$.
- If in addition f is convex, set $f^* = \inf_{x \in \mathbb{R}^p} f(x)$ and assume that it is attained at x^* , we have for any $t \in \mathbb{R}$, $t > 0$,

$$f(x(t)) - f^* \leq \frac{\|x_0 - x^*\|_2^2}{2t}.$$

And $x(t) \xrightarrow[t \rightarrow \infty]{} \bar{x}$ where \bar{x} is a global minimizer of f .

Gradient algorithm: $f: \mathbb{R}^p \mapsto \mathbb{R}$, iteration cost of the order of p .

$$x_{k+1} = x_k - s_k \nabla f(x_k) \quad (3)$$

Lemma

Let $f: \mathbb{R}^p \mapsto \mathbb{R}$ be continuously differentiable with L -Lipschitz gradient ($L > 0$), then for any $x, y \in \mathbb{R}^p$,

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \leq \frac{L}{2} \|y - x\|_2^2.$$

Proposition

Let $f: \mathbb{R}^p \mapsto \mathbb{R}$ be continuously differentiable with L -Lipschitz gradient and such that $\inf_{x \in \mathbb{R}^p} f(x) > -\infty$. Consider the algorithm, for $x_0 \in \mathbb{R}^p$ and

$$x_{k+1} = x_k - \frac{1}{L} \nabla f(x_k). \quad (4)$$

Then

- $\lim_{k \rightarrow \infty} \|\nabla f(x_k)\| = 0$, (any accumulation point \bar{x} of the trajectory satisfies $\nabla f(\bar{x}) = 0$).
- If in addition f is convex, set $f^* = \inf_{x \in \mathbb{R}^p} f(x)$ and assume that it is attained at x^* , we have for any $k \in \mathbb{N}$, $k > 0$,

$$f(x_k) - f^* \leq \frac{L \|x_0 - x^*\|_2^2}{2k}.$$

Furthermore x_k converges to \bar{x} a global minimum of f

- If in addition f is μ -strongly convex, then we have for any $k \in \mathbb{N}$

$$f(x_{k+1}) - f^* \leq \left(1 - \frac{\mu}{L}\right) (f(x_k) - f^*).$$

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How to deal with ℓ_1 norm penalty? We need a generalization of the notion of gradient.

Lower semicontinuity: f denotes a lower semi-continuous convex function on \mathbb{R}^p . Lower semi-continuity: epigraph is closed:

$$\text{epi}_f = \left\{ (x, z) \in \mathbb{R}^{p+1}, z \geq f(x) \right\}.$$

equivalently as for any $x \in \mathbb{R}^p$

$$\liminf_{y \rightarrow x} f(y) \geq f(x).$$

Domain: f is allowed to take value $+\infty$, we denote its domain by

$$\text{dom}_f = \{x \in \mathbb{R}^p, f(x) < +\infty\},$$

which is a convex set.

For example:

$$\min_{\|\theta\|_1 \leq 1} \|\mathbb{X}\theta - y\|_2^2 = \min_{\theta \in \mathbb{R}^d} \|\mathbb{X}\theta - y\|_2^2 + \delta(x)$$

where $\delta(\theta) = 0$ if $\|\theta\|_1 \leq 1$, and $+\infty$ otherwise (indicator of the ℓ_1 unit ball).

Show that a convex function is continuous on the interior of its domain.

Definition

For any $x \in \text{dom}_f$, the subgradient of f denotes the set

$$\partial f(x) = \{v \in \mathbb{R}^p, f(y) \geq f(x) + \langle v, y - x \rangle, \forall y \in \mathbb{R}^p\}.$$

For $x \notin \text{dom}_f$, $\partial f(x)$ is set to be empty.

We deduce from the definition the generalization of Fermat rule

Theorem

$x^* \in \arg \min_x f(x)$ if and only if $0 \in \partial f(x^*)$.

Exercise, indicator: Let C be compact convex and $\delta(x) = 0$ for $x \in C$ and $+\infty$ otherwise. Describe $\partial \delta$.

Proposition

For any $x \in \mathbb{R}^p$, $\partial f(x)$ is a closed convex set. Furthermore, at any $x \in \text{int}(\text{dom}_f)$, $\partial f(x)$ is non empty and bounded.

Exercise, sequential closedness: Let $f: \mathbb{R}^p \mapsto \mathbb{R}$ be a convex function, show that ∂f is sequentially closed in the sense that, for any \bar{x}

$$\{v \in \mathbb{R}^p, \exists (x_k, v_k)_{k \in \mathbb{N}}, x_k \rightarrow \bar{x}, v_k \rightarrow v, v_k \in \partial f(x_k), f(x_k) \rightarrow f(\bar{x})\} \subset \partial f(\bar{x})$$

Exercise, lipschitzness: Let $f: \mathbb{R}^p \mapsto \mathbb{R}$, show that f is L -Lipschitz if and only if $\sup_{x \in \mathbb{R}^p, v \in \partial f(x)} \|v\|_2 \leq L$.

Exercise, sum rule: Let f and g be convex. Show that $\partial(f+g)(x) \supset \partial f(x) + \partial g(x)$ for every x such that $\partial f(x)$ and $\partial g(x)$ are non empty. What do you think about the reverse inclusion?

Theorem

Let f be convex and lower semicontinuous and finite at least at one point, then f is the supremum of all its affine minorants: for any $x \in \mathbb{R}^p$

$$f(x) = \sup_{r \in \mathbb{R}, v \in \mathbb{R}^p} r + v^T x \quad \text{s.t.} \quad f(y) \geq r + v^T y, \forall y \in \mathbb{R}^p.$$

Theorem

For any $x \in \text{int}(\text{dom}_f)$ and any $h \in \mathbb{R}^p$,

$$D_h f(x) = \sup_{v \in \partial f(x)} \langle v, h \rangle,$$

where D_h denotes the directional derivative of f ,

$$D_h f(x) = \lim_{t > 0, t \rightarrow 0} \frac{f(x + th) - f(x)}{t}.$$

Consequence: if f is differentiable at \bar{x} then $\partial f(\bar{x}) = \{\nabla f(\bar{x})\}$

Definition

Given f convex, the Fenchel-Legendre transform of f is given as follows

$$f^* : z \mapsto \sup_{y \in \mathbb{R}^p} z^T y - f(y)$$

Theorem

For any f convex, f^* is convex and for any $x, z \in \mathbb{R}^p$

$$f(x) + f^*(z) \geq z^T x$$

and the preceding inequality holds if and only if $z \in \partial f(x)$. This is called Fenchel-Young's inequality. Furthermore, f is lower semicontinuous if and only if $(f^*)^* = f$.

Set $f: x \mapsto \|x\|_1$. Compute f^* and the subgradient of f .

Plan

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Proposition

Let $f: \mathbb{R}^p \mapsto \mathbb{R}$ be a convex function which attains its infimum and has full domain. Consider the algorithm, for $x_0 \in \mathbb{R}^p$, a sequence of positive numbers $\alpha_k > 0$, $k \in \mathbb{N}$, iterate

$$x_{k+1} = x_k - \alpha_k v_k \tag{5}$$

$$v_k \in \partial f(x_k). \tag{6}$$

Then for any global minimizer x^* , setting, $y_k = \sum_{i=0}^k \alpha_i x_i / \left(\sum_{i=0}^k \alpha_i \right)$

$$\min_{i=1, \dots, k} f(x_k) - f^* \leq \frac{\|x_0 - x^*\|^2 + \sum_{i=0}^k \alpha_i^2 \|v_i\|_2^2}{2 \sum_{i=0}^k \alpha_i}$$

$$f(y_k) - f^* \leq \frac{\|x_0 - x^*\|^2 + \sum_{i=0}^k \alpha_i^2 \|v_i\|_2^2}{2 \sum_{i=0}^k \alpha_i}.$$

Corollary

If f is L -Lipschitz, we have the following convergence result for subgradient method.

- If $\alpha_k = \alpha$ is constant, we have

$$\min_{i=1, \dots, k} f(x_k) - f^* \leq \frac{\|x_0 - x^*\|^2}{2(k+1)\alpha} + \frac{L^2\alpha}{2}.$$

- In particular, choosing $\alpha_i = \frac{\|x_0 - x^*\|/L}{\sqrt{k+1}}$, we have

$$\min_{i=1, \dots, k} f(x_k) - f^* \leq \frac{\|x_0 - x^*\|L}{\sqrt{k+1}}.$$

- Choosing $\alpha_k = \|x_0 - x^*\|/(L\sqrt{k})$ for all k , we obtain for all k

$$\min_{i=1, \dots, k} f(x_k) - f^* = O\left(\frac{\|x_0 - x^*\|_2 L(1 + \log(k))}{\sqrt{k}}\right).$$

- Very generic, applies to any convex function (all purpose tool).
- Requires computing subgradient (interior of the domain).
- The convergence rate is optimal among all Lipschitz function.
- Hard to tune (decreasing step size).
- Quite slow in practice.

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Lasso estimator

$$\hat{\theta}^{\ell_1} \in \arg \min_{\theta \in \mathbb{R}^d} \frac{1}{2n} \|\mathbb{X}\theta - Y\|^2 + \lambda \|\theta\|_1.$$

Composite structure: “Smooth + non smooth”

$$F = f + g$$

where f is smooth and g is convex, non smooth.

This additional structure can be leveraged. This model includes constrained optimization problems.

Definition

Given a closed convex function, $g: \mathbb{R}^d \mapsto \mathbb{R}$, the proximity operator of g is defined as follows

$$\text{prox}_g: z \mapsto \arg \min_{y \in \mathbb{R}^d} g(y) + \frac{1}{2} \|y - z\|_2^2.$$

By strong convexity, the minimum is attained and is strict.

Note that we have $x = \text{prox}_g(z)$ if and only if $z = \partial g(x) + x$ and the proximity operator is sometimes denoted $(\partial g + I)^{-1}$.

Indicator: Let C be compact convex and $\delta(x) = 0$ for $x \in C$ and $+\infty$ otherwise. What is prox_δ ?

$$\min_{x \in \mathbb{R}^p} f(x) + g(x)$$

Lemma

Let $f: \mathbb{R}^p \mapsto \mathbb{R}$ be convex continuously differentiable with L -Lipschitz gradient and g be convex lower semicontinuous. Fix any $x \in \mathbb{R}^p$ and set

$$y = \text{prox}_{g/L} \left(x - \frac{1}{L} \nabla f(x) \right).$$

Then, for any $z \in \mathbb{R}^d$,

$$f(z) + g(z) + \frac{L}{2} \|x - z\|_2^2 \geq f(y) + g(y) + \frac{L}{2} \|y - z\|_2^2.$$

$$\min_{x \in \mathbb{R}^p} f(x) + g(x)$$

Proposition

Let $f: \mathbb{R}^p \mapsto \mathbb{R}$ be convex continuously differentiable with L -Lipschitz gradient and g be convex lower semicontinuous such that $\rho = \inf_{x \in \mathbb{R}^p} f(x) + g(x) > -\infty$ is attained at x^* . Consider the algorithm, for $x_0 \in \mathbb{R}^p$ and

$$x_{k+1} = \text{prox}_{g/L} \left(x_k - \frac{1}{L} \nabla f(x_k) \right). \quad (7)$$

Then x_k converges to a global minimum and we have for any $k \in \mathbb{N}$, $k > 0$,

$$f(x_k) + g(x_k) - \rho \leq \frac{L \|x_0 - x^*\|_2^2}{2k}.$$

If in addition $f + g$ is μ -strongly convex, we have in addition

$$\|x_{k+1} - x^*\|_2^2 \leq \frac{L}{L + \mu} \|x_k - x^*\|_2^2.$$

- More efficient way to handle nonsmooth convex functions.
- Easier to implement.
- Faster in practice (similar as gradient descent).
- Require to compute prox operators (not always possible).

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$O(1/k)$ convergence rate?

Can we do better? What is the limit?

Definition

A first order method to minimize a smooth convex function f when initiated at $x_1 = 0$, produces a sequence of points $(x_i)_{i \in \mathbb{N}}$ such that for any $k \in \mathbb{N}$,

$$x_{k+1} \in \text{span}(\nabla f(x_0), \dots, \nabla f(x_k)).$$

Theorem

Let $k \leq (d - 1)/2$, $L > 0$. There exists a convex function f with L -Lipschitz gradient over \mathbb{R}^d , such that for any first order method satisfying definition (11),

$$\min_{1 \leq s \leq k} f(x_s) - f(x^*) \geq \frac{3L}{32} \frac{\|x_0 - x^*\|^2}{(k + 1)^2}.$$

For $h : \mathbb{R}^d \rightarrow \mathbb{R}$ we denote $h^* = \inf_{x \in \mathbb{R}^d} h(x)$.

For $k \leq d$ let $A_k \in \mathbb{R}^{d \times d}$ be the symmetric and tridiagonal matrix defined by

$$(A_k)_{i,j} = \begin{cases} 2, & i = j, i \leq k \\ -1, & j \in \{i-1, i+1\}, i \leq k, j \neq k+1 \\ 0, & \text{otherwise.} \end{cases}$$

We verify that $0 \preceq A_k \preceq 4I$ since for any $x \in \mathbb{R}^d$,

$$\begin{aligned} x^T A_k x &= 2 \sum_{i=1}^k x(i)^2 - 2 \sum_{i=1}^{k-1} x(i)x(i+1) = x(1)^2 + x(k)^2 + \sum_{i=1}^{k-1} (x(i) - x(i+1))^2 \\ &\leq 4 \sum_{i=1}^k x(i)^2 \geq 0 \end{aligned}$$

Lower bound: proof (from Bubeck's book)

$$A_k = \left(\begin{array}{cccccc} 2 & -1 & 0 & & & \\ -1 & 2 & -1 & & 0 & \\ & \dots & & & \dots & \\ & 0 & & -1 & 2 & -1 \\ & & & 0 & -1 & 2 \\ & & & & & & 0_{d-k,k} & & & & 0_{d-k,d-k} \end{array} \right) \begin{array}{l} \\ \\ \\ k \text{ lines} \\ \\ \\ \end{array}$$

We consider now the following convex function:

$$f(x) = \frac{L}{8} x^\top A_{2k+1} x - \frac{L}{4} x^\top e_1.$$

For any $s = 1, \dots, k$, x_s must lie in the linear span of e_1, \dots, e_{s-1} (assumption). In particular for $s \leq k$, $x_s(i) = 0$ for $i = s, \dots, d$, which implies $x_s^\top A_{2k+1} x_s = x_s^\top A_k x_s$. Set

$$f_k(x) = \frac{L}{8} x^\top A_k x - \frac{L}{4} x^\top e_1,$$

We proved that, for all $s \leq k$

$$f(x_s) - f^* = f_k(x_s) - f_{2k+1}^* \geq f_k^* - f_{2k+1}^*.$$

Thus it remains to compute the minimizer x_k^* of f_k , its norm, and the corresponding function value f_k^* .

The point x_k^* is the unique solution in the span of e_1, \dots, e_k of $A_k x = e_1$. One can verify (Exercise) that it is defined by $x_k^*(i) = 1 - \frac{i}{k+1}$ for $i = 1, \dots, k$. Thus we have:

$$f_k^* = \frac{L}{8} (x_k^*)^\top A_k x_k^* - \frac{L}{4} (x_k^*)^\top e_1 = -\frac{L}{4} (x_k^*)^\top e_1 = -\frac{L}{4} \left(1 - \frac{1}{k+1} \right).$$

Furthermore note that

$$\|x_k^*\|^2 = \sum_{i=1}^k \left(1 - \frac{i}{k+1} \right)^2 = \sum_{i=1}^k \left(\frac{i}{k+1} \right)^2 \leq \frac{k+1}{3}.$$

Thus one obtains:

$$f_k^* - f_{2k+1}^* = \frac{L}{4} \left(\frac{1}{k+1} - \frac{1}{2k+2} \right) \geq \frac{3L}{16} \frac{\|x_{2k+1}^*\|^2}{(k+1)^2},$$

Gradient descent achieves $1/k$ and the lower bound is $1/k^2$. Which one is tight?

Theorem

Let $f: \mathbb{R}^p \mapsto \mathbb{R}$ be convex continuously differentiable with L -Lipschitz gradient $\inf_{x \in \mathbb{R}^p} f(x) > -\infty$. Consider the algorithm, for $x_{-1} \in \mathbb{R}^p$, set $y_0 = x_{-1}$, $t_1 = 1$ and for $k \in \mathbb{N}$,

$$\begin{aligned} x_k &= y_k - \frac{1}{L} \nabla f(y_k) \\ t_{k+1} &= \frac{1 + \sqrt{1 + 4t_k^2}}{2} \\ y_{k+1} &= x_k + \left(\frac{t_k - 1}{t_{k+1}} \right) (x_k - x_{k-1}). \end{aligned} \tag{8}$$

Then for any $k \in \mathbb{N}$

$$f(x_k) - f^* \leq \frac{4L \|x_0 - x^*\|_2^2}{(k+2)^2}.$$

Set for any $k \in \mathbb{N}$,

$$p_k := (t_k - 1)(x_{k-1} - x_k) \quad \text{so that} \quad y_{k+1} = x_k - \frac{p_k}{t_{k+1}}$$

Momentum term: for any $k \geq 1$

$$t_k \geq \frac{1 + \sqrt{4t_{k-1}^2 + 1}}{2} \geq t_{k-1} + \frac{1}{2} \geq t_0 + \frac{k}{2} = 1 + \frac{k}{2}. \quad (9)$$

$$(t_{k+1}^2 - t_{k+1}) = t_k^2. \quad (10)$$

Main argument: the sequence $\{z_k\}_{k \in \mathbb{N}}$,

$$z_k := \frac{2t_k^2}{L} (f(x_k) - f^*) + \|p_k - x_k + x^*\|^2, \quad (11)$$

is non-increasing and $z_0 \leq 2\|x_0 - x^*\|^2$. The result can be deduced by combining (9) and (11).

We have a series of three inequalities.

$$p_{k+1} - x_{k+1} = p_k - x_k + \frac{t_{k+1}}{L} \nabla f(y_{k+1})$$

This implies

$$\begin{aligned} \|p_{k+1} - x_{k+1} + x^*\|_2^2 &= \|p_k - x_k + x^*\|_2^2 + 2 \frac{(t_{k+1} - 1)}{L} \langle p_k, \nabla f(y_{k+1}) \rangle \\ &\quad + 2 \frac{t_{k+1}}{L} \langle x^* - y_{k+1}, \nabla f(y_{k+1}) \rangle + \frac{t_{k+1}^2}{L^2} \|\nabla f(y_{k+1})\|_2^2 \end{aligned}$$

From the Lipschitz gradient assumption, we obtain

$$\begin{aligned} f(x_{k+1}) - f^* &\leq f(y_{k+1}) - f^* - \frac{1}{2L} \|\nabla f(y_{k+1})\|_2^2 \\ &\leq \langle \nabla f(y_{k+1}), y_{k+1} - x^* \rangle - \frac{1}{2L} \|\nabla f(y_{k+1})\|_2^2 \\ \frac{1}{2L} \|\nabla f(y_{k+1})\|_2^2 &\leq f(y_{k+1}) - f(x_{k+1}) \leq f(x_k) - f(x_{k+1}) - \frac{1}{t_{k+1}} \langle p_k, \nabla f(y_{k+1}) \rangle \end{aligned}$$

Using the last three identities, we obtain

$$\begin{aligned}
 & \|p_{k+1} - x_{k+1} + x^*\|_2^2 - \|p_k - x_k + x^*\|_2^2 \\
 &= 2 \frac{(t_{k+1} - 1)}{L} \langle p_k, \nabla f(y_{k+1}) \rangle + 2 \frac{t_{k+1}}{L} \langle x^* - y_{k+1}, \nabla f(y_{k+1}) \rangle + \frac{t_{k+1}^2}{L^2} \|\nabla f(y_{k+1})\|_2^2 \\
 &\leq 2t_{k+1} \frac{(t_{k+1} - 1)}{L} \left(f(x_k) - f(x_{k+1}) - \frac{1}{2L} \|\nabla f(y_{k+1})\|_2^2 \right) \\
 &\quad + 2 \frac{t_{k+1}}{L} \left(f^* - f(x_{k+1}) - \frac{1}{2L} \|\nabla f(y_{k+1})\|_2^2 \right) + \frac{t_{k+1}^2}{L^2} \|\nabla f(y_{k+1})\|_2^2 \\
 &= 2t_{k+1} \frac{(t_{k+1} - 1)}{L} (f(x_k) - f^* + f^* - f(x_{k+1})) + 2 \frac{t_{k+1}}{L} (f^* - f(x_{k+1})) \\
 &= 2 \frac{t_k^2}{L} (f(x_k) - f^*) - 2 \frac{t_{k+1}^2}{L} (f(x_{k+1}) - f^*)
 \end{aligned}$$

This proves that the sequence $(z_k)_{k \in \mathbb{N}}$ is non increasing. It remains to compute z_0 ,

$$z_0 = \frac{2}{L} (f(x_0) - f^*) + \|x^* - x_0\|_2^2 \leq 2 \|x_0 - x^*\|_2^2.$$

Putting things together

$$f(x_k) - f^* \leq \frac{Lz_0}{2t_k^2} \leq \frac{4L \|x_0 - x^*\|_2^2}{(k+2)^2}.$$

- When available prefer proximal method.
- Acceleration works well in practice.
- Extension of Nesterov's algorithm to the proximal decomposition setting (Beck and Teboulle, FISTA).