Optimization for Data Science — Robin Sieber — FS24 — ETH Zürich

Basics

(! General!)

Constrained opt: $\nabla f(x^*) = 0$ not required \rightarrow optimality cond! Check that x^* and iterates are feasible! Remove const terms in minimization.

For upper bounds: Remove subtractions of non-neg terms & use monotonicity of functions.

split norm sum $||x \pm y||^2 = ||x||^2 + ||y||^2 \pm 2\langle x, y \rangle$ max \geq avg: $\max_i x_i^2 \geq \frac{1}{d} ||x||_2^2 = \frac{1}{d} \sum_i x_i^2$

Ineq. with e.g. indicator func: make case distinction.

(Triangle ineq.) $||x + y|| \le ||x|| + ||y||$ (reverse tri ineq) $|||x|| - ||y||| \le ||x - y||$

(Parallelogram law)

$$||x + y||^2 + ||x - y||^2 = 2 ||x||^2 + 2 ||y||^2$$

(Law of cosines)

$$||x - y||^2 = ||x||^2 + ||y||^2 - 2\langle x, y \rangle$$

(Cauchy-Schwarz) $|\langle x, y \rangle| \le ||x|| ||y||$

(Jensen's inequality) f conv, $\sum \lambda_i = 1$, $x_i \in \text{dom}(f)$ $f\left(\sum \lambda_i x_i\right) \leq \sum \lambda_i f(x_i)$ $\Rightarrow f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)]$

(Convex set) $\lambda x + (1 - \lambda)y \in C \quad \forall x, y \in C, \lambda \in [0, 1]$

(Spectral norm) $||A|| = \max_{\|x\|=1} ||Ax||$ Consequence: $||Ax|| \le ||A|| ||x||$

(Differentiability) $f: \text{dom}(f) \subseteq \mathbb{R}^d \to \mathbb{R}^m$ is called diff'able at x in the interior of dom(f) if $\exists A \in \mathbb{R}^{m \times d}$ and $r: \mathbb{R}^d \to \mathbb{R}^m$ s.t. $\forall y$ in neighborhood of x:

 $f(y) = f(x) + A(y - x) + r(y - x) \text{with } \lim_{v \to 0} \frac{\|r(v)\|}{\|v\|} = 0$ We then define $D f(x)_{ij} = (\partial f_i / \partial x_j)(x)$.

(Lipschitz) f diff'able, dom(f) convex, $B \in \mathbb{R}_+$. Following is equiv:

 $||f(x) - f(y)|| \le B ||x - y||$ (f is B-Lipschitz) $||Df(x)|| \le B$ (bounded differential)

(Young's inequality) p, q > 0 s.t. 1/p + 1/q = 1 and $a, b \ge 0$

$$ab \leq \frac{a^p}{p} + \frac{b^q}{q}, \quad ab \leq \frac{a^2}{2} + \frac{b^2}{2}$$

2nd part p = q = 2. Equality holds iff $a^p = b^q$.

Hölder's ineq: $u^{\top}v \leq \|u\|_{\infty} \|v\|_{1}$ **AM-GM:** $n^{-1} \sum x_{i} \geq \sqrt[n]{\Pi x_{i}} \Rightarrow w/$ CS: $|x^{\top}y| \leq (\|x\|/\sqrt{c})(\|y\|\sqrt{c}) \leq$

$$\frac{1}{2}(\|x\|^2/c + c\|y\|^2)$$

Norms and seminorms are convex.

Basic inequalities: $\ln(1+x) \le x; 1-x \le e^{-x}; ||x||_2 \le ||x||_1 \le \sqrt{d} ||x||_2; ||x||_\infty \le ||x||_2 \le \sqrt{d} ||x||_\infty$

Hypograph: hyp $f = \{(x,t) \mid f(x) \le t\}$, epigraph: epi $f = \{(x,t) \mid f(x) \ge t\}$

Differentiation: $g = Ax + b \Rightarrow \nabla(f \circ g)(x) = A^{\top} \nabla f (Ax + b); f = x^{\top} Qx + b^{\top} x + c \Rightarrow \nabla f (x) = 2Qx + b; \nabla x^{\top} A = A; \nabla a^{\top} x = \nabla x^{\top} a = a; \nabla b^{\top} Ax = A^{\top} b; \nabla x^{\top} x = 2x; \nabla_w \|y - Xw\|_2^2 = 2X^{\top} (Xw - y)$

Basic diff: $(fg)' = f'g + fg'; (f/g)' = (f'g - fg')/g^2; (f \circ g)' = f'(g)g'$

Convex Functions

Convex functions are continuous: dom(f) open, f convex $\Rightarrow f$ continuous. (proof not obv)

(Convex function)
$$\forall x, y \in \text{dom}(f) \text{ conv}, \lambda \in [0, 1]$$

$$f(\lambda x + (1 - \lambda)y) \le \lambda f(x) + (1 - \lambda)f(y)$$

$$f(y) \ge f(x) + \nabla f(x)^{\top}(y - x)$$

$$y^{\top} \nabla^2 f(x) y \ge 0$$

1oc requires ∇f to exist at every point and $\operatorname{dom}(f)$ open. 1oc is equivalent to **monotonicity of the gradient** $(\nabla f(y) - \nabla f(x))^{\mathsf{T}}(y-x) \geq 0$. 2oc requires $\nabla^2 f$ to exist at every point and $\operatorname{dom}(f)$ open.

(Convexity preserving operations) $\lambda_i \in \mathbb{R}_+$, f_i convex, $g: \mathbb{R}^m \to \mathbb{R}^d$ $f:= \max_i f_i \lor f := \sum_i \lambda_i f_i \text{ convex on } \text{dom}(f) = \bigcap_i \text{dom}(f_i)$ $g(x) = Ax + b \Rightarrow f(x) = f(g(x)) \text{ convex if } f \text{ convex on } \{x \in \mathbb{R}^m : g(x) \in \text{dom}(f)\}$

f, g convex $\Rightarrow f \circ g$ convex! E.g. $f = -\ln, g = x^2 - 1$, domain will not be convex. f co, g co + non-decreasing $\Rightarrow g(f(x))$ co. f, g co, positive & monotonically incr. $\Rightarrow fg$ co.

(Global minimum) Let f conv, dom(f) open, $x \in dom(f)$. Then:

x is global minimum of $f \Leftrightarrow \nabla f(x) = 0$ (\Rightarrow) doesn't require convexity

If f is **strictly convex**, there is at most one global minimum. $\nabla f(x) > 0 \ \forall x \Rightarrow f$ strictly co. \Leftarrow : $f(x) = x^4$.

(Constr. opt.) $f: \operatorname{dom}(f) \to \mathbb{R}$ co+diff. $X \subseteq \operatorname{dom}(f)$ co. $x^* \in X$ is a min $\Leftrightarrow \nabla f(x^*)^{\mathsf{T}}(x-x^*) \geq 0 \ \forall x \in X$.

W'strass: f cont. If sublvl set $f^{\leq \alpha}$ nonempty and bounded, then f has glob min.

Convex programming: $\min f_0(x)$, s.t. $f_i(x) \le 0$, $h_j(x) = 0$, (i = 1..m, j = 1..p). Feasible region: $X = \{x \in \mathbb{R}^d : f_i(x) \le 0, h_j(x) = 0 \forall i, j\}$.

Lagrangian: $L: \mathcal{D} \times R^m \to \mathbb{R}$, $L(x,\lambda,\nu) = f_0(x) + \sum_{i=1}^m \lambda_i f_i(x) + \sum_{j=1}^p \nu_j h_j(x)$. λ_i, ν_i are Langrange multipliers.

Dual function: $g: \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R} \cup \{-\infty\}, g(\lambda, \nu) = \inf_{x \in D} L(x, \lambda, \nu).$

Weak duality: If x feasible, then $g(\lambda, \nu) \le f_0(x)$ for all $\lambda \in \mathbb{R}^m \ge 0, \nu \in \mathbb{R}^p$.

Dual problem: $\max g(\lambda, \nu)$, s.t. $\lambda \ge 0$. Always conv (even if primal isn't).

Slater point: Suppose a conv prog with feasible solution \tilde{x} in addition satisfies $f_i(\tilde{x}) < 0$, i = 1..m (a Slater point). Then the infimum value of the primal equals the supremum value of the dual. Moreover, if the value is finite, it is attained by a feasible solution of the dual. Note: Strong duality ($\inf f_0(x) = \sup g(\lambda, \nu)$) may also hold when there is no Slater point or even when it's not a conv prog. The stated Slater point condition provides one particular sufficient condition.

KKT conditions: When strong duality holds, KKT provide necessary and –under convexity– sufficient conditions. Let \tilde{x} , $(\tilde{\lambda}, \tilde{v})$ be primal and dual optimal solutions with 0 duality gap $(f_0(\tilde{x}) = g(\tilde{\lambda}, \tilde{v}))$. If all f_i , h_j are differentiable, then (necessary):

$$\tilde{\lambda}_i f_i(\tilde{x}) = 0, \quad i = 1..m$$

$$\nabla f_0(\tilde{x}) + \sum_{i=1}^m \tilde{\lambda}_i \nabla f_i(\tilde{x}) + \sum_{j=1}^p \tilde{v}_j \nabla h_j(\tilde{x}) = 0$$

Sufficient: All f_i , h_j diff, all f_i conv, h_j affine and the above equations hold. Then \tilde{x} , $(\tilde{\lambda}, \tilde{v})$ have 0 duality gap.

L-smoothness

(L-smoothness)
$$f : \mathbb{R}^d \to \mathbb{R}$$
, conv not req. (!)
$$f(y) \le f(x) + \nabla f(x)^\top (y - x) + \frac{L}{2} \|y - x\|^2$$

If *f* co, the following are equiv.:

$$\begin{split} \|\nabla f(x) - \nabla f(y)\| &\leq L \|x - y\| \\ f(y) &\geq f(x) + \nabla f(x)^{\mathsf{T}} (y - x) + \frac{1}{2L} \|\nabla f(x) - \nabla f(y)\|^2 \\ (\nabla f(x) - \nabla f(y))^{\mathsf{T}} (x - y) &\geq \frac{1}{L} \|\nabla f(x) - \nabla f(y)\|^2 \\ (\nabla f(x) - \nabla f(y))^{\mathsf{T}} (x - y) &\leq L \|x - y\|^2 \end{split}$$

Also these: $f(\lambda x + (1 - \lambda)y) \ge \lambda f(x) + (1 - \lambda)f(y) - \frac{\lambda(1-\lambda)L}{2} \|x - y\|^2$ and $f(\lambda x + (1 - \lambda)y) \le \lambda f(x) + (1 - \lambda)f(y) - \frac{\lambda(1-\lambda)}{2L} \|\nabla f(x) - \nabla f(y)\|^2$.

For $f \ge diff$, also $\nabla^2 f(x) \le L\mathbf{I}$ is equiv.

f L-smooth $\Leftrightarrow g(x) := \frac{L}{2}x^{\top}x - f(x)$ is convex on dom(f). All $f(x) = x^{\top}Qx + b^{\top}x + c$ are $2 \|Q\|$ -smooth.

 $f = \sum \lambda_i f_i$ is $\sum \lambda_i L_i$ -smooth. f(Ax+b) is $L ||A||^2$ -smooth.

μ-strong convexity

(
$$\mu$$
-strong convexity) $f : \mathbb{R}^d \to \mathbb{R}$

$$f(y) \ge f(x) + \nabla f(x)^{\top} (y - x) + \frac{\mu}{2} \|y - x\|^2$$

 $f \mu$ -sc $\Leftrightarrow g(x) = f(x) - \frac{\mu}{2}x^{T}x$ is convex on dom(f).

 $f \mu$ -sc $\Leftrightarrow (\nabla f(x) - \nabla f(y))^{\top} (x - y) \ge \mu ||x - y||^2$.

 $f \text{ μ-sc} \Leftrightarrow f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y) - \frac{\alpha(1-\alpha)\mu}{2} \|x - y\|^2.$

 $f \mu$ -sc $\Leftrightarrow \nabla^2 f(x) \ge \mu \mathbf{I}$.

 $f \mu$ -sc $\Rightarrow \|\nabla f(x) - \nabla f(y)\| \ge \mu \|x - y\|$.

 $\begin{array}{lll} f & \mu\text{-sc} & \Rightarrow & f(y) & \leq & f(x) & + & \nabla f(x)^\top (y & - & x) & + \\ \frac{1}{2\mu} \left\| \nabla f(x) - \nabla f(y) \right\|^2. \end{array}$

 $f \mu$ -sc $\Rightarrow (\nabla f(x) - \nabla f(y))^{\top} (x - y) \le \frac{1}{\mu} \|\nabla f(x) - \nabla f(y)\|^2$.

 $f \mu$ -sc \Rightarrow f strictly convex + has unique global minimum.

f is μ -smooth and μ -sc \Rightarrow $f(x) = \frac{\mu}{2} ||x - b||^2 + c$.

 $\begin{array}{ll} f \text{ L-sm and } \mu\text{-sc } \Rightarrow (\nabla f(x) - \nabla f(y))^\top (x - y) & \geq \\ \frac{\mu L}{\mu + L} \left\| x - y \right\|^2 + \frac{1}{\mu + L} \left\| \nabla f(x) - \nabla f(y) \right\|^2. \end{array}$

Convergence

Always w.r.t. $f(x) - f(x^*) < \varepsilon$, as there could be several minima $y^* \neq x^*$. $O(1/\varepsilon)$ better than $O(1/\varepsilon^2)$, but $O(1/T^2)$ better than O(1/T).

Convergence rates (must hold only for sufficiently large t): $\varepsilon_t = f(x_t) - f(x^*)$.

Linear: $\varepsilon_{t+1} \le c \varepsilon_t, c \in (0,1) \implies O(\log(1/\varepsilon)).$

Sup.: $\varepsilon_{t+1} \leq c \varepsilon_t^r, c > 0, r > 1; r = 2 \Rightarrow O(\log \log(1/\varepsilon)).$

Sublinear: Anything below linear.

Gradient Descent (GD)

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

Vanilla analysis: Bound for avg. error since x_T is not necessarily close to best. Result follows from 1oc, UR and cos-thm.

 $f \text{ conv: } \sum_{t=0}^{T-1} \varepsilon_t \le \frac{\gamma}{2} \sum_{t=0}^{T-1} \|g_t\|^2 + \frac{1}{2\gamma} \|x_0 - x^*\|^2$

 $\begin{array}{ll} f \text{ conv, } \|x_0 - x^*\| \leq R, \|\nabla f(x)\| \leq B, \gamma = R/(B\sqrt{T}): \\ \frac{1}{T} \sum_{t=0}^{T-1} \varepsilon_t \leq \frac{RB}{\sqrt{T}} \text{ and } \min_{t=0}^{T-1} \varepsilon_t \leq \varepsilon \Rightarrow T \geq \frac{R^2B^2}{\varepsilon^2} \end{array}$

(Sufficient decrease) f L-smooth, $\gamma := 1/L$

$$f(x_{t+1}) \le f(x_t) - \frac{1}{2L} \|\nabla f(x_t)\|^2, \ t \ge 0$$

f conv, L-smooth: $f(x_T) - f(x^*) \le \frac{L}{2T} \|x_0 - x^*\|^2$ and $T \ge \frac{R^2 L}{2s}$

f conv, *L*-sm, μ-sc: vanilla: $\varepsilon_t \le \frac{1}{2\gamma} (\gamma^2 \|\nabla f(x_t)\|^2 + \|x_t - x^*\|^2 - \|x_{t+1} - x^*\|^2) - \frac{\mu}{2} \|x_t - x^*\|^2$. With $\gamma = 1/L$ we get (i) geometrically decr dist to x^* and (ii) exp small

abs error after T iter.

$$||x_{t+1} - x^*||^2 \le (1 - \mu/L) ||x_t - x^*||^2, t \ge 0$$

 $f(x_T) - f(x^*) \le \frac{L}{2} (1 - \mu/L)^T ||x_0 - x^*||^2, T > 0$

It follows $T \geq \frac{L}{\mu} \ln \left(\frac{R^2 L}{2\varepsilon} \right)$

Projected Gradient Descent (Proj. GD)

Choose $x_0 \in X$ arb. Proj is well-defined for squared dist, even sc and unique min for closed conv set *X*.

$$\begin{aligned} y_{t+1} &:= x_t - \gamma \nabla f(x_t) \\ x_{t+1} &:= \Pi_X(y_{t+1}) := \mathop{\arg\min}_{x \in X} \|x - y_{t+1}\|^2 \end{aligned}$$

For $X \subseteq \mathbb{R}^d$ closed and conv, $x \in X$, $y \in \mathbb{R}^d$, it holds:

- $(x \Pi_X(y))^{\top} (y \Pi_X(y)) \le 0 \text{ (angle } \ge 90^{\circ})$
- $||x \Pi_X(y)||^2 + ||y \Pi_X(y)||^2 \le ||x y||^2$

Proj is **non-expansive**: $\|\Pi_X(x) - \Pi_X(y)\| \le \|x - y\|$.

 $f \operatorname{co}, X \subseteq \operatorname{dom}(f) \operatorname{closed} \& \operatorname{co}, ||x_0 - x^*|| \le R, ||\nabla f(x)|| \le$ $B, \gamma := R/(B\sqrt{T}): \frac{1}{T} \sum_{t=0}^{T-1} \varepsilon_t \le (RB)/\sqrt{T}. \Rightarrow O(1/\varepsilon^2).$

f L-sm, $X \subseteq dom(f)$ closed & co, $\gamma := 1/L$: $f(x_{t+1}) \le$ $f(x_t) - \frac{1}{2L} \|\nabla f(x_t)\|^2 + \frac{L}{2} \|y_{t+1} - x_{t+1}\|^2$.

f co, L-sm, $X \subseteq dom(f)$ closed & co, $\gamma := 1/L$: $\varepsilon_t \le$ $\frac{L}{2T} \|x_0 - x^*\|^2$.

f co, L-sm, μ -sc, $X \subseteq dom(f)$ closed & co. With $\gamma :=$ 1/L we get (i) geometrically decr dist to x^* and (ii) exp small abs error after *T* iter. Constrained optimization $\Rightarrow \nabla f(x^*) \neq 0$ possible!

$$\|x_{t+1} - x^*\|^2 \le (1 - \mu/L) \|x_t - x^*\|^2, \ t \ge 0$$

$$\text{Proj in Proj GD can be expensive even for convex s}$$

$$\varepsilon_T \le \|\nabla f(x^*)\| \left(1 - \frac{\mu}{L}\right)^{T/2} \|x_0 - x^*\| + \frac{L}{2} \left(1 - \frac{\mu}{L}\right)^T \|x_0 - x^*\|_{\text{linear Min. Oracle: LMO}_X(g)}$$

$$\text{erg in Proj GD can be expensive even for convex s}$$

Coordinate Descent (CD)

For GD proved $x_t \to x^*$, here only $f(x_t) \to f(x^*)$.

(PL inequality)
$$f$$
 diff w/ glob min x^* . $\exists \mu > 0$ s.t.:
$$\frac{1}{2} \|\nabla f(x)\|^2 \ge \mu(f(x) - f(x^*)), \quad \forall x \in \mathbb{R}^d$$

 μ -sc \Rightarrow PL holds. (PL is a strictly weaker condition, e.g. $f(x_1, x_2) = x_1^2$ satisfies PL but not μ -sc.) Even some nonconv funcs can satisfy PL.

f L-sm, PL holds, $\gamma := 1/L$: $\varepsilon_T \leq (1 - \mu/L)^T \varepsilon_0$, T > 0.

(Coord.-wise smooth) f diff, $\mathcal{L} = (L_1, \dots, L_d) \in \mathbb{R}_d^+$.

$$f(x + \lambda e_i) \le f(x) + \lambda \nabla_i f(x) + \frac{L_i}{2} \lambda^2, \ \forall x \in \mathbb{R}^d, \lambda \in \mathbb{R}$$

holds, cw-sm w/ \mathcal{L} . If $L_i = L$, then w/ param L .

Algorithm: Choose $i \in [d]$: $x_{t+1} := x_t - \gamma_i \nabla_i f(x_t) e_i$ $f \mathcal{L}$ -cw-sm, $\gamma_i = 1/L_i$: $f(x_{t+1}) \le f(x_t) - \frac{1}{2L_i} |\nabla_i f(x_t)|^2$. Randomized CD: $i \in [d]$ chosen uniformly at random in step t. f L-sm, PL holds, $\gamma_i = 1/L$: $\mathbb{E}[\varepsilon_T] \leq (1 - 1)$ $\mu/(dL)^T \varepsilon_0, T > 0.$

Importance Sampling: choose coordinate actively, sample $i \in [d]$ with prob. $p_i = \frac{L_i}{\sum_{i=1}^{d} L_i}$. CD-step: $x_{t+1} :=$ $x_t - \frac{1}{L_i} \nabla_i f(x_t) e_i$.

Theorem: f diff with gl. min. x^* . Suppose f cw-sm with param $\mathbb{L} = (L_1, ..., L_d)$, PL holds with $\mu > 0$. Let $\overline{L} = \frac{1}{d} \sum_{i=1}^{d} L_i$. Then CD with IS and arbitrary x_0 satisfies $\mathbb{E}[f(x_T) - f(x^*)] \le (1 - \frac{\mu}{d\overline{t}})^T (f(x_0) - f(x^*)), T > 0.$

Steepest CD: $i = \arg \max_{i} |\nabla_{i} f(x_{t})| f$ L-cw-sm, PL holds, $\gamma_i = 1/L$. No \mathbb{E} since alg is deterministic: $\varepsilon_T \leq$ $(1 - \mu/(dL))^T \varepsilon_0$, T > 0. \Rightarrow Difference to GD is that only cw-sm instead of global smoothness is needed. In case f μ -sc wrt ℓ_1 -norm (stronger cond.), then d can be dropped in the bound.

Greedy CD: f diff not required. Choose $i \in [d]: x_{t+1} :=$ $\arg\min_{\lambda\in\mathbb{R}} f(x_t - \lambda e_i)$. But now additional 1D opt. problem in each step.

Non-convex functions

 $f \ge \text{diff}, \|\nabla^2 f(x)\| \le L \forall x \in X. \text{ Then } f \text{ is } L\text{-sm.}$

f L-sm, $\gamma := 1/L$, GD yields: $\frac{1}{T} \sum_{t=0}^{T-1} \|\nabla f(x_t)\|^2 \leq \frac{2L}{T} \varepsilon_0$ and $\lim_{t\to\infty} \|\nabla f(x_t)\|^2 = 0$. Proof using sufficient decr. which doesn't require conv.

Lemma: For *f L*-sm, GD cannot overshoot a critial point Performance of AGD vs Subgr. D:

Frank-Wolfe

Constrained opt. $\min_{x \in X} f(x)$

Proj in Proj GD can be expensive even for convex sets.

Algorithm ($\gamma_t \in [0, 1]$):

$$s := \text{LMO}_X(\nabla f(x_t))$$

$$x_{t+1} := (1 - \gamma_t)x_t + \gamma_t s$$

In each step, alg. minimizes the linear approximation over the set X and makes a step in the direction of the minimizer. Iterates are always feasible.

Duality gap / Hearn gap: $g(x) := \nabla f(x)^{\mathsf{T}}(x-s)$. $g(x) := \nabla f(x)^{\mathsf{T}}(x-s)$ can be interpreted as opt gap of the linear subproblem $\nabla f(x)^{\mathsf{T}} x - \nabla f(x)^{\mathsf{T}} s. \ g(x) \ge 0.$

Duality gap is an upper bound for the optimality gap: $g(x) \ge f(x) - f(x^*)$. I.e. $g(x_t)$ always gives a guaranteed upper bound on the optimality gap.

f co, L-sm, X closed+bounded, $\mu_t = \gamma_t := 2/(t+2)$, then: $\varepsilon_T \le \frac{2L \operatorname{diam}(X)^2}{T+1}, \ T \ge 1, \ \operatorname{diam}(X) := \max_{x,y \in X} \|x - y\|.$

Descent lemma for $\gamma_t \in [0,1]$: $f(x_{t+1}) \leq f(x_t) - \gamma_t g(x_t) +$ $\gamma_t^2 \frac{L}{2} \|s - x_t\|^2$.

Stepsize variants:

Line search s.t. progress is maximal: γ_t := $\arg\min_{y \in [0,1]} f((1-y)x_t + ys)$. For $h(x) = f(x) - f(x^*)$, we then obtain: $h(x_{t+1}) \leq h(y_{t+1}) \leq (1 - \mu_t)h(x_t) +$ $\mu_t^2 \frac{L}{2} \operatorname{diam}(X)^2$, where y_{t+1} is the iterate obtained using standard stepsize μ_t

Gap-based $\gamma_t := \min\{1, \frac{g(x_t)}{L\|s-x_t\|^2}\}$ and progress is guaranteed in every iteration: $h(x_{t+1}) \leq$ $h(x_t) - (1 - \frac{\gamma_t}{2}), \quad \gamma_t < 1$ $h(x_t),$

(f, X), (f', X') affinely equiv if f'(x) = f(Ax + b) for A inv. $X' = \{A^{-1}(x - b) : x \in X\}$. LMO+FW return same

Random

Unconstrained optimization:

	Lip+co	L+co	μ +co	$L+\mu+co$
GD	$\mathcal{O}(\varepsilon^{-2})$	$\mathcal{O}(\varepsilon^{-1})$		$O(\log(\varepsilon^{-1}))$
AGD		$\mathcal{O}(1/\sqrt{\varepsilon})$		
Proj. GD	$\mathcal{O}(\varepsilon^{-2})$	$\mathcal{O}(\varepsilon^{-1})$		$O(\log(\varepsilon^{-1}))$
Subgr. D	$\mathcal{O}(\varepsilon^{-2})$		$\mathcal{O}(\varepsilon^{-1})$	
SGD	$\mathcal{O}(\varepsilon^{-2})$		$\mathcal{O}(\varepsilon^{-1})$	

LMO: Let $X := conv(\mathcal{A})$, then:

Ex.	\mathcal{A}	$ \mathcal{A} $	dim.	$LMO_X(g)$
L1-ball	$\{\pm e_i\}$	2d	d	$\pm e_i$, $i = \arg \max_i g_i $
Simplex	$\{e_i\}$	d	d	$e_i, i = \arg \min_i g_i$
Spectahedron	$\{xx^{\top}, x = 1\}$	∞	d^2	$\arg \min_{\ x\ =1} x^{\top} G x$
Norms	$\{x, x \le 1\}$	∞	d	$\arg\min_{\ s\ \leq 1} \langle s, g \rangle$
Nuclear norm	$\{Y,\ Y\ _*\leq 1\}$	∞	d^2	

	Convex	Strongly Convex
Subgr. D	$\mathcal{O}\left(\frac{BR}{\sqrt{t}}\right)$	$\mathcal{O}\left(rac{B^2}{\mu t} ight)$
AGD	$\mathcal{O}\left(\frac{LR^2}{t^2}\right)$	$\mathcal{O}\left(\left(\frac{1-\sqrt{\kappa}}{1+\sqrt{\kappa}}\right)^{2t}\right)$

→ Subgr. D is always slower, even in sc case only sublinear cvg.

Complexity for SGD:

	iteration complexit	y iteration cos	t total		
Smooth and strongly convex problems $(\kappa = L/\mu)$					
GD SGD	$ \frac{\mathcal{O}(\kappa \log(1/\varepsilon))}{\mathcal{O}(1/\varepsilon)} $	$\mathcal{O}(n)$ $\mathcal{O}(1)$	$\begin{array}{c c} \mathcal{O}(n\kappa\log(1/\varepsilon)) \\ \mathcal{O}(1/\varepsilon) \end{array}$		
Nonconvex problems					
GD SGD	$\mathcal{O}(1/\varepsilon^2)$ $\mathcal{O}(1/\varepsilon^4)$	$\mathcal{O}(n)$ $\mathcal{O}(1)$	$\mathcal{O}(n/\varepsilon^2)$ $\mathcal{O}(1/\varepsilon^4)$		

Vanilla Analysis (GD & Proj. GD):

- 1. Use 1oc: $f(y) \ge f(x) + \nabla f(x)^{\mathsf{T}} (y x)$
- 2. Set $y = x^*$, $x = x_t$: $\varepsilon_t \leq \nabla f(x_t)^{\top} (x_t x^*)$
- 3. Use update rule: $x_t x^* = (z_{t+1} x^*) + \gamma \nabla f(x_t)$ where $z_{t+1} = x_{t+1}$ for GD, $z_{t+1} = y_{t+1}$ for Proj.
- 4. Apply cosine theorem: $2v^{T}w = ||v||^{2} + ||w||^{2} ||v v||^{2}$
- 5. For Proj. GD: Use projection property $||x_{t+1}|$ $|x^*|^2 \le ||y_{t+1} - x^*||^2$

6. Sum over t, telescope: $\frac{\gamma}{2} \sum_{t=0}^{T-1} \|\nabla f(x_t)\|^2 + \frac{1}{2\gamma} \|x_0 - x^*\|^2$

- 1. Use smoothness: $f(y) \leq f(x) + \nabla f(x)^{\mathsf{T}} (y x) +$ $\frac{L}{2}||y-x||^2$
- 2. Šet $y = z_{t+1}$, $x = x_t$, use update rule where $z_{t+1} = x_{t+1}$ for GD, $z_{t+1} = y_{t+1}$ for Proj.
- 3. For Proj. GD: Use projection property $f(x_{t+1}) \le$
- 4. Minimize RHS w.r.t. γ : $\gamma = 1/L$
- 5. Get sufficient decrease: GD: $f(x_{t+1}) \le f(x_t) - \frac{1}{2I} \|\nabla f(x_t)\|^2$ Proj. GD: $f(x_{t+1}) \le f(x_t) - \frac{1}{2L} \|\nabla f(x_t)\|^2 + \frac{L}{2} \|y_{t+1} - y_{t+1}\|^2$ $|x_{t+1}||^2$

μ -strongly convex:

- 1. Use strong convexity: $f(y) \ge f(x) + \nabla f(x)^{\mathsf{T}} (y y)^{\mathsf{T}} (y y)^{\mathsf{$ $(x) + \frac{\mu}{2} ||y - x||^2$
- 2. Set $y = x^*$, $x = x_t$, combine with vanilla analysis
- 3. Use sufficient decrease to bound/eliminate gradi-
- 4. For Proj. GD: Apply projection property $||x_{t+1}||$ $|x^*|^2 \le ||y_{t+1} - x^*||^2$
- 5. Get recursive inequality for $||x_t x^*||^2$

Working with iterate distances: $||x_{t+1} - x^*||^2 =$ $\|x_t - \gamma \nabla f(x_t) - x^*\|^2 = \|x_t - x^*\|^2 - 2\gamma \nabla f(x_t)^\top (x_t - x^*) +$ $\gamma^2 \|\nabla f(x_t)\|^2$ (use update rule and expand norm). Then bound middle term with μ -sc and L-sm or similar properties. For projections in UR: use non-expansive prop.

Telescoping sum: $\sum_{t=0}^{T-1} (f(x_t) - f(x_{t+1})) = f(x_0) - f(x_T)$ Matrix diff example:

$$f(x) = \log(a^\top x) \Rightarrow \nabla f(x) = \frac{a}{a^\top x} \Rightarrow \nabla^2 f(x) = -\frac{aa^\top}{(a^\top x)^2}$$
 $(a_i > 0)$

$$\begin{array}{lll} f(x) &=& \sum_{i=1}^d \log(x_i) \implies \nabla f(x) &=& (\frac{1}{x_1}, \dots, \frac{1}{x_d}) \\ \nabla^2 f(x) &=& -\mathrm{diag}(\frac{1}{x_1^2}, \dots, \frac{1}{x_d^2}) \end{array}$$

Stochastic: $F(x) := \mathbb{E}_{\xi}[f_{\xi}(x)]$. unbiased grad estimator: $\mathbb{E}[\nabla f_{\varepsilon}(x)] = \nabla F(x)$. Then: $\nabla F(x^*) = \mathbb{E}[\nabla f_{\varepsilon}(x^*)] = 0$. But: $\nabla f_{\xi}(x^*) \neq 0, \mathbb{E}[\|\nabla f_{\xi}(x^*)\|^2] \neq 0.$ Jensen: $\|\nabla F(x)\|^2 =$ $\|\mathbb{E}[\nabla f_{\mathcal{E}}(x)]\|^2 \leq \mathbb{E}[\|\nabla f_{\mathcal{E}}(x)\|^2]$

Probability: $\mathbb{E}[X] = \sum x_i p(x_i)$, $Var[X] = \mathbb{E}[(X - \sum x_i p(x_i))]$ $\mathbb{E}[X])^2 = \mathbb{E}[X^2] - \mathbb{E}[X]^2, \operatorname{Cov}[X, Y] = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[X])$ $\mathbb{E}[Y])] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y].$

 $\mathbb{E}[XY|Z] = \mathbb{E}[X|Z]\mathbb{E}[Y|Z]$ if X, Y indep given Z. P(B) = $\sum P(B|A_i)P(A_i), P(A|B) = \frac{P(B|A)P(A)}{P(B)}$

Newton's method

 $(x_t)^\top \nabla^2 f(x_t)(x-x_t).$

1D:
$$x_{t+1} := x_t - f'(x_t)/f''(x_t), t \ge 0.$$

For optimization apply to
$$f'$$
: $x_{t+1} := x_t - f'(x_t)/f''(x_t)$, $t \ge 0$, resp. $x_{t+1} := x_t - \nabla^2 f(x_t)^{-1} \nabla f(x_t)$. f co, $2 \times \text{diff}$, $\nabla^2 f(x) > 0$ inv, then x_{t+1} from Newton satisfies $x_{t+1} = \arg\min_{x \in \mathbb{R}^d} f(x_t) + \nabla f(x_t)^{\top} (x - x_t) + \frac{1}{2}(x - x_t)$

Let there be a ball $X \subseteq \operatorname{dom}(f)$ with center x^* such that $\|\nabla^2 f(x)^{-1}\| \le 1/\mu$ and $\|\nabla^2 f(x) - \nabla^2 f(y)\| \le B \|x - y\|$, then for x_t, x_{t+1} resulting from a Newton step, the following holds: $\|x_{t+1} - x^*\| \le \frac{2B}{\mu} \|x_t - x^*\|^2$.

 $f \ge x$ diff, μ -sc over open conv $X \subseteq \text{dom}(f)$. Then $\nabla^2 f(x)$ is inv and $\|\nabla^2 f(x)^{-1}\| \le 1/\mu$ for all $x \in X$.

Quasi-Newton methods

Secant method (2nd derivative free!): Replace f''(x) with $\frac{f'(x_t) - f'(x_{t-1})}{x_t - x_{t-1}}$.

Subgradient methods

(Subgradient) $f : \text{dom}(f) \to \mathbb{R} \cup \{+\infty\}$, co. $g \in \mathbb{R}^d$ is a subgradient of f at x if

 $f(y) \ge f(x) + g^{\mathsf{T}}(y - x), \ \forall y \in \text{dom}(f)$ Set of all subgradients at x is called subdifferential

If f co and diff at x, then $\partial f(x) = {\nabla f(x)}$.

f co, dom(f) open, $B \in \mathbb{R}_+$. The following are equiv:

- $||g|| \le B$, $\forall x \in \text{dom}(f)$, $\forall g \in \partial f(x)$.
- $|f(x) f(y)| \le B ||x y||, \forall x, y \in \text{dom}(f).$

If $\mathbf{0} \in \partial f(x)$, $x \in \text{dom}(f)$, then x is a *global* minimum.

f co, $x \in dom(f)$. Then $\partial f(x)$ is co and closed.

f func where dom(f) is co and $\partial f(x) \neq \emptyset \ \forall x \in dom(f)$. Then f is co over dom(f).

Directional derivatives: $f'(x;d) = \lim_{\delta \to 0^+} \frac{f(x+\delta d) - f(x)}{\delta}$. For f diff $f'(x;d) = \nabla f(x)^{\mathsf{T}} d$. For subgr: $f'(x;d) = \max_{g \in \partial f(x)} g^{\mathsf{T}} d$.

Calculating subgradients:

- Conic combination: $h(x) = \lambda f(x) + \mu g(x); \lambda, \mu \ge 0; f, g$ co, then $\partial h(x) = \lambda \partial f(x) + \mu \partial g(x) \ \forall x \in \text{int}(\text{dom}(h)).$
- Affine compos.: h(x) = f(Ax + b); f co, then $\partial h(x) = A^{\mathsf{T}} \partial f(Ax + b)$.
- Supremum: $h(x) = \sup_{\alpha \in \mathcal{A}} f_{\alpha}(x)$ and f_{α} co, then: $\partial h(x) \supseteq \operatorname{conv} \{\partial f_{\alpha}(x) \mid \alpha \in \alpha(x)\}$ where $\alpha(x) = \{\alpha : h(x) = f_{\alpha}(x)\}$
- Superposition: $h(x) = F(f_1(x), ..., f_m(x))$ where $F(y_1, ..., y_m)$ is non-decr and co, then $\partial h(x) \supseteq \{\sum_{i=1}^m d_i \partial f_i(x) : (d_1, ..., d_m) \in \partial F(y_1, ..., y_m)\}.$

Subgradient method: f co, possibly non-diff. Goal $\min f(x)$ s.t. $x \in X \subseteq \text{dom}(f)$. X closed+co. Let $R^2 = \max_{x,y \in X} \|x-y\|_2^2$, $B = \sup_{x,y \in X} \frac{|f(x)-f(y)|}{\|x-y\|_2}$. Init $x_1 \in X$. For $t = 1, \ldots, T$:

$$x_{t+1} = \Pi_X(x_t - \gamma_t g_t), g_t \in \partial f(x_t)$$

For f diff, this reduces to Proj GD. Subgr. Descent is not necessarily a descent method and moving along the negative direction of g_t is not guaranteed to decrease the function value.

Stepsize choices:

- Constant: $\gamma_t \equiv \gamma > 0$
- Scaled: $\gamma_t = \gamma/\|g_t\|_2$
- Diminishing, non-summable: $\sum \gamma_t$ ∞ , $\lim_{t\to\infty} \gamma_t = 0$
- Sq-summable: $\sum \gamma_t = \infty$, $\sum \gamma_t^2 < \infty$ (e.g. 1/t)
- *Polyak:* Assuming $f(x^*)$ known. $\gamma_t = \varepsilon_t / ||g_t||_2^2$

f co, then SubgrD satisfies

$$\min \varepsilon_t \le \left(\sum_{t=1}^T \gamma_t\right)^{-1} \left(\frac{1}{2} \|x_1 - x^*\|_2^2 + \frac{1}{2} \sum_{t=1}^T \gamma_t^2 \|g_t\|_2^2\right)$$
$$f(\hat{x}_T) - f(x^*) \le \left(\sum_{t=1}^T \gamma_t\right)^{-1} \left(\frac{1}{2} \|x_1 - x^*\|_2^2 + \frac{1}{2} \sum_{t=1}^T \gamma_t^2 \|g_t\|_2^2\right)$$

where
$$\hat{x}_T = \left(\sum_{t=1}^T \gamma_t\right)^{-1} \left(\sum_{t=1}^T \gamma_t x_t\right) \in X$$
.

Using bounds R, B and changing summation to $T_0 \ge 1$:

$$\min_{T_0 \le 1 \le T} f(x_t) - f(x^*) \le \frac{\frac{R^2}{2} + \frac{1}{2} \sum_{t=T_0}^{T} \gamma_t^2 B^2}{\sum_{t=T_0}^{T} \gamma_t}$$

Mirror Descent

Goal: Generalize SubgrD to non-Euclid. distances.

(Bregman divergence) $\omega: X \to \mathbb{R}$ strictly(!) conv, continuously diff on closed conv X.

$$V_{\omega}(x, y) = \omega(x) - \omega(y) - \nabla \omega(y)^{\mathsf{T}}(x - y)$$

 V_{ω} is not a valid distance: asymmetric and triangle inequal may not hold–it is called distance-generating function.

If ω σ -sc wrt some norm, then it holds $V_{\omega}(x,y) \ge \frac{\sigma}{2} ||x-y||^2$.

For well-defined V_{ω},V_{ψ} and a,b>0 it holds $V_{a\omega+b\psi}(x,y)=aV_{\omega}(x,y)+bV_{\psi}(x,y)$.

Generalized Pythagorean: Let x^* be Bregman proj of x_0 onto conv set $C \subset X$, $x^* = \arg\min_{x \in C} V_{\omega}(x, x_0)$. Then for all $y \in C$: $V_{\omega}(y, x_0) \ge V_{\omega}(y, x^*) + V_{\omega}(x^*, x_0)$.

Prox-mapping: $\operatorname{Prox}_{x}(\xi) = \arg\min_{u \in X} \{V_{\omega}(u, x) + \langle \xi, u \rangle\}$, where ω is 1-sc wrt some norm.

Mirror descent:

$$\begin{split} x_{t+1} &= \operatorname{Prox}_{x_t}(\gamma_t g_t) = \underset{x \in X}{\arg\min} \{V_{\omega}(x, x_t) + \langle \gamma_t g_t, x \rangle\} \\ &= \underset{x \in X}{\arg\min} \{\omega(x) + \langle \gamma_t g_t - \nabla \omega(x_t), x \rangle\} \end{split}$$

Example setups

 $\ell_2: X \subseteq R^n, \omega(x) = \frac{1}{2} \|x\|_2^2, \|\cdot\| = \|\cdot\|_2: V_{\omega}(x, y) = \frac{1}{2} \|x - y\|_2^2; \operatorname{Prox}_x(\xi) = \Pi_X(x - \xi) \Rightarrow \operatorname{SubgrD}.$

$$\ell_1: X = \Delta_n, \omega(x) = \sum_{i=1}^n x_i \ln(x_i), \|\cdot\| = \|\cdot\|_1: V_{\omega}(x, y) = \sum_{i=1}^n x_i \ln(x_i/y_i) \\ \text{(Kullback-Leibler)}; \text{Prox}_x(\xi) = \left(\sum_{i=1}^n x_i \exp(-\xi_i)\right)^{-1} \left[x_1 \exp(-\xi_1), \dots, x_n \exp(-\xi_n)\right]^{\mathsf{T}} \\ \text{Good for multiplicative updates with normalization.}$$

(Three point iden.) $\forall x,y,z \in \text{dom}(\omega): V_{\omega}(x,z) = V_{\omega}(x,y) + V_{\omega}(y,z) - \langle \nabla \omega(z) - \nabla \omega(y), x - y \rangle$

Convex conjugate

 $f: \operatorname{dom}(f) \to \mathbb{R}$, conv conj: $f^*(y) = \sup_{x \in \operatorname{dom}(f)} \{x^{\mathsf{T}}y - f(x)\}$. f conv is not necessary!

Fenchel inequality follows from def.: $x^{T}y \leq f(x) + f^{*}(y)$, which is a generalization of Young's ineq $x^{T}y \leq \|x\|^{2}/2 + \|y\|^{2}/2$.

If f co, lower semi-continuous and proper, then $(f^*)^* = f$. That is $\liminf_{x \to x_0} f(x) \ge f(x_0)$ and $f(x) > -\infty$.

 $f \mu$ -sc $\Rightarrow f^*$ is $1/\mu$ -Lipschitz smooth and continuously diff.

For f, g proper, conv, semi-cont:

$$(\hat{f} + g)^*(x) = \inf_{y} \{ f^*(y) + g^*(x - y) \}$$

 $(\alpha f)^*(x) = \alpha f^*(x/\alpha), \ \alpha > 0$

Smoothing techniques

Goal: Approximate non-sm/diff f with smooth f_{μ} s.t. GD and AGD can be applied.

Nesterov's smoothing: $f_{\mu}(x) = \max_{y \in \text{dom}(f^*)} \{x^{\top}y - f^*(y) - \mu \cdot d(y)\} = (f + \mu d)^*(x)$, where d(y) is a sc, nonnegative proximity function. f_{μ} is continuously diff and Lipschitz smooth.

Moreau-Yosida: $f_{\mu}(x) = \min_{y \in \text{dom}(f)} \{f(y) + \frac{1}{2\mu} ||x - y||_2^2\}$ for $\mu > 0$. It is equiv to Nesterov with $d(y) = \frac{1}{2} ||y||_2^2$.