CME 307: Optimization

CME 307 / MS&E 311 / OIT 676

Lecture 11: Gradient Descent

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#### 1 Setup and conventions

We study gradient descent (GD) for unconstrained smooth optimization

 $\min_{x \in \mathbb{R}^n} f(x)$ , f differentiable, with an attained optimal value  $f^* := \min_x f(x)$ .

The basic iteration with constant step size t > 0 is

$$x^{k+1} = x^k - t\nabla f(x^k).$$

We also discuss line search strategies (e.g., Armijo backtracking) that choose  $t^k$  adaptively.

First-order optimality (recall). If  $x^*$  minimizes a differentiable f, then  $\nabla f(x^*) = 0$ .

#### 2 Quadratic upper bound: L-smoothness

**Definition 2.1** (Smoothness). A differentiable function  $f: \mathbb{R}^n \to \mathbb{R}$  is L-smooth if for all x, y, y

$$f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{L}{2} ||y - x||^2.$$

Equivalently (when  $\nabla^2 f$  exists),  $\|\nabla f(y) - \nabla f(x)\| \le L\|y - x\|$  and  $\nabla^2 f(x) \le LI$  for all x in the domain.

**Example 2.2** (Quadratic). For  $f(x) = \frac{1}{2}x^T A x$  with  $A \succeq 0$ , f is L-smooth with  $L = \lambda_{\max}(A)$ .

### 3 Quadratic lower bound: $\mu$ -strong convexity

**Definition 3.1** (Strong convexity). A differentiable function  $f: \mathbb{R}^n \to \mathbb{R}$  is  $\mu$ -strongly convex if for all x, y,

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

Equivalently (when  $\nabla^2 f$  exists),  $\nabla^2 f(x) \succeq \mu I$ ; and the gradient is  $\mu$ -coercive in the sense  $\|\nabla f(y) - \nabla f(x)\| \ge \mu \|y - x\|$ .

**Example 3.2** (Quadratic). For  $f(x) = \frac{1}{2}x^T A x$  with  $A \succeq 0$ , f is  $\mu$ -strongly convex with  $\mu = \lambda_{\min}(A)$  if and only if  $A \succ 0$ .

#### 4 Some important losses: smoothness and strong convexity

**Example 4.1** (Least squares and logistic regression). Let  $A \in \mathbb{R}^{m \times n}$ ,  $b \in \mathbb{R}^m$ .

- Quadratic loss:  $f(x) = ||Ax b||^2$  is smooth, and is strongly convex if A has full column rank  $(\lambda_{\min}(A^TA) > 0)$ .
- Logistic loss:  $f(x) = \sum_{i=1}^{m} \log(1 + \exp(b_i a_i^T x))$  is smooth; it is strongly convex on any compact set when A has full column rank.

Worked details. For logistic loss,  $\nabla^2 f(x) = A^T D(x) A$  with  $D(x) = \operatorname{diag}(\sigma(s_i)(1 - \sigma(s_i)))$  and  $s_i = b_i a_i^T x$ , so  $0 \leq D(x) \leq \frac{1}{4} I$ , giving  $L \leq \frac{1}{4} \lambda_{\max}(A^T A)$ . On bounded sets that keep  $\sigma(s_i) \in [\delta, 1 - \delta]$ ,  $D(x) \succeq \delta(1 - \delta) I$ , giving  $\mu \geq \delta(1 - \delta) \lambda_{\min}(A^T A)$ .

#### 5 Choosing the next iterate by optimizing the upper bound

Minimizing the quadratic upper model at  $x^k$  yields

$$x^{k+1} = \underset{y}{\operatorname{argmin}} \left\{ f(x^k) + \nabla f(x^k)^T (y - x^k) + \frac{L}{2} ||y - x^k||^2 \right\} = x^k - \frac{1}{L} \nabla f(x^k).$$

Thus t=1/L is the natural stepsize when L is known. (We will prove it guarantees decrease.) Remark 5.1 (Quadratic approximation viewpoint). Replacing the Hessian by  $H=\frac{1}{t}I$  in the local quadratic model yields  $x^+=x-t\nabla f(x)$ , i.e., gradient descent.

## 6 The Polyak-Łojasiewicz (PL) condition

**Definition 6.1** (PL). A differentiable function f satisfies the  $\mu$ -PL inequality if

$$\frac{1}{2}\|\nabla f(x)\|^2 \ge \mu \big(f(x) - f^*\big) \qquad \text{for all } x.$$

PL does *not* require convexity and does *not* imply uniqueness of minimizers; under PL, objective convergence does not necessarily imply iterate convergence.

**Proposition 6.2** (Strong convexity  $\Rightarrow$  PL). If f is  $\mu$ -strongly convex, then f is  $\mu$ -PL.

*Proof sketch.* Minimize the strong convexity lower bound over y:

$$f^* \ge \min_{y} \left\{ f(x) + \nabla f(x)^T (y - x) + \frac{\mu}{2} ||y - x||^2 \right\} = f(x) - \frac{1}{2\mu} ||\nabla f(x)||^2,$$

where the minimum is attained at  $y = x - \nabla f(x)/\mu$ . Rearranging gives the PL inequality.

**Example 6.3** (Compositions that are PL). If f(x) = g(Ax) with g strongly convex and A linear, then f satisfies a PL inequality (even when f is not strongly convex or convex) [?]. This covers least squares, and logistic regression on compact sets when A has full column rank.

#### 7 Types and rates of convergence

**Definition 7.1** (Objective and iterate convergence). We say GD achieves *objective convergence* if  $f(x^k) \to f^*$  and *iterate convergence* if  $x^k \to x^*$ . Under strong convexity, objective convergence implies iterate convergence; under PL, not necessarily (the minimizer set may be a manifold).

**Definition 7.2** (Rates). We say  $f(x^k) - f^* \leq c^k(f(x^0) - f^*)$  for some  $c \in (0,1)$  is *linear* (geometric) convergence, which appears as a straight line on a semilog plot; rates like O(1/k) are *sublinear* and curve upward in semilog.

#### 8 Main theorem: GD under L-smoothness and PL

**Theorem 8.1** (GD is linearly convergent under PL). If f is L-smooth and  $\mu$ -PL, and  $x^*$  exists, then GD with t = 1/L satisfies

$$f(x^k) - f^* \le \left(1 - \frac{\mu}{L}\right)^k \left(f(x^0) - f^*\right).$$

*Proof.* By L-smoothness with  $x = x^k$  and  $y = x^{k+1} = x^k - \frac{1}{L}\nabla f(x^k)$ ,

$$f(x^{k+1}) \le f(x^k) + \nabla f(x^k)^T (x^{k+1} - x^k) + \frac{L}{2} ||x^{k+1} - x^k||^2 = f(x^k) - \frac{1}{2L} ||\nabla f(x^k)||^2.$$

By PL,  $\|\nabla f(x^k)\|^2 \ge 2\mu \left(f(x^k) - f^{\star}\right)$ ; combine to get

$$f(x^{k+1}) - f^{\star} \le \left(1 - \frac{\mu}{L}\right) \left(f(x^k) - f^{\star}\right)$$

and iterate.  $\Box$ 

Remark 8.2 (What improves with exact line search). Exact line search always does at least as well as t = 1/L in function decrease, so the same linear rate bound holds (and can be faster in practice).

#### 9 Sublinear rate on smooth convex functions

For completeness, we include the standard O(1/k) rate for convex L-smooth f (no PL).

**Theorem 9.1** (GD on L-smooth convex f). If f is convex and L-smooth, GD with t = 1/L satisfies

$$f(x^k) - f^* \le \frac{L}{2k}, ||x^0 - x^*||^2.$$

Proof sketch. Combine the descent lemma  $f(x^{k+1}) \leq f(x^k) - \frac{1}{2L} \|\nabla f(x^k)\|^2$  with convexity,  $f(x^k) - f^* \leq \nabla f(x^k)^T (x^k - x^*)$ , and nonexpansiveness of the GD step, to telescope  $\|x^{k+1} - x^*\|^2 \leq \|x^k - x^*\|^2 - \frac{2}{L} (f(x^k) - f^*)$ . Summing over k yields the bound.

#### 10 Line search and guaranteed decrease

**Definition 10.1** (Armijo backtracking). Given  $c \in (0,1)$  and shrinkage factor  $\beta \in (0,1)$ , set  $t \leftarrow 1$  and decrease  $t \leftarrow \beta t$  until

$$f(x - t\nabla f(x)) \le f(x) - ct \|\nabla f(x)\|^2.$$

**Proposition 10.2** (Armijo accepts small enough steps). If f is L-smooth, then Armijo with any  $c \leq \frac{1}{2}$  accepts any  $t \leq 1/L$ . In particular, the procedure always terminates.

*Proof.* By L-smoothness,  $f(x-tg) \leq f(x) - t\|g\|^2 + \frac{L}{2}t^2\|g\|^2$  with  $g = \nabla f(x)$ . If  $t \leq 1/L$ , then  $-t + \frac{L}{2}t^2 \leq -\frac{1}{2}t$ , hence  $f(x-tg) \leq f(x) - \frac{1}{2}t\|g\|^2$ , which is Armijo with  $c \leq \frac{1}{2}$ .

### 11 Quadratics: spectral viewpoint and exact line search

Consider  $f(x) = \frac{1}{2}x^T A x - b^T x$  with A > 0 (unique minimizer  $x^* = A^{-1}b$ ).

• With constant  $t \in (0, \frac{2}{\lambda_{\max}(A)})$ ,

$$x^{k+1} - x^* = (I - tA)(x^k - x^*), \quad ||x^k - x^*||_A \le \rho^k ||x^0 - x^*||_A, \quad \rho = \max_i |1 - t\lambda_i(A)|.$$

• With exact line search,

$$t_k = \operatorname*{argmin}_{\alpha \ge 0} f(x^k - \alpha \nabla f(x^k)) = \frac{\|\nabla f(x^k)\|^2}{\nabla f(x^k)^T A \nabla f(x^k)}.$$

These formulas make the role of the condition number  $\kappa = \lambda_{\text{max}}/\lambda_{\text{min}}$  explicit and explain zig-zagging in elongated valleys.

#### 12 Practical convergence and local vs. global

Remark 12.1 (Exact line search dominates fixed t). For t = 1/L, the exact-line-search iterate satisfies

$$f(x^{k+1}) = \min_{\alpha > 0} f(x^k - \alpha \nabla f(x^k)) \le f(x^k - \frac{1}{L} \nabla f(x^k)),$$

so it never does worse (and is typically better) in function decrease.

Remark 12.2 (Local vs. global). Rates like Theorem ?? are global under PL. For general nonconvex f, PL may only hold in a neighborhood of a minimum (a local linear rate), even when iterates globally decrease.

#### 13 Worked examples

**Example 13.1** (Least squares step sizes). Let  $f(x) = \frac{1}{2} ||Ax - b||^2$ . Then  $L = \lambda_{\max}(A^T A)$ . If A has full column rank,  $\mu = \lambda_{\min}(A^T A)$ , so GD with t = 1/L has linear rate  $(1 - \mu/L)^k = (1 - 1/\kappa)^k$ . (Compute L and  $\mu$  from the spectrum of  $A^T A$ .)

**Example 13.2** (Logistic regression step sizes). For  $f(x) = \sum_i \log(1 + \exp(b_i a_i^T x))$ ,  $\nabla^2 f(x) = A^T D(x) A$  with  $0 \leq D(x) \leq \frac{1}{4}I$ , hence  $L \leq \frac{1}{4}\lambda_{\max}(A^T A)$ . On bounded domains with A full column rank,  $\mu > 0$  exists, giving linear convergence with GD. (Empirically, backtracking picks steps near 1/L early on.)

Gotcha 13.3 (Units and step size). Gradients live in the dual space and carry units;  $x^{k+1} = x^k - t\nabla f(x^k)$  implies t has units of (variable units)<sup>2</sup>. Mismatched units make t hard to tune; standardize features.

### 14 Summary: what to remember

- L-smooth  $\Rightarrow$  quadratic upper bound;  $\mu$ -strongly convex  $\Rightarrow$  quadratic lower bound.
- PL strictly generalizes strong convexity in the sense of convergence proofs; it applies beyond convex functions.
- Under L-smooth + PL, GD with t = 1/L converges linearly with rate  $(1 \mu/L)^k$ .
- For convex L-smooth f without PL, GD achieves O(1/k) sublinear rate.
- Backtracking Armijo guarantees sufficient decrease and terminates; exact line search often accelerates.

### Appendix A. The descent lemma (proof and variations)

**Lemma 14.1** (Descent lemma). If f is L-smooth, then for all x, y,

$$f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{L}{2} ||y - x||^2.$$

*Proof.* Define  $\phi(t) = f(x + t(y - x))$ . Then  $\phi'(t) = (y - x)^T \nabla f(x + t(y - x))$  and

$$\phi(1) - \phi(0) = \int_0^1 \phi'(t), dt = \int_0^1 \left[ \nabla f(x) + (\nabla f(x + t(y - x)) - \nabla f(x)) \right]^T (y - x), dt.$$

Apply Cauchy-Schwarz and Lipschitz continuity of  $\nabla f$  to bound the second term by  $\frac{L}{2}||y-x||^2$ .

**Corollaries.** (i) For GD with  $t \le 1/L$ ,  $f(x^{k+1}) \le f(x^k) - (t - \frac{L}{2}t^2)\|\nabla f(x^k)\|^2$ . (ii) With t = 1/L,  $f(x^{k+1}) \le f(x^k) - \frac{1}{2L}\|\nabla f(x^k)\|^2$  (used in Theorem ??).

#### Appendix B. Equivalent smoothness characterizations

Under twice differentiability, the following are equivalent:

L-smooth; 
$$\iff$$
;  $\nabla^2 f(x) \leq LI \ \forall x \iff \|\nabla f(y) - \nabla f(x)\| \leq L\|y - x\| \ \forall x, y.$ 

(See Definition ??.)

## Appendix C. Quadratics in detail

For  $f(x) = \frac{1}{2}x^T A x - b^T x$  with A > 0:

$$L = \lambda_{\max}(A), \quad \mu = \lambda_{\min}(A), \quad x^{k+1} - x^* = (I - tA)(x^k - x^*).$$

The optimal fixed t minimizes  $\max_i \|1 - t\lambda_i(A)\|$ , attained at  $t = \frac{2}{\lambda_{\max} + \lambda_{\min}}$ , with rate  $\rho = \frac{\kappa - 1}{\kappa + 1}$  in the A-norm; exact line search uses  $t_k = \frac{\|\nabla f(x^k)\|^2}{\nabla f(x^k)^T A \nabla f(x^k)}$ .

# Appendix D. Backtracking always terminates

From Appendix A,  $f(x - t\nabla f(x)) \le f(x) - t\|\nabla f(x)\|^2 + \frac{L}{2}t^2\|\nabla f(x)\|^2$ . For  $t \le \min 1, L^{-1}$ , the Armijo condition with  $c \le 1/2$  holds. Hence halving will eventually find an acceptable t. (This formalizes the slide's "A: yes!" remark.)

## Appendix E. PL without convexity

**Example 14.2** (A nonconvex PL function). Let  $f(x) = \frac{1}{2} \operatorname{dist}(x, \mathcal{M})^2$  where  $\mathcal{M}$  is a closed subspace; PL holds with  $\mu = 1$  though f is flat along  $\mathcal{M}$  and not strongly convex. Under PL, GD still decreases linearly in objective to  $f^* = 0$ , but  $x^k$  may converge only to the set  $\mathcal{M}$  (not to a unique point). (Compare the slides' "river valley" comment.)

## Appendix F. When GD diverges

For  $f(x) = \frac{1}{2}Lx^2$  in 1D, the GD map is  $x^{k+1} = (1 - tL)x^k$ . If t > 2/L, then ||1 - tL|| > 1 and iterates diverge even though f is convex and smooth. This illustrates the tight stability range  $t \in (0, 2/L)$  for quadratics.

#### Appendix G. Units, scaling, and step-size choice

Gradients inhabit the dual space: if x has units "meters,"  $\nabla f$  can have units "1/meters," so t carries "meters<sup>2</sup>." Poor scaling across coordinates makes a single global t awkward; standardizing features and rescaling variables can make L and  $\mu$  more benign and GD more stable.