CS257 Linear and Convex Optimization Lecture 8

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Recap: QP, QCQP

Quadratic program (QP)

$$\min_{x} \frac{1}{2}x^{T}Qx + c^{T}x$$
s.t. $Bx \le d$

$$Ax = b$$

Quadratically constrained quadratic program (QCQP)

$$\min_{\mathbf{x}} \quad \frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x} + \mathbf{c}^T \mathbf{x}$$
s.t.
$$\frac{1}{2} \mathbf{x}^T \mathbf{Q}_i \mathbf{x} + \mathbf{c}_i^T \mathbf{x} + \mathbf{d}_i \le 0, \quad i = 1, 2, \dots, m$$

$$\mathbf{A} \mathbf{x} = \mathbf{b}$$

Recap: LS, Lasso, and Ridge Regressions

Given $\mathbf{y} \in \mathbb{R}^n$, $\mathbf{X} \in \mathbb{R}^{n \times p}$.

Linear least squares regression

$$\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2$$

Lasso

$$\min_{\mathbf{w}} \quad \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_{2}^{2}$$

s. t. $\|\mathbf{w}\|_{1} < t$

Ridge regression

$$\begin{aligned} & \min_{\boldsymbol{w}} & & \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2 \\ & \text{s. t.} & & \|\boldsymbol{w}\|_2^2 \leq t \end{aligned}$$

Recap: GP

Posynomial form

$$\begin{aligned} & \min_{\boldsymbol{x}} & & \sum_{k=1}^{p_0} \gamma_{0k} x_1^{a_{0k1}} x_2^{a_{0k2}} \cdots x_n^{a_{0kn}} \\ & \text{s. t.} & & \sum_{k=1}^{p_i} \gamma_{ik} x_1^{a_{ik1}} x_2^{a_{ik2}} \cdots x_n^{a_{ikn}} \leq 1, \quad i = 1, \dots, m \\ & & & \eta_j x_1^{c_{j1}} x_2^{c_{j2}} \cdots x_n^{c_{jn}} = 1, \quad j = 1, \dots, r \end{aligned}$$

Convex form

$$\min_{\mathbf{y}} \quad \log \left(\sum_{k=1}^{p_0} e^{\mathbf{a}_{0k}^T \mathbf{y} + b_{0k}} \right)$$
s. t.
$$\log \left(\sum_{k=1}^{p_i} e^{\mathbf{a}_{ik}^T \mathbf{y} + b_{ik}} \right) \le 0, \quad i = 1, \dots, m$$

$$\mathbf{c}_j^T \mathbf{y} + d_j = 0, \quad j = 1, \dots, r$$

Contents

1. Gradient Descent

Unconstrained Optimization Problems

Consider an unconstrained, smooth convex optimization problem

$$\min_{\mathbf{x}} f(\mathbf{x})$$

where f is convex and differentiable on \mathbb{R}^n .

The optimal solution satisfies the first-order optimality condition

$$\nabla f(\mathbf{x}^*) = \mathbf{0}$$

In some rare cases, this yields closed-form solutions, e.g.

$$\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2$$

has closed-form solution

$$\mathbf{w}^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

But in most cases we need numerical algorithms.

Descent Method

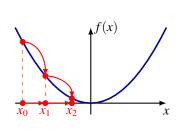
1: choose initial point $x_0 \in \mathbb{R}^n$

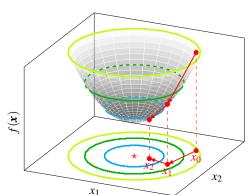
2: repeat

3: choose descent direction $d_k \in \mathbb{R}^n$ and step size $t_k > 0$

4: $x_{k+1} = x_k + t_k d_k$ s.t. $f(x_{k+1}) < f(x_k)$

5: until stopping criterion is satisfied





Questions

- How to choose d_k and t_k ?
- Does x_k converge to x^* ?

Descent Direction

 d_k is a descent direction at x_k if for all small enough t > 0

$$g(t) \triangleq f(\mathbf{x}_k + t\mathbf{d}_k) < f(\mathbf{x}_k) = g(0)$$

For differentiable f (not necessarily convex),

- if d_k is a descent direction, then $g'(0) = d_k^T \nabla f(x_k) \leq 0$;
- if $g'(0) = d_k^T \nabla f(x_k) < 0$, then d_k is a descent direction.

For convex f, by the first-order condition for convexity,

$$f(\mathbf{x}_k) > f(\mathbf{x}_k + t\mathbf{d}_k) \ge f(\mathbf{x}_k) + t\mathbf{d}_k^T \nabla f(\mathbf{x}_k).$$

 $d_k^T \nabla f(\mathbf{x}_k) < 0$ is also necessary for d_k to be a descent direction.

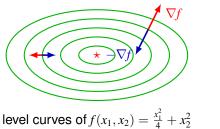
For convex differentiable f,

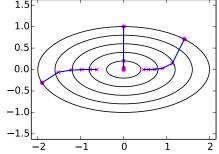
$$d_k$$
 is a descent direction $\iff d_k^T \nabla f(x_k) < 0$

Gradient Descent

Choose
$$d_k = -\nabla f(\mathbf{x}_k)$$
, $d_k^T \nabla f(\mathbf{x}_k) = -\|\nabla f(\mathbf{x}_k)\|_2^2 < 0$ unless $\nabla f(\mathbf{x}_k) = 0$.

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - t_k \nabla f(\boldsymbol{x}_k)$$





Question. What happens if $\nabla f(\mathbf{x}_k) = \mathbf{0}$?

Max-rate Descending Direction

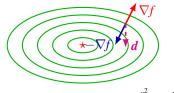
- $-\nabla f(\mathbf{x}_k)$ is the max-rate descending direction
 - If $||d_k||_2 = 1$, the rate of change of f at x_k along the direction d_k is

$$\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k) = g'(0) = \lim_{t \downarrow 0} \frac{f(\boldsymbol{x}_k + t\boldsymbol{d}_k) - f(\boldsymbol{x}_k)}{t} = \boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k)$$

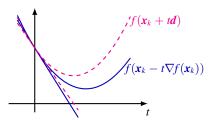
by the Cauchy-Schwarz inequality,

$$d_k^T \nabla f(x_k) \ge -\|d_k\|_2 \cdot \|\nabla f(x_k)\|_2 = -\|\nabla f(x_k)\|_2$$

with equality iff $d_k = -\nabla f(\mathbf{x}_k) / \|\nabla f(\mathbf{x}_k)\|$



level curves of $f(x_1, x_2) = \frac{x_1^2}{4} + x_2^2$



Gradient Descent Algorithm

- 1: initialization $x \leftarrow x_0 \in \mathbb{R}^n$
- 2: while $\|\nabla f(x)\| > \delta$ do
- 3: $\mathbf{x} \leftarrow \mathbf{x} t \nabla f(\mathbf{x})$
- 4: end while
- 5: return x

Step size (aka learning rate in machine learning)

- the above algorithm uses constant step size t for all iterations
- there are other methods for choosing *t* for each iteration, e.g. exact line search, backtracking line search

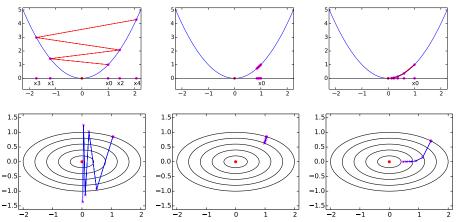
Stopping criterion

- ideally, stop if $\nabla f(\mathbf{x}) = 0$ (optimality condition), but impractical
- more practical: stop when $\|\nabla f(x)\| \le \delta$ for some small δ
- other criteria: $|f(x_{\sf new}) f(x_{\sf old})| \le \delta$, $\frac{|f(x_{\sf new}) f(x_{\sf old})|}{|f(x_{\sf old})|} \le \delta$, ...
- in practice, also stop if maximum # of iterations is reached

Large vs. Small Step Size

Consider constant step size. How large should the step size be?

- Too large: may oscillate and diverge
- Too small: may be too slow
- "Just right": fast convergence



1D Example

Consider $f(x) = \frac{1}{2}ax^2$, where a > 0.

- gradient at x_k is $f'(x_k) = ax_k$, so $d_k = -ax_k$ in gradient descent
- update

$$x_{k+1} = x_k - tf'(x_k) = (1 - at)x_k$$

• in order for $f(x_{k+1}) < f(x_k)$, the step size should satisfy

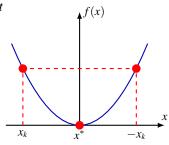
$$|x_{k+1}| < |x_k| \implies |1 - at| < 1 \implies 0 < t < \frac{2}{a}$$

• $x_k \to x^* = 0$ geometrically for such t

Note f satisfies

- $\bullet |f'(x) f'(y)| = a|x y|$
- f''(x) = a

f' is Lipschitz continuous



Lipschitz Continuity

A function $f: \mathbb{R}^n \to \mathbb{R}^m$ is Lipschitz continuous with Lipschitz constant L>0, or simply L-Lipschitz, if

$$||f(\mathbf{x}) - f(\mathbf{y})|| \le L||\mathbf{x} - \mathbf{y}||, \quad \forall \mathbf{x}, \mathbf{y}$$

Note. Lipschitz continuity can be defined with respect to any norms. But we will assume the norms in the above definition are the 2-norms in \mathbb{R}^n and \mathbb{R}^m , respectively, unless stated otherwise.

Note. Lipschitz continuity implies uniform continuity.

Example.
$$f(x) = ax$$
 is $|a|$ -Lipschitz, $|f(x) - f(y)| = |a| \cdot |x - y|$

Example.
$$f(x) = |x|$$
 is 1-Lipschitz, $|f(x) - f(y)| = ||x| - |y|| \le |x - y|$

Example. $f(x) = a^T x$ is ||a||-Lipschitz, $|a^T x - a^T y| \le ||a|| \cdot ||x - y||$ by the Cauchy-Schwarz inequality.

Lipschitz Continuity (cont'd)

Example. Let
$$\mathbf{Q} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$
. $f(\mathbf{x}) = \mathbf{Q}\mathbf{x} = (x_1, 2x_2)^T$ is 2-Lipschitz.

$$f(\mathbf{x}) - f(\mathbf{y}) = (x_1 - y_1, 2x_2 - 2y_2)^T = (d_1, 2d_2)^T$$
$$\|f(\mathbf{x}) - f(\mathbf{y})\| = \sqrt{d_1^2 + 4d_2^2} \le 2\sqrt{d_1^2 + d_2^2} = 2\|\mathbf{x} - \mathbf{y}\|$$

More generally, f(x) = Qx with $Q \succeq O$ is $\lambda_{\max}(Q)$ -Lipschitz, where $\lambda_{\max}(Q)$ is the largest eigenvalue of Q^1 .

Proof. Let d = x - y.

$$||f(x) - f(y)|| = ||Qd|| = \sqrt{d^T Q^2 d} \le \sqrt{\lambda_{\max}(Q^2) ||d||^2} = \lambda_{\max}(Q) ||x - y||$$

The last equality uses the fact $\lambda_{\max}(\mathbf{Q}^2) = \lambda_{\max}^2(\mathbf{Q})$.

¹if we do not assume $Q \succeq O$, then we should replace $\lambda_{\max}(Q)$ by $\sigma_{\max}(Q)$, the largest singular value of Q

Appendix: Bounds on Quadratic Forms

Proposition. For a symmetric matrix $Q \in \mathbb{R}^{n \times n}$,

$$\lambda_{\min} \|\mathbf{x}\|_2^2 \le \mathbf{x}^T \mathbf{Q} \mathbf{x} \le \lambda_{\max} \|\mathbf{x}\|_2^2, \quad \forall \mathbf{x} \in \mathbb{R}^n$$

where λ_{\max} and λ_{\min} are the largest and the smallest eigenvalues of ${\bf Q}$, respectively.

Proof. Recall that Q can be orthogonally diagonalized, i.e. $Q = U\Lambda U^T$, where $\Lambda = \text{diag}\{\lambda_1, \dots, \lambda_n\}$ and $U^TU = I$ (Lecture 2, slide 24). Let x = Uy.

$$\mathbf{x}^T \mathbf{Q} \mathbf{x} = \mathbf{y}^T (\mathbf{U}^T \mathbf{Q} \mathbf{U}) \mathbf{y} = \mathbf{y}^T \mathbf{\Lambda} \mathbf{y} = \sum_{i=1}^n \lambda_i y_i^2 \le \sum_{i=1}^n \lambda_{\max} y_i^2 = \lambda_{\max} ||\mathbf{y}||_2^2$$

Then use the fact that orthogonal transformations preserves 2-norms, i.e.

$$||x||_2^2 = x^T x = (Uy)^T (Uy) = y^T (U^T U)y = y^T y = ||y||_2^2.$$

Similarly for $x^T Q x \ge \lambda_{\min} ||x||_2^2$.

Lipschitz Continuity of Gradient

A function is L-smooth if it is differentiable and its gradient is L-Lipschitz, i.e.

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \le L\|\mathbf{x} - \mathbf{y}\|, \quad \forall \mathbf{x}, \mathbf{y}$$

Note. L upper bounds the rate of change of ∇f

Example.
$$f(x) = \frac{1}{2}ax^2$$
 is $|a|$ -smooth, since $f'(x) = ax$ is $|a|$ -Lipschitz

Example. $f(x) = \frac{1}{2}x^TQx$ with $Q \succeq O$ is $\lambda_{\max}(Q)$ -smooth, since $\nabla f(x) = Qx$ is $\lambda_{\max}(Q)$ -Lipschitz.

With
$$\mathbf{Q} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$
, we obtain $f(\mathbf{x}) = \frac{1}{2}x_1^2 + x_2^2$ is 2-smooth.

Lemma. A twice continuously differentiable convex $f: \mathbb{R}^n \to \mathbb{R}$ is L-smooth iff $\nabla^2 f(x) \leq L I$, meaning $L I - \nabla^2 f(x) \succeq O$, or equivalently $\lambda_{\max}(\nabla^2 f(x)) \leq L$.

Lipschitz Continuity of Gradient (cont'd)

Lemma. A twice continuously differentiable $f: \mathbb{R}^n \to \mathbb{R}$ is L-smooth iff for any x, $-LI \leq \nabla^2 f(x) \leq LI$, or equivalently $|\lambda| \leq L$ for all eigenvalues λ of $\nabla^2 f(x)$.

Proof. " \Leftarrow ". Assume $-LI \leq \nabla^2 f(x) \leq LI$ for all x.

By the Mean Value Theorem, there exists z = y + t(x - y) for some $t \in [0, 1]$ s.t.

$$\nabla f(\mathbf{x}) - \nabla f(\mathbf{y}) = \nabla^2 f(\mathbf{z})(\mathbf{x} - \mathbf{y})$$

Since $-L\mathbf{I} \preceq \nabla^2 f(\mathbf{x}) \preceq L\mathbf{I}$,

$$\|\nabla f(x) - \nabla f(y)\| = \|\nabla^2 f(z)(x - y)\| \le L\|x - y\|$$

by the proof on slide 15.

Lipschitz Continuity of Gradient (cont'd)

Proof (cont'd). " \Rightarrow ". Assume f is L-smooth. Fix a direction d. Let $h(t) = \nabla f(x + td)$. Since f is L-smooth,

$$||g(t) - g(0)|| = ||\nabla f(x + td) - \nabla f(x)|| \le L||td||$$

SO

$$\left\| \frac{g(t) - g(0)}{t} \right\| \le L \|\boldsymbol{d}\|$$

Letting $t \to 0$ and using the chain rule

$$\|\nabla^2 f(\mathbf{x})\mathbf{d}\| = \|g'(0)\| \le L\|\mathbf{d}\|$$

Let *d* be an eigenvector of $\nabla^2 f(x)$ with associated eigenvalue λ ,

$$|\lambda| \cdot ||\boldsymbol{d}|| = ||\lambda \boldsymbol{d}|| \le L||\boldsymbol{d}|| \implies |\lambda| \le L$$

Quadratic Upper Bound

Lemma. If f is L-smooth, then

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

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

$$f(\mathbf{y})$$

$$f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x})$$

Note. The upper bound does not assume the convexity of f.

If $\nabla^2 f(x) \leq LI$, this is intuitive from the second-order Taylor expansion

$$f(\mathbf{y}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) + \frac{1}{2} (\mathbf{y} - \mathbf{x})^T \nabla^2 f(\mathbf{z}) (\mathbf{y} - \mathbf{x})$$

for some z on the line segment between x and y. (Check $f(x) = \frac{1}{2}x^T Qx$)

Proof

Let
$$z(t) = \mathbf{x} + t(\mathbf{y} - \mathbf{x})$$
 and $g(t) = f(z(t))$. Then $g(0) = f(\mathbf{x})$, $g(1) = f(\mathbf{y})$, $g'(t) = \nabla f(z(t))^T (\mathbf{y} - \mathbf{x})$, $g'(0) = \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x})$.

1. By the Newton-Leibniz formula,

$$g(1) - g(0) - g'(0) = \int_0^1 [g'(t) - g'(0)]dt \le \int_0^1 |g'(t) - g'(0)|dt$$

2. By the Cauchy-Schwarz inequality and L-smoothness

$$|g'(t) - g'(0)| = |[\nabla f(z(t)) - \nabla f(x)]^T (y - x)|$$

$$\leq ||\nabla f(z(t)) - \nabla f(x)|| \cdot ||y - x||$$

$$\leq L||z(t) - x|| \cdot ||y - x||$$

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

3. Plugging $|g'(t) - g'(0)| \le tL ||x - y||^2$ into step 1,

$$f(\mathbf{y}) - f(\mathbf{x}) - \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) = g(1) - g(0) - g'(0) \le \frac{L}{2} ||\mathbf{x} - \mathbf{y}||^2$$

Consequence of Quadratic Upper Bound

For *L*-smooth f, the sequence $\{x_k\}$ produced by gradient descent satisfies

$$f(\mathbf{x}_{k+1}) \le f(\mathbf{x}_k) - t\left(1 - \frac{Lt}{2}\right) \|\nabla f(\mathbf{x}_k)\|^2$$

Proof. Plugging in $x = x_k$ and $y = x_{k+1} = x_k - t\nabla f(x_k)$ in the quadratic upper bound,

$$f(\mathbf{x}_{k+1}) \le f(\mathbf{x}_k) - t \|\nabla f(\mathbf{x}_k)\|^2 + \frac{L}{2}t^2 \|\nabla f(\mathbf{x}_k)\|^2$$
$$= f(\mathbf{x}_k) - t \left(1 - \frac{Lt}{2}\right) \|\nabla f(\mathbf{x}_k)\|^2$$

Note. If $\nabla f(\mathbf{x}_k) \neq 0$ and $0 < t < \frac{2}{L}$, then $f(\mathbf{x}_{k+1}) < f(\mathbf{x}_k)$, so gradient descent with step size $t \in (0, 2/L)$ is indeed a descent method.

Note. We can lower bound the decrease in function value in each step. In particular, for $0 < t \le \frac{1}{L}$,

$$f(\mathbf{x}_k) - f(\mathbf{x}_{k+1}) \ge \frac{t}{2} \|\nabla f(\mathbf{x}_k)\|^2$$

Convergence Analysis

Theorem. If f is convex and L-smooth, and x^* is a minimum of f, then for step size $t \in (0, \frac{1}{L}]$, the sequence $\{x_k\}$ produced by the gradient descent algorithm satisfies

$$f(\mathbf{x}_k) - f(\mathbf{x}^*) \le \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|^2}{2tk}$$

Notes.

- $f(\mathbf{x}_k) \downarrow f^*$ as $k \to \infty$.
- Any limiting point of x_k is an optimal solution.
- The rate of convergence is O(1/k), i.e. # of iterations to guarantee $f(\mathbf{x}_k) f(\mathbf{x}^*) \le \epsilon$ is $O(1/\epsilon)$. For $\epsilon = 10^{-p}$, $k = O(10^p)$, exponential in the number of significant digits!
- Faster convergence with larger t; best $t = \frac{1}{L}$, but L is unknown.
- Good initial guess helps.

Proof

1. By the basic gradient step $x_{k+1} = x_k - t\nabla f(x_k)$,

$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\|^2 = \|\mathbf{x}_k - t\nabla f(\mathbf{x}_k) - \mathbf{x}^*\|^2$$

= $\|\mathbf{x}_k - \mathbf{x}^*\|^2 + t^2 \|\nabla f(\mathbf{x}_k)\|^2 + 2t\nabla f(\mathbf{x}_k)^T (\mathbf{x}^* - \mathbf{x}_k)$

2. By the first-order condition for convexity,

$$\nabla f(\mathbf{x}_k)^T(\mathbf{x}^* - \mathbf{x}_k) \le f(\mathbf{x}^*) - f(\mathbf{x}_k)$$

3. Plugging 2 into 1,

$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\|^2 \le \|\mathbf{x}_k - \mathbf{x}^*\|^2 + t^2 \|\nabla f(\mathbf{x}_k)\|^2 + 2t[f(\mathbf{x}^*) - f(\mathbf{x}_k)]$$

4. Plugging in $\frac{t}{2} \|\nabla f(\mathbf{x}_k)\|^2 \le f(\mathbf{x}_k) - f(\mathbf{x}_{k+1})$ from slide 21,

$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\|^2 \le \|\mathbf{x}_k - \mathbf{x}^*\|^2 + 2t[f(\mathbf{x}^*) - f(\mathbf{x}_{k+1})]$$

Proof (cont'd)

5. Rearranging,

$$f(\mathbf{x}_{k+1}) - f(\mathbf{x}^*) \le \frac{\|\mathbf{x}_k - \mathbf{x}^*\|^2 - \|\mathbf{x}_{k+1} - \mathbf{x}^*\|^2}{2t}$$

6. Summing over k from 0 to N-1,

$$\sum_{k=0}^{N-1} [f(\mathbf{x}_{k+1}) - f(\mathbf{x}^*)] \le \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|^2 - \|\mathbf{x}_N - \mathbf{x}^*\|^2}{2t} \le \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|^2}{2t}$$

7. Recalling the descent property $f(x_{k+1}) \leq f(x_k)$,

$$f(\mathbf{x}_N) - f(\mathbf{x}^*) \le \frac{1}{N} \sum_{k=0}^{N-1} [f(\mathbf{x}_{k+1}) - f(\mathbf{x}^*)] \le \frac{\|\mathbf{x}_0 - \mathbf{x}^*\|^2}{2tN}$$