AMA 505: Optimization Methods

Subject Lecturer: Ting Kei Pong

Lecture 2

Unconstrained Optimization

Optimality conditions and gradient descent

Problem setting

Aim: Given $f \in C^1(\mathbb{R}^n)$, solve

$$\operatorname*{Minimize}_{x \in \mathbb{R}^n} \quad f(x)$$

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  - ⋆ Nelder-Mead method; etc.

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  - ⋆ Newton's method (if f is C^2);
  - ⋆ quasi-Newton method; etc.

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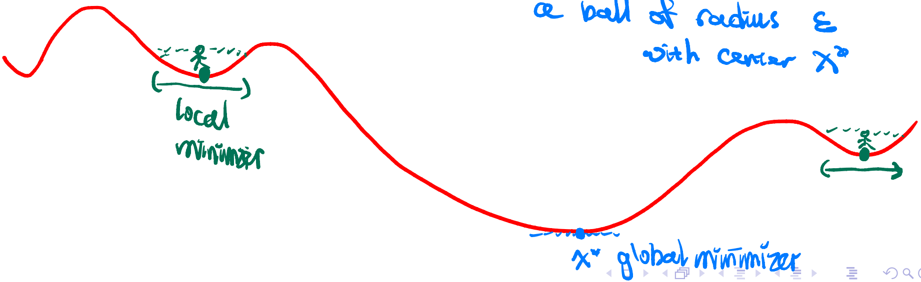
In general, finding global minimizers for f is NP-hard.

Minimizers

Definition:

- We say that x^* is a global minimizer of f if $f(x) \geq f(x^*)$ for all $x \in \mathbb{R}^n$.
- We say that x^* is a local minimizer of f if there exists $\epsilon > 0$ so that $f(x) \geq f(x^*)$ for all x satisfying $\|x - x^*\|_2 < \epsilon$.

a ball of radius ε with center x^*



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Remarks:

- Finding local minimizers is also NP-hard in general.
- In order to set a modest goal, we look at more properties of local minimizers.

1st-order necessary conditions

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Proof: Fix any $h \in \mathbb{R}^n$. Then for all sufficiently small $t > 0$, there exists $\xi^t \in \{x^* + sth : \; s \in (0,1)\}$ such that we have

$$f(x^*) \le f(x^* + th) = f(x^*) + t[\nabla f(\xi^t)]^T h.$$

Hence,

$$[\nabla f(\xi^t)]^T h \ge 0.$$

Passing to the limit and noting that $\xi^t \to x^*$, we conclude that $[\nabla f(x^*)]^T h \ge 0.$

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Passing to the limit and noting that $\xi^t \to x^*$, we conclude that $[\nabla f(x^*)]^T h \geq 0$.

Set $h = -\nabla f(x^*)$ to obtain the desired conclusion.

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Theorem 2.2. Let $f \in C^2(\mathbb{R}^n)$.

1. If x^* is a local minimizer of f, then $\nabla^2 f(x^*) \succeq 0$.
2. If x^* is a stationary point of f and $\nabla^2 f(x^*) \succ 0$, then x^* is a local minimizer.

Proof: We first prove part 1. Fix any $h \in \mathbb{R}^n$. Then for all sufficiently small $t > 0$, there exists $\xi^t \in \{x^* + t\alpha h : \ \alpha \in (0, 1)\}$ such that

$$f(x^*) \leq f(x^* + th) = f(x^*) + t \underbrace{[\nabla f(x^*)]^T}_{=0} h + \frac{t^2}{2} h^T \nabla^2 f(\xi^t) h$$

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Hence, $h^T \nabla^2 f(\xi^t) h \geq 0$. Passing to the limit as $t \downarrow 0$, we obtain $h^T \nabla^2 f(x^*) h \geq 0$. Since this is true for any $h \in \mathbb{R}^n$, it follows that $\nabla^2 f(x^*) \succeq 0$.

2nd-order conditions cont.

Proof of Theorem 2.2 cont.: We now prove part 2. Since $\nabla^2 f(x^*) \succ 0$ and $f \in C^2(\mathbb{R}^n)$, there exists $\epsilon > 0$ so that $\nabla^2 f(y) \succ 0$ whenever $\|y - x^*\|_2 < \epsilon$.

2nd-order conditions cont.

Proof of Theorem 2.2 cont.: We now prove part 2. Since $\nabla^2 f(x^*) \succ 0$ and $f \in C^2(\mathbb{R}^n)$, there exists $\epsilon > 0$ so that $\nabla^2 f(y) \succ 0$ whenever $\|y - x^*\|_2 < \epsilon$.

Consider any nonzero h with $\|h\|_2 < \epsilon$. Then

$$\begin{aligned} f(x^* + h) &= f(x^*) + \int_0^1 \nabla f(x^* + th)^T h \, dt \\ &= f(x^*) + \int_0^1 [\underbrace{\nabla f(x^* + th)^T h}_{\varphi(t)} - \underbrace{\nabla f(x^*)^T h}_{\varphi(0)}] dt \\ &= f(x^*) + \int_0^1 t h^T \nabla^2 f(x^* + \xi_t h) h dt \end{aligned}$$

for some $\xi_t \in [0, t] \subseteq [0, 1]$. Hence, $h^T \nabla^2 f(x^* + \xi_t h) h > 0$ and thus $f(x^* + h) \geq f(x^*)$.

Example 1

Example: Consider the function $f(x_1, x_2) = x_1^2 + (x_1 + 1)x_2^2$. Then

$$\nabla f(x) = \begin{bmatrix} 2x_1 + x_2^2 \\ 2x_2(x_1 + 1) \end{bmatrix}.$$

Hence, $\nabla f(x) = 0$ gives stationary points:

$$(0, 0), \ \ (-1, \sqrt{2}), \ \ (-1, -\sqrt{2}).$$

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Next,

$$\nabla^2 f(x) = \begin{bmatrix} 2 & 2x_2 \\ 2x_2 & 2x_1 + 2 \end{bmatrix}.$$

Example 1 cont.

Example cont.: Then

$$\nabla^2 f(0,0) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \succ 0 \quad \Rightarrow (0,0) \text{ is a local minimizer.}$$

$$\nabla^2 f(-1,\sqrt{2}) = \begin{bmatrix} 2 & 2\sqrt{2} \\ 2\sqrt{2} & 0 \end{bmatrix} \text{ is indefinite}$$

$$\Rightarrow (-1,\sqrt{2}) \text{ is not a local minimizer nor maximizer.}$$

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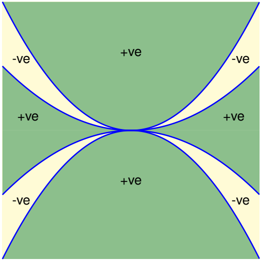
Example 2

Example: Consider the function $f(x_1, x_2) = (x_2^2 - x_1^4)\left(x_2^2 - \frac{x_1^4}{4}\right)$ at the stationary point $(0, 0)$. Then for any $h \in \mathbb{R}^2 \backslash \{0\}$, there exists $t_0 > 0$ such that

$$f(th) > 0 \ \text{ for all } t \in (0, t_0).$$

However, (0, 0) is not a local minimizer of f! Note, however, that $\nabla^2 f(0, 0) = 0 \succeq 0$.



Example 2 cont.

Example cont.: Details: We show that for any $h \in \mathbb{R}^2 \backslash \{0\}$, there exists $t_0 > 0$ such that

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Case 1: $h = (h_1, h_2)$ for some $h_2 \neq 0$. Then

$$f(th) = t^4(h_2^2 - t^2 h_1^4)\left(h_2^2 - t^2 \frac{h_1^4}{4}\right)$$

is positive for all sufficiently small $t > 0$.

Case 2: $h = (h_1, 0)$ for some $h_1 \neq 0$. Then

$$f(th) = (-t^4 h_1^4)\left(-t^4 \frac{h_1^4}{4}\right)$$

is positive for all $t > 0$.

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$$(x_1, x_2) = (\sqrt{3}\epsilon, 2\epsilon^2)$$

Then $\|(x_1, x_2)\|_2 < 3\epsilon$ and

$$f(x_1, x_2) = \epsilon^8(4 - 9)\left(4 - \frac{9}{4}\right) < 0.$$

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Since $\epsilon > 0$ is arbitrary, we have shown that:

No matter how small we shrink the neighborhood $\{x : \|x\|_2 < 3\epsilon\}$, there is always a point in it such that f goes negative.

Thus, $(0, 0)$ is not a local minimizer.

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Aim (Revised): Given $f \in C^1(\mathbb{R}^n)$:

- Find a stationary point of f (i.e., x^* so that $\nabla f(x^*) = 0$).
- Test whether it is a local minimizer by looking at $\nabla^2 f(x^*)$ if $f \in C^2(\mathbb{R}^n)$ and if Hessian is not too hard to compute.

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Newton's method
Let $x^0 \in \mathbb{R}^n$. For $k = 0, 1, 2, \ldots$, update

$$x^{k+1} = x^k - [\nabla^2 f(x^k)]^{-1} \nabla f(x^k).$$

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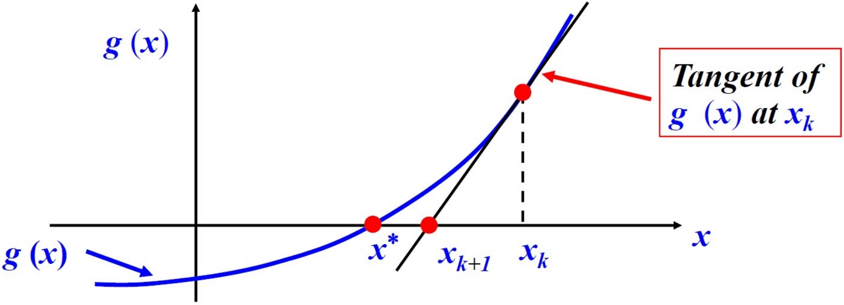
Note:

- The above iterates require that $\nabla^2 f(x^k)$ is invertible for each k. The method fails if $\nabla^2 f(x^k)$ is singular.
- In practice, computing $[\nabla^2 f(x^k)]^{-1} \nabla f(x^k)$ can be expensive.

Newton's method

- In $\mathbb{R}$, to solve $g(x) = 0$ with $g \in C^1(\mathbb{R})$, the Newton's method takes the form

$$x_{k+1} = x_k - \frac{g(x_k)}{g'(x_k)}.$$



Newton's method cont.

Under certain conditions, Newton's method enjoys fast local convergence. For simplicity, we only state and prove the case for $\mathbb{R}$.

Theorem 2.3. (Quadratic convergence of Newton's method)
Let $g \in C^2(\mathbb{R})$ and x_* satisfies $g(x_*) = 0$ and $g'(x_*) \neq 0$. Then there exists $\epsilon > 0$ so that if $|x_0 - x_*| < \epsilon$, then the Newton's iterate $x_{k+1} = x_k - g(x_k)/g'(x_k)$ is well defined and there exists $M > 0$ so that

$$|x_{k+1} - x_*| \leq M|x_k - x_*|^2.$$

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- This means that if x_0 is initialized sufficiently close to a nice solution, the Newton's method is well defined and converges very fast: roughly doubling the number of correct digits every iteration.

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Note:

- This means that if x_0 is initialized sufficiently close to a nice solution, the Newton's method is well defined and converges very fast: roughly doubling the number of correct digits every iteration.
- Using a more delicate analysis, one can replace "$g \in C^2(\mathbb{R})$" by "$g \in C^1(\mathbb{R})$ and $\exists L > 0$ with $|g'(x) - g'(y)| \leq L|x - y|$ for all x and y close to x_*".

Newton's method cont.

Proof of Theorem 2.3: Since $g'(x_*) \neq 0$, there exist $\epsilon_1 > 0$ and $\delta > 0$ so that $|g'(x)| > \delta$ whenever $|x - x_*| \leq \epsilon_1$. Moreover, since g'' is continuous, there exists τ so that $\tau \geq |g''(x)|$ for these x.
Now, for each such x, by Taylor's theorem, there exists ξ_x between x_* and x so that

$$0 = g(x_*) = g(x) + g'(x)(x_* - x) + 0.5g''(\xi_x)(x_* - x)^2.$$

This means

$$x - \frac{g(x)}{g'(x)} - x_* = \frac{g''(\xi_x)}{2g'(x)}(x_* - x)^2.$$

Thus

$$\left| x - \frac{g(x)}{g'(x)} - x_* \right| \leq \frac{\tau}{2\delta}|x_* - x|^2.$$

Hence, if $|x_0 - x_*| < \min\{\epsilon_1, \frac{2\delta}{\tau}\} =: \epsilon$, an induction shows that $|x_k - x_*| \leq \epsilon_1$ for all k and the desired inequality holds with $M = \frac{\tau}{2\delta}$.

Newton's method cont.

Applying Newton's method to $g(x) = x^3 - 3$ starting at $x_0 = 1.5$:

$$x_{k+1} = x_k - \frac{x_k^3 - 3}{3x_k^2}.$$

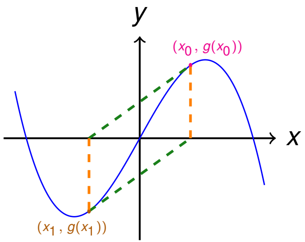
We have (in 10 s.f.)

x_1	1.444444444e+00
x_2	1.442252904e+00
x_3	1.442249570e+00
x_4	1.442249570e+00

Thus, $x_* = 1.4422$, rounded to 4 decimal places.

Failure of Newton's method

Failure of Newton's method: Besides failing when $g'(x_k) = 0$, if x^0 is too far away from x^*, Newton's method can also fail due to cycling:



Newton's method fails for $g(x) = x - x^3$, starting at $x_0 = \frac{1}{\sqrt{5}}$.

Steepest descent

- Instead of just solving for $\nabla f(x) = 0$, we take advantage of the function values of f.
- Since $f \in C^1(\mathbb{R}^n)$, we have

$$f(x+d) = f(x) + [\nabla f(x)]^T d + [\nabla f(\xi) - \nabla f(x)]^T d,$$

where $\xi \in \{x + td : \ t \in (0,1)\}$.

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where $\xi \in \{x + td : \ t \in (0,1)\}$. Thus, if $\nabla f(x) \neq 0$ (i.e., x is not stationary) and we take $d = -\alpha \nabla f(x)$ for some $\alpha > 0$, then

$$f(x - \alpha \nabla f(x)) = f(x) - \alpha \|\nabla f(x)\|_2^2 - \alpha \underbrace{([\nabla f(\xi) - \nabla f(x)]^T \nabla f(x))}_{\to 0 \text{ as } \alpha \to 0}.$$

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Hence, for sufficiently small $\alpha > 0$, it holds that

$$f(x - \alpha \nabla f(x)) < f(x).$$

Steepest descent cont.

- $-\nabla f(x)$ is called the steepest descent direction.
- A natural greedy algorithm is

Steepest descent with exact line search
Start at $x^0 \in \mathbb{R}^n$. For each $k = 0, 1, 2, \ldots,$

⋆ Set $d^k = -\nabla f(x^k)$.
⋆ Pick α_k so that

$$\alpha_k \in \operatorname{Arg\,min}\{f(x^k + \alpha d^k) : \ \alpha \geq 0\}. \tag{1}$$

⋆ Set $x^{k+1} = x^k + \alpha_k d^k$.

Note: The update $x^{k+1} = x^k + \alpha_k d^k$ is prototypical in optimization.

- d^k is called the search direction. In the above algorithm, $d^k = -\nabla f(x^k)$.
- α_k is called the step size. In the above algorithm, it is chosen according to the exact line search criterion (1).

Steepest descent cont.

- In Steepest descent with exact line search, it is implicitly assumed that a minimizer α_k exists for the exact line search subproblem (1).
  If α_k exists and $\nabla f(x^k) \neq 0$, then $\alpha_k > 0$. Why? Hence, we have

$$0 = \frac{d}{d\alpha} f(x^k + \alpha d^k)\Big|_{\alpha=\alpha_k} = (d^k)^T \nabla f(x^{k+1}) = -(\nabla f(x^k))^T \nabla f(x^{k+1}).$$

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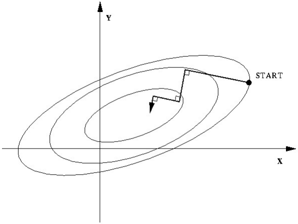
  New direction $\perp$ old direction: Creating zigzag path!
- Exact line search can be hard to perform.



Picture downloaded from http://trond.hjorteland.com/thesis/node26.html.

Armijo rule

In contrast to exact line search, usually inexact line search strategy is performed. One commonly used rule is:

Armijo rule:
Let $\sigma \in (0, 1)$, $x \in \mathbb{R}^n$ and $d \in \mathbb{R}^n$. Find $\alpha > 0$ so that

$$f(x + \alpha d) \leq f(x) + \alpha\sigma[\nabla f(x)]^T d.$$

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Examples: At an x that is not stationary,

- $d = -\nabla f(x)$ is a descent direction;
- More generally, if $D \succ 0$, then $d = -D\nabla f(x)$ is a descent direction.

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Let $\sigma \in (0, 1)$, $x \in \mathbb{R}^n$ and $d \in \mathbb{R}^n$. Find $\alpha > 0$ so that

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Definition. Let $f \in C^1(\mathbb{R}^n)$ and $x \in \mathbb{R}^n$. A $d \in \mathbb{R}^n$ is said to be a descent direction of f at x if

$$[\nabla f(x)]^T d < 0.$$

Examples: At an x that is not stationary,

- $d = -\nabla f(x)$ is a descent direction;
- More generally, if $D \succ 0$, then $d = -D\nabla f(x)$ is a descent direction.

Is the Newton direction $-[\nabla^2 f(x)]^{-1}\nabla f(x)$ a descent direction?

Armijo rule cont.

The next theorem shows that Armijo rule is not void.

Theorem 2.4:
Let $f \in C^1(\mathbb{R}^n)$, $x \in \mathbb{R}^n$, and $d \in \mathbb{R}^n$ be a descent direction at x. Let $\sigma \in (0, 1)$. Then there exists $\alpha_1 > 0$ so that for all $\alpha \in [0, \alpha_1]$,

$$f(x + \alpha d) \leq f(x) + \alpha\sigma[\nabla f(x)]^T d.$$

Armijo rule cont.

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$$f(x + \alpha d) \leq f(x) + \alpha\sigma[\nabla f(x)]^T d.$$

Proof: Since $f \in C^1(\mathbb{R}^n)$, we have for any $\alpha > 0$ that

$$f(x + \alpha d) = f(x) + \alpha[\nabla f(x)]^T d + \alpha[\nabla f(\xi) - \nabla f(x)]^T d$$
$$= f(x) + \sigma\alpha[\nabla f(x)]^T d + \alpha\Big\{(1-\sigma)[\nabla f(x)]^T d + [\nabla f(\xi) - \nabla f(x)]^T d\Big\},$$

where $\xi \in \{x + \alpha t d : \ t \in (0,1)\}$. Since $(1-\sigma)[\nabla f(x)]^T d < 0$ and $\lim_{\alpha \downarrow 0}[\nabla f(\xi) - \nabla f(x)]^T d = 0$, the green part is negative for all sufficiently small $\alpha > 0$.

Armijo rule cont.

How to execute Armijo rule in practice?

Armijo line search by backtracking:
Fix $\sigma \in (0, 1)$ and $\beta \in (0, 1)$. Given $x \in \mathbb{R}^n$, $d \in \mathbb{R}^n$ and $\bar{\alpha} > 0$.
Find the smallest nonnegative integer $j = j_0$ so that

$$f(x + \bar{\alpha}\beta^j d) \leq f(x) + \bar{\alpha}\beta^j \sigma [\nabla f(x)]^T d. \tag{2}$$

The stepsize generated is then $\bar{\alpha}\beta^{j_0}$.

Note:

- According to Theorem 2.4, if d is a descent direction, then (2) is satisfied for all sufficiently large j.
- In practice, one test the validity of (2) for $j = 0, 1, 2, \ldots$ successively. This is called backtracking because the stepsize $\bar{\alpha}\beta^j$ being tested keeps decreasing.
- The choice of $\bar{\alpha}$ is crucial for the efficiency of such scheme.

Convergence under Armijo rule

Theorem 2.5:
Let $f \in C^1(\mathbb{R}^n)$ with $\inf f > -\infty$. Let $\{\bar{\alpha}_k\} \subset \mathbb{R}$ satisfy $0 < \inf_k \bar{\alpha}_k \leq \sup_k \bar{\alpha}_k < \infty$, and fix $\sigma \in (0,1)$ and $\beta \in (0,1)$. Suppose $\{x^k\}$ is generated as

$$x^{k+1} = x^k + \alpha_k d^k,$$

where

- $d^k := -D_k \nabla f(x^k)$; here $\{D_k\}$ is a bounded sequence of positive definite matrices with $D_k - \delta I \succeq 0$ for some $\delta > 0$;
- α_k is generated via the Armijo line search by backtracking with $x = x^k$, $d = d^k$ and $\bar{\alpha} = \bar{\alpha}_k$, and σ and β defined above.

Then any accumulation point of $\{x^k\}$ is a stationary point of f.

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Then any accumulation point of $\{x^k\}$ is a stationary point of f.

Remark:

- If x^k is non-stationary, then d^k is a descent direction.
- The condition $D_k - \delta I \succeq 0$ implies that for any $y \in \mathbb{R}^n$, we have $y^T(D_k - \delta I)y \geq 0$. Hence $y^T D_k y \geq \delta \|y\|_2^2$.

Convergence under Armijo rule cont.

Proof sketch of Theorem 2.5: If x^k is a stationary point for some finite $k \geq 0$, then $x^l \equiv x^k$ whenever $l \geq k$ and we are done.

Assume that x^k is not stationary for each k. Then according to Armijo line search by backtracking, we have $\alpha_k > 0$ for all k and

$$f(x^{k+1}) \leq f(x^k) + \sigma\alpha_k[\nabla f(x^k)]^T d^k.$$

Note that $[\nabla f(x^k)]^T d^k < 0$ for each k. Rearranging terms and summing from $k = 0$ to ∞, we have

$$0 \leq -\sigma \sum_{k=0}^{\infty} \alpha_k[\nabla f(x^k)]^T d^k \leq f(x^0) - \inf f < \infty.$$

Thus,

$$\lim_{k\to\infty} \alpha_k[\nabla f(x^k)]^T d^k = 0. \tag{3}$$

Convergence under Armijo rule cont.

Proof sketch of Theorem 2.5 cont.: Let $\bar{x}$ be an accumulation point of $\{x^k\}$. By definition, there is a subsequence $\{x^{k_i}\}$ with $\lim_{i\to\infty} x^{k_i} = \bar{x}$.

If $\liminf_{i\to\infty} \alpha_{k_i} > 0$, then (3) implies

$$\lim_{i\to\infty} [\nabla f(x^{k_i})]^T d^{k_i} = 0.$$

Recall that $d^k = -D_k \nabla f(x^k)$ for some bounded sequence $\{D_k\}$. By passing to a further subsequence if necessary, we may assume that

(Bolzano-Weierstrass theorem is invoked)

$$\lim_{i\to\infty} D_{k_i} = D_*$$

for some matrix D_*. This implies

$$\begin{aligned} 0 &= -\lim_{i\to\infty} [\nabla f(x^{k_i})]^T D_{k_i} \nabla f(x^{k_i}) = -[\nabla f(\bar{x})]^T D_* \nabla f(\bar{x}) \\ &= -\lim_{i\to\infty} [\nabla f(\bar{x})]^T D_{k_i} \nabla f(\bar{x}) \leq -\delta \|\nabla f(\bar{x})\|_2^2. \end{aligned}$$

Thus, we have $\nabla f(\bar{x}) = 0$ as desired.

Convergence under Armijo rule cont.

Proof sketch of Theorem 2.5 cont.: Now it remains to consider the case that $\liminf_{i\to\infty} \alpha_{k_i} = 0$.

By passing to a further subsequence if necessary, we may assume that $\lim_{i\to\infty} \alpha_{k_i} = 0$.

Since $\inf_k \bar{\alpha}_k > 0$ and $\lim_{i\to\infty} \alpha_{k_i} = 0$, the Armijo line search by backtracking must have been invoked when i is sufficiently large.

Then for all large i

$$f(x^{k_i} + [\alpha_{k_i}/\beta]d^{k_i}) > f(x^{k_i}) + \sigma(\alpha_{k_i}/\beta)[\nabla f(x^{k_i})]^T d^{k_i}.$$

Convergence under Armijo rule cont.

Proof sketch of Theorem 2.5 cont.: Then

$$\frac{f(x^{k_i} + [\alpha_{k_i}/\beta]d^{k_i}) - f(x^{k_i})}{(\alpha_{k_i}/\beta)} > \sigma[\nabla f(x^{k_i})]^T d^{k_i}. \tag{4}$$

Recall that $d^k = -D_k \nabla f(x^k)$ for some bounded sequence $\{D_k\}$. By passing to a further subsequence if necessary, we may assume that

(Bolzano-Weierstrass theorem is invoked)

$$\lim_{i\to\infty} d^{k_i} = -D_* \nabla f(\bar{x}) =: d^*$$

for some $D_* := \lim_{i\to\infty} D_{k_i}$. Passing to the limit in (4), we have $[\nabla f(\bar{x})]^T d^* \geq \sigma[\nabla f(\bar{x})]^T d^*$. Since $\sigma \in (0,1)$, this implies

$$\begin{aligned} 0 \leq [\nabla f(\bar{x})]^T d^* &= -[\nabla f(\bar{x})]^T D_* \nabla f(\bar{x}) \\ &= -\lim_{i\to\infty}[\nabla f(\bar{x})]^T D_{k_i} \nabla f(\bar{x}) \leq -\delta\|\nabla f(\bar{x})\|_2^2. \end{aligned}$$

Hence, $\nabla f(\bar{x}) = 0$ also in the case that $\liminf_{i\to\infty} \alpha_{k_i} = 0$.

Convergence under Armijo rule cont.

Some remarks on parameters:

- σ is chosen to be small so that (2) may be satisfied with a small number of backtracking steps: note that each backtracking requires an evaluation of $f(x^k + \alpha d^k)$, which adds to the main computational cost. A typical choice is $\sigma = 10^{-4}$.
- β is typically $\frac{1}{2}$.
- The choice of $\{\bar{\alpha}_k\}$ is crucial. Ideally, it should be chosen so that (2) may be satisfied with a small number of backtracking steps. Possible choices are:
  - ⋆ $\bar{\alpha}_k \equiv 1$ for "Newton-like" directions.
  - ⋆ $\bar{\alpha}_k = \max\{u, \min\{\ell, \alpha_{k-1}\}\}$, where u and ℓ are positive.
  - ⋆ (Projected) Barzilai-Borwein stepsize (see the next lecture).
- One can terminate when $\|\nabla f(x^k)\|_2 \leq tol \cdot \max\{|f(x^k)|, 1\}$, i.e., when the gradient is small relative to the function value.

Special case

Corollary 2.1: (Steepest descent with constant stepsize)
Let $f \in C^2(\mathbb{R}^n)$ with $\inf f > -\infty$. Suppose that there exists $L > 0$ so that

$$L \geq \|\nabla^2 f(x)\|_2 \;\text{ for all } x.$$

Fix any $\gamma \in (0, 2)$ and consider the sequence generated as

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

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Then any accumulation point of $\{x^k\}$ is a stationary point of f.

Remark:

- Given L, the above algorithm can be written in one line.
- While the algorithm avoids line search (which can be costly), it can be potentially slow because the constant stepsize can be too conservative in making progress.

Special case cont.

Proof of Corollary 2.1: It suffices to show that if one sets $\sigma = 1 - \frac{\gamma}{2} \in (0,1)$, $D_k = \frac{\gamma}{L} I$ and $\bar{\alpha}_k \equiv 1$ in Theorem 2.5, then backtracking is not invoked in (2).

To this end, note that for each x, with $d := -\frac{\gamma}{L}\nabla f(x)$, there exists ξ such that

$$
\begin{aligned}
f(x+d) &= f(x) + \nabla f(x)^T d + \tfrac{1}{2} d^T \nabla^2 f(\xi) d \\
&\leq f(x) + \nabla f(x)^T d + \tfrac{1}{2}\|d\|_2 \|\nabla^2 f(\xi) d\|_2 \\
&\leq f(x) + \nabla f(x)^T d + \tfrac{1}{2}\|d\|_2 \|\nabla^2 f(\xi)\|_2 \|d\|_2 \\
&\leq f(x) + \nabla f(x)^T d + \tfrac{L}{2}\|d\|_2^2 \\
&= f(x) + \nabla f(x)^T d - \tfrac{\gamma}{2}\nabla f(x)^T d \\
&= f(x) + (1 - \tfrac{\gamma}{2})\nabla f(x)^T d \\
&= f(x) + \sigma \nabla f(x)^T d.
\end{aligned}
$$

This shows that the Armijo rule is satisfied with $\alpha = 1$.

Example

Example: Let $f(x_1, x_2) = x_1^2 + 3x_1x_2 + 8x_2^2$.

- Show that $\|\nabla^2 f(x)\|_2 \leq 18$ for all x.
- Write down the general update formula and the first 2 iterations of the steepest descent with constant stepsize, starting at $(x_1, x_2) = (0, 1)$ and using $\gamma = 0.9$.

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Remarks: For a symmetric matrix A, it holds that

$$\|A\|_2 = \max\{|\lambda_{\max}(A)|, |\lambda_{\min}(A)|\}.$$

Example cont.

Solution:

$$\nabla f(x) = \begin{bmatrix} 2x_1 + 3x_2 \\ 3x_1 + 16x_2 \end{bmatrix}, \quad \nabla^2 f(x) = \begin{bmatrix} 2 & 3 \\ 3 & 16 \end{bmatrix}.$$

The eigenvalues of $\nabla^2 f(x)$ are $9 \pm \sqrt{58}$. Hence

$$\|\nabla^2 f(x)\|_2 \leq 9 + \sqrt{58} \approx 16.62 < 18.$$

The iterative scheme is given by

$$x^{k+1} = x^k - \frac{0.9}{18} \begin{bmatrix} 2x_1^k + 3x_2^k \\ 3x_1^k + 16x_2^k \end{bmatrix}.$$

Hence,

$$x^1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} - 0.05 \begin{bmatrix} 3 \\ 16 \end{bmatrix} = \begin{bmatrix} -0.15 \\ 0.2 \end{bmatrix},$$

$$x^2 = \begin{bmatrix} -0.15 \\ 0.2 \end{bmatrix} - 0.05 \begin{bmatrix} -0.3 + 0.6 \\ -0.45 + 3.2 \end{bmatrix} = \begin{bmatrix} -0.165 \\ 0.0625 \end{bmatrix}.$$

A chain rule

Let $h \in C^2(\mathbb{R}^m)$ and let $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$.

Define $f(x) := h(Ax - b)$. Then $f \in C^2(\mathbb{R}^n)$ and

$$\nabla f(x) = A^T \nabla h(Ax - b) \;\text{ and }\; \nabla^2 f(x) = A^T \nabla^2 h(Ax - b) A.$$

A chain rule

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Define $f(x) := h(Ax - b)$. Then $f \in C^2(\mathbb{R}^n)$ and

$$\nabla f(x) = A^T \nabla h(Ax - b) \;\text{ and }\; \nabla^2 f(x) = A^T \nabla^2 h(Ax - b) A.$$

In particular, if there exists L such that $L \geq \|\nabla^2 h(y)\|_2$ for all y, then

$$\begin{aligned} \|\nabla^2 f(x)\|_2 &\leq \|A^T\|_2 \|\nabla^2 h(Ax - b)\|_2 \|A\|_2 \\ &\leq L \|A^T\|_2 \|A\|_2 = L \lambda_{\max}(A^T A). \end{aligned}$$

Example

Example: Let $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and

$$h(y) = \sum_{i=1}^{m} \ln\left(1 + y_i^2\right).$$

Fix any $\mu > 0$ and consider the problem of minimizing

$$f(x) := h(Ax - b) + \frac{\mu}{2}\|x\|_2^2.$$

Discuss how the parameters can be chosen for implementing steepest descent with constant stepsize.

Remark: The function h is related to Cauchy measurement noise in b, and $\mu > 0$ is a tuning parameter for ridge regression.

Example cont.

Solution: We first compute an upper estimate of $\|\nabla^2 h(y)\|_2$. Notice that $\nabla^2 h(y)$ is a diagonal matrix with the ith diagonal entry given by

$$\frac{\partial^2}{\partial y_i^2} \ln\left(1 + y_i^2\right) = \frac{\partial}{\partial y_i}\left(\frac{2y_i}{y_i^2 + 1}\right) = \frac{2(1 - y_i^2)}{(y_i^2 + 1)^2}$$

Thus,

$$|(\nabla^2 h(y))_{ii}| \leq \frac{2(1 + y_i^2)}{(y_i^2 + 1)^2} = \frac{2}{y_i^2 + 1} \leq 2.$$

Hence, $\|\nabla^2 h(y)\|_2 \leq 2$. Since $\nabla^2 f(x) = A^T \nabla^2 h(Ax - b)A + \mu I$, it follows that

$$\|\nabla^2 f(x)\|_2 \leq 2\lambda_{\max}(A^T A) + \mu.$$

Consequently, we can take $L = 2\lambda_{\max}(A^T A) + \mu$ and any $\gamma \in (0, 2)$ in the algorithm.

Example cont.

Remark on computation cost: Using flop counts, we can make the following observations.

- Note that computing Ax requires $m(2n-1)$ flops. This is the dominant computation in computing f.
- Since $\nabla f(x) = A^T \nabla h(Ax - b)$, computing ∇f requires computing one Au and $A^T v$. The former can be saved during the computation of $f(x)$, the latter requires another $n(2m-1)$ flops.
- Thus, if the algorithm in Theorem 2.5 is used with $D_k \equiv I$ and if no backtracking is invoked in the line search, then each iteration requires computing one Au and $A^T v$. Any additional backtrack step requires recomputing $f(x + \alpha d)$.