Chapter 7: Optimization for Data Science
Gradient Descent

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October 8, 2022

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Unconstrained Optimization Problem

Unconstrained Minimization Problem

$$\min_{x\in\mathbb{R}^n} f(x) = f(x^*)$$

- $f : \mathbb{R}^n \to \mathbb{R}$ convex and differentiable.
- Necessary and sufficient conditions $\nabla f(x^*) = 0 \implies$ Set of n (nonlinear) equations with n variables

Goal: Find an approximate solution $\tilde{x} \in \mathbb{R}^n$ such that

$$f(\tilde{x}) - f(x^*) < \varepsilon$$

- compute $\tilde{x}$ iteratively via an algorithm (e.g., gradient descent)

Gradient Descent

- Iterative algorithm $x_{t+1} = x_t + v_t$
- Choose step v_t such that $f(x_{t+1}) < f(x_t)$
- Taylor series

$$f(x_t + v_t) = f(x_t) + \nabla f(x_t)^\top v_t + \underbrace{r(v_t)}_{o(\|v_t\|)} \approx f(x_t) + \nabla f(x_t)^\top v_t$$

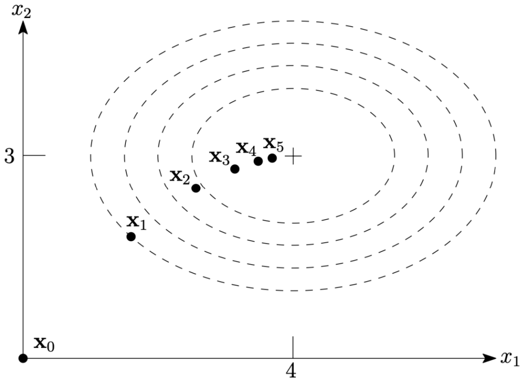
  - " $\approx$ " requires step size $||v_t||$to be small.
  - want $\nabla f(x_t)^T v_t <) \implies v_t = -\nabla f(x_t)$ not small

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

- Step size $\gamma > 0$, how to choose it?
  - γ "too small" $\implies$ gradient descent takes long to converge.
  - γ "too large" $\implies$ gradient descent might overshoot.

Gradient Descent Cont'd

Example: Run of gradient descent on the quadratic function $f(x_1, x_2) = 2(x_1 - 4)^2 + 3(x_2 - 3)^2$ with global minimum $x^* = (4, 3)$; we have choose $x_0 = (0, 0), \gamma = 0.1$; dashed lines represent level sets of f (points of constant f-value).



Theoretical Analysis

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

Lemma 1 (Property of Gradient Descent):

$$\sum_{t=0}^{T-1} (f(x_t) - f(x^*)) \leq \frac{\gamma}{2} \sum_{t=0}^{T-1} ||\nabla f(x_t)||^2 + \frac{1}{2\gamma} ||x_0 - x^*||^2$$

- Clearly, $\min_{t-0,\ldots,T-1} f(x_t) - f(x^*) \leq \frac{1}{T} \sum_{t=0}^{T-1} (f(x_t) - f(x^*))$
- Dependence on $||x_0 - x^*||$ to be expected (if we start far away, we need more steps).
- Need to control the gradient $||\nabla f(x_t)||^2$

Proof of Lemma 1

The gradient descent can be equivalently written as

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

Recall for any $v, w \in \mathbb{R}^n, 2v^T w = ||v||^2 + ||w||^2 - ||v - w||^2$. Hence

$$\begin{aligned}
\nabla f(x_t)^T (x_t - x^*) &= \frac{1}{\gamma}(x_t - x_{t+1})^T (x_t - x^*) \\
&= \frac{1}{2\gamma}(||x_t - x_{t+1}||^2 + ||x_t - x^*||^2 - ||x_{t+1} - x^*||^2) \\
&= \frac{\gamma}{2}||\nabla f(x_t)||^2 + \frac{1}{2\gamma}(||x_t - x^*||^2 - ||x_{t+1} - x^*||^2)
\end{aligned}$$

Proof of Lemma 1 Cont'D

Hence, applying a telescopic sum

$$\sum_{t=0}^{T-1} \nabla f(x_t)^T (x_t - x^*) = \frac{\gamma}{2} \sum_{t=0}^{T-1} ||\nabla f(x_t)||^2 + \frac{1}{2\gamma}(||x_0 - x^*||^2 - ||x^T - x^*||^2)$$

$$= \frac{\gamma}{2} \sum_{t=0}^{T-1} ||\nabla f(x_t)||^2 + \frac{1}{2\gamma}||x_0 - x^*||^2 \qquad (\star)$$

Since f is convex the first-order convexity conditions state

$$f(x_t) - f(x^*) \leq \nabla f(x_t)^T (x_t - x^*)$$

which combined with $(\star)$ leads to

$$\sum_{t=0}^{T-1} (f(x_t) - f(x^*)) \leq \frac{\gamma}{2} \sum_{t=0}^{T-1} ||\nabla f(x_t)||^2 + \frac{1}{2\gamma}||x_0 - x^*||^2$$

This proves **Lemma 1**.

Lipschitz Continuous Functions

Definition: A function $f : \mathbb{R}^n \to \mathbb{R}$ is Lipschitz continuous with Lipschitz constant $l > 0$ if $|f(x) - f(y)| \leq l||x - y||, \forall x, y \in \mathbb{R}^n$

- f is l Lipschitz $\iff ||\nabla f(x)|| \leq l, \forall x \in \mathbb{R}^n$
- Ex: $f(x) = x^2$ is not Lipschitz cont. as $\nabla f(x) = 2x$ is unbounded.

Lipschitz Continuous Functions Cont'd

Theorem (Gradient Descent for Lipschitz Function): Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex and differentiable with global minimum x^*. Suppose that $||x_0 - x^*|| \leq R$ and $||\nabla f(x)|| \leq B, \forall x \in \mathbb{R}^n$. Choosing the step size $\gamma = \frac{R}{B\sqrt{T}}$, the gradient descent yields.

$$\frac{1}{T}\sum_{t=0}^{T-1}(f(x_t) - f(x^*)) \leq \frac{RB}{\sqrt{T}}$$

- For achieving $\min_{t=0,\dots,T-1} f(x_t) - f(x^*) \leq \varepsilon$, we need $T \geq \frac{R^2B^2}{\varepsilon^2}$ $\implies$ # of iterations scale as $\mathcal{O}(1/\varepsilon^2)$.
- No specific dependence on n.

Proof of Theorem

Using Lemma 1 directly leads to

$$\sum_{t=0}^{T-1}(f(x_t) - f(x^\star)) \leq \underbrace{\frac{\gamma}{2}TB^2 + \frac{1}{2\gamma}R^2}_{=:q(\gamma)},$$

which holds for any $\gamma > 0$. Solving $\min_{\gamma>0} q(\gamma)$ gives the optimal step size as $\gamma^* = \dfrac{R}{L\sqrt{T}}$ and $q(\gamma^*) = RB\sqrt{T}$. Hence,

$$\frac{1}{T}\sum_{t=0}^{T-1}(f(x_t) - f(x^*)) \leq \frac{RB}{\sqrt{T}}$$

which completes the proof.

- What happen if we do not know R and/or B?
- Can we improve the $\mathcal{O}(1/\varepsilon^2)$ complexity?

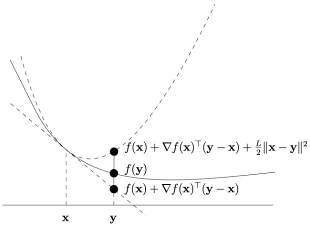
Smooth Convex Functions

Recall the first order convexity conditions

$$f(y) \geq f(x) + \nabla f(x)^T (y - x), \forall x, y \in \mathbb{R}^n$$

Definition: Let $f : \mathbb{R}^n \to \mathbb{R}$ be differentiable and $\mathbb{X} \subset \mathbb{R}^n$ be convex and $L > 0$. Then function f is called L-smooth over $\mathbb{X}$, if

$$f(y) \leq f(x) + \nabla f(x)^T (y - x) + \frac{L}{2} ||y - x||^2, \forall x, y \in \mathbb{X}$$



- No convexity of f required
- Ex: $f(x) = x^2$ is smooth with $L = 2$
- How can we easily check smoothness of a function?

Properties of Smooth Functions

Lemma: Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex and differentiable. The following are equivalent

(i) f is L-smooth.

(ii) $||\nabla f(x) - \nabla f(y)|| \leq L||x - y||, \forall x, y \in \mathbb{R}^n$

(iii) (ii) $\implies$ (i) holds without convexity

Lemma (Smoothness Preserving Operation):

(i) Let $f_1, ..., f_m$ be smooth with parameters $L_1, ..., L_m$, let $\lambda_1, ..., \lambda_m > 0$. Then the function $f = \sum_{i=1}^{m} \lambda_i f_i$ is L-smooth with $L = \sum_{i=1} \lambda_i L_i$ over $\text{dom}(f) = \cap_{i=1}^{m} \text{dom}(f_i)$.

(ii) Consider $f : \mathbb{R}^n \to \mathbb{R}$ L-smooth and $g : \mathbb{R}^m \to \mathbb{R}^n$ affine, i.e., $g(x) = Ax + b$. Then $f(g(x)) = f(Ax + b)$ is smooth with parameter $L||A||^2$, where $||A||$ = the spectral norm.

Convergence analysis for smooth functions

Lemma 2 (Sufficient Decrease): Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex, differentiable and L-smooth. For $\gamma = 1/L$, gradient descent yields

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

- GD (with suitable stepsize γ) makes progress in function value on smooth functions in every step.

Proof:

$$\begin{aligned} f(x_{t+1}) &\overset{L\text{-smooth}}{\leq} f(x_t) + \nabla f(x_t)^\top \underbrace{(x_{t+1} - x_t)}_{-1/L\nabla f(x_t)} + \frac{L}{2}\underbrace{\|x_t - x_{t+1}\|^2}_{1/L^2\|\nabla f(x_t)\|^2} \\ &= f(x_t) - \frac{1}{L}\|\nabla f(x_t)\|^2 + \frac{1}{2L}\|\nabla f(x_t)\|^2 \\ &= f(x_t) - \frac{1}{2L}\|\nabla f(x_t)\|^2 \end{aligned}$$

Convergence analysis for smooth functions Cont'd

Theorem (Gradient Descent for Smooth Functions): Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex with global minimum x^*, differentiable and L-smooth. For $\gamma = 1/L$, gradient descent yields

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

- For $R = ||x_0 - x^*||$, to get $f(x_T) - f(x^*) \leq \varepsilon$, we need $T \geq \dfrac{R^2 L}{2\varepsilon}$
  $\implies$ complexity $\mathcal{O}(1/\varepsilon)$

Lipschitz functions:	Smooth functions:
$T = \mathcal{O}(1/\varepsilon^2)$	$T = \mathcal{O}(1/\varepsilon)$

- Could we do even better? E.g., we could achieve $\mathcal{O}(1/\sqrt{\varepsilon})$ or $\mathcal{O}(1/\log \varepsilon)$?

Proof of Theorem

$$\sum_{t=0}^{T-1}(f(x_t) - f(x^\star)) \overset{\text{Lemma 1}}{\leq} \frac{\gamma}{2}\sum_{t=0}^{T-1} \underbrace{\|\nabla f(x_t)\|^2}_{\overset{\text{Lemma 2}}{\leq} 2L(f(x_t)-f(x_{t+1}))} + \frac{1}{2\gamma}\|x_0 - x^\star\|^2$$

$$\leq \quad f(x_0) - f(x_T) + \frac{L}{2}\|x_0 - x^\star\|^2$$

This is equivalent to

$$\sum_{t=1}^{T}(f(x_t) - f(x^*)) \leq \frac{L}{2}||x_0 - x^*||^2 \qquad (1)$$

Recall that from Lemma 2, we know that $f(x_{t+1}) \leq f(x_t)$. Hence, take averages in (1) gives

$$f(x_T) - f(x^*) \leq \sum_{t=1}^{T}(f(x_t) - f(x^*) \leq \frac{L}{2T}||x_0 - x^*||^2$$

Acceleration for Smooth Convex Functions

Accelerated gradient descent[1]:
Choose $z_0 = y_0 = x_0$ arbitrarily.
For $t \geq 0$ set

$$
\begin{aligned}
y_{t+1} &= x_t - \frac{1}{L}\nabla f(x_t) \\
z_{t+1} &= z_t - \frac{t+1}{2L}\nabla f(x_t) \\
x_{t+1} &= \frac{t+1}{t+3} y_{t+1} + \frac{2}{t+3} z_{t-1}
\end{aligned}
$$

[1] Yurii Nesterov 1983

Acceleration for Smooth Convex Functions Cont'd

Theorem (Accelerated Gradient Descent): Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex with global minimum x^*, differentiable and L-smooth. Accelerated gradient descent yields

$$f(y_T) - f(x^*) \leq \frac{2L||z_0 - x^*||^2}{T(T+1)}, \quad T > 0$$

- To reach error ε, we need $\mathcal{O}(1/\sqrt{\varepsilon})$ steps.

An Observation

- Consider the smooth function $f(x) = x^2$. Gradient descent according to our theorem ensures.

$$f(x_T) \leq \frac{1}{T} x_0^2$$

- For $\gamma = 1/L = 1/2$, gradient descent yields

$$x_{t+1} = x_t - 1/2 \nabla f(x_t) = x_t - x_t = 0$$

$\implies$ we converge in only one step

- For a suboptimal (valid) step size $\gamma = 1/4$, gradient descent yields

$$x_{t+1} = x_t - 1/4 \nabla f(x_t) = \frac{x_t}{2} \implies f(x_T) = f(x_0/2^T) = \frac{x_0^2}{2^{2^T}}$$

To achieve $f(x_T) \leq \varepsilon$, we require $T \approx \frac{1}{2} \log(x_0^2/\varepsilon)$

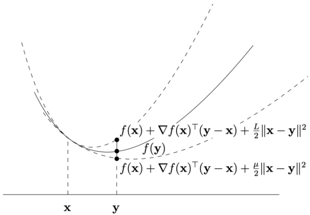
Strong Convexity

Recall the first order convexity conditions

$$f(y) \geq f(x) + \nabla f(x)^T (y - x), \quad \forall x, y \in \mathbb{R}^n$$

Definition: Let $f : \mathbb{R}^n \to \mathbb{R}$ be differentiable and $\mathbb{X} \subset \mathbb{R}^n$ be convex and $L > 0$. The function f is called μ-strongly convex over $\mathbb{X}$, if

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{\mu}{2}||x - y||^2, \forall x, y \in \mathbb{X}$$



- Smooth and strongly convex function
- Smooth $\rightarrow$ “not too curved"
- Strongly convex $\rightarrow$ “not too flat"
- Ex: $f(x) = x^2$ is smooth and strongly convex

Smooth and Strongly Convex Case

Theorem (Smooth and Strongly Convex Function): Let $f : \mathbb{R}^n \to \mathbb{R}$ be μ-strongly convex with global minimum x^*, differentiable and L-smooth. For a step size $\gamma = 1/L$, gradient descent yields

(i) $||x_{t+1} - x^*||^2 \leq (1 - \frac{\mu}{L})||x_t - x^*||^2, t \geq 0$

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

- For $R = ||x_0 - x^*||$, to achieve $f(x_T) - f(x^*) \leq \varepsilon$, using (i) one can chooseT $\log(1 - \frac{\mu}{L}) \leq \log(\frac{2\varepsilon}{LR^2}) \qquad (2)$
  Using the bound $\log(1 - \frac{\mu}{L}) \leq -\frac{\mu}{L}$, the condition (2) is implied by

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

- Hence, the over iteration complexity is $\mathcal{O}(\log(1/\varepsilon))$.

Proof of Theorem

We first show (i):

$$
\begin{aligned}
& f(x_t) - f(x^\star) + \frac{\mu}{2}\|x_t - x^\star\|^2 \\
& \overset{\mu \text{ strongly convex}}{\leq} \quad \nabla f(x_t)^\top (x_t - x^\star) \\
& \overset{\text{Proof of Lemma 1}}{\leq} \quad \frac{\gamma}{2}\|\nabla f(x_t)\|^2 + \frac{1}{2\gamma}(\|x_t - x^\star\|^2 - \|x_{t+1} - x^\star\|^2)
\end{aligned}
$$

Therefore,

$$
f(x_t) - f(x^\star) \leq \frac{1}{2\gamma}(\gamma^2\|\nabla f(x_t)\|^2 + \|x_t - x^\star\|^2 - \|x_{t+1} - x^\star\|^2) - \frac{\mu}{2}\|x_t - x^\star\|^2,
$$

which is equivalent to

$$
\|x_{t+1} - x^\star\|^2 \leq 2\gamma(f(x_t) - f(x^\star)) + \gamma^2\|\nabla f(x_t)\|^2 + (1 - \mu\gamma)\|x_t - x^\star\|^2 \quad (3)
$$

Proof of Theorem

$$f(x^\star) - f(x_t) \le f(x_{t+1}) - f(x_t) \overset{\text{Lemma 2}}{\le} -\frac{\gamma}{2}\|\nabla f(x_t)\|^2$$

$$\begin{aligned}
&\Longrightarrow 2\gamma(f(x^\star) - f(x_t)) + \gamma^2\|\nabla f(x_t)\|^2 \le 0 \\
&\overset{(3)}{\Longrightarrow} \|x_{t+1} - x^\star\|^2 \le (1-\mu\gamma)\|x_t - x^\star\|^2 = (1 - \tfrac{\mu}{L})\|x_t - x^\star\|^2 \\
&\Longrightarrow \|x_T - x^\star\|^2 \le (1 - \tfrac{\mu}{L})^T\|x_0 - x^\star\|^2,
\end{aligned}$$

which shows (i). To show (ii), note that

$$\begin{aligned}
f(x_T) - f(x^\star) &\overset{\text{smooth}}{\le} \nabla f(x^\star)(x_T - x^\star) + \tfrac{L}{2}\|x_T - x^\star\|^2 \\
&\overset{\nabla f(x^\star)=0}{=} \tfrac{L}{2}\|x_T - x^\star\|^2 \\
&\overset{(i)}{\le} \tfrac{L}{2}(1 - \tfrac{\mu}{L})^T\|x_0 - x^\star\|^2,
\end{aligned}$$

Main Take-Away Points

- **Definitions:** smooth convex functions, strongly convex functions
- **Iteration complexity analysis for gradient descent:** For a convex function f.

	Lipschitz	smooth	smooth & strongly con.
gradient descent	$\mathcal{O}(1/\varepsilon^2)$	$\mathcal{O}(1/\varepsilon)$	$\mathcal{O}(\log(1/\varepsilon))$
acc. gradient desc.		$\mathcal{O}(1/\sqrt{\varepsilon})$	