Optimization in Machine Learning

Lecture 15: Algorithms for Optimization, Convergence Analysis of Gradient Descent under Lipschitz Continuity and Convexity, Enhancements via Smoothness and Strong Convexity

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[Recap] Convergence Rate For Smooth + Strongly Convex

- Setting $R^2 = ||x_0 - x^*||^2$, we get:

$$f(x_T) - f(x^*) \leq \frac{L}{2}\left(1 - \frac{\mu}{L}\right)^T R^2$$

- To get an error of ϵ, we require $\frac{L}{2}\left(1 - \frac{\mu}{L}\right)^T R^2 \leq \epsilon$ which implies $T \geq \frac{L}{\mu}\log(\frac{R^2 L}{2\epsilon})$.
- To get an error of $\epsilon = 0.01$, we now need only $L/\mu \log(50R^2L)$ iterations as opposed to $50R^2L$ iterations in the smooth case!

Summary of Results so Far...(with convexity by default)

- Lipschitz continuous functions (C). With $\gamma = \frac{R}{B\sqrt{T}}$, achieve an ϵ-approximate solution in R^2B^2/ϵ^2 iterations
- Smooth Functions (S): With $\gamma = 1/L$, achieve an ϵ-approximate solution in $\frac{R^2L}{\epsilon}$ iterations.
- Smooth + Strongly Convex (SS): With $\gamma = 1/L$, achieve an ϵ-approximate solution in $\frac{L}{\mu}\log(\frac{R^2L}{2\epsilon})$ iterations.
- Concrete examples. Let $L = B = 10, R = 1, \mu = 1$. Then, we have the following:
  - $\epsilon = 0.1$, C: 10000, S $=$ 50, SS $=$ 8.49 iterations
  - $\epsilon = 0.01$, C: 1000000, S $=$ 500, SS $=$ 13.49 iterations
  - $\epsilon = 0.001$, C: 100000000, S $=$ 5000, SS $=$ 18.49 iterations
- As ϵ reduces by 10, the number of iterations of strongly + smooth case increases only by a additive constant! This is linear convergence!

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worst case for some intermediate ineq.

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Revisist optional slides and notice that this is Q-linear convergence

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==> We cannot insist on L-smoothness
But we could add a regularizer and get strong convexity nevertheless!

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- Unfortunately No!!!!

Unless we consider restriction of the fn

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Within a bounded set eg: $\|w\|^2 \leq R^2$

Very often (especially in ML) we cannot insist on differentiability
==> We cannot insist on L-smoothness
But we could add a regularizer and get strong convexity nevertheless!

$$\text{Hinge}(w^T x, y) + \lambda \|w\|^2$$
$$\text{s.t. } \|w\|^2 \leq R$$

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- Can we get an improved convergence rate in such a case?

improvement upon $O(\frac{1}{\epsilon^2})$

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- But on a bounded set, we can assume that they are (and the gradients are upper bounded)
- Can we get an improved convergence rate in such a case?
- We can obtain an improved $\boxed{O(1/\epsilon)}$ bound!!

Lipschitz Continuity + Strong Convexity I

- Recall: $g_t^T(x_t - x^*) = \frac{\gamma_t}{2}||g_t||^2 + \frac{1}{2\gamma_t}\left(||x_t - x^*||^2 - ||x_{t+1} - x^*||^2\right)$
- Recall: Using stronger lower bound on the above expression(s) via strong convexity:
  $g_t^T(x_t - x^*) \geq f(x_t) - f(x^*) + \frac{\mu}{2}||x_t - x^*||^2$
- Combining, we obtained:
  $||x_{t+1} - x^*||^2 \leq 2\gamma\left(f(x^*) - f(x_t)\right) + \gamma^2||g_t||^2 + (1 - \mu\gamma)||x_t - x^*||^2$

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$g_t^T(x_t - x^*) \geq f(x_t) - f(x^*) + \frac{\mu}{2}||x_t - x^*||^2$ } we used this for L-smoothness only.

- Combining, we obtained:

$$\left[\,||x_{t+1} - x^*||^2 \leq \underline{2\gamma\,(f(x^*) - f(x_t))} + \overset{\mathbf{O}}{\underline{\gamma^2||g_t||^2}} + \underline{(1-\mu\gamma)||x_t - x^*||^2}\,\right] * \frac{1}{2\gamma}$$

$\leq \gamma^2 B^2$

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- Now, with Lipschitz continuity, assume the gradients $||g_t|| \leq B \implies ||g_t||^2 \leq B^2$. Combining with strong convexity we get,

$$f(x_t) - f(x^*) \leq \frac{B^2\gamma_t}{2} + \left(\frac{1}{2\gamma_t} - \frac{\mu}{2}\right)||x_t - x^*|| - \frac{1}{2\gamma_t}||x_{t+1} - x^*||^2$$

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To LHS

≤ 0 To make this disappear do I need specific choice of γ_t?

$$f(x_t) - f(x^*) \leq \frac{B^2\gamma_t}{2} + \left(\frac{1}{2\gamma_t} - \frac{\mu}{2}\right)||x_t - x^*|| - \frac{1}{2\gamma_t}||x_{t+1} - x^*||^2$$

We will do a scheme with γ_t to make things work! t-specific

Telescopic summing?

Lipschitz Continuity + Strong Convexity II

- So Far:

$$\boxed{f(x_t) - f(x^*)} \leq \boxed{\frac{B^2\gamma_t}{2}} + \boxed{\left(\frac{1}{2\gamma_t} - \frac{\mu}{2}\right) ||x_t - x^*||} - \boxed{\frac{1}{2\gamma_t}||x_{t+1} - x^*||^2}$$

- So Far:

$$\sum_t f(x_t) - f(x^*) \leq \frac{B^2\gamma_t}{2} + \left(\frac{1}{2\gamma_t} - \frac{\mu}{2}\right)||x_t - x^*|| - \frac{1}{2\gamma_t}||x_{t+1} - x^*||^2$$

if $\gamma_t \propto \frac{1}{t}$

Lipschitz Continuity + Strong Convexity II

- So Far:

$$f(x_t) - f(x^*) \leq \frac{B^2\gamma_t}{2} + \left(\frac{1}{2\gamma_t} - \frac{\mu}{2}\right)||x_t - x^*|| - \frac{1}{2\gamma_t}||x_{t+1} - x^*||^2$$

- For the specific case of $\gamma_t^{-1} = \mu(1+t)/2$ and multiplying both sides by t:

$$t\left[f(x_t) - f(x^*)\right] \leq \frac{B^2 t}{\mu(t+1)} + \frac{\mu}{4}\left\{t(t-1)\,||x_t - x^*||^2 - (t+1)t\,||x_{t+1} - x^*||^2\right\}$$

$$\leq \frac{B^2}{\mu} + \frac{\mu}{4}\{t(t-1)\,||x_t - x^*||^2 - (t+1)t\,||x_{t+1} - x^*||^2\}$$

Lipschitz Continuity + Strong Convexity II

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$\Gamma_t = \frac{2}{\mu(1+t)}$

- For the specific case of $\boxed{\gamma_t^{-1} = \mu(1+t)/2}$ and multiplying both sides by t:

$$\sum_{t=0}^{T-1}\left[\underbrace{t[f(x_t) - f(x^*)]}_{=0 \text{ for } t=0} \le \frac{B^2 t}{\mu(t+1)} + \frac{\mu}{4}\left\{t(t-1)\,||x_t - x^*||^2 - (t+1)t\,||x_{t+1} - x^*||^2\right\}\right.$$

$$\left.\le \frac{B^2}{\mu} + \frac{\mu}{4}\{\underbrace{t(t-1)}_{=0 \text{ for } t=0 \,\&\, t=1}\,||x_t - x^*||^2 - (t+1)\underbrace{t}_{=0 \text{ for } t=0}\,||x_{t+1} - x^*||^2\}\right]$$

Lowerbnd based on $f(x_T) - f(x^*)$ $\le \sum_{t=1}^{T-1} t[f(x_t) - f(x^*)] \le \frac{TB^2}{\mu} - T(T-1)||x_T - x^*||^2 \cdot \frac{\mu}{4} \le \frac{TB^2}{\mu}$

Lipschitz Continuity + Strong Convexity II

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$$f(x_t) - f(x^*) \le \frac{B^2\gamma_t}{2} + \left(\frac{1}{2\gamma_t} - \frac{\mu}{2}\right)||x_t - x^*|| - \frac{1}{2\gamma_t}||x_{t+1} - x^*||^2$$

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$$\le \frac{B^2}{\mu} + \frac{\mu}{4}\{t(t-1)\,||x_t - x^*||^2 - (t+1)t\,||x_{t+1} - x^*||^2\}$$

- Now we can use the telescoping sum and obtain...

$$\sum_{t=1}^{T} t(f(x_t) - f(x^*)) \le \frac{TB^2}{\mu} + \mu/4(\,0 - T(T+1)\,||x_{T+1} - x^*||^2) \le \frac{TB^2}{\mu}$$

Lipschitz + Strongly Convex III

- So Far:

$$\boxed{\sum_{t=1}^{T} t(f(x_t) - f(x^*))} \leq \boxed{\frac{TB^2}{\mu}}$$

$f(x^*) \leq f(x_T) \leq f(x_{T-1}) \leq \dots \leq f(x_1)$

$0 \leq f(x_T) - f(x^*) \leq \dots \leq f(x_1) - f(x^*)$

- So Far:

$$\boxed{\sum_{t=1} t\,(f(x_T) - f(x^*))} < \sum_{t=1}^{T} t(f(x_t) - f(x^*)) \leq \frac{TB^2}{\mu}$$

$$\geq \left(\sum_{t=1}^{T-1} t\right)(f(x_T) - f(x^*))$$

$$= \frac{T(T-1)}{2}(f(x_T) - f(x^*))$$

Lipschitz + Strongly Convex III

- So Far:

$$\boxed{\sum_{t=1}^{T} t(f(x_t) - f(x^*))} \leq \boxed{\frac{TB^2}{\mu}}$$

- Multiply by $2/(T(T+1))$ on both sides to make it a convex combination:

$$\sum_{t=1}^{T} \frac{2t}{T(T+1)}(f(x_t) - f(x^*)) \leq \frac{2B^2}{\mu(T+1)}$$

Lipschitz + Strongly Convex III

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- Thus, for the error $\leq \epsilon$, we need $T \geq \frac{2B^2}{\mu\epsilon} - 1$

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Side note: Smoothness has yeilded overall less wall clock time (however the dependence is still $1/\epsilon$ } Like CS

Lower Bounds with convexity (No proof will be discussed in the class)

- Case I: Lipschitz Continuous Functions: Any black-box procedure will have an error of at least $\frac{RB}{2(1+\sqrt{T})}$ (GD: $\frac{RB}{\sqrt{T}}$)
- Case II: Lipschitz Continuous + Strongly Convex Functions: Any black-box procedure have an error of at least $\frac{B^2}{2\mu T}$ (GD: $\frac{2B^2}{\mu(T-1)}$)
- Case III: Smooth Functions: Any black box procedure will have an error of at least $\frac{3L}{32}\frac{R^2}{(T+1)^2}$ (GD: $\frac{LR^2}{2T}$) - notice the gap between lower bound and actual time!
  - Can some improvement to the GD algorithm help bridge this? Ans: YES - Accelerated GD
- Case IV: Smooth + Strongly Convex Functions: Define $\kappa = \frac{L}{\mu}$. Then, any black box procedure will have an error of at least $\frac{\mu}{2}\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{2(T-1)}$

  (contrast with GD: $\frac{L}{2}\left(1-\frac{\mu}{L}\right)^T = \frac{L}{2}(\frac{\kappa-1}{\kappa})^T$)

For proofs, see Section 3.5 (page 53 onwards of) `https://arxiv.org/pdf/1405.4980.pdf`

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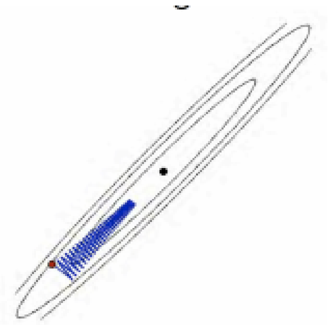
Accelerated GD? Why could GD be slow?

- GD has suboptimal rates for smooth (and to a smaller extent for smooth + strongly convex).
- GD relies just on local gradient information
- Can we add some momentum from the progress made so far to push it faster towards the optimal?



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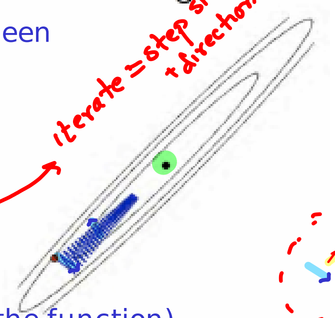
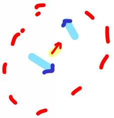
Motivation1: Bridging the gap
Concern: The gap could have been worse for some other function that Nesterov would have come up with?

Motivation2: Emperically could the next iterate have been influenced by the series of previous iterates (which also account for some curvature of the function)

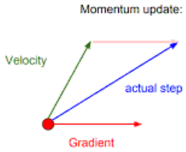
iterate = step size + direction





Avg movement

Efficient alternatives to GD: Momentum



- **Momentum Accelerated GD:** $x_{act} = x_{old} + \hat{\mathbf{v}}$ where $\hat{\mathbf{v}} = \mu \mathbf{v} - \eta_k \frac{\partial f}{\partial x}$

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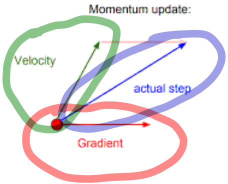

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Accounting for momentum

$\propto$

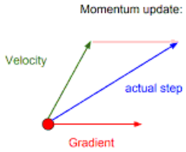
Multipicative factor associated with the history (captured through the velocity)

$\cancel{\mu > 1}$?

$\cancel{\mu < 0}$?

$\mu \in (0,1)$ ✓

Efficient alternatives to GD: Momentum



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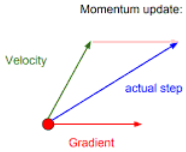
- Set to an exponentially decaying average of the negative gradient: Decay factor will be

$\mu \in [0,1)$

Efficient alternatives to GD: Momentum



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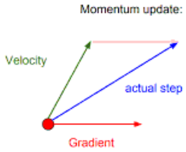
  - Set to an exponentially decaying average of the negative gradient: Decay factor will be $\mu \in [0, 1)$. Common values of μ used in practice are .5, .9, and .99.
- Physical analogy $\Rightarrow$ negative gradient is a force moving a particle through parameter space, according to Newton's laws of motion
- Step size largest when

Efficient alternatives to GD: Momentum



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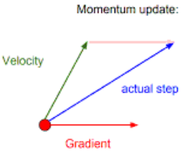
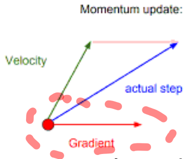
Suggestion: When the gradient and velocity are in the same direction
More generally: When successive gradients are in the same direction



- **Momentum Accelerated GD:** $x_{act} = x_{old} + \hat{\mathbf{v}}$ where $\hat{\mathbf{v}} = \mu \mathbf{v} - \eta_k \frac{\partial f}{\partial x}$
- $\mathbf{v}$ plays the role of velocity - it is the direction and speed at which the parameter x_i moves through parameter space.
- Set to an exponentially decaying average of the negative gradient: Decay factor will be $\mu \in [0, 1)$. Common values of μ used in practice are .5, .9, and .99.

- Physical analogy $\Rightarrow$ negative gradient is a force moving a particle through parameter space, according to Newton's laws of motion
- Step size largest when many successive gradients point in exactly the same direction

Efficient alternatives to GD: Momentum



option 2: $\frac{\partial f}{\partial x_{new}}$

option 1: $\frac{\partial f}{\partial x_{old}}$

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  Q: x is x_{old} OR x_{new}

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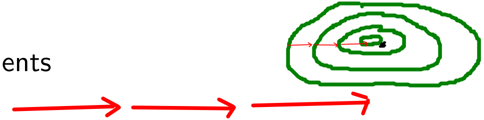
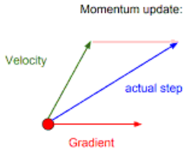


Efficient alternatives to GD: Momentum



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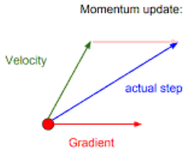

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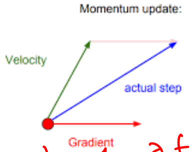
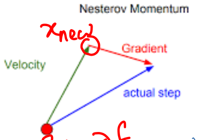
Heavy-ball/Polyak



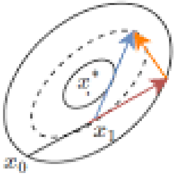


option 1: $\frac{\partial f}{\partial x_{old}}$ option 2: $\frac{\partial f}{\partial x_{new}}$

Momentum and its variants

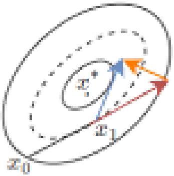
- Modified Nesterov momentum $\Rightarrow$ gradient is evaluated after the current velocity is applied. Speeds up rate of convergence from $O(1/T)$ to $O(1/T^2)$

Polyak's Momentum



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

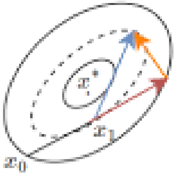
Nesterov Momentum



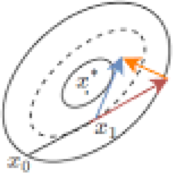
$$x_{t+1} = x_t + \mu(x_t - x_{t-1}) \\ - \gamma\nabla f(x_t + \mu(x_t - x_{t-1}))$$

- Modified Nesterov momentum $\Rightarrow$ gradient is evaluated after the current velocity is applied. Speeds up rate of convergence from $O(1/T)$ to $O(1/T^2)$ for L-continuity and strong convexity case

Polyak's Momentum



Nesterov Momentum



$$x_{t+1} = x_t \underbrace{- \alpha\nabla f(x_t)}_{} + \mu(x_t - x_{t-1})$$

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

$-\alpha \nabla f(x_t) \leftarrow$ Difference $\rightarrow -r\nabla f(x_t + u(x_t - x_{t-1})) = -r\nabla f(x_{new})$

Attempt 1: Polyak's Heavy Ball Momentum

- Recall standard gradient descent: $x_{t+1} = x_t - \alpha_t \nabla f(x_t)$
- Polyak's Heavy Ball Momentum adds inertia: $x_{t+1} = x_t - \alpha_t \nabla f(x_t) + \mu_t(x_t - x_{t-1})$
- Heavy Ball result: For smooth + strongly convex functions, the heavy ball algorithm converges in $\frac{R^2}{2}\left(1 - \sqrt{\frac{1}{\kappa}}\right)^T = \frac{L}{2}\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}}\right)^T$ in comparison with GD's $\frac{R^2}{2}\left(1 - \frac{1}{\kappa}\right)^T = \frac{L}{2}\left(\frac{\kappa-1}{\kappa}\right)^T$ iterations.
- Heavy Ball momentum is not optimal for the Smooth case (though it is optimal for the strongly convex + smooth class)

Attempt 1: Polyak's Heavy Ball Momentum

Conservatively exploits curvature

In this term which is standard GD
the curvature is not being exploited

Velocity exploits
curvature empirically

Exponential Decay μ_t

- Recall standard gradient descent: $x_{t+1} = x_t - \alpha_t \nabla f(x_t)$
- Polyak's Heavy Ball Momentum adds inertia: $x_{t+1} = x_t - \alpha_t \nabla f(x_t) + \mu_t(x_t - x_{t-1})$
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Comparable and Commensurate with Lower Bo

- Heavy Ball momentum is not optimal for the Smooth case (though it is optimal for the strongly convex + smooth class)

+ vanilla convexity

We have both an upper bound
and a lower bound on the curvature
We might have to be a bit careful in going aggressively in exploiting curvature