CS7301: Advanced Topics in Optimization for Machine Learning

Lecture 2.2: Gradient Descent and Family

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https://github.com/rishabhk108/AdvancedOptML

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Outline

- Lipschitz Continuity, Strong Convexity and Lipschitz Smoothness
- Gradient Descent and Analysis: Continuous, Smooth and Strongly Convex (and their combinations)
- Accelerated Gradient Descent and Lower Bounds

Recap

Lipschitz Continuity

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  - If f_1 is L_1-Lipschitz continuous and f_2 is L_2-Lipschitz continuous, then $f_1 + f_2$ is $L_1 + L_2$ Lipschitz continuous
  - Product of two Lipschitz continuous and bounded functions is also Lipschitz continuous.

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- Lemma: If a convex function f is smooth (i.e. has Lipschitz continuous gradients) then:

$$f(\mathrm{y}) \leq f(\mathrm{x}) + \nabla^\top f(\mathrm{x})(\mathrm{y} - \mathrm{x}) + \frac{L}{2}||\mathrm{y} - \mathrm{x}||^2$$

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- Is $f(x) = x^4$ Lipschitz smooth? What about $f(x) = x^3/3$? Lets study the latter. $\nabla f(x) = x^2$. Lipschitz continuity implies does there exists a L such that $|x^2 - y^2| \leq L|x - y|$ which implies $|x + y| \leq L$. This means that globally, this is not Lipschitz continuous though it can be locally!

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- Message: Only functions of asymptotically at most quadratic growth can be smooth globally.

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- However, it is not differentiable everywhere (not at 0). Such functions are called differentiable almost everywhere.
- Is every sub-quadratic function Lipschitz smooth? Consider $f(x) = |x|^{3/2}$ on a closed set X s.t. $0 \in X$. Is this function smooth? Note that the gradient of $f'(x)$ is ∞ at $x = 0$.

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- Recall that a function is Lipschitz continuous if the norm of the (sub)gradient is bounded!
- Also it holds that over a closed and bounded subset of $\Re^n$ that f is Lipschitz continuous $\supseteq$ f is convex

More reading on Lipschitz Continuity

- Juha Heinonen, *Lectures on Lipschitz Analysis*, `http://www.math.jyu.fi/research/reports/rep100.pdf`
- `https://ljk.imag.fr/membres/Anatoli.Iouditski/cours/convex/chapitre_3.pdf`
- Wikipedia: `https://en.wikipedia.org/wiki/Lipschitz_continuity`
- Nice Blog on Lipschitz Continuity: `https://xingyuzhou.org/blog/notes/Lipschitz-gradient`. The author has a similar blog on Strong Convexity: `http://xingyuzhou.org/blog/notes/strong-convexity`

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- Multi-class Logistic Regression: $L(\theta_1, \cdots, \theta_k) = \sum_{i=1}^{n} -\theta_{y_i}^T x_i + \log(\sum_{c=1}^{k} \exp(\theta_c^T x_i))\}$: Lipschitz Smooth

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- L2 Regularization: Lipschitz Smooth and Strongly Convex!

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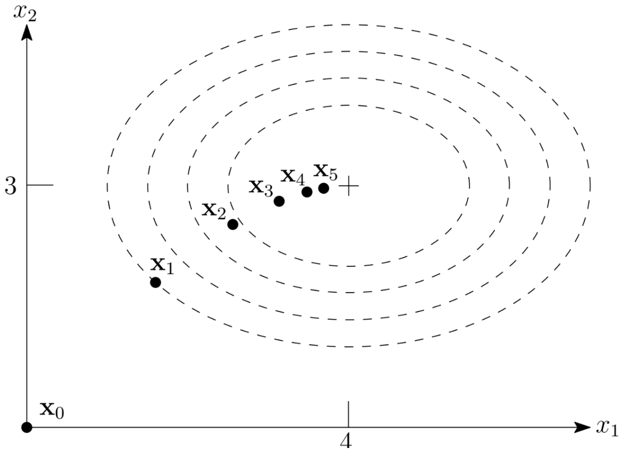
- Let f be Lipschitz continuous with parameter B. If f is smooth, let ∇f be Lipschitz continuous with parameter L.

Gradient Descent Illustration



Source: Martin Jaggi (CS 439)

Acknowledgements

In the following slides, I heavily borrow from the notes of Sebastian Bubeck and the slides of Martin Jaggi (EPFL).

Analysis I

- Define $g_t = \nabla f(x_t)$. From the definition of GD:

$$g_t^T(x_t - x^*) = \frac{1}{\gamma}(x_t - x_{t+1})^T(x_t - x^*)$$

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- We can then rewrite the RHS as:

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- Summing this up over

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t iterations:

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- Combining both, we have:

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- Choose $\hat{x} = \text{argmin}_i f(x_i)$ as the final iterate. Show that $|f(\hat{x}) - f(x^*)|$ satisfies the above bound (**exercise**).

UT DALLAS

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- Which implies:

$$T \geq \frac{R^2 B^2}{\epsilon^2}$$

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- If we need $|f(\hat{x}) - f(x^*)| \leq \epsilon$, this implies

$$\frac{RB}{\sqrt{T}} \leq \epsilon$$

- Which implies:

$$T \geq \frac{R^2 B^2}{\epsilon^2}$$

- Final Result: Given a Lipschitz continuous function f, Gradient descent with step size $\gamma = \frac{R}{B\sqrt{T}}$ achieves a solution $\hat{x}$ s.t $|f(\hat{x}) - f(x^*)| \leq \epsilon$ in $\frac{R^2 B^2}{\epsilon^2}$ iterations.

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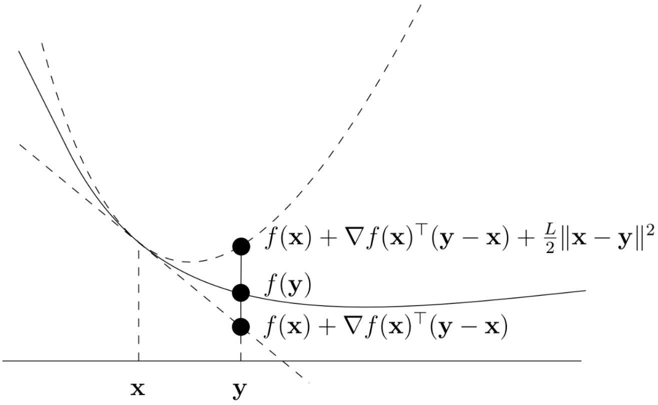
- Advantages of this bound: a) Goes to zero as T gets large, and b) Dimension Independent!
- Disadvantages: Slow convergence. To achieve a an error of 0.01, we require $10^4 R^2 B^2$ iterations. To achieve an error of 0.0001, the number of iterations is $10^8 R^2 B^2$!



Source: Martin Jaggi (CS 439)

Recap: Smoothness vs Continuity

- Bounded gradients $\Longleftrightarrow$ Lipschitz continuous f

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- Recall:

$$f(\mathrm{y}) \leq f(\mathrm{x}) + \nabla^\top f(\mathrm{x})(\mathrm{y} - \mathrm{x}) + \frac{L}{2}||\mathrm{y} - \mathrm{x}||^2$$

Gradient Descent for Smooth Functions: I

- Recall:

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- This means GD is guaranteed to decrease the function value at every iteration!

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- Summing this from $t = 1$ to $T - 1$:

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- Next, recall from Analysis II (and after setting $\gamma = 1/L$

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

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- This implies that (**why?**):

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

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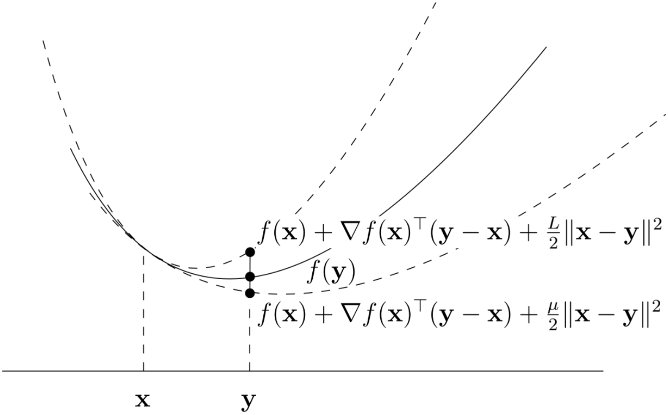
Smooth + Strongly Convex Functions



Source: Martin Jaggi (CS 439)

Fastest Convergence with Smooth + Strongly Convex I

- Recall from Analysis I:

$$g_t^T(x_t - x^*) = \gamma_t/2||g_t||^2 + 1/2\gamma_t(||x_t - x^*||^2 - ||x_{t+1} - x^*||^2)$$

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- We can use a stronger lower bound on the LHS via strong convexity: $g_t^T(x_t - x^*) \geq f(x_t) - f(x^*) + \frac{\mu}{2}||x_t - x^*||^2$

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- Putting both together and next rearranging terms:

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

$$\Rightarrow ||x_{t+1} - x^*||^2 \leq 2\gamma(f(x^*) - f(x_t)) + \gamma^2||g_t||^2 + (1 - \mu\gamma)||x_t - x^*||^2$$

Fastest Convergence with Smooth + Strongly Convex II

- From previous slide:

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$$\begin{aligned} 2\gamma(f(x^*) - f(x_t)) + \gamma^2||g_t||^2 &\leq \frac{2}{L}(f(x_{t+1}) - f(x_t)) + \frac{1}{L^2}||g_t||^2 \\ &\leq -\frac{1}{L^2}||g_t||^2 + \frac{1}{L^2}||g_t||^2 = 0 \end{aligned}$$

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- Packing everything together:

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- Final step: Lets combine smoothness and the fact that $\nabla f(x^*) = 0$:

$$f(x_T) - f(x^*) \leq \nabla f(x^*)^T (x_T - x^*) + \frac{L}{2}||x_T - x^*||^2 = \frac{L}{2}||x_T - x^*||^2$$

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

Convergence Rate For Smooth + Strongly Convex

- Set $R^2 = ||x_0 - x^*||^2$. We get:

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- To get an error of $\epsilon = 0.01$, we now need only $L/\mu \log(50R^2 L)$ iterations as opposed to $50R^2 L$ iterations in the smooth case!

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  - $\epsilon = 0.001$, 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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- What if we have strong convexity? Can a function be **both** Lipschitz Continuous and Strongly Convex?
- Unfortunately No!!!!
- 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 $O(1/\epsilon)$ bound!!

Lipschitz + Strongly Convex I

- Assume the gradients $||g_t|| \leq B$.

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- Recall Analysis I:

$$g_t^T(x_t - x^*) = \gamma_t/2||g_t||^2 + 1/2\gamma_t(||x_t - x^*||^2 - ||x_{t+1} - x^*||^2)$$

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- Combining with strong convexity we get (after $||g_t|| \leq B^2$)

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

Lipschitz + Strongly Convex II

- So Far:

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- Plug in $\gamma_t^{-1} = \mu(1+t)/2$ and multily by t on both sides:

$$\begin{aligned} t[f(x_t) - f(x^*)] &\leq \frac{B^2 t}{\mu(t+1)} + \frac{\mu}{4}\{t(t-1)||x_t - x^*||^2 - (t+1)t||x_{t+1} - x^*||^2\} \\ &\leq \frac{B^2}{\mu} + \frac{\mu}{4}\{t(t-1)||x_t - x^*||^2 - (t+1)t||x_{t+1} - x^*||^2\} \end{aligned}$$

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

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

Lipschitz + Strongly Convex III

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

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- This implies if the error $\leq \epsilon$ implies $T \geq \frac{2B^2}{\mu\epsilon} - 1$

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- Case IV: Smooth + Strongly Convex: Define $\kappa = \frac{L}{\mu}$. Then Any black box procedure will have an error of at least $\frac{\mu}{2}(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1})^{2(T-1)}$ (GD: $\frac{L}{2}(1-\frac{\mu}{L})^T = \frac{L}{2}(\frac{\kappa-1}{\kappa})^T$)

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- Difference between Theory and Practice and the need to connect the two!
- Next, we will implement some of these algorithms for various ML Loss Functions!

Gradient Descent in Practice: Basic Version

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[python]

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Gradient Descent in Practice: Basic Version

```
def gd(funObj,w,maxEvals,alpha,X,y,lam, verbosity):
    [f,g] = funObj(w,X,y,lam)
    funEvals = 1
    funVals = []
    while(1):
        [f,g] = funObj(w,X,y,lam)
        optCond = LA.norm(g, np.inf)
        if (verbosity > 0):
            print(funEvals,alpha,f,optCond)
        w = w - alpha*g
        funEvals = funEvals+1
        if ((optCond < 1e-2) and (funEvals > maxEvals)
            break
        funVals.append(f)
    return funVals
```

Gradient Descent in Practice: Basic Version

- Run this by invoking:

```
funV = gd(LogisticLoss,w,200,1e-1,X,y,1,1,10)
```

- Try running this with different values of learning rates: $\alpha = 1e-1, 1e-3, 1e-5, ...$
- How do we find the optimal learning rate every time?
- Can there be better strategies to adapt the learning rates?
- Next, we shall see a few line search based strategies.

Armijo Backtracking Line-Search V1

- We don't want to tune α every time
- This is the idea behind line search
- Simple Line search strategy:
  - Start with a large value of α
  - Divide α by 1/2 if it doesn't satisfy Armijo's condition:

$$f(w - \alpha g) \leq f(w) - \gamma\alpha||g||^2$$

  - Basically find α such that there is a reduction in function value by atleast $\gamma\alpha||g||^2$
  - Idea: Choose α and γ such that this happens.

Armijo Backtracking Line-Search V2

- Danger with the simple backtracking is that α may quickly become very small quickly
- Easy fix: Reset α every time!
- Issue with this: Too many function evaluations lost in repeated backtracking!

Armijo Backtracking Line-Search V3

- Just halving the step size ignores the information collected during line search!
- Reduce the number of backtracks using a polynomial interpolation!
- Minimize a quadratic passing through $f(w), f'(w)$ and $f(w - \alpha g)$
- Choose α using a polynomial interpolation as follows:

$$\alpha = \frac{\alpha^2 g^T g}{2(fcurr + \alpha g^T g - f)}$$

- Here *fcurr* is the function evaluation with the current value of α and f is the function value before starting backtracking!

Armijo Backtracking Line-Search V4

- Final Issue to fix is better initialization of α.
- Initializing $\alpha = 1$ is too large in practice
- Wasted backtracks because of this.
- Use a hueristic like $\alpha = 1/||g||$
- On subsequent iterations again use a polynomial interpolation:

$$\alpha = \min(1, 2(f_{old} - f)/g^T g)$$

- A lot of this is tried empirically and based on empirical knowledge..