

CMPT 409/981: Optimization for Machine Learning

Lecture 18

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Adaptive step-sizes

- Recall the claim we proved earlier: If the convex set \mathcal{C} has diameter D , for an arbitrary sequence of losses such that each f_k is convex and differentiable, OGD with the update $w_{k+1} = \Pi_{\mathcal{C}}[w_k - \eta_k \nabla f_k(w_k)]$ such that $\eta_k \leq \eta_{k-1}$ and $w_1 \in \mathcal{C}$ has the following regret for $u \in \mathcal{C}$,

$$R_T(u) \leq \frac{D^2}{2\eta_T} + \sum_{k=1}^T \frac{\eta_k}{2} \|\nabla f_k(w_k)\|^2 = \frac{D^2}{2\eta} + \frac{\eta}{2} \sum_{k=1}^T \|\nabla f_k(w_k)\|^2 \quad (\text{If } \eta_k = \eta \text{ for all } k)$$

In order to find the optimal η , differentiating the RHS w.r.t η and setting it to zero,

$$-\frac{D^2}{2\eta^2} + \frac{1}{2} \sum_{k=1}^T \|\nabla f_k(w_k)\|^2 = 0 \implies \eta^* = \frac{D}{\sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2}}$$

Since the second derivative equal to $\frac{2D^2}{\eta^3} > 0$, η^* minimizes the RHS. Setting $\eta = \eta^*$,

$$R_T(u) \leq D \sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2}$$

Adaptive step-sizes

- Choosing $\eta = \eta^* = \frac{D}{\sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2}}$ minimizes the upper-bound on the regret. However, this is not practical since setting η requires knowing $\nabla f_k(w_k)$ for all $k \in [T]$.
- To approximate η^* to have a practical algorithm, we can set η_k as follows:

$$\eta_k = \frac{D}{\sqrt{\sum_{s=1}^k \|\nabla f_s(w_s)\|^2}}$$

Hence, at iteration k , we only use the gradients upto that iteration.

- Algorithmically, we only need to maintain the running sum of the squared gradient norms.
- Moreover, this choice of step-size ensures that $\eta_k \leq \eta_{k-1}$ (since we are accumulating gradient norms in the denominator so the step-size cannot increase) and hence we can use our general result for bounding the regret.

Scalar AdaGrad

Hence, we have the following update for any $\eta > 0$,

$$w_{k+1} = \Pi_C[w_k - \eta_k \nabla f_k(w_k)] \quad ; \quad \eta_k = \frac{\eta}{\sqrt{\sum_{s=1}^k \|\nabla f_s(w_s)\|^2}}$$

This is exactly the AdaGrad update without a per-coordinate scaling and is referred to as scalar AdaGrad or AdaGrad Norm [WWB20].

- For a sequence of convex, differentiable losses, using the general result,

$$R_T(u) \leq \frac{D^2}{2\eta_T} + \sum_{k=1}^T \frac{\eta_k}{2} \|\nabla f_k(w_k)\|^2 = \frac{D^2}{2\eta} \sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2} + \frac{\eta}{2} \sum_{k=1}^T \frac{\|\nabla f_k(w_k)\|^2}{\sqrt{\sum_{s=1}^k \|\nabla f_s(w_s)\|^2}}$$

In order to bound the regret for AdaGrad, we need to bound the last term.

Scalar AdaGrad

We prove the following general claim and will use it for $a_s = \|\nabla f_s(w_s)\|^2$.

Claim: For all T and $a_s \geq 0$, $\sum_{k=1}^T \frac{a_k}{\sqrt{\sum_{s=1}^k a_s}} \leq 2\sqrt{\sum_{k=1}^T a_k}$.

Proof: Let us prove by induction. **Base case:** For $T = 1$, LHS = $\sqrt{a_1} < 2\sqrt{a_1} =$ RHS.

Inductive Hypothesis: If the statement is true for $T - 1$, we need to prove it for T .

$$\sum_{k=1}^T \frac{a_k}{\sqrt{\sum_{s=1}^k a_s}} = \sum_{k=1}^{T-1} \frac{a_k}{\sqrt{\sum_{s=1}^k a_s}} + \frac{a_T}{\sqrt{\sum_{s=1}^T a_s}} \leq 2\sqrt{\sum_{s=1}^{T-1} a_s} + \frac{a_T}{\sqrt{\sum_{s=1}^T a_s}} = 2\sqrt{Z-x} + \frac{x}{\sqrt{Z}}$$

$(x := a_T, Z := \sum_{s=1}^T a_s)$

The derivative of the RHS w.r.t to x is $-\frac{1}{\sqrt{Z-x}} + \frac{1}{\sqrt{Z}} < 0$ for all $x \geq 0$ and hence the RHS is maximized at $x = 0$. Setting $x = 0$ completes the induction proof.

$$\Rightarrow \sum_{k=1}^T \frac{a_k}{\sqrt{\sum_{s=1}^k a_s}} \leq 2\sqrt{Z} = 2\sqrt{\sum_{s=1}^T a_s}$$

Scalar AdaGrad

Recall that $R_T(u) \leq \frac{D^2}{2\eta} \sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2} + \frac{\eta}{2} \sum_{k=1}^T \frac{\|\nabla f_k(w_k)\|^2}{\sqrt{\sum_{s=1}^k \|\nabla f_s(w_s)\|^2}}$.

Using the claim in the previous slide with $a_s := \|\nabla f_s(w_s)\|^2 \geq 0$,

$$R_T(u) \leq \frac{D^2}{2\eta} \sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2} + \eta \sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2} = \left(\frac{D^2}{2\eta} + \eta \right) \sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2}.$$

The step-size that minimizes the above bound is equal to $\eta^* = \frac{D}{\sqrt{2}}$. With this choice,

$$R_T(u) \leq \sqrt{2}D \sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2}$$

Comparing to the regret for the optimal (impractical) constant step-size on Slide 1,

$$R_T(u) \leq \sqrt{2} \min_{\eta} \left[\frac{D^2}{2\eta} + \frac{\eta}{2} \sum_{k=1}^T \|\nabla f_k(w_k)\|^2 \right]$$

Hence, AdaGrad is only sub-optimal by $\sqrt{2}$ when compared to the best constant step-size!

Scalar AdaGrad - Convex, Lipschitz functions

Claim: If the convex set \mathcal{C} has diameter D i.e. for all $x, y \in \mathcal{C}$, $\|x - y\| \leq D$, for an arbitrary sequence of losses such that each f_k is convex, differentiable and G -Lipschitz, scalar AdaGrad with $\eta_k = \frac{\eta}{\sqrt{\sum_{s=1}^k \|\nabla f_s(w_s)\|^2}}$ and $w_1 \in \mathcal{C}$ has the following regret for all $u \in \mathcal{C}$,

$$R_T(u) \leq \left(\frac{D^2}{2\eta} + \eta \right) G \sqrt{T}$$

Proof: Using the general result from the previous slide,

$$R_T(u) \leq \left(\frac{D^2}{2\eta} + \eta \right) \sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2} \leq \left(\frac{D^2}{2\eta} + \eta \right) \sqrt{G^2 T} = \left(\frac{D^2}{2\eta} + \eta \right) G \sqrt{T}$$

(Since each f_k is G -Lipschitz)

With $\eta = \frac{D}{\sqrt{2}}$, $R_T(u) \leq \sqrt{2} D G \sqrt{T}$.

- Hence, for convex, Lipschitz functions, AdaGrad achieves the same regret as OGD but is adaptive to G .

Scalar AdaGrad - Convex, Smooth functions

Claim: If the convex set \mathcal{C} has diameter D , for an arbitrary sequence of losses such that each f_k is convex, differentiable and L -smooth and $\zeta^2 := \max_{k \in [T]} [f_k(u) - f_k^*]$ where $f_k^* = \min_{w \in \mathcal{C}} f_k(w)$, scalar AdaGrad with $\eta_k = \frac{\eta}{\sqrt{\sum_{s=1}^k \|\nabla f_s(w_s)\|^2}}$ and $w_1 \in \mathcal{C}$ has the following regret for all $u \in \mathcal{C}$,

$$R_T(u) \leq 2L \left(\frac{D^2}{2\eta} + \eta \right)^2 + \sqrt{2L} \left(\frac{D^2}{2\eta} + \eta \right) \zeta \sqrt{T},$$

- The regret depends on ζ^2 which depends on u . Such bounds that depend on the fixed decision that we are comparing against are called *first-order regret bounds*.
- If the learner is competing against a fixed decision u that minimizes each f_k , i.e. $u \in \arg \min_w f_k(w)$ for all k , then $\zeta^2 = 0$. Hence, ζ^2 characterizes the analog of interpolation in the online setting. In this setting, AdaGrad only incurs a *constant regret* that is independent of T . This observation has been used to explain the good performance of IL algorithms when using over-parameterized (convex) models [YBC20, LVS22].
- Note that the above bound holds for all $\eta > 0$ and AdaGrad does not need to know ζ or L .

Scalar AdaGrad - Convex, Smooth functions

Proof: Using the general result for scalar AdaGrad,

$$R_T(u) \leq \left(\frac{D^2}{2\eta} + \eta \right) \sqrt{\sum_{k=1}^T \|\nabla f_k(w_k)\|^2}.$$

Using L -smoothness of f_k to bound the gradient norm term (for each k) in the regret expression,

$$\|\nabla f_k(w_k)\|^2 \leq 2L[f_k(w_k) - f_k^*] = 2L[f_k(w_k) - f_k(u)] + 2L[f_k(u) - f_k^*] \leq 2L[f_k(w_k) - f_k(u)] + 2L\zeta^2$$

$$\implies \sum_{k=1}^T \|\nabla f_k(w_k)\|^2 \leq 2L \sum_{k=1}^T [f_k(w_k) - f_k(u)] + 2L \sum_{k=1}^T \zeta^2 = 2L [R_T(u) + \zeta^2 T]$$

$$\implies R_T(u) \leq \left(\frac{D^2}{2\eta} + \eta \right) \sqrt{2L [R_T(u) + \zeta^2 T]}$$

Scalar AdaGrad - Convex, Smooth functions

Recall that $R_T(u) \leq \left(\frac{D^2}{2\eta} + \eta\right) \sqrt{2L[R_T(u) + \zeta^2 T]}$. Squaring this expression,

$$\begin{aligned} [R_T(u)]^2 &\leq \underbrace{2L \left(\frac{D^2}{2\eta} + \eta\right)^2}_{:=\alpha} \underbrace{[R_T(u)]}_{:=x} + \underbrace{\zeta^2 T}_{:=\beta} \\ \implies x^2 &\leq \alpha(x + \beta) \implies x \leq \frac{\alpha + \sqrt{\alpha^2 + 4\alpha\beta}}{2} \leq \alpha + \sqrt{\alpha\beta} \\ \implies R_T(u) &\leq 2L \left(\frac{D^2}{2\eta} + \eta\right)^2 + \sqrt{2L} \left(\frac{D^2}{2\eta} + \eta\right) \zeta \sqrt{T} \end{aligned}$$

Scalar AdaGrad - Strongly-Convex, Lipschitz functions




Claim: If the convex set \mathcal{C} has diameter D i.e. for all $x, y \in \mathcal{C}$, $\|x - y\| \leq D$, for an arbitrary sequence of losses such that each f_k is μ strongly-convex, differentiable and G -Lipschitz, scalar AdaGrad with $\eta_k = \frac{G^2/\mu}{1 + \sum_{s=1}^k \|\nabla f_s(w_s)\|^2}$ and $w_1 \in \mathcal{C}$ has the following regret for all $u \in \mathcal{C}$,

$$R_T(u) \leq \frac{D^2 \mu}{2 G^2} + \frac{G^2}{2 \mu} [1 + \log(1 + G^2 T)]$$

Proof: Need to prove this in Assignment 4!

- Though AdaGrad can achieve logarithmic regret for strongly-convex, Lipschitz functions similar to OGD and FTL, it requires knowledge of both G and μ .

Questions?

-  Jonathan Wilder Lavington, Sharan Vaswani, and Mark Schmidt, *Improved policy optimization for online imitation learning*, arXiv preprint arXiv:2208.00088 (2022).
-  Rachel Ward, Xiaoxia Wu, and Leon Bottou, *Adagrad stepsizes: Sharp convergence over nonconvex landscapes*, *The Journal of Machine Learning Research* **21** (2020), no. 1, 9047–9076.
-  Xinyan Yan, Byron Boots, and Ching-An Cheng, *Explaining fast improvement in online policy optimization*, arXiv preprint arXiv:2007.02520 (2020).