CS6301: Optimization in Machine Learning
Lecture 16: SGD and Adaptive Gradient Methods

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https://sites.google.com/view/cs-6301-optml/home

March 30th, 2020

Announcements

- First of All, Hope all of you are Safe!
- Please practice Social Distancing! Till the end of this semester, all classes will be held remotely.
- Assignment 2 was due last week.
- Given the situation with Covid-19, I decided to only have two assignments. We will however be having the course project, so please continue working on it.

Plan for the Next 5 Weeks

- March 30th (Today): SGD & Adaptive Gradient Methods
- March 30th (Today): Non-Convex Optimization
- April 1st (Wed): Duality, Lagrangians and Barrier Methods
- April 6th (Mon): Introduction to Submodular Optimization: Definition, Motivation and Applications
- April 8th (Wed): Submodular Optimization Problems
- April 13th/15th: Submodular Optimization Algorithms (Minimization and Maximization)
- April 20th - 29th: Project Presentations.

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- Nesterov's Accelerated Gradient (NAG): $\gamma_k = \beta_k$.

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- Fix: Adapt learning rate based on gradient information until now.

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- Define:
$$H_k = \text{diag}(\{\sum_{i=1}^{k} \eta_i g_i \circ g_i\}^{1/2})$$

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	SGD	HB	NAG	AdaGrad	RMSProp	Adam
G_k	I	I	I	$G_{k-1} + D_k$	$\beta_2 G_{k-1} + (1-\beta_2) D_k$	$\frac{\beta_2}{1-\beta_2^k} G_{k-1} + \frac{(1-\beta_2)}{1-\beta_2^k} D_k$
α_k	α	α	α	α	α	$\alpha \frac{1-\beta_1}{1-\beta_1^k}$
β_k	0	β	β	0	0	$\frac{\beta_1(1-\beta_1^{k-1})}{1-\beta_1^k}$
γ	0	0	β	0	0	0

More on ADAM

- Adam is basically HB Momentum + Adaptive.
- Define $m_k = \beta_1 m_{k-1} + (1 - \beta_1) g_k$
- Define $v_k = \beta_2 v_{k-1} + (1 - \beta_2) g_k \circ g_k$
- Intuition of m_k and v_k are estimates of first moment (mean) and second moment (uncentered variance) of the gradients.
- Since m_k and v_k are initialized to 0, they are biased towards zero when the decay rates are small. To counter this, they are further normalized by $1 - \beta^k$.
- Define $\hat{m}_k = m_k/(1 - \beta_1^k)$ and $\hat{v}_k = v_k/(1 - \beta_2^k)$.
- The ADAM update is $w_{k+1} = w_k - \alpha_k \hat{m}_k \circ \hat{v}_k^{-1/2}$
- Parameters used in practice: $\beta_1 = 0.9, \beta_2 = 0.999$.

Extensions

Numerous extensions of the above techniques

- AdaMax is an extension of ADAM to use the l_{infty} norm (i.e. max) instead of square.
- NADAM applies Nesterovs momentum instead of HB Momentum to Adaptive Methods.
- ADADelta is an extension of RMSProp to use the RMS operator on the weight differences as well.
- Recent Algorithm (AMSGrad) by Reddi et al (ICLR 2018) which fixes a theoretical error in ADAM (causing it to not converge even for convex functions) simply by ensuring v_t's remain positive!
- See more details to compare the different optimization algorithms (and also what they are) here: `https://ruder.io/optimizing-gradient-descent/`.

Theoretical Results

Numerous extensions of the above techniques

- The first theoretical result was shown for AdaGrad. The convergence result there is a *Regret* bound which is common for online algorithms.
- As mentioned above, the paper introducing ADAM actually had a bug in its analysis. The same also holds for RMSProp, AdaDelta and NADAM etc. They do not have **theoretical Regret bounds** backing them.
- Paper introducing AMSGrad showed regret bounds with a modified version of ADAM (and correspondingly RMSProp, NADAM, ...)
- All this only holds for convex functions. No results known for Non-Convex Functions.

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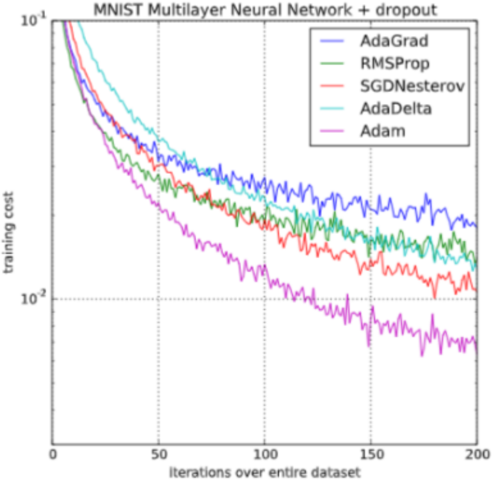
- The starting point of numerous new techniques for adaptive methods.
- There is really no one technique that is provably better than the other. Each technique has its own pros and cons!
- In the next few slides, I'll try to put together a few takeaways from some recent papers which have studied this specifically for non-convex optimization.

Kingma et al, ICLR 2015 – Original ADAM paper



Adaptive vs Non Adaptive Techniques: Comparisons

- Benefits of AdaGrad: AdaGrad can significantly improve upon SGD in sparse feature sets! It automatically sets the learning rate, and secondly, automatically updates the learning rates with a decay schedule! Also, it has a per coordinate learning rate!

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- Though adaptive gradient methods tend to minimize training loss better, they do so by obtaining more complex and less generalizable solutions!
- They gave a few synthetic examples (particularly in over0parameterized scenarios) where SGD and its variants obtain the less complex solutions but Adaptive variants obtain solutions which do not generalize well!

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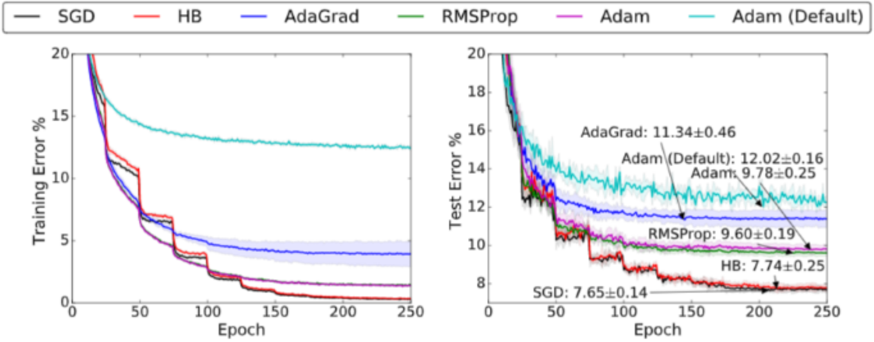
See Wilson et al, The Marginal Value of Adaptive Gradient Methodsin Machine Learning, NeurIPS 2017



(a) CIFAR-10 (Train) (b) CIFAR-10 (Test)

Additional Reading

- Wilson et al, The Marginal Value of Adaptive Gradient Methodsin Machine Learning, NeurIPS 2017
- Reddi et al, On the Convergence of ADAM and Beyond, ICLR 2018.
- Kingma and Ba, ADAM: A Method for Stochastic Optimization, ICLR 2015
- Duchi et al, Adaptive subgradient methods for online learningand stochastic optimization, Journal of Machine Learning Research 2011.
- Zeiler. ADADELTA: An Adaptive Learning Rate Method, ArXiv 2012
- `https://ruder.io/optimizing-gradient-descent/`