CS6375: Machine Learning

Lecture 21: Summary Of Optimization Algorithms in Machine Learning

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Announcements

- Assignment 4 due on November 30th
- Finals will be December 2nd. Timing is 7:30pm - 10pm CST which is 7am to 9:30am IST.
- The examination will be for 2.5 hours, similar to the QE exam
- The number of questions etc. will be similar to the the mid-term (consisting of short answers, true/false questions and the questions will cover through all the topics covered until today).
- Roughly the split will be 50% pre-midterm and 50% post-midterm.
- Try to focus on the fundamentals!

Recap: General Machine Learning Problem

- Given training data $\{(x_1, y_1), \cdots, (x_N, y_N)\}$
- Assume Parameters are w (weights)
- General ML Optimization Problem:

$$\min_w \sum_{i=1}^{N} L(x_i, y_i, w) + \lambda R(w) \tag{1}$$

- $R(w)$ is a regularizer (either L1 or L2 regularization)

Gradient Descent

- General ML Optimization Problem:

$$\min_{w} \sum_{i=1}^{N} L(x_i, y_i, w) + \lambda R(w) \tag{2}$$

- Gradient Descent computes the full gradient!
- Update equation: $w_{k+1} = w_k - \alpha_k \sum_{i=1}^{N} \nabla_w L(x_i, y_i, w) - \lambda \nabla_w R(w)$
- What is the problem with gradient descent?

Stochastic Gradient Descent

- Computing full gradient can be time consuming if N is very large!
- Idea of SGD: Compute an approximation of the full gradient and then move in that direction
- Idea: At iteration k, pick a random index i_k and then perform the following update:

$$w_{k+1} = w_k - \alpha_k \nabla f_{i_k}(w_k)$$

- Can be extended to minibatch setting as well.

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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

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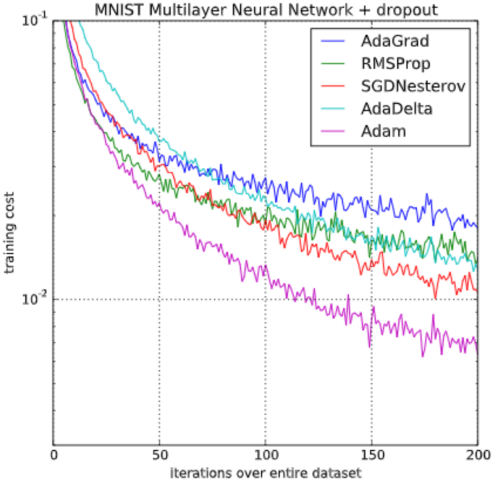
- The starting point of numerous new techniques for adaptive methods.
- There is really no one technique that is provably better than the other. Each technique has its own pros and cons!
- In the next few slides, I'll try to put together a few takeaways from some recent papers which have studied this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

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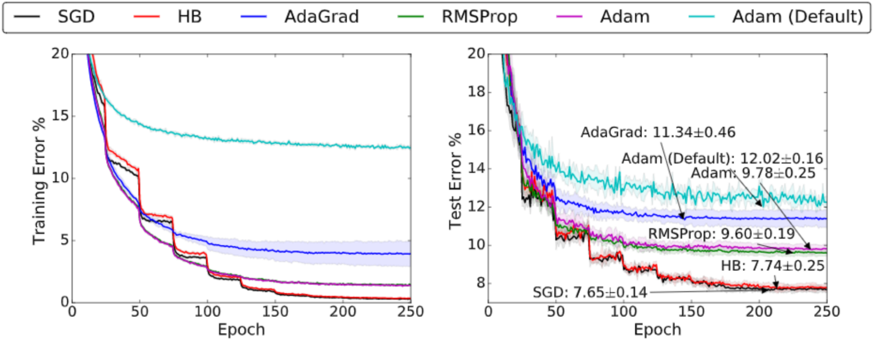
- Though adaptive gradient methods tend to minimize training loss better, they do so by obtaining more complex and less generalizable solutions!
- They gave a few synthetic examples (particularly in over0parameterized scenarios) where SGD and its variants obtain the less complex solutions but Adaptive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

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/`