Adaptive Gradient Methods AdaGrad / Adam

Machine Learning for Big Data
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Announcements:

- HW3 posted
  - Dual coordinate ascent
  - (some review of SGD and random features)
- Projects: the term end is approaching!
- Today:
  - Review: adaptive gradient methods
  - Today: momentum; parallelization

Review

Curvature approximation:

- One idea:

$$\nabla^2 \hat{L}(w) \overset{?}{\approx} \frac{1}{t} \sum_t g_t(w) g_t(w)^\top$$

where g_t(w) is the gradient of the t-th data point

P.S.D.

- Many ideas try to use this approximation
  - Quasi-Newton methods, Gauss newton methods
  - Ellipsoid method (sort of)

Mahalanobis Regret Bounds

$$\mathbf{w}^{(t+1)} = \arg\min_{\mathbf{w}\in\mathcal{W}} ||\mathbf{w} - (\mathbf{w}^{(t)} - \eta A^{-1} g_t)||_A^2$$

- **What *A* to choose?**
- Regret bound now:

$$\sum_{t=1}^{T} \ell_t(\mathbf{w}^{(t)}) - \ell_t(\mathbf{w}^*) \leq \frac{1}{2\eta}||\mathbf{w}^{(1)} - \mathbf{w}^*||_2^2 + \frac{\eta}{2}\sum_{t=1}^{T}||g_t||_{A^{-1}}^2$$

- What if we minimize upper bound on regret w.r.t. *A* in hindsight?

$$\min_A \sum_{t=1}^{T} g_t^T A^{-1} g_t$$

Mahalanobis Regret Minimization

- Objective:

$$\min_A \sum_{t=1}^{T} g_t^T A^{-1} g_t \qquad \text{subject to } A \succeq 0, \text{tr}(A) \leq C$$

$$= \text{Tr}\left(\left(\sum_t g_t g_t^T\right) A^{-1}\right)$$

- Solution:

$$A = c\left(\sum_{t=1}^{T} g_t g_t^T\right)^{\frac{1}{2}}$$

For proof, see Appendix E, Lemma 15 of Duchi et al. 2011.
Uses "trace trick" and Lagrangian.

- *A* defines the norm of the metric space we should be operating in

AdaGrad Algorithm

- At time *t*, estimate optimal (sub)gradient modification *A* by

$$A_t = \left(\sum_{\tau=1}^{t} g_\tau g_\tau^T\right)^{\frac{1}{2}}$$

- For *d* large, A_t is computationally intensive to compute. Instead,

$$\text{diag}(A_t) = \begin{pmatrix} A_{11} & & 0 \\ & \ddots & \\ 0 & & A_{dd} \end{pmatrix} \qquad (A_t)_{ii} = \sqrt{\sum_{\tau=1}^{t} g_{\tau,i}^2}$$

- Then, algorithm is a simple modification of normal updates:

$$\mathbf{w}^{(t+1)} = \arg\min_{\mathbf{w}\in\mathcal{W}} ||\mathbf{w} - (\mathbf{w}^{(t)} - \eta\text{diag}(A_t)^{-1} g_t)||^2_{\text{diag}(A_t)}$$

AdaGrad in Euclidean Space

with diagonal approx.

- For $\mathcal{W} = \mathbb{R}^d$,

- For each feature dimension,

$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \eta_{t,i} g_{t,i}$$

where

$$\eta_{t,i} =$$

- That is,

$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \frac{\eta}{\sqrt{\sum_{\tau=1}^{t} g_{\tau,i}^2}} g_{t,i}$$

- Each feature dimension has it's own learning rate!
  - Adapts with *t*
  - Takes geometry of the past observations into account
  - Primary role of η is determining rate the first time a feature is encountered

AdaGrad Theoretical Guarantees

- AdaGrad regret bound:

$$R_\infty := \max_t ||\mathbf{w}^{(t)} - \mathbf{w}^*||_\infty$$

$$\sum_{t=1}^{T} \ell_t(\mathbf{w}^{(t)}) - \ell_t(\mathbf{w}^*) \leq 2R_\infty \sum_{i=1}^{d} ||g_{1:T,i}||_2$$

  - In stochastic setting:

$$\mathbb{E}\left[\ell\left(\frac{1}{T}\sum_{t=1}^{T} w^{(t)}\right)\right] - \ell(\mathbf{w}^*) \leq \frac{2R_\infty}{T}\sum_{i=1}^{d}\mathbb{E}[||g_{1:T,j}||_2]$$

with diag scaling.

- This is used in practice.
- Many cool examples. Let's just examine one…

AdaGrad Theoretical Example

- Expect to out-perform when gradient vectors are *sparse*
- SVM hinge loss example:

$$\ell_t(\mathbf{w}) = [1 - y^t \langle \mathbf{x}^t, \mathbf{w} \rangle]_+$$

$$\mathbf{x}^t \in \{-1, 0, 1\}^d$$

- If $x_j^t \neq 0$ with probability $\propto j^{-\alpha}, \quad \alpha > 1$

$$\mathbb{E}\left[\ell\left(\frac{1}{T}\sum_{t=1}^{T} \mathbf{w}^{(t)}\right)\right] - \ell(\mathbf{w}^*) = \mathcal{O}\left(\frac{||\mathbf{w}^*||_\infty}{\sqrt{T}} \cdot \max\{\log d, d^{1-\alpha/2}\}\right)$$

- (sort of) previously bound: $\mathbb{E}\left[\ell\left(\frac{1}{T}\sum_{t=1}^{T} \mathbf{w}^{(t)}\right)\right] - \ell(\mathbf{w}^*) = \mathcal{O}\left(\frac{||\mathbf{w}^*||_\infty}{\sqrt{T}} \cdot \sqrt{d}\right)$

ADAM

- Like AdaGrad but with "forgetting"
- The algo has component-wise updates

Adam update rule consists of the following steps

- Compute gradient g_t at current time t
- Update biased first moment estimate

$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$$

- Update biased second raw moment estimate

$$v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$$

- Compute bias-corrected first moment estimate

$$\hat{m}_t = \frac{m_t}{1-\beta_1^t}$$

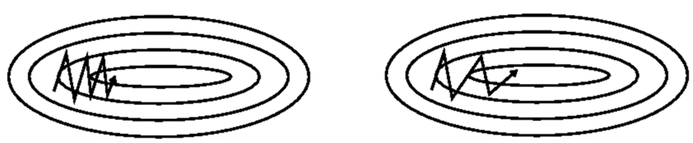
- Compute bias-corrected second raw moment estimate

$$\hat{v}_t = \frac{v_t}{1-\beta_2^t}$$

- Update parameters

$$\theta_t = \theta_{t-1} - \alpha \frac{\hat{m}_t}{\sqrt{\hat{v}_t} + \epsilon}$$

Momentum Algorithm

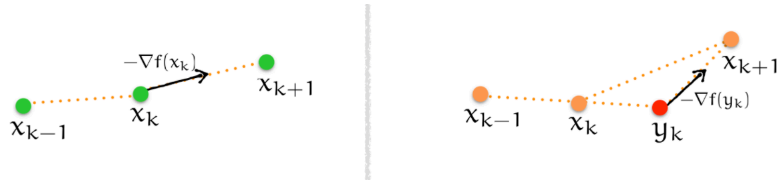


- (Polyak 1964) The Heavy Ball method
- Two step procedure:

$$p_k = -\nabla f(x_k) + \beta_k p_{k-1}$$
$$x_{k+1} = x_k + \alpha_k p_k$$

- Theory: asymptotically, it replaces condition number κ with root(κ).
- Practice: Used with stochastic gradients. The results are mixed (both in the exact and stochastic case).

Nesterov's Acceleration Algorithm

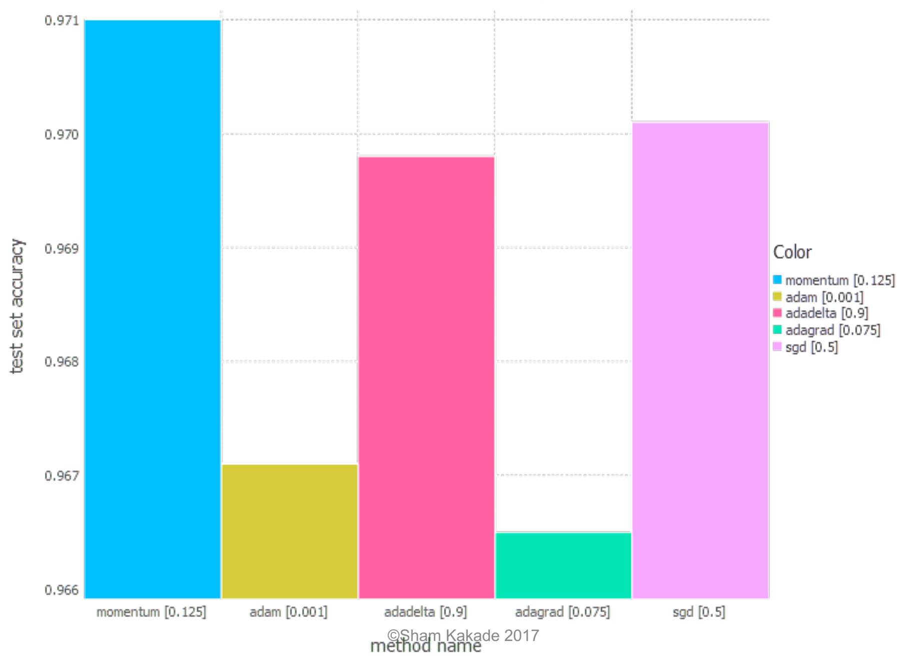


- (Nesterov 1983) Momentum done right:
- Two step procedure:

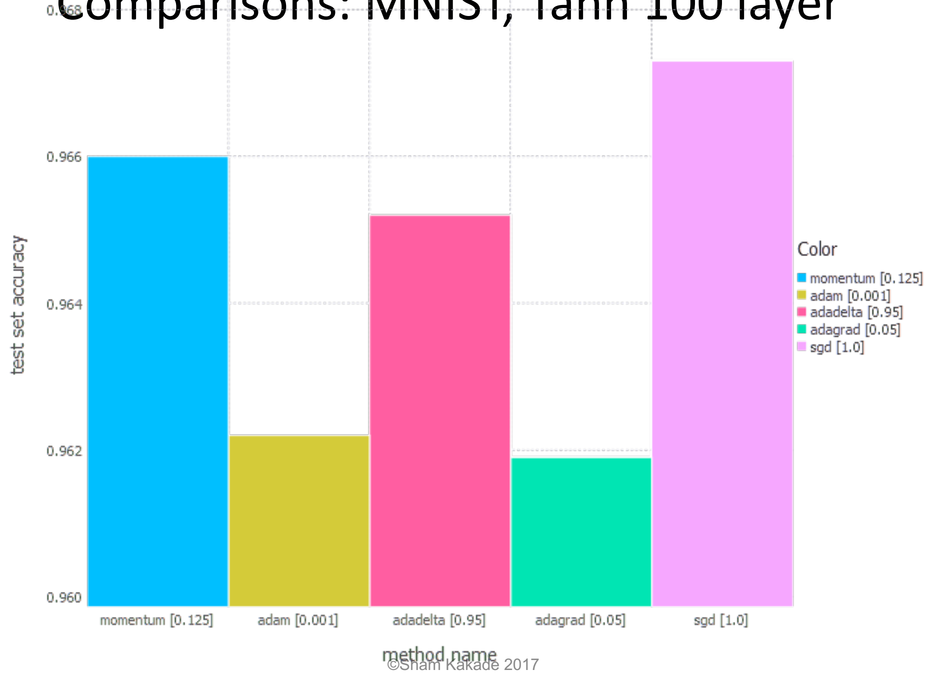
$$y_{k+1} \leftarrow x_k + \beta_k (x_k - x_{k-1})$$
$$x_{k+1} \leftarrow y_{k+1} - \frac{1}{L} \nabla f(y_{k+1}),$$

- Theory: It replaces condition number κ with root(κ).
- Practice: We need a stochastic variant. (It's "great" in the determistic case)

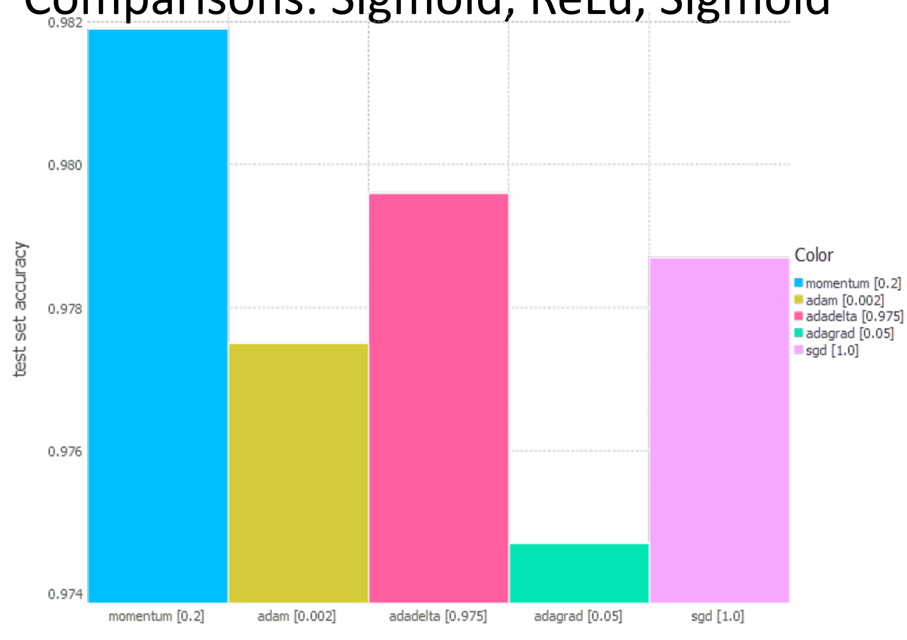
Comparisons: MNIST, Sigmoid 100 layer



Comparisons: MNIST, Tanh 100 layer



Comparisons: Sigmoid, ReLu, Sigmoid



Take Aways / Perspective

- Curvature adaptive methods can (in principle and in practice) speed up the optimization
  - For exact gradient methods, they are widely used
- With regards to SGD, the empirical results are more mixed.
- Scalar learning rate case: In practice, we often need to turn the learning rate down. What is the "right" way to do this?
  - Sadly, there isn't a clear "universal" picture in the convex case (1/T, 1/Root(t), constant, etc depending on the setting)
  - So how do we expect reasonable adaptive algorithms in the non-convex case?
- Using "matrix" valued curvature: Often use diagonal scalings
  - The 'choice' is problem dependent (scale subsets of coordinates/nodes jointly, scale individual coordinates, etc)
  - How to effectively turn down learning rates?
- Can we get a clearer picture?

Acknolwedgments

- Some figs taken from: http://int8.io/comparison-of-optimization-techniques-stochastic-gradient-descent-momentum-adagrad-and-adadelta/
- http://awibisono.github.io/2016/06/20/accelerated-gradient-descent.html
- http://sebastianruder.com/optimizing-gradient-descent/