Case Study 1: Estimating Click Probabilities

Adaptive Gradient Methods
AdaGrad / Adam

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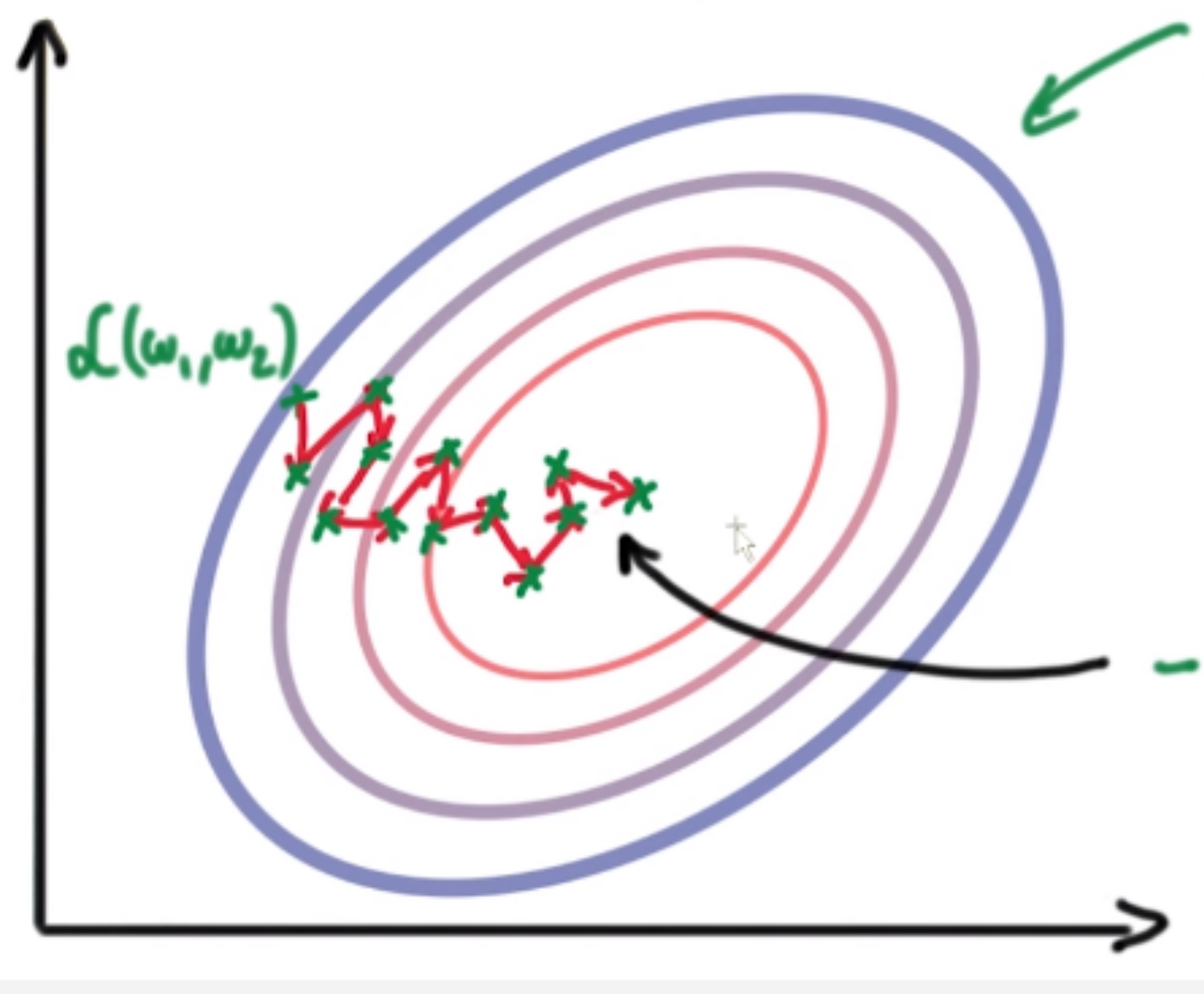
The Problem with GD (and SGD)



Adaptive Gradient Methods: Convex Case

- What we want?
- Newton's method:

$$w \leftarrow w - [\nabla^2 L(w)]^{-1} \nabla L(w)$$

- Why is this a good idea?
  - Guarantees?
  - Stepsize?
- Related ideas:
  - Conjugate Gradient/Acceleration:
  - L-BFGS
  - Quasi-Newton methods

Adaptive Gradient Methods: Non-Cvx Case

- What do we want?
  - Hessian may not be PSD, so is Newton's method a descent method?

- Other ideas:
  - Natural Gradient methods:
  - Curvature adaptive:
    - Adagrad, AdaDelta, RMS prop, ADAM, l-BFGS, heavy ball gradient, momemtum
  - Noise injection:
    - Simulated annealing, dropout, Langevin methods

- Caveats:
  - Batch methods may be poor: "On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima"

Natural Gradient Idea

- Probabilistic models and maximum likelihood estimation:

$$\hat{L}(w) = -\log Pr(\text{data}|w)$$

- True likelihood function:

$$L(w) = -E_{z\sim D} \log\ Pr(z|w)$$

  where z is sampled form the underling data distribution D.

- Suppose the model is correct, i.e. $z\sim \Pr(z|w^*)$ for some w^*
  - Let's look at the Hessian at w^*

$$\begin{aligned} \nabla^2 L(w^*) &= \mathbb{E}_{z\sim\Pr(z|w^*)}[-\nabla^2 \log \Pr(z|w^*)] \\ &= \mathbb{E}_{z\sim\Pr(z|w^*)}[\nabla \log \Pr(z|w^*)(\nabla \log \Pr(z|w^*))^\top] \end{aligned}$$

- How do we approximate the Hessian at w?

Fisher Information Matrix

- Define the Fisher matrix:

$$F(w) \quad := \quad \mathbb{E}_{z\sim \Pr(z|w)}[\nabla \log \Pr(z|w)(\nabla \log \Pr(z|w))^\top]$$

- If the model is correct and if $w -> w^*$, then $F(w) \rightarrow F(w^*)$
- Natural Gradient: Use the update rule:

$$w \leftarrow w - [F(w)]^{-1} \nabla L(w)$$

- Empirically, use L^(w) and

$$\hat{F}(w) \quad := \quad \frac{1}{t} \sum_t g_t(w) g_t(w)^\top$$

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

Curvature approximation:

- One idea:

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

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

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

Motivating AdaGrad (Duchi, Hazan, Singer 2011)

- Assuming $\mathbf{w} \in \mathbb{R}^d$, standard stochastic (sub)gradient descent updates are of the form:

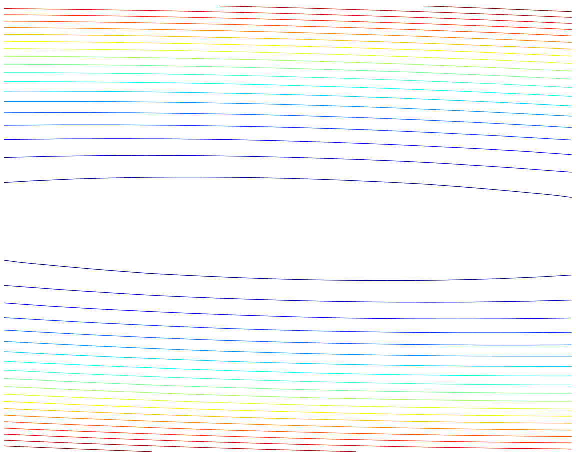
$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \eta_t g_{t,i}$$

- Should all features share the same learning rate?

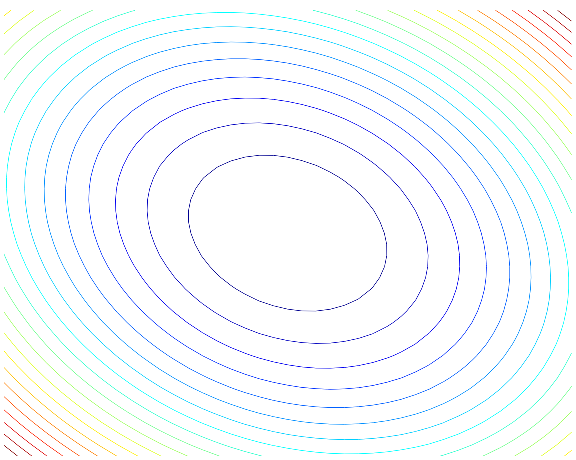
- Motivating AdaGrad (Duchi, Hazan, Singer 2011):
  Often have high-dimensional feature spaces
  - Many features are irrelevant
  - Rare features are often very informative

- Adagrad provides a feature-specific adaptive learning rate by incorporating knowledge of the geometry of past observations

Why Adapt to Geometry?



Hard



Nice

y_t	$x_{t,1}$	$x_{t,2}$	$x_{t,3}$
1	1	0	0
-1	.5	0	1
1	-.5	1	0
-1	0	0	0
1	.5	0	0
-1	1	0	0
1	-1	1	0
-1	-.5	0	1

Examples from Duchi et al. ISMP 2012 slides

1. Frequent, irrelevant
2. Infrequent, predictive
3. Infrequent, predictive

Not All Features are Created Equal

- Examples:

Text data:

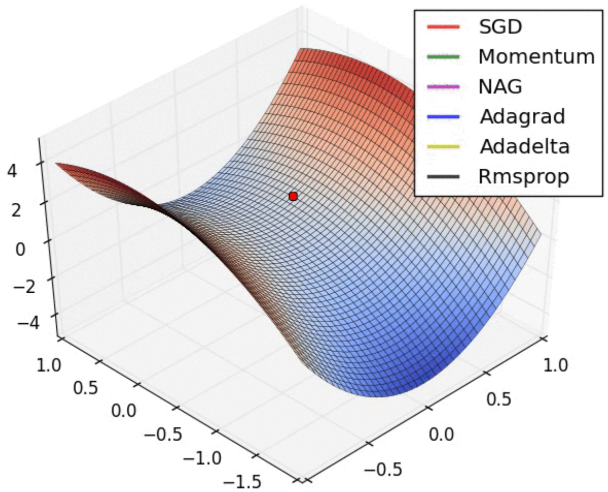
The most unsung birthday in American business and technological history this year may be the 50th anniversary of the Xerox 914 photocopier.[a]

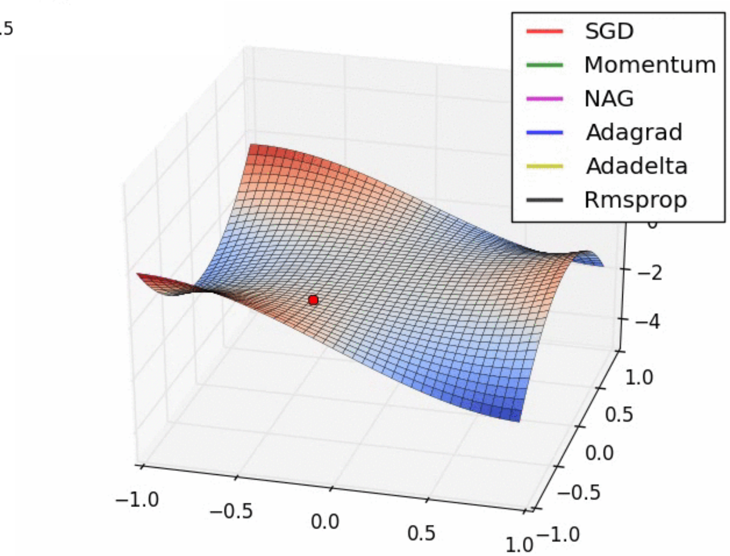
[a] *The Atlantic*, July/August 2010.

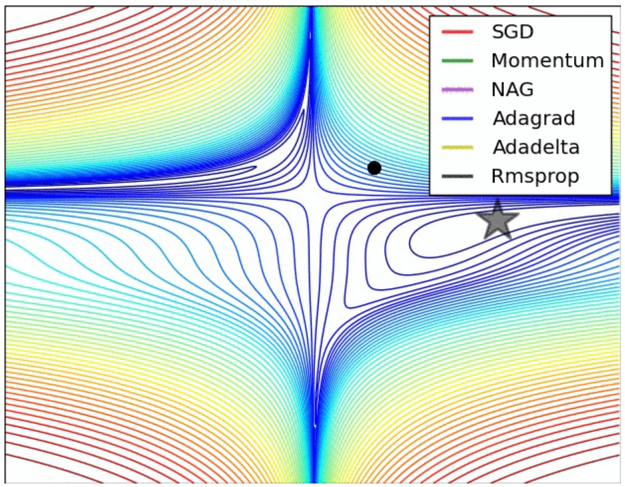
High-dimensional image features

Images from Duchi et al. ISMP 2012 slides

Visualizing Effect







Credit:
http://imgur.com/a/Hqolp

Regret Minimization

- How do we assess the performance of an online algorithm?

- Algorithm iteratively predicts $\mathbf{w}^{(t)}$
- Incur ***loss*** $\ell_t(\mathbf{w}^{(t)})$
- ***Regret***:
  What is the total incurred loss of algorithm relative to the best choice of $\mathbf{w}$ that could have been made ***retrospectively***

$$R(T) = \sum_{t=1}^{T} \ell_t(\mathbf{w}^{(t)}) - \inf_{\mathbf{w} \in \mathcal{W}} \sum_{t=1}^{T} \ell_t(\mathbf{w})$$

Regret Bounds for Standard SGD

- Standard projected gradient stochastic updates:

$$\mathbf{w}^{(t+1)} = \arg\min_{\mathbf{w}\in\mathcal{W}} ||\mathbf{w} - (\mathbf{w}^{(t)} - \eta g_t)||_2^2$$

- Standard regret bound:

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

Projected Gradient using Mahalanobis

- Standard projected gradient stochastic updates:

$$\mathbf{w}^{(t+1)} = \arg\min_{\mathbf{w}\in\mathcal{W}} ||\mathbf{w} - (\mathbf{w}^{(t)} - \eta g_t)||_2^2$$

- What if instead of an L_2 metric for projection, we considered the ***Mahalanobis*** norm

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

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:

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

- 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,

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

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

AdaGrad in Euclidean Space

- 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:

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

- This really 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 $\propto j^{-\alpha}, \quad \alpha > 1$

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

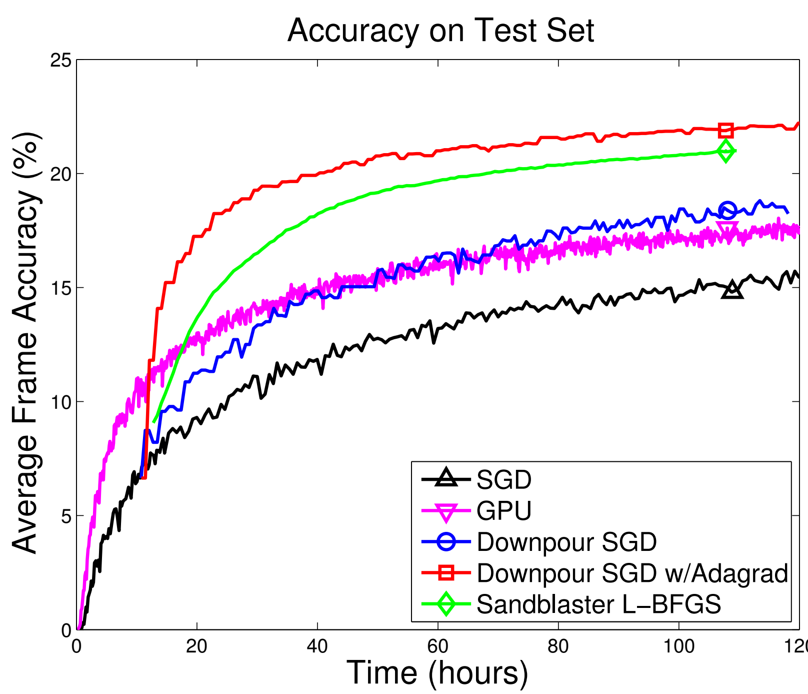
- (sort of) previously bound: $\mathbb{E}\left[\ell\left(\frac{1}{T}\sum_{t=1}^{T}\mathbf{w}^{(t)}\right)\right] - \ell(\mathbf{w}^*) = \mathcal{O}\left(\frac{||\mathbf{w}^*||_\infty}{\sqrt{T}} \cdot \sqrt{d}\right)$

Neural Network Learning

- Very non-convex problem, but use SGD methods anyway

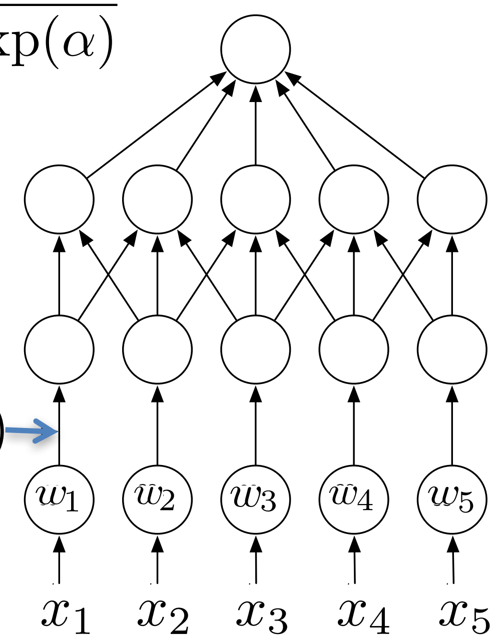
$$\ell(w, x) = \log(1 + \exp(\langle [p(\langle w_1, x_1 \rangle) \cdots p(\langle w_k, x_k \rangle)], x_0 \rangle))$$

$$p(\alpha) = \frac{1}{1 + \exp(\alpha)}$$



(Dean et al. 2012)

$p(\langle w_1, x_1 \rangle)$



Distributed, $d = 1.7 \cdot 10^9$ parameters. SGD and AdaGrad use 80 machines (1000 cores), L-BFGS uses 800 (10000 cores)

Images from Duchi et al. ISMP 2012 slides

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

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

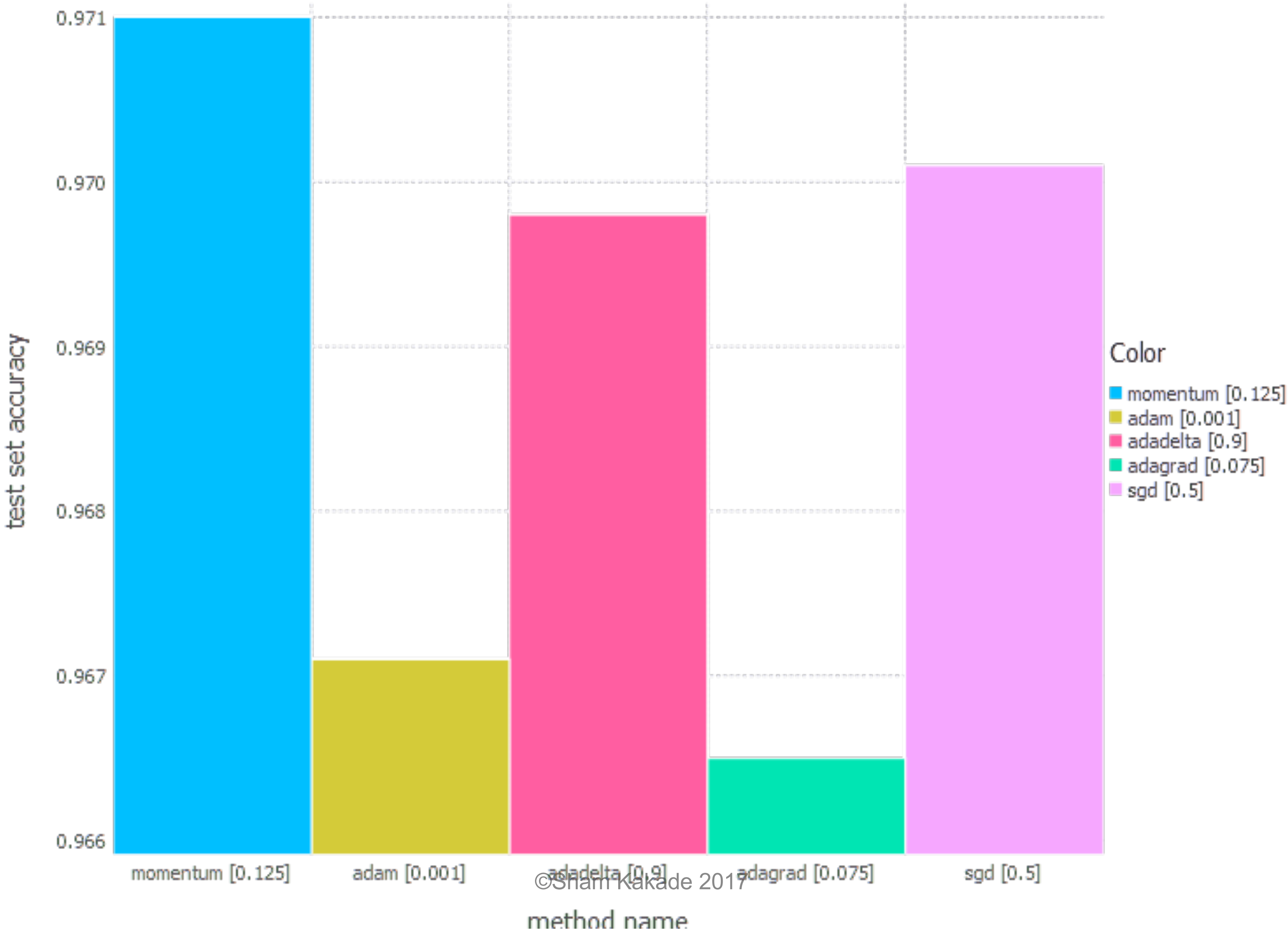
- Compute bias-corrected second raw moment estimate

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

- Update parameters

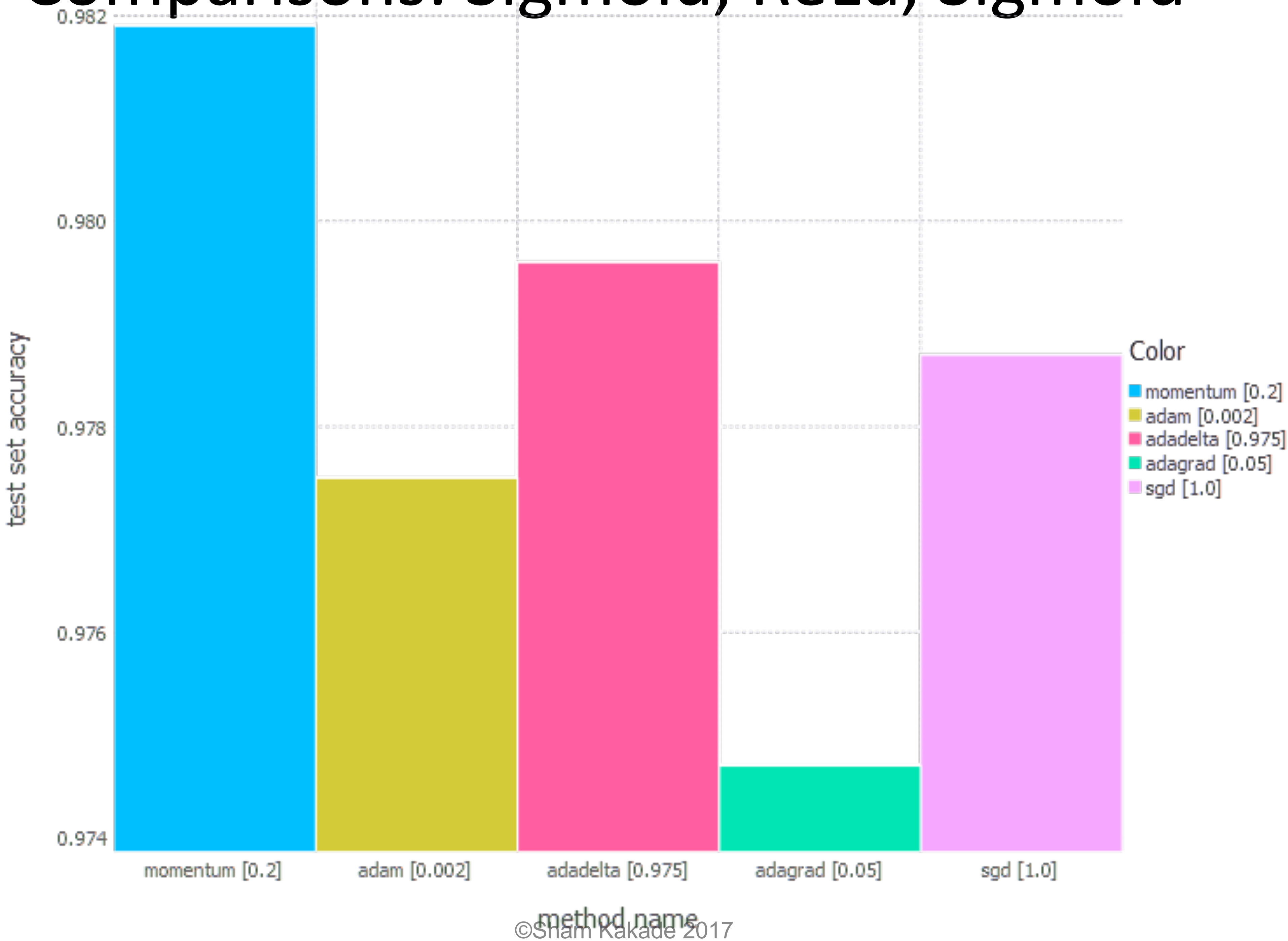
$$\theta_t = \theta_{t-1} - \alpha \frac{\hat{m}_t}{\sqrt{\hat{v}_t} + \epsilon}$$

Comparisons: MNIST, Sigmoid 100 layer



Comparisons: MNIST, Tanh 100 layer

Comparisons: Sigmoid, ReLu, Sigmoid



Acknolwedgments

- Some figs taken from: http://int8.io/comparison-of-optimization-techniques-stochastic-gradient-descent-momentum-adagrad-and-adadelta/