Modern Computational Statistics

Lecture 3: Advanced Gradient Descent

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Overview

- While gradient descent is simple and intuitive, it has many problems as well.
  - Saddle-point problem
  - Not applicable to non-differential objectives
  - Could be slow
  - How to scale to big data problems
- In this lecture, we will discuss some advanced techniques that can alleviate these problems

Momentum Method

- Introduced in 1964 by Polyak, momentum method is a technique that can accelerate gradient descent by taking accounts of previous gradients in the update rule at each iteration.

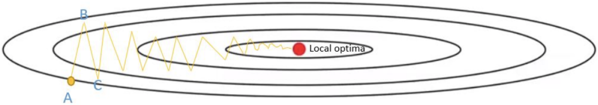
$$
\begin{aligned}
m^{(k)} &= \mu m^{(k-1)} + (1-\mu)\nabla f(x^{(k)}) \\
x^{(k+1)} &= x^{(k)} - \alpha m^{(k)}
\end{aligned}
$$

  where $0 \le \mu < 1$

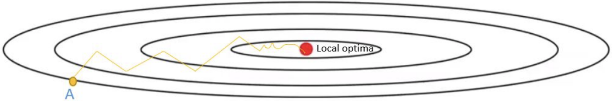
- When $\mu = 0$, gradient descent is recovered.

How Does Momentum Work?

- The vanilla gradient descent may suffer from oscillations when the magnitudes of gradient varies a lot across different directions.



- Using the exponential weighted gradient (momentum), those oscillations are more likely to be damped out, resulting in faster rate of convergence.



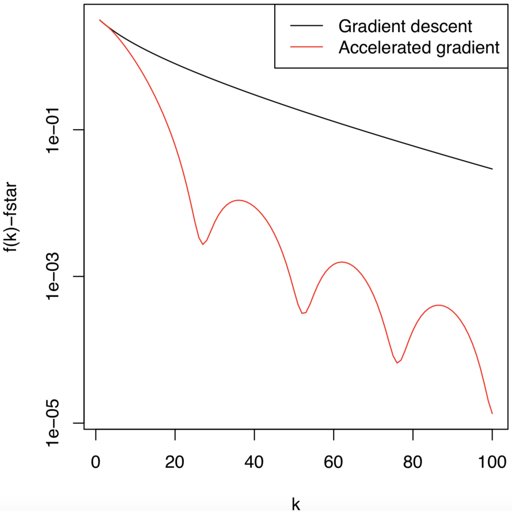
- Choose any initial $x^{(0)} = x^{(-1)}$, $\forall\, k = 1, 2, 3, \ldots$

$$y = x^{(k-1)} + \frac{k-2}{k+1}(x^{(k-1)} - x^{(k-2)})$$
$$x^{(k)} = y - t_k \nabla f(y)$$

- The first two steps are the usually gradient updates
- After that, $y = x^{(k-1)} + \frac{k-2}{k+1}(x^{(k-1)} - x^{(k-2)})$ carries some "momentum" from previous iterations, and $x^{(k)} = y - t_k \nabla f(y)$ uses *lookahead* gradient at y.

Example

Logistic regression



Assumptions

- f is convex and continuously differentiable on $\mathbb{R}^n$
- $\nabla f(x)$ is L-Lipschitz continuous w.r.t Euclidean norm: for any $x, y \in \mathbb{R}^n$

$$\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$$

- optimal value $f^* = \inf_x f(x)$ is finite and attained at x^*.

Theorem: Gradient descent with $0 < t \leq 1/L$ satisfies

$$f(x^{(k)}) - f^* \leq \frac{1}{2kt}\|x^{(0)} - x^*\|^2$$

Some Useful Lemma and Strong Convexity

- If f is L-Lipschitz, then for any $x, y \in \mathbb{R}^n$

$$f(y) \leq f(x) + \nabla f(x)^T (y - x) + \frac{L}{2} \|y - x\|^2$$

- If f is differentiable and m-strongly convex, then

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{m}{2} \|y - x\|^2$$

  If $m = 0$, we cover the standard(weak) convexity

- In other words, f is *sandwiched* between two quadratic functions

Proof

- If $x^+ = x - t\nabla f(x)$ and $0 < t \leq 1/L$

$$f(x^+) \leq f(x) - t\|\nabla f(x)\|^2 + \frac{t^2 L}{2}\|\nabla f(x)\|^2$$
$$\leq f(x) - \frac{t}{2}\|\nabla f(x)\|^2$$

- From convexity

$$f(x) \leq f^* + \nabla f(x)^T(x - x^*) - \frac{m}{2}\|x - x^*\|^2$$

- Add the above two inequalities

$$f(x^+) - f^* \leq \nabla f(x)^T(x - x^*) - \frac{t}{2}\|\nabla f(x)\|^2 - \frac{m}{2}\|x - x^*\|^2$$

Proof

- Continue ...

$$\begin{aligned}
&\le \frac{1}{2t}(\|x - x^*\|^2 - \|x^+ - x^*\|^2) - \frac{m}{2}\|x - x^*\|^2 \\
&= \frac{1}{2t}\left((1 - mt)\|x - x^*\|^2 - \|x^+ - x^*\|^2\right) \qquad (1) \\
&\le \frac{1}{2t}(\|x - x^*\|^2 - \|x^+ - x^*\|^2) \qquad (2)
\end{aligned}$$

- For gradient descent updates

$$\begin{aligned}
\sum_{i=1}^{k}(f(x^{(i)}) - f^*) &\le \frac{1}{2t}\sum_{i=1}^{k}(\|x^{(i-1)} - x^*\|^2 - \|x^{(i)} - x^*\|^2) \\
&= \frac{1}{2t}(\|x^{(0)} - x^*\|^2 - \|x^{(k)} - x^*\|^2)
\end{aligned}$$

Proof

- Since $f(x^{(i)})$ is non-increasing

$$f(x^{(k)}) - f^* \leq \frac{1}{2kt}\|x^{(0)} - x^*\|^2$$

- If f is m-strongly convex, and $m > 0$, from (1)

$$\|x^{(i)} - x^*\|^2 \leq (1 - mt)\|x^{(i-1)} - x^*\|^2, \quad \forall i = 1, 2, \ldots$$

- Therefore

$$\|x^{(k)} - x^*\|^2 \leq (1 - mt)^k\|x^{(0)} - x^*\|^2$$

i.e., linear convergence if f is strongly convex ($m > 0$)

- First order method: any iterative algorithm that selects $x^{(k+1)}$ in the set

$$x^{(0)} + \text{span}\{\nabla f(x^{(0)}), \nabla f(x^{(1)}), \ldots, \nabla f(x^{(k)})\}$$

- **Theorem** (Nesterov): for every integer $k \leq (n-1)/2$ and every $x^{(0)}$, there exist functions that satisfy the assumptions such that for any first-order method

$$f(x^{(k)}) - f^* \geq \frac{3}{32} \frac{L\|x_0 - x^*\|^2}{(k+1)^2}$$

- Therefore, $1/k^2$ is the best convergence rate for all first-order methods.

- Accelerated gradient descent with fixed step size $t \leq 1/L$ satisfies

$$f(x^{(k)}) - f^* \leq \frac{2\|x^{(0)} - x^*\|^2}{t(k+1)^2}$$

- Nesterov's accelerated gradient (**NAG**) descent achieve the oracle convergence rate of first-order methods!

Reformulation of NAG

- Initialize $x^{(0)} = u^{(0)}$, and for $k = 1, 2, \ldots$

$$y = (1 - \theta_k) x^{(k-1)} + \theta_k u^{(k-1)}$$
$$x^{(k)} = y - t_k \nabla f(y)$$
$$u^{(k)} = x^{(k-1)} + \frac{1}{\theta_k}(x^{(k)} - x^{(k-1)})$$

  with $\theta_k = 2/(k+1)$.

- This is equivalent to the formulation of NAG presented earlier (slide 5), and makes convergence analysis easier

Proof

- If $y = (1-\theta)x + \theta u,\ x^+ = y - t\nabla f(y)$, and $0 < t \leq 1/L$

$$f(x^+) \leq f(y) + \nabla f(y)^T(x^+ - y) + \frac{1}{2t}\|x^+ - y\|^2$$

- From convexity, $\forall z \in \mathbb{R}^n$

$$f(y) \leq f(z) + \nabla f(y)^T(y - z)$$

- Add these together

$$f(x^+) \leq f(z) + \frac{1}{t}(x^+ - y)(z - x^+) + \frac{1}{2t}\|x^+ - y\|^2 \qquad (3)$$

- Let $u^+ = x + \frac{1}{\theta}(x^+ - x)$, using bound (3) at $z = x$ and $z = x^*$

$$
\begin{aligned}
& f(x^+) - f^* - (1-\theta)(f(x) - f^*) \\
& \qquad \leq \frac{1}{t}(x^+ - y)^T(\theta x^* + (1-\theta)x - x^+) + \frac{1}{2t}\|x^+ - y\|^2 \\
& \qquad = \frac{\theta^2}{2t}\left(\|u - x^*\|^2 - \|u^+ - x^*\|^2\right)
\end{aligned}
$$

- *i.e.*, at iteration k

$$
\begin{aligned}
& \frac{t}{\theta_k^2}(f(x^{(k)}) - f^*) + \frac{1}{2}\|u^{(k)} - x^*\|^2 \\
& \qquad \leq \frac{(1-\theta_k)t}{\theta_k^2}(f(x^{(k-1)}) - f^*) + \frac{1}{2}\|u^{(k-1)} - x^*\|^2
\end{aligned}
$$

Proof

- Using $(1-\theta_i)/\theta_i^2 \le 1/\theta_{i-1}^2$, and iterating this inequlity

$$
\begin{aligned}
&\frac{t}{\theta_k^2}(f(x^{(k)}) - f^*) + \frac{1}{2}\|u^{(k)} - x^*\|^2 \\
&\quad \le \frac{(1-\theta_1)t}{\theta_1^2}(f(x^{(0)}) - f^*) + \frac{1}{2}\|u^{(0)} - x^*\|^2 \\
&\quad = \frac{1}{2}\|x^{(0)} - x^*\|^2
\end{aligned}
$$

- Therefore

$$
f(x^{(k)}) - f^* \le \frac{\theta_k^2}{2t}\|x^{(0)} - x^*\|^2 = \frac{2}{t(k+1)^2}\|x^{(0)} - x^*\|^2
$$

Why NAG works?

- Although the algebraic manipulations of the proof is beautiful, the acceleration effect in NAG has been mysterious and hard to understand
- Recent works reinterpreted the NAG algorithm from different point of views, including Zhu et al (2017) and Su et al (2014)
- Here we introduce the ODE explanation from Su et al (2014)

An ODE Explanation

- Su et al (2014) proposed an ODE based explanation where NAG can be viewed as a discretization of the following ordinary differential equation

$$\ddot{X} + \frac{3}{t}\dot{X} + \nabla f(X) = 0, \quad t > 0 \tag{4}$$

  with initial conditions $X(0) = x^{(0)}, \dot{X}(0) = 0$.

- **Theorem** (Su et al): For any $f \in \mathcal{F}_\infty \triangleq \cap_{L>0}\mathcal{F}_L$ and any $x^{(0)} \in \mathbb{R}^n$, the ODE (4) with initial conditions $X(0) = x^{(0)}, \dot{X}(0) = 0$ has a unique global solution $X \in C^2((0,\infty);\mathbb{R}^n) \cap C^1([0,\infty);\mathbb{R}^n)$.

- **Theorem** (Su et al): For any $f \in \mathcal{F}_\infty$, let $X(t)$ be the unique global solution to (4) with initial conditions $X(0) = x^{(0)}, \dot{X}(0) = 0$. For any $t > 0$,

$$f(X(t)) - f^* \leq \frac{2\|x^{(0)} - x^*\|^2}{t^2}$$

- Consider the energy functional defined as

$$\mathcal{E}(t) \triangleq t^2(f(X(t)) - f^*) + 2\|X + \frac{t}{2}\dot{X} - x^*\|^2$$

- The derivative of the energy function is

$$\dot{\mathcal{E}} = 2t(f(X) - f^*) + t^2\langle \nabla f, \dot{X} \rangle + 4\langle X + \frac{t}{2}\dot{X} - x^*, \frac{3}{2}\dot{X} + \frac{t}{2}\ddot{X} \rangle$$

Convergence Rate of The ODE Solution

- Substituting $3\dot{X}/2 + t\ddot{X}/2$ with $-t\nabla f(X)/2$

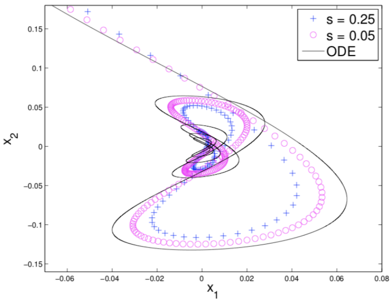
$$\begin{aligned}\dot{\mathcal{E}} &= 2t(f(X) - f^*) + 4\langle X - x^*, -\frac{t}{2}\nabla f(X)\rangle \\ &= 2t(f(X) - f^*) - 2t\langle X - x^*, \nabla f(X)\rangle \\ &\leq 0\end{aligned}$$

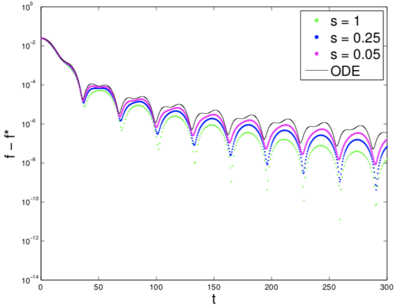
  where the last inequality follows from the convexity of f.
- Therefore,

$$f(X(t) - f^*) \leq \mathcal{E}(t)/t^2 \leq \mathcal{E}(0)/t^2 = \frac{2\|x^{(0)} - x^*\|^2}{t^2}$$

Example

$$f(x) = 0.02x_1^2 + 0.005x_2^2, \quad x^{(0)} = (1, 1)$$





The objective in many unconstrained optimization problems can be split in two components

$$\text{minimize } f(x) = g(x) + h(x)$$

- g is convex and differentiable on $\mathbb{R}^n$
- h is convex and simple, but may be non-differentiable

Examples

- Indicator function of closed convex set C

$$h(x) = \mathbf{1}_C(x) = \begin{cases} 0, & x \in C \\ +\infty, & x \notin C \end{cases}$$

- L_1 regularization (LASSO): $h(x) = \|x\|_1$

The **proximal mapping** (or **proximal-operator**) of a convex function h is defined as

$$\mathrm{prox}_h(x) = \arg\min_u \left(h(u) + \frac{1}{2}\|u - x\|_2^2 \right)$$

Examples

- $h(x) = 0$: $\mathrm{prox}_h(x) = x$
- $h(x) = \mathbf{1}_C(x)$: prox_h is projection on C

$$\mathrm{prox}_h(x) = \arg\min_{u \in C} \|u - x\|_2^2 = P_C(x)$$

- $h(x) = \|x\|_1$: prox_h is the "soft-threshold" (shrinkage) operation

$$\mathrm{prox}_h(x)_i = \begin{cases} x_i - 1 & x_i \geq 1 \\ 0 & |x_i| \leq 1 \\ x_i + 1 & x_i \leq -1 \end{cases}$$

- **Proximal gradient algorithm**

$$x^{(k+1)} = \text{prox}_{t_k h}(x^{(k)} - t_k \nabla g(x^{(k)})), \quad k = 0, 1, \ldots$$

- Interpretation. If $x^+ = \text{prox}_{th}(x - t\nabla g(x))$, from the definition of proximal mapping

$$\begin{aligned} x^+ &= \arg\min_u \left(h(u) + \frac{1}{2t} \|u - x + t\nabla g(x)\|_2^2 \right) \\ &= \arg\min_u \left(h(u) + g(x) + \nabla g(x)^T (u - x) + \frac{1}{2t} \|u - x\|_2^2 \right) \end{aligned}$$

- x^+ minimizes $h(u)$ plus a simple quadratic local approximation of $g(u)$ around x

- **Gradient Descent**: special case with $h(x) = 0$

$$x^+ = x - t\nabla g(x)$$

- **Projected Gradient Descent**: special case with $h(x) = \mathbf{1}_C(x)$

$$x^+ = P_C(x - t\nabla g(x))$$

- **ISTA** (Iterative Shrinkage-Thresholding Algorithm): special case with $h(x) = \|x\|_1$

$$x^+ = \mathcal{S}_t(x - t\nabla g(x))$$

where

$$\mathcal{S}_t(u) = (|u| - t)_+ \mathrm{sign}(u)$$

- If h is convex and closed,

$$\text{prox}_h(x) = \arg\min_u \left(h(u) + \frac{1}{2}\|u - x\|_2^2 \right)$$

exists and is unique for all x. Moreover, it has the following useful properties

$$\begin{aligned} u = \text{prox}_h(x) &\iff x - u \in \partial h(u) \\ &\iff h(z) \geq h(u) + (x - u)^T (z - u), \ \forall z \end{aligned}$$

- Proximal gradient descent has the same convergence rate as gradient descent when $0 < t \leq 1/L$

$$f(x^{(k)}) - f^* \leq \frac{1}{2kt}\|x^{(0)} - x^*\|_2^2$$

- Similarly, we can apply Nesterov's acceleration for proximal gradient descent. Choose any initial $x^{(0)} = x^{(-1)}$, $\forall\ k = 1, \dots$

$$y = x^{(k-1)} + \frac{k-2}{k+1}(x^{(k-1)} - x^{(k-2)})$$
$$x^{(k)} = \mathrm{prox}_{t_k h}(y - t_k \nabla g(y))$$

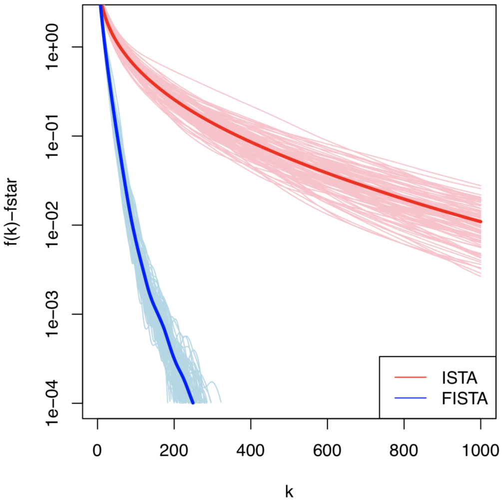
- Convergence rate is the same with NAG if $0 < t \leq 1/L$

$$f(x^{(k)}) - f^* \leq \frac{2\|x^{(0)} - x^*\|^2}{t(k+1)^2}$$

- When applied to LASSO, this is called **FISTA** (Fast Iterative Shrinkage-Thresholding Algorithm)

Example: ISTA vs FISTA

LASSO Logistic regression: 100 instances



Consider the following stochastic optimization problem

$$\min_{x} \; f(x) = \mathbb{E}_{\xi}(F(x,\xi)) = \int F(x,\xi)p(\xi)d\xi$$

- ξ is a random variable
- The challenge: evaluation of the expectation/integration

Example

- Supervised Learning

$$\min_{w} f(w) = \mathbb{E}_{(x,y)\sim D(x,y)}(\ell(h_w(x),y))$$

where $D(x,y)$ is the data distribution, $\ell(\cdot,\cdot)$ is certain loss, w is the model parameter

- Gradient descent with stochastic approximation (SA)

$$x^{(k+1)} = x^{(k)} - t_k g(x^{(k)})$$

where $\mathbb{E}(g(x)) = \nabla f(x), \ \forall x$

- Example. Consider supervised learning with observations $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$

$$\min_w f(w) = \frac{1}{N} \sum_{i=1}^N \ell(h_w(x^{(i)}, y^{(i)}))$$

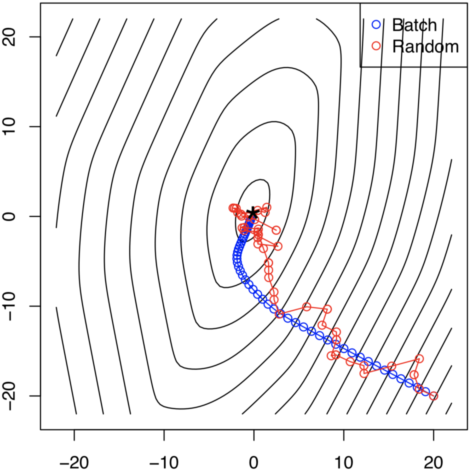
SGD

$$w^{(k+1)} = w^{(k)} - t_k \nabla \ell(h_w(x^{(i_k)}, y^{(i_k)}))$$

where $i_k \in \{1, \ldots, m\}$ is some chosen index at iteration k.

Example

Stochastic logistic regression



Convergence Rate of SGD

- Assume that $\mathbb{E}(\|g(x)\|^2) \leq M^2$ and $f(x)$ is convex

$$\mathbb{E}f(\tilde{x}^{[0:k]}) - f^* \leq \frac{\|x^{(0)} - x^*\|_2^2 + M^2 \sum_{j=0}^{k} t_j^2}{2 \sum_{j=0}^{k} t_k}$$

  where $\tilde{x}^{[0:k]} = \sum_{j=1}^{k} t_j x^{(j)} / \sum_{j=1}^{k} t_j$

- Fix the number of iterations K and constant step sizes $t_j = \frac{\|x^{(0)} - x^*\|}{M\sqrt{K}}$, $j = 0, 1, \ldots, K$, we have

$$\mathbb{E}(f(\bar{x}^K)) - f^* \leq \frac{\|x^{(0)} - x^*\| M}{\sqrt{K}}$$

  where $\bar{x}^K = \frac{1}{K+1} \sum_{j=0}^{K} x^{(j)}$

Proof

By convexity, we have $f(x^{(k)}) - f^* \leq \nabla f(x^{(k)})^T(x^{(k)} - x^*)$

$$
\begin{aligned}
t_k \mathbb{E}(f(x^{(k)})) - t_k f^* &\leq t_k \mathbb{E}(g(x^{(k)})^T(x^{(k)} - x^*)) \\
&= \frac{1}{2}(\mathbb{E}\|x^{(k)} - x^*\|_2^2 - \mathbb{E}\|x^{(k+1)} - x^*\|_2^2) + \frac{1}{2}t_k^2 \mathbb{E}\|g(x^{(k)})\|_2^2 \\
&\leq \frac{1}{2}(\mathbb{E}\|x^{(k)} - x^*\|_2^2 - \mathbb{E}\|x^{(k+1)} - x^*\|_2^2) + \frac{1}{2}t_k^2 M^2
\end{aligned}
$$

$\forall k \geq 0$. Therefore

$$
\sum_{j=0}^{k} t_j \mathbb{E}(f(x^{(j)})) - \sum_{j=0}^{k} t_j f^* \leq \frac{1}{2}\|x^{(0)} - x^*\|_2^2 + \frac{M^2}{2}\sum_{j=0}^{k} t_j^2
$$

Dividing both size with $\sum_{j=0}^{k} t_j$ together with convexity complete the proof

Pros and Cons of Vanilla SGD

What We Love About SGD

- Efficient in computation and memory usage, naturally scalable for big data problems
- Less likely to be trapped at local modes

What Needs to Be Improved

- In general, vanilla SGD is slow to converge (only $1/k$ even with strong convexity). Variance reduction seems to be a good remedy, see algorithms like SVRG, SAGA, etc.
- Choosing a proper learning rate can be difficult, require much effort in hyperparameter tuning to get good results
- The same learning rate applies to all parameter updates

Inspiration From Fisher Scoring

- Assume that f can be related to a probabilistic model, *i.e.*

$$f(\theta) = -\mathbb{E}_{y\sim P_{data}} L(y|\theta) = -\mathbb{E}_{y\sim P_{data}} \log p(y|\theta)$$

- Recall that Fisher information is defined as

$$\mathcal{I}(\theta) = \mathbb{E}_{y\sim p(y|\theta)}(\nabla L(y|\theta)(\nabla L(y|\theta))^T) \tag{5}$$

- We can use Fisher information to adapt the learning rate according to the local curvature. (5) inspire us to use some average of $g(\theta^{(t)})(g(\theta^{(t)}))^T$

- Previously, we performed an update for all parameters using the same learning rate
- Duchi et al (2011) proposed an improved version of SGD, AdaGrad, that adapts the learning rate to the parameters, according to the frequencies of their associated features
- Denote the vector of parameters as θ and the gradient at iteration t as g_t. Let η be the usual learning rate for SGD. AdaGrad's update rule:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t$$

  where G_t is a diagonal matrix where each diagonal element is the sum of the squares of the corresponding gradients up to time step t

RMSprop

- A potential weakness about AdaGrad is its accumulation of the squared gradients in G_t, which in turn cause the learning rate to shrink and eventually become very small
- RMSprop (Geoff Hinton): resolve AdaGrad's diminishing learning rate via the exponentially decaying average

$$\mathbb{E}(g^2)_t = 0.9\mathbb{E}(g^2)_{t-1} + 0.1 g_t^2$$
$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\mathbb{E}(g^2)_t + \epsilon}} g_t$$

- Presumably the most popular stochastic gradient methods in machine learning, proposed by D.P. Kingma et al (2014).
- In addition to the squared gradients, Adam also keeps an exponentially decaying average of the past gradients

$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t, \quad v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$$

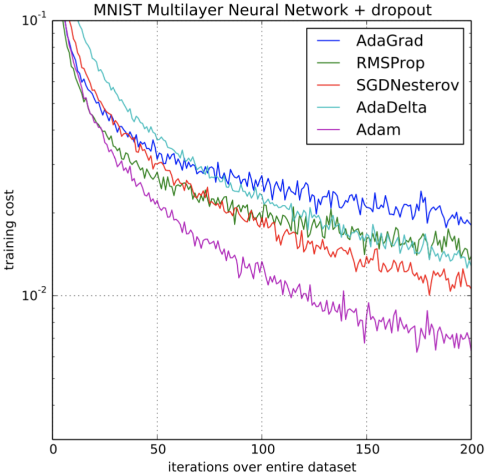
- Bias correction for zero initialization

$$\hat{m}_t = \frac{m_t}{1-\beta_1^t}, \quad \hat{v}_t = \frac{v_t}{1-\beta_2^t}$$

- Adam uses the same update rule

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

Test on MNIST Images



Pros

- Faster training speed and smoother learning curve
- Easier to choose hyperparameters
- Better when data are very sparse

Cons

- Worse performance on unseen data (Wilson et al., 2017)
- Convergence issue: non-decreasing learning rates, extreme learning rates

Some recent proposals for improvement: AMSGrad (Reddi et al., 2018), AdaBound (Luo et al., 2019), etc.

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