

Statistical Models & Computing Methods

Lecture 3: Advanced Gradient Descent



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- ▶ 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

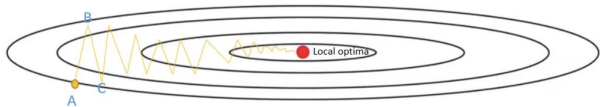
- ▶ Introduced in 1964 by Polyak, momentum method is a technique that can accelerate gradient descent by taking accounts of previous gradients in the update rule at each iteration.

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

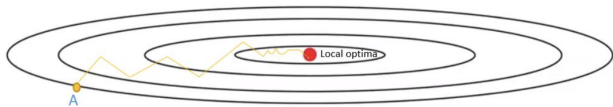
where $0 \leq \mu < 1$

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

- ▶ 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.



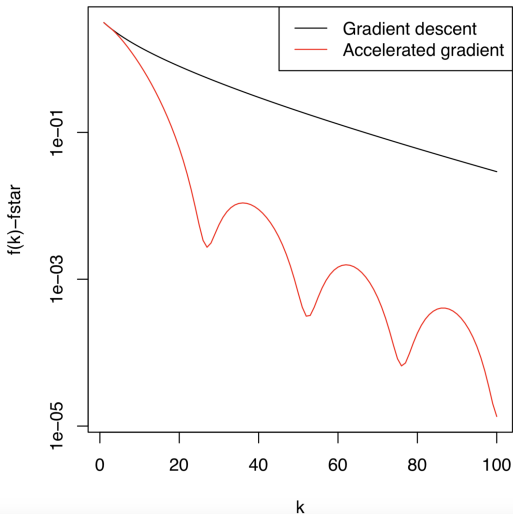
- ▶ Choose any initial $x^{(0)} = x^{(-1)}$, $\forall k = 1, 2, 3, \dots$

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

- ▶ 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 .



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

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

- ▶ 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



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

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

- From convexity

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

- Add the above two inequalities

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

► Continue ...

$$\begin{aligned} &\leq \frac{1}{2t} (\|x - x^*\|^2 - \|x^+ - x^*\|^2) - \frac{m}{2} \|x - x^*\|^2 \\ &= \frac{1}{2t} ((1 - mt) \|x - x^*\|^2 - \|x^+ - x^*\|^2) \quad (1) \end{aligned}$$

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

► For gradient descent updates

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



- ▶ 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)

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

- ▶ 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

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

- ▶ **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!



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

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

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

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

- 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

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



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

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

- *i.e.*, at iteration k

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



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

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

- Therefore

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



- ▶ 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)

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

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

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

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



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

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

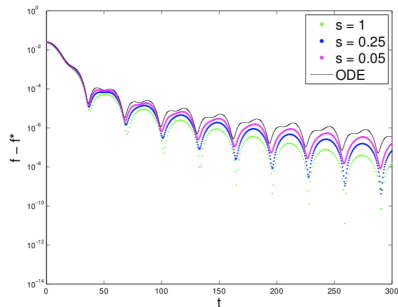
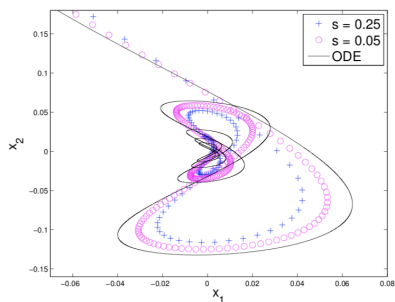
where the last inequality follows from the convexity of f .

- ▶ Therefore,

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



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



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

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

Examples

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

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

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

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



► **Proximal gradient algorithm**

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

- 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

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



- ▶ If h is convex and closed,

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

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

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

- ▶ 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 $x^{(0)} = x^{(-1)}$, $\forall k = 1, \dots$

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

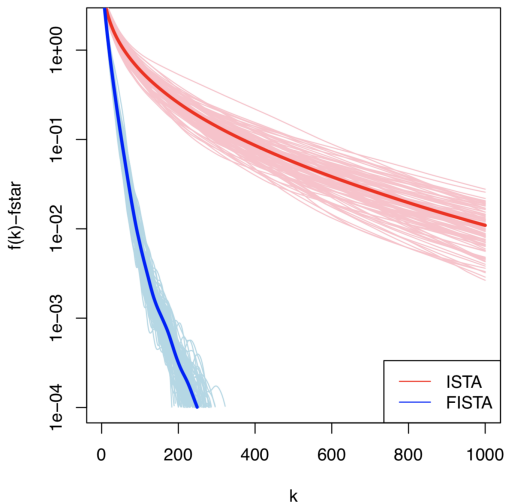
- ▶ Convergence rate is the same with NAG if $0 < t \leq 1/L$

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

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



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 $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$

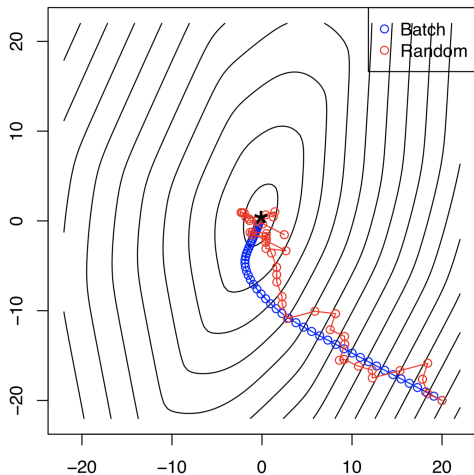
$$\min_w f(w) = \frac{1}{N} \sum_{i=1}^N \ell(h_w(x^{(i)}, y^{(i)}))$$

SGD

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

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

Stochastic logistic regression



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

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

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

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

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

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



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



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

- ▶ 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

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

- ▶ 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



- ▶ 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

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



- ▶ 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

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

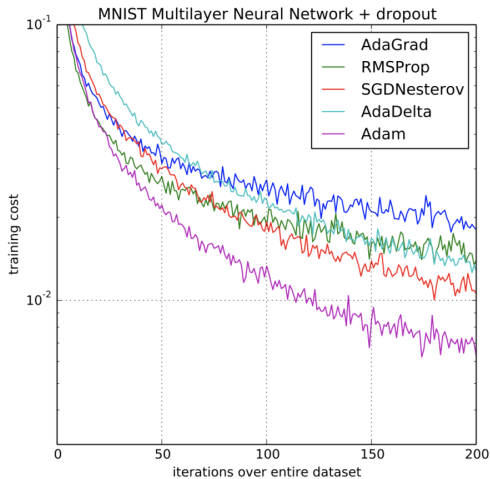
- ▶ Bias correction for zero initialization

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

- ▶ Adam uses the same update rule

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





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), AdaBelief (Zhuang et al., 2020), etc.

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