Optimization for Machine Learning

Lecture 5: Newton's Method & Adaptive Gradient Methods

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May 14, 2024

Quiz Week 5

i-th coordinate of $\nabla f(x)$

Recall the coordinate-wise smoothness condition:

$$\|\nabla_i f(\mathbf{x}) - \nabla_i f(\mathbf{y})\|^2 \leq L_i \|\mathbf{x} - \mathbf{y}\|^2 \qquad \text{vs.} \qquad \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|^2 \leq L \|\mathbf{x} - \mathbf{y}\|^2$$

1. It holds $L \leq L_i$. ✗
2. It holds $L = \max_i L_i$. ✗
3. It holds $L = \sum_{i=1}^n L_i$. ✗
4. It holds $L \geq \frac{1}{n} \sum_{i=1}^n L_i$. ✓

$f(x) = \frac{1}{2} x^T A x$

$\nabla^2 f(x) = A = \begin{pmatrix} \ddots & & \\ & L_i & \\ & & \ddots \end{pmatrix}$

$L = \|A\|$

Quiz Week 5 (II)

Example: $f_1(x) = x^2$

$f_2(x) = -x^2$

Consider

$$f(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} f_i(\mathbf{x})$$

where each $f_i\colon \mathbb{R}^d \to \mathbb{R}$ is L_i-smooth, and let L denote the smoothness constant of f.

1. Then $L \geq \max_i L_i$. ✗

2. Then $L = \sum_{i=1}^{n} L_i$. ✗

3. Then $L \geq \frac{1}{n}\sum_{i=1}^{n} L_i$. ✗

   $\leq$ ✓

Theory-Practice Gap

- In theory, without imposing additional assumption or structure, it is impossible to achieve an (asymptotically!) better rate than SGD.

  $O\left(\frac{1}{T} + \frac{\sigma}{\sqrt{T}}\right)$

- In practice, acceleration techniques such as momentum, adaptive pre-conditioning are heavily used.
  - difficult to analyze!

- this lecture:
  - Newton's method (part I)
  - overview of some adaptive methods used in practice (part II)
  - (appendix: a method that adapts the stepsize)

Chapter 8

Newton's Method

1-dimensional case: Newton-Raphson method

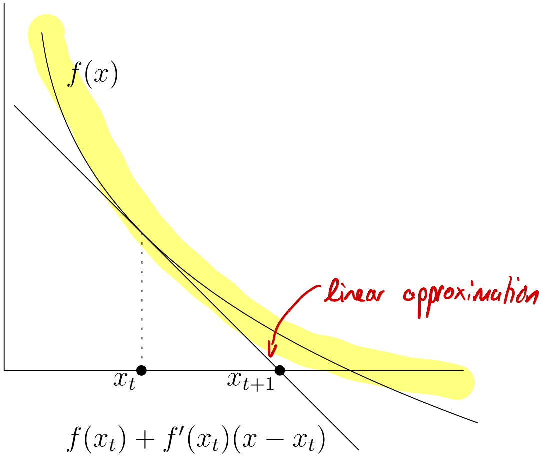
Goal: find a zero of differentiable $f : \mathbb{R} \to \mathbb{R}$.

Method:

$$x_{t+1} := x_t - \frac{f(x_t)}{f'(x_t)}, \quad t \geq 0.$$

x_{t+1} solves

$$f(x_t) + f'(x_t)(x - x_t) = 0,$$



The Babylonian method

Computing square roots: find a zero of $f(x) = x^2 - R$, $R \in \mathbb{R}_+$.

Newton-Raphson step:

$$x_{t+1} = x_t - \frac{f(x_t)}{f'(x_t)} = x_t - \frac{x_t^2 - R}{2x_t} = \frac{1}{2}\left(x_t + \frac{R}{x_t}\right).$$

Starting far (large $x_0 > 0$), we move slowly:

$$x_{t+1} = \frac{1}{2}\left(x_t + \frac{R}{x_t}\right) \geq \frac{x_t}{2}.$$

E.g., from $x_0 = R \geq 1$, it takes $\mathcal{O}(\log R)$ steps to get $x_t - \sqrt{R} < 1/2$ (Exercise 38).

The Babylonian method - Takeoff

Starting close, $x_0 - \sqrt{R} < 1/2$ (achievable after $\mathcal{O}(\log R)$ steps), things will speed up:

$$x_{t+1} - \sqrt{R} = \frac{1}{2}\left(x_t + \frac{R}{x_t}\right) - \sqrt{R} = \frac{x_t}{2} + \frac{R}{2x_t} - \sqrt{R} = \frac{1}{2x_t}\left(x_t - \sqrt{R}\right)^2.$$

Assume $R \geq 1/4$.Then all iterates have value at least $\sqrt{R} \geq 1/2$. Hence we get

$$\underbrace{x_{t+1} - \sqrt{R}}_{\text{error at step } t+1} \leq \left(x_t - \sqrt{R}\right)^2.$$

(error at step t)^2

$$x_T - \sqrt{R} \leq \left(x_0 - \sqrt{R}\right)^{2^T} < \left(\frac{1}{2}\right)^{2^T}, \quad T \geq 0.$$

To get $x_T - \sqrt{R} < \varepsilon$, we only need $T = \log\log(\frac{1}{\varepsilon})$ steps!

The Babylonian method - Example

$R = 1000$, IEEE 754 double arithmetic

- 7 steps to get $x_7 - \sqrt{1000} < 1/2$
- 3 more steps to get x_{10} equal to $\sqrt{1000}$ up to machine precision (53 binary digits).
- First phase: $\approx$ one more correct digit per iteration
- Last phase, $\approx$ double the number of correct digits in each iteration!

Once you're close, you're there...

Newton's method for optimization

1-dimensional case: Find a global minimum $x^\star$ of a differentiable convex function $f : \mathbb{R} \to \mathbb{R}$.

$\Longleftrightarrow \quad \nabla f(x^*) = 0 = f'(x^*)$

Can equivalently search for a zero of the derivative f': Apply the Newton-Raphson method to f'.

Gradient descent: $x_{t+1} = x_t - \gamma \cdot f'(x)$ with $\gamma = \frac{1}{f''(x)}$

Update step:

$$x_{t+1} := x_t - \frac{f'(x_t)}{f''(x_t)} = x_t - f''(x_t)^{-1} f'(x_t)$$

(needs f twice differentiable).

***d*-dimensional case:** Newton's method for minimizing a convex function $f : \mathbb{R}^d \to \mathbb{R}$:

$$\mathbf{x}_{t+1} := \mathbf{x}_t - \nabla^2 f(\mathbf{x}_t)^{-1} \nabla f(\mathbf{x}_t)$$

Newton's method = adaptive gradient descent

General update scheme:

$$\mathbf{x}_{t+1} = \mathbf{x}_t - H(\mathbf{x}_t)\nabla f(\mathbf{x}_t),$$

where $H(\mathbf{x}) \in \mathbb{R}^{d\times d}$ is some matrix.

Newton's method: $H = \nabla^2 f(\mathbf{x}_t)^{-1}$. $\to$ compute $d \times d$ matrix ↯

Gradient descent: $H = \underline{\gamma I}$.

Newton's method: "adaptive gradient descent", adaptation is w.r.t. the local geometry of the function at $\mathbf{x}_t$.

$f(x) = \frac{1}{2} x^T A x$

$$x_1 = x_0 - (A^{-1}) \cdot A x_0 = x_0 - \mathbb{1} \cdot x_0 = 0$$

Convergence in one step on quadratic functions

A nondegenerate quadratic function is a function of the form

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top M\mathbf{x} - \mathbf{q}^\top \mathbf{x} + c,$$

where $M \in \mathbb{R}^{d\times d}$ is an invertible symmetric matrix, $\mathbf{q} \in \mathbb{R}^d, c \in R$. Let $\mathbf{x}^\star = M^{-1}\mathbf{q}$ be the unique solution of $\nabla f(\mathbf{x}) = \mathbf{0}$.

- $\mathbf{x}^\star$ is the unique global minimum if f is convex.

Lemma (Lecture-5).1

On nondegenerate quadratic functions, with any starting point $\mathbf{x}_0 \in \mathbb{R}^d$, Newton's method yields $\mathbf{x}_1 = \mathbf{x}^\star$.

Proof.

We have $\nabla f(\mathbf{x}) = M\mathbf{x} - \mathbf{q}$ (this implies $\mathbf{x}^\star = M^{-1}\mathbf{q}$) and $\nabla^2 f(\mathbf{x}) = M$. Hence,

$$\mathbf{x}_1 = \mathbf{x}_0 - \nabla^2 f(\mathbf{x}_0)^{-1}\nabla f(\mathbf{x}_0) = \mathbf{x}_0 - M^{-1}(M\mathbf{x}_0 - \mathbf{q}) = M^{-1}\mathbf{q} = \mathbf{x}^\star.$$

□

Minimizing the second-order Taylor approximation

Alternative interpretation of Newton's method:

Each step minimizes the local second-order Taylor approximation.

Lemma (Lecture-5).2 (Exercise 42)

Let f be convex and twice differentiable at $\mathbf{x}_t \in \mathbf{dom}(f)$, with $\nabla^2 f(\mathbf{x}_t) \succ 0$ being invertible. The vector $\mathbf{x}_{t+1}$ resulting from the Netwon step satisfies

$$\mathbf{x}_{t+1} = \underset{\mathbf{x}\in\mathbb{R}^d}{\operatorname{argmin}}\ f(\mathbf{x}_t) + \nabla f(\mathbf{x}_t)^\top(\mathbf{x} - \mathbf{x}_t) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_t)^\top \nabla^2 f(\mathbf{x}_t)(\mathbf{x} - \mathbf{x}_t).$$

Downside of Newton's method

Computational bottleneck in each step:

- compute and invert the Hessian matrix
- or solve the linear system $\nabla^2 f(\mathbf{x}_t)\Delta\mathbf{x} = -\nabla f(\mathbf{x}_t)$ for the next step $\Delta\mathbf{x}$.

Matrix / system has size $d \times d$, taking up to $\mathcal{O}(d^3)$ time to invert / solve.

In many applications, d is large...

Discussion

- Newton's Method
  - fast local convergence, $\mathcal{O}(\log\log\frac{1}{\epsilon})$
  - slow (or might even diverge) when initialized far-away from the optimal solution
- a method with global convergence guarantees:
  Cubic Regularized Newton's Method [NP06]
- computationally more efficient versions based on the secant-equation:
  quasi-Newton methods (see also [JJM24])

A First Adaptive Method (without proof)

Stochastic Gradient Descent

$$\min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x})$$

$$\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma_t \mathbf{g}_t$$
$$\text{with } \mathbb{E}[\mathbf{g}_t] = \nabla f(\mathbf{x}_t)$$

Recall Lecture 3:

- Under the assumptions of convexity & $\mathbb{E}[\|\mathbf{g}_t\|^2] \leq B^2$, $\forall t$
- $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$ convergence
- for the constant stepsize $\gamma_t = \gamma = \mathcal{O}\left(\frac{1}{B\sqrt{T}}\right)$

Estimating $\gamma = \frac{c}{B\sqrt{T}}$

- in practice we do not know B (or T)
- if we set $\gamma_t = \frac{c}{B\sqrt{t}}$ (for a constant c), we only need to estimate B
- empirical estimate:

$$B^2 \approx \frac{1}{t}\sum_{i=0}^{t} \|\mathbf{g}_i\|^2$$

- this leads to

$$\gamma_t = \frac{c}{\sqrt{\sum_{i=0}^{t} \|\mathbf{g}_i\|^2}}$$

The resulting method is quite tricky to analyze, as γ_t depends on $\mathbf{g}_t$.

Main Theorem

Theorem (Lecture-5).3 ([LO19, Cut22])

Let $f : \mathbb{R}^d \to \mathbb{R}$ be L-smooth, B-Lipschitz and let $\Delta = f(\mathbf{x}_0) - f^\star$. Suppose $\mathbb{E}[\max_{t \le T} \|\mathbf{g}_t\|] \le B$ and $\mathbb{E}[\|\mathbf{g}_t - \nabla f(\mathbf{x}_t)\|^2] \le \sigma^2$ for all t. Then Adaptive SGD guarantees:

$$\frac{1}{T+1}\mathbb{E}\left[\sqrt{\sum_{t=0}^{T} \|\nabla f(\mathbf{x}_t)\|^2}\right]^2 \le \tilde{\mathcal{O}}\left(\frac{\sigma}{\sqrt{T}}\right) .$$

See appendix for more details.

Adaptive Methods in Practice

Adaptive Stochastic Gradient Methods

- Some limitations of SGD:
  - learning rate tuning
  - uniform learning rate for all coordinates
- Adaptive stepsizes are widely used in practice to improve the performance of SGD:
  - AdaGrad [DHS11]
  - RMSProp [TH12]
  - ADAM [KB14]
  - AMSGrad [RKK19]
  - ....

Popular Variants

- Momentum SGD

reduce the variance of stochastic gradients

$$\begin{cases} \mathbf{m}_t &= \alpha \mathbf{m}_{t-1} + (1-\alpha)\overbrace{\nabla f(\mathbf{x}_t, \xi_t)} \\ \mathbf{x}_{t+1} &= \mathbf{x}_t - \gamma_t \mathbf{m}_t \end{cases}$$

- AdaGrad

estimate the stepsize

AdaGrad-Norm:

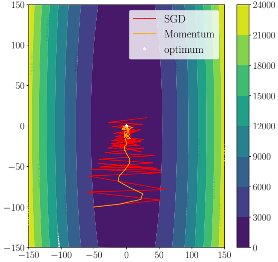
$v_t = v_{t-1} + \|\nabla f(\xi)\|^2$

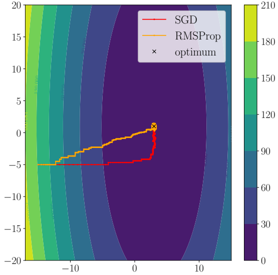
$$\begin{cases} \mathbf{v}_t &= \mathbf{v}_{t-1} + \nabla f(\mathbf{x}_t, \xi_t)^{\odot 2} \\ \mathbf{x}_{t+1} &= \mathbf{x}_t - \frac{\gamma_0}{\epsilon + \sqrt{\mathbf{v}_t}} \odot \nabla f(\mathbf{x}_t, \xi_t) \end{cases}$$

- RMSProp

AdaGrad + momentum

$$\begin{cases} \mathbf{v}_t &= \beta \mathbf{v}_{t-1} + (1-\beta)\nabla f(\mathbf{x}_t, \xi_t)^{\odot 2} \\ \mathbf{x}_{t+1} &= \mathbf{x}_t - \frac{\gamma_0}{\varepsilon + \sqrt{\mathbf{v}_t}} \odot \nabla f(\mathbf{x}_t, \xi_t) \end{cases}$$





ADAM

ADAM $\approx$ RMSProp + Momentum ($>$100K citations)

$$\begin{cases} \mathbf{v}_t & = \beta \mathbf{v}_{t-1} + (1-\beta)\nabla f(\mathbf{x}_t, \boldsymbol{\xi}_t)^{\odot 2} \\ \mathbf{m}_t & = \alpha \mathbf{m}_{t-1} + (1-\alpha)\nabla f(\mathbf{x}_t, \boldsymbol{\xi}_t) \\ \mathbf{x}_{t+1} & = \mathbf{x}_t - \frac{\gamma_0}{\varepsilon + \sqrt{\tilde{\mathbf{v}}_t}} \odot \tilde{\mathbf{m}}_t \end{cases}$$

- Exponential decay of previous information $\mathbf{m}_t, \mathbf{v}_t$.
- Note $\tilde{\mathbf{v}}_t = \frac{\mathbf{v}_t}{1-\beta^t}$ and $\tilde{\mathbf{m}}_t = \frac{\mathbf{m}_t}{1-\alpha^t}$ are bias-corrected estimates.
- In practice, α and β are chosen to be close to 1.

Numerical Illustration

for an animation: CS231n (`https://cs231n.github.io/neural-networks-3/`)

Generic Adaptive Scheme

The following scheme encapsulates these popular adaptive methods in a unified framework. [RKK19]

$$
\begin{aligned}
\mathbf{g}_t &= \nabla f(\mathbf{x}_t, \boldsymbol{\xi}_t) \\
\mathbf{m}_t &= \phi_t(\mathbf{g}_1, \ldots, \mathbf{g}_t) \\
V_t &= \psi_t(\mathbf{g}_1, \ldots, \mathbf{g}_t) \\
\hat{\mathbf{x}}_t &= \mathbf{x}_t - \alpha_t V_t^{-1/2} \mathbf{m}_t \\
\mathbf{x}_{t+1} &= \underset{\mathbf{x} \in X}{\operatorname{argmin}} \{ (\mathbf{x} - \hat{\mathbf{x}}_t)^T V_t^{1/2} (\mathbf{x} - \hat{\mathbf{x}}_t) \}
\end{aligned}
$$

Popular Examples

- **SGD**

$$\phi_t(\mathbf{g}_1, \ldots, \mathbf{g}_t) = \mathbf{g}_t, \quad \psi_t(\mathbf{g}_1, \ldots, \mathbf{g}_t) = \mathbb{I}$$

- **AdaGrad**

$$\phi_t(\mathbf{g}_1, \ldots, \mathbf{g}_t) = \mathbf{g}_t, \quad \psi_t(\mathbf{g}_1, \ldots, \mathbf{g}_t) = \frac{\mathrm{diag}(\sum_{\tau=1}^{t} \mathbf{g}_\tau^2)}{t}$$

- **Adam**

$$\phi_t(\mathbf{g}_1, \ldots, \mathbf{g}_t) = (1-\beta_1)\sum_{\tau=1}^{t} \beta_1^{t-\tau}\mathbf{g}_\tau, \quad \psi_t(\mathbf{g}_1, \ldots, \mathbf{g}_t) = (1-\beta_2)\mathrm{diag}(\sum_{\tau=1}^{t} \beta_2^{t-\tau}\mathbf{g}_\tau^2)$$

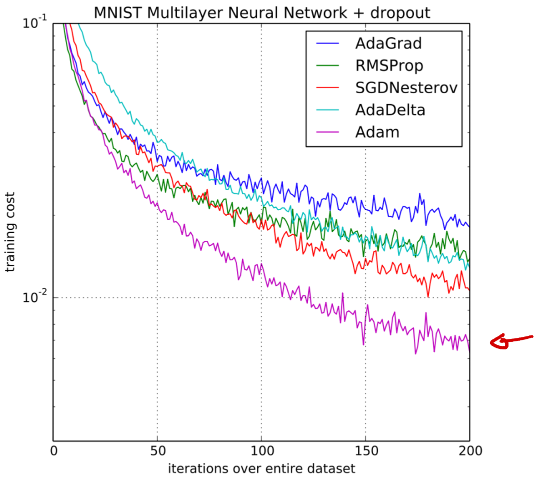
In other words, $\mathbf{m}_t = \beta_1 \mathbf{m}_{t-1} + (1-\beta_1)\mathbf{g}_t$, $V_t = \beta_2 V_{t-1} + (1-\beta_2)\mathrm{diag}(\mathbf{g}_t^2)$.

What do we know in practice?

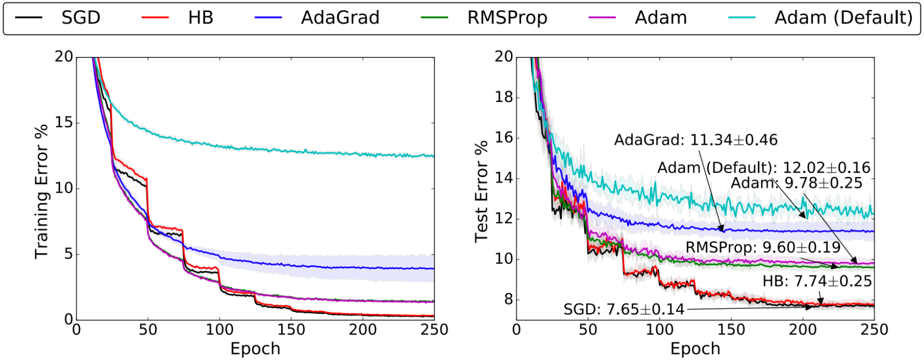
Adaptive methods

- Less sensitive to parameter tuning and adapt to sparse gradients.
- Outperform SGD for NLP tasks, training generative adversarial networks (GANs), deep reinforcement learning, etc., but are less effective in computer vision tasks.
- Tend to overfit and generalize worse than their non-adaptive counterparts [WRS+17].
- Often display faster initial progress on the training set, but their performance quickly plateaus on the testing set [WRS+17].

Some Good Stories



Some Bad Stories



(a) CIFAR-10 (Train) **(b) CIFAR-10 (Test)**

What do we know in theory?

- SGD with momentum has no acceleration even for some convex quadratic functions.
- For convex problems, Adagrad does converge, but RMSProp and Adam may not converge when $\beta_1 < \sqrt{\beta_2}$ (same for decreasing β_1 over time).

The Non-Convergence of Adam

Counterexample: consider a one-dimensional problem:

$$X = [-1, 1], \quad f(x,\xi) = \begin{cases} Cx, & \text{if } \xi = 1 \\ -x, & \text{if } \xi = 0 \end{cases}, \text{ where } P(\xi = 1) = p = \frac{1+\delta}{C+1}.$$

- Here $F(x) = \mathbb{E}[f(x,\xi)] = \delta x$ and $x^\star = -1$.
- The Adam step is $x_{t+1} = x_t - \gamma_0 \Delta_t$ with $\Delta_t = \frac{\alpha m_t + (1-\alpha) g_t}{\sqrt{\beta v_t + (1-\beta) g_t^2}}$
- For large enough $C > 0$, one can show that $\mathbb{E}[\Delta_t] \leq 0$.
- The Adam steps keep drifting away from the optimal solution $x^\star = -1$.

A Convergent Adam-type Algorithm

AMSGrad [RKK19]

Algorithm 2 AMSGRAD

Input: $x_1 \in \mathcal{F}$, step size $\{\alpha_t\}_{t=1}^T$, $\{\beta_{1t}\}_{t=1}^T$, β_2

Set $m_0 = 0$, $v_0 = 0$ and $\hat{v}_0 = 0$

for $t = 1$ **to** T **do**

$\quad g_t = \nabla f_t(x_t)$

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

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

$\quad \hat{v}_t = \max(\hat{v}_{t-1}, v_t)$ and $\hat{V}_t = \mathrm{diag}(\hat{v}_t)$

$\quad x_{t+1} = \Pi_{\mathcal{F}, \sqrt{\hat{V}_t}}(x_t - \alpha_t m_t / \sqrt{\hat{v}_t})$

end for

- Use maximum value for normalizing the running average of the gradient.
- Ensure non-increasing stepsize and avoid pitfalls of Adam and RMSProp.
- Allow long-term memory of past gradients.

Lecture 5 Recap

- introduction to Newton's method

- overview of adaptive methods used in practice

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Discussion

$$f(x) = x^2 + xy + y^2$$

$$\begin{pmatrix} [x_{t+1}]_1 \\ [x_{t+1}]_2 \end{pmatrix} = x_{t+1} = x_t - \frac{1}{\sqrt{v_t}} \odot \nabla f(x_t)$$

$$= \begin{pmatrix} \\ \end{pmatrix} - \begin{pmatrix} \gamma_1 \cdot [\nabla f(x_t)]_1 \\ \gamma_2 [\nabla f(x_t)]_2 \end{pmatrix}$$

Discussion

Discussion

Appendix

An Adaptive Method (with Proof)

*Not part of the course materials/exam.

Adaptive Stochastic Gradient Descent

Input: $\mathbf{x}_0$, scaling c, a small constant $\epsilon > 0$

Repeat:

$$
\begin{aligned}
&\text{sample stochastic gradient } \mathbf{g}_t \\
&\gamma_t = \frac{c}{\sqrt{\epsilon^2 + \sum_{i=0}^{t} \|\mathbf{g}_i\|^2}} \\
&\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \mathbf{g}_t
\end{aligned}
$$

Remark:

- this an (almost) parameter-free method, rate depends 'mildly' on c, ϵ
- small issue: correct choice of the remaining hyper-parameters, e.g. $\epsilon \approx B^2$

Auxiliary Theorem (Lecture-5).4

Theorem (Lecture-5).4 (A)

Let $f : \mathbb{R}^d \to \mathbb{R}$ be B-Lipschitz, L-smooth and for every t let $\mathbf{g}_t$ denote a stochastic gradient $\mathbb{E}_t[\mathbf{g}_t] = \nabla f(\mathbf{x}_t)$, with $\mathbb{E}[\max_{t \le T} \|\mathbf{g}_t\|] \le B$. Let $\gamma_0, \ldots, \gamma_T$ be any sequence of learning rates such that (1) $\gamma_t \ge 0$, (2) $\gamma_0 \ge \gamma_1 \ge \cdots \ge \gamma_T$, and (3) the sequence is 'causual' in the sense that γ_t is not allowed to depend on $\mathbf{g}_{t+1}, \ldots, \mathbf{g}_T$. Let γ_{-1} be a deterministic quantity such that $\gamma_{-1} \ge \gamma_0$. Consider the SGD update: $\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \mathbf{g}_t$. Then we have

$$\mathbb{E}\left[f(\mathbf{x}_{T+1})\right] \le \mathbb{E}\left[f(\mathbf{x}_0) - \sum_{t=0}^{T} \gamma_{t-1} \left\|\nabla f(\mathbf{x}_t)\right\|^2 + \frac{L}{2} \sum_{t=0}^{T} \gamma_t^2 \left\|\mathbf{g}_t\right\|^2\right] + \gamma_{-1} B^2$$

Main Theorem

Theorem (Lecture-5).5 ([LO19, Cut22])

Let $f\colon \mathbb{R}^d \to \mathbb{R}$ be L-smooth, B-Lipschitz and let $\Delta = f(\mathbf{x}_0) - f^\star$. Suppose $\mathbb{E}[\max_{t\le T}\|\mathbf{g}_t\|] \le B$ and $\mathbb{E}[\|\mathbf{g}_t - \nabla f(\mathbf{x}_t)\|^2] \le \sigma^2$ for all t. Define

$$K = \frac{\Delta}{c} + \frac{Lc\log\left(1 + \frac{(T+1)(B^2+\sigma^2)}{\epsilon^2}\right)}{2} + \frac{B^2}{\epsilon} = \mathcal{O}(\log(T))\,.$$

Then Adaptive SGD guarantees:

$$\frac{1}{T+1}\mathbb{E}\left[\sqrt{\sum_{t=0}^{T}\|\nabla f(\mathbf{x}_t)\|^2}\right]^2 \le \frac{8K^2 + 4K\epsilon}{T+1} + \frac{4K\sigma}{\sqrt{T+1}} = \tilde{\mathcal{O}}\left(\frac{\sigma}{\sqrt{T}}\right)\,.$$

Proof I

Applying Theorem A with $\gamma_{-1} = \frac{c}{\epsilon}$ gives

$$\mathbb{E}\left[f(\mathbf{x}_{T+1})\right] \leq \mathbb{E}\left[f(\mathbf{x}_0) - \sum_{t=0}^{T} \gamma_{t-1} \left\|\nabla f(\mathbf{x}_t)\right\|^2 + \frac{L}{2} \sum_{t=0}^{T} \gamma_t^2 \left\|\mathbf{g}_t\right\|^2\right] + \gamma_{-1} B^2$$

With the definition of γ_t:

$$\begin{aligned}
\mathbb{E}\left[\sum_{t=0}^{T} \gamma_t^2 \left\|\mathbf{g}_t\right\|^2\right] &= \mathbb{E}\left[c^2 \sum_{t=0}^{T} \frac{\left\|\mathbf{g}_t\right\|^2}{\epsilon^2 + \sum_{i=0}^{t} \left\|\mathbf{g}_t\right\|^2}\right] \\
&\overset{\text{Lemma (Lecture-5).6}}{\leq} \mathbb{E}\left[c^2 \log\left(1 + \frac{\sum_{t=0}^{T} \left\|\mathbf{g}_t\right\|^2}{\epsilon^2}\right)\right] \\
&\overset{\text{Jensen ineq.}}{\leq} c^2 \log\left(1 + \frac{\sum_{t=0}^{T} \mathbb{E}\left\|\mathbf{g}_t\right\|^2}{\epsilon^2}\right) \\
&\leq c^2 \log\left(1 + \frac{(T+1)(B^2+\sigma^2)}{\epsilon^2}\right)
\end{aligned}$$

Proof II

Thus, we have

$$\mathbb{E}\left[f(\mathbf{x}_{T+1})\right] \leq \mathbb{E}\left[f(\mathbf{x}_0) - \sum_{t=0}^{T} \gamma_{t-1} \left\|\nabla f(\mathbf{x}_t)\right\|^2\right] + \frac{Lc^2 \log\left(1 + \frac{(T+1)(B^2+\sigma^2)}{\epsilon^2}\right)}{2} + \frac{cB^2}{\epsilon}$$

rearranging:

$$\mathbb{E}\left[\sum_{t=0}^{T} \gamma_{t-1} \left\|\nabla f(\mathbf{x}_t)\right\|^2\right] \leq \mathbb{E}\left[f(\mathbf{x}_0) - f(\mathbf{x}_T)\right] + \frac{Lc^2 \log\left(1 + \frac{(T+1)(B^2+\sigma^2)}{\epsilon^2}\right)}{2} + \frac{cB^2}{\epsilon}$$

and using $\gamma_T \leq \gamma_t$:

$$\mathbb{E}\left[\sum_{t=0}^{T} \gamma_T \left\|\nabla f(\mathbf{x}_t)\right\|^2\right] \leq \Delta + \frac{Lc^2 \log\left(1 + \frac{(T+1)(B^2+\sigma^2)}{\epsilon^2}\right)}{2} + \frac{cB^2}{\epsilon} = cK$$

A technical Lemma

Lemma (Lecture-5).6 (Exercise)

Suppose $x_0, \ldots, x_T$ are arbitrary non-negative values. And let $f : \mathbb{R} \to \mathbb{R}$ be an arbitrary decreasing function. Then

$$\sum_{t=1}^{T} x_t f\left(\sum_{i=0}^{t} x_i\right) \leq \int_{x_0}^{\sum_{i=0}^{T} x_i} f(x) dx\,.$$

As a corollary:

$$\sum_{t=0}^{T} \frac{\|\mathbf{g}_t\|^2}{\epsilon^2 + \sum_{i=0}^{t} \|\mathbf{g}_t\|^2} \leq \int_{\epsilon^2}^{\epsilon^2 + \sum_{t=0}^{T} \|\mathbf{g}_t\|^2} \frac{dx}{x} = \log\left(1 + \frac{\sum_{t=0}^{T} \|\mathbf{g}_t\|^2}{\epsilon^2}\right)$$

Proof cont. III

Define random variables

$$A^2 = \sum_{t=0}^{T} \gamma_T \left\|\nabla f(\mathbf{x}_t)\right\|^2 \qquad\qquad B^2 = \frac{1}{\gamma_T}$$

Then by Cauchy-Schwarz for random variables (Exercise)

$$\mathbb{E}[AB] \le \sqrt{\mathbb{E}[A^2]\mathbb{E}[B^2]}$$

$$\frac{\mathbb{E}[AB]^2}{\mathbb{E}[B^2]} \le \mathbb{E}[A^2]$$

$$\frac{\mathbb{E}\left[\sqrt{\sum_{t=0}^{T} \left\|\nabla f(\mathbf{x}_t)\right\|^2}\right]^2}{\mathbb{E}[\gamma_T^{-1}]} \le \mathbb{E}\left[\sum_{t=0}^{T} \gamma_T \left\|\nabla f(\mathbf{x}_t)\right\|^2\right]$$

Proof IV

With this, it now follows

$$\mathbb{E}\left[\sqrt{\sum_{t=0}^{T}\|\nabla f(\mathbf{x}_t)\|^2}\right]^2 \leq cK\mathbb{E}\left[\gamma_T^{-1}\right] = K\mathbb{E}\left[\sqrt{\epsilon^2 + \sum_{t=0}^{T}\|\mathbf{g}_t\|^2}\right]$$

Define $X = \mathbb{E}\left[\sqrt{\sum_{t=0}^{T}\|\nabla f(\mathbf{x}_t)\|^2}\right]$ and note

$\|\mathbf{g}_t\|^2 = \|\mathbf{g}_t - \nabla f(\mathbf{x}_t) + \nabla f(\mathbf{x}_t)\|^2 \leq 2\|\mathbf{g}_t - \nabla f(\mathbf{x}_t)\|^2 + 2\|\mathbf{g}_t\|^2$. Therefore

$$\begin{aligned}
X^2 &\leq K\mathbb{E}\left[\sqrt{\epsilon^2 + 2\sum_{t=0}^{T}\|\mathbf{g}_t - \nabla f(\mathbf{x}_t)\|^2 + 2\sum_{t=0}^{T}\|\nabla f(\mathbf{x}_t)\|^2}\right] \\
&\leq K\mathbb{E}\left[\sqrt{\epsilon^2 + 2\sum_{t=0}^{T}\|\mathbf{g}_t - \nabla f(\mathbf{x}_t)\|^2}\right] + K\sqrt{2}\mathbb{E}\left[\sqrt{\sum_{t=0}^{T}\|\nabla f(\mathbf{x}_t)\|^2}\right] \\
&= K\mathbb{E}\left[\sqrt{\epsilon^2 + 2\sum_{t=0}^{T}\|\mathbf{g}_t - \nabla f(\mathbf{x}_t)\|^2}\right] + K\sqrt{2}X
\end{aligned}$$

Proof IV

And with Jensen:

$$X^2 \leq K\sqrt{\epsilon^2 + 2\sum_{t=0}^{T}\mathbb{E}[\|\mathbf{g}_t - \nabla f(\mathbf{x}_t)\|^2]} + K\sqrt{2}X \leq K\sqrt{\epsilon^2 + 2(T+1)\sigma^2} + K\sqrt{2}X$$

Now, by the quadratic formula $(ax^2 + bx + c = 0,\ x \leq \frac{-b+\sqrt{b^2-4ac}}{2a})$

$$\begin{aligned} X &\leq \frac{K\sqrt{2} + \sqrt{2K^2 + 4K\sqrt{\epsilon^2 + 2(T+1)\sigma^2}}}{2} \\ &\leq K\sqrt{2} + \sqrt{K}(\epsilon^2 + 2(T+1)\sigma^2)^{1/4} \\ &\leq K\sqrt{2} + \sqrt{K\epsilon} + \sqrt{2K\sigma}(T+1)^{1/4} \end{aligned}$$

Finally, from

$$\frac{1}{\sqrt{T+1}}X \leq \frac{K\sqrt{2} + \sqrt{K\epsilon}}{\sqrt{T+1}} + \frac{\sqrt{2K\sigma}}{(T+1)^{1/4}}$$

and squaring both sides the theorem follows. (Note $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$, $(a+b)^2 \leq 2a^2 + 2b^2$)

Proof of Theorem (Lecture-5).4

By smoothness:

$$f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \gamma_t \nabla f(\mathbf{x}_t)^\top \mathbf{g}_t + \frac{L}{2}\gamma_t^2 \left\|\mathbf{g}_t\right\|^2$$
$$= f(\mathbf{x}_t) - \gamma_{t-1} \nabla f(\mathbf{x}_t)^\top \mathbf{g}_t + (\gamma_{t-1} - \gamma_t)\nabla f(\mathbf{x}_t)^\top \mathbf{g}_t + \frac{L}{2}\gamma_t^2 \left\|\mathbf{g}_t\right\|^2$$

Summing up:

$$f(\mathbf{x}_{T+1}) \leq f(\mathbf{x}_0) - \sum_{t=0}^{T} \gamma_{t-1} \left\|\nabla f(\mathbf{x}_t)\right\|^2 + \frac{L}{2}\sum_{t=0}^{T} \gamma_t^2 \left\|\mathbf{g}_t\right\|^2 + A$$

where

$$A = \sum_{t=0}^{T} (\gamma_{t-1} - \gamma_t)\nabla f(\mathbf{x}_t)^\top \mathbf{g}_t \leq \max_{t \leq T} \left|\nabla f(\mathbf{x}_t)^\top \mathbf{g}_t\right| \sum_{t=0}^{T} (\gamma_{t-1} - \gamma_t)$$
$$\leq \max_{t \leq T} \left\|\nabla f(\mathbf{x}_t)\right\| \max_{t \leq T} \left\|\mathbf{g}_t\right\| \sum_{t=0}^{T} (\gamma_{t-1} - \gamma_t) \leq \max_{t \leq T} \left\|\nabla f(\mathbf{x}_t)\right\| \max_{t \leq T} \left\|\mathbf{g}_t\right\| \gamma_{-1}$$

And the proof follows by taking expectation.