Mathematics of Data: From Theory to Computation

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Lecture 10: Structures in non-convex optimization

Laboratory for Information and Inference Systems (LIONS)
École Polytechnique Fédérale de Lausanne (EPFL)

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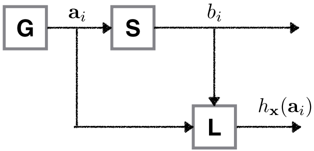
Outline

- Scalable non-convex optimization with emphasis on deep learning

Recall: The general setting...



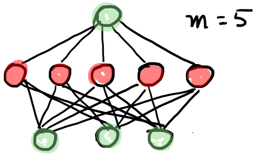
Definition (Optimization formulation)

The deep-learning training problem is given by

$$\mathbf{x}^\star_{\text{DL}} \in \arg\min_{\mathbf{x}\in\mathcal{X}} \left\{ f(\mathbf{x}) := \frac{1}{n}\sum_{i=1}^{n} L(h_{\mathbf{x}}(\mathbf{a}_i), b_i) \right\},$$

where $\mathcal{X}$ denotes the constraints on the parameters.

- A single hidden layer neural network with params $\mathbf{x} := [\mathbf{X}_1, \mathbf{X}_2, \mu_1, \mu_2]$



$$h_{\mathbf{x}}(\mathbf{a}) := \left[\ \mathbf{X}_2\ \right] \underbrace{\overset{\text{activation}}{\sigma}\left(\left[\ \overset{\text{weight}}{\mathbf{X}_1}\ \right] \left[\overset{\text{input}}{\mathbf{a}}\right] + \left[\overset{\text{bias}}{\mu_1}\right] \right) + \left[\overset{\text{bias}}{\mu_2}\right]}_{\text{hidden layer} \,=\, \text{learned features}}$$

Towards training with neural networks

◦ What do we have at hand?

1. The optimization objective $f(\mathbf{x})$ from multi-layer, multi-class, convolutions, transformers, etc.
2. First-order gradient via backpropagation $\nabla f(\mathbf{x})$

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◦ Barriers to training of neural networks:

1. Curse-of-dimensionality
2. Non-convexity
3. Ill-conditioning

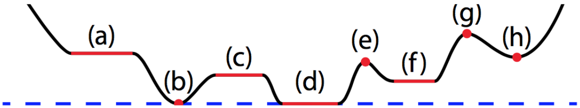

Figure: A non-convex function. (a) and (c) are plateaus, (b) and (d) are global minima, (f) and (h) are local minima, (e) and (g) are local maxima. [23]

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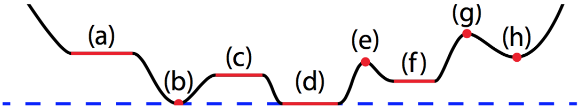
- Barriers to training of neural networks:
  1. Curse-of-dimensionality $\rightarrow$ first-order methods, see lectures 4–5
  2. Non-convexity $\rightarrow$ stochasticity $+$ momentum, this lecture
  3. Ill-conditioning $\rightarrow$ adaptive gradient methods, this lecture



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Stochastic Gradient Descent (SGD) and some key variants

Vanilla (Minibatch) SGD
Input: Stochastic gradient oracle $\mathbf{g}$, initial point $\mathbf{x}^0$, step size α_k
1. For $k = 0, 1, \ldots$:   obtain the (minibatch) stochastic gradient $\mathbf{g}^k$ update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k - \gamma_k \mathbf{g}^k$

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Perturbed Stochastic Gradient Descent [19]
Input: Stochastic gradient oracle $\mathbf{g}$, initial point $\mathbf{x}^0$, step size α_k
1. For $k = 0, 1, \ldots$:   sample noise ξ uniformly from unit sphere   update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k - \alpha_k(\mathbf{g}^k + \xi)$

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*Stochastic Gradient Langevin Dynamics [47]
Input: Stochastic gradient oracle g, initial point $\mathbf{x}^0$, step size α_k
1. For $k = 0, 1, \ldots$ sample noise ξ standard Gaussian   update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^l - \alpha_k \mathbf{g}^k + \sqrt{2\alpha_k}\xi$

Basic questions:

1. Does SGD converge with probability 1?
2. Does SGD avoid non-minimum points with probability 1?
3. How fast does SGD converge to local minimizers?
4. Can SGD converge to global minimizers?

Critical points

Recall (Classification of critical points)

Let $f : \mathbb{R}^d \to \mathbb{R}$ be twice differentiable and let $\bar{\mathbf{x}}$ be a critical point. Let $\{\lambda_i\}_{i=1}^d$ be the eigenvalues of the hessian $\nabla^2 f(\bar{\mathbf{x}})$, then

- $\lambda_i > 0$ for all $i \Rightarrow \bar{\mathbf{x}}$ is a local minimum
- $\lambda_i < 0$ for all $i \Rightarrow \bar{\mathbf{x}}$ is a local maximum
- $\lambda_i > 0$, $\lambda_j < 0$ for some i, j and $\lambda_i \neq 0$ for all $i \Rightarrow \bar{\mathbf{x}}$ is a saddle point
- Other cases $\Rightarrow$ inconclusive

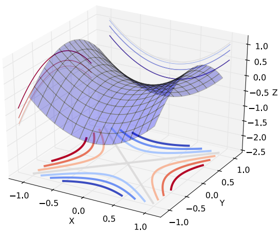


Figure: Minmax saddle ($\lambda_i \neq 0$ for all i)

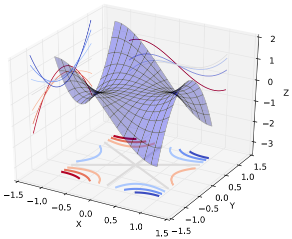


Figure: Monkey saddle ($\lambda_i = 0$ for some i)

The strict saddle property

Definition (Strict saddle)

A twice differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ *is* $(\alpha, \beta, \epsilon, \delta)$*-strict saddle if for any point* $\mathbf{x}$ *at least one of the following is true*

1. $\| \nabla f(\mathbf{x}) \| \geq \epsilon$.
2. $\lambda_{\min} (\nabla^2 f(\mathbf{x})) \leq -\beta$.
3. *There is a local minimum* $\mathbf{x}^*$ *such that* $\| \mathbf{x} - \mathbf{x}^* \| \leq \delta$ *and the function* f *restricted to a* 2δ *neighborhood of* $\mathbf{x}^*$ *is* α *strongly convex.*

(Informal)

For any point whose gradient is small, it is either close to a local minimum, or is a saddle point (or local maximum) with a significant negative eigenvalue.

Q1: Does SGD converge?

◦ SGD converges to the critical points of f as $k \to \infty$.

1. GD converges from any intialization with constant step-size and full gradients
2. With probability 1, (P)SGD does not converge with constant step-size γ [5, 41]
3. With probability 1, SGD converges with vanishing step-size if $\mathbf{x}^k$ is bounded with probability 1 [36, 5]

Boundedness is not required (Theorem 1 of [38])

Assume Lipschitzness, **sublevel regularity**, $\mathbb{E}\|\mathbf{g}\|^q \leq \sigma^q$ and $\sum_k \gamma_k^{1+q/2} < \infty$ $(q \geq 2)$. Then, $\mathbf{x}^k$ converges with probability 1.

Q2: Does SGD avoid saddle points?

∘ SGD avoids strict saddles $(\lambda_{\min}(\nabla^2 f(\mathbf{x}^\star)) < 0)$

1. GD avoids strict saddles from almost all initializations [30]
2. With probability $1-\zeta$, PSGD with constant γ escapes strict saddles after $\Omega\left(\log(1/\zeta)/\gamma^2\right)$ iterations [20]
   - However, SGD does not converge with constant γ
   - We cannot take $\zeta = 0$

SGD avoids traps almost surely (Theorem 3 of [38])

Assume bounded uniformly exciting noise and $\gamma_k = \mathcal{O}\left(\frac{1}{k^\kappa}\right)$ for $\kappa \in (0,1]$. Then, SGD avoids strict saddles from any initial condition with probability 1.

Remark

However, there are LIONS™ hidden in the tall grass: converging to sharp minima or even local *maxima* and other undesirable behaviours are unfortunately possible [53]...

Q3: How fast does SGD converge to local minimizers?

◦ SGD remains close to Hurwicz minimizers (i.e., $\mathbf{x}^\star : \lambda_{\min}(\nabla^2 f(\mathbf{x}^\star)) > 0$)

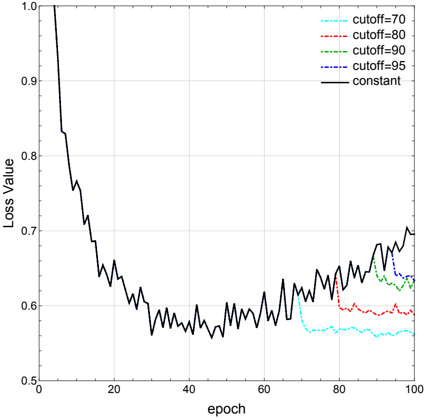
1. SGD with constant γ can obtain objective value ϵ-close to a Hurwicz minimizer in $\mathcal{O}(1/\epsilon^2)$-iterations [20, 21]
   - However, SGD does not converge with constant γ
   - Need averaging which is problematic in non-convex optimization

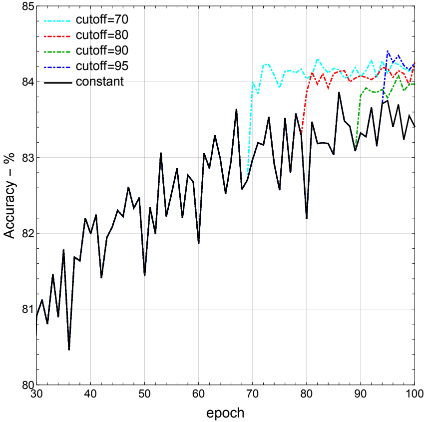
Using a vanishing step-size helps! (Theorem 4 of [38])

Using $\gamma_k = \mathcal{O}\left(\frac{1}{k}\right)$, SGD enjoys a $\mathcal{O}\left(\frac{1}{k}\right)$ convergence rate in objective value.

Using $1/k$ step-size decrease helps in practice

◦ ResNet training at different cool-down cut-offs





Q4: Can SGD converge to global minimizers?

- A few phenomena about neural networks [51]:
  - Deep neural networks can fit random labels
  - First-order methods can find global minimizers

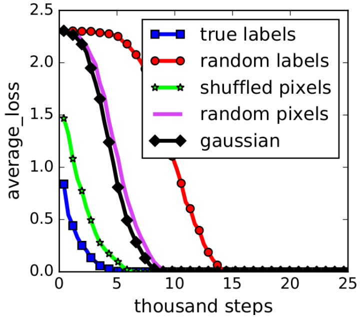


Figure: DNN Training curves on CIFAR10, from [51]

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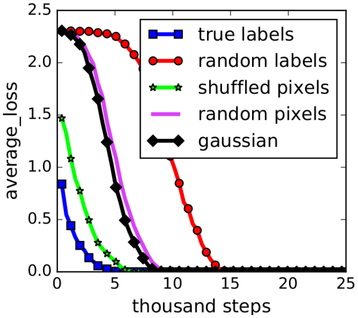


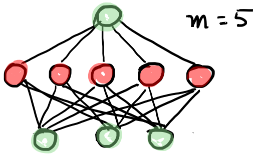
Figure: DNN Training curves on CIFAR10, from [51]

- Overparametrization can explain these mysteries!

Overparametrization

Number of parameters $\gg$ number of training data.

GD finds global minimizers of overparametrized networks



activation, weight, input, bias, bias

$$h_{\mathbf{x}}(\mathbf{a}) := \left[\ \mathbf{X}_2\ \right] \sigma \left(\left[\ \mathbf{X}_1\ \right] \left[\mathbf{a}\right] + \left[\mu_1\right] \right) + \left[\mu_2\right]$$

hidden layer = learned features

Theorem (Linear convergence of Gradient Descent [14])

- $f(\mathbf{a}; \mathbf{X}_1, \mathbf{X}_2)$: *1-hidden-layer network with width* m,*hidden layer weights* $\mathbf{X}_1$, *output layer weights* $\mathbf{X}_2$ *and ReLu activation.*
- $m = \Omega(\frac{n^6}{\delta^3})$ *where* n *=number of samples.*
- $\mathbf{X}_1^0$ *is initialized with a normal distribution,* $\mathbf{X}_2^0 \sim$ *Unif*$[-1, 1]^m$.
- *Stepsize* $\eta = O(n^{-2})$.

With probability at least $1 - \delta$, *for the empirical risk* R_n *we have*

$$R_n(\beta_t, W_t, b_t) \leq (1 - \eta)^t R_n(\beta_0, W_0, b_0) \tag{1}$$

Optimization landscape of overparametrized neural networks

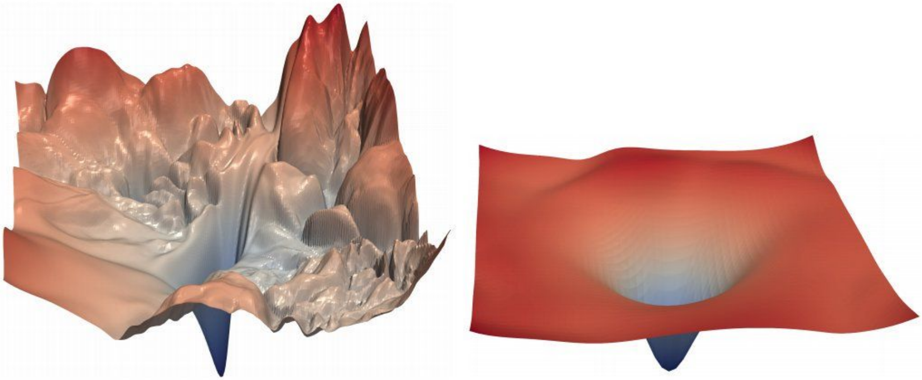


Figure: Intuitive comparison, loss landscape with few parameters (left) vs overparametrized regime (right). From [34], originally skip connections vs. no skip connections

Overparametrization is an active area of research

Reference	Number of parameters	Depth d	Result
[25, 26, 22]	$\tilde{\Omega}(n)$	1, 2	Existence of zero error
[49, 24, 39]	$\tilde{\Omega}(n)$	Any d	Existence of zero error
[35]	$\tilde{\Omega}(\text{poly}(n))$	1	(S)GD global convergence
[14]	$\tilde{\Omega}(n^6)$	1	(S)GD global convergence
[43]	$\tilde{\Omega}(n^2)$	1	(S)GD global convergence
[2, 54]	$\tilde{\Omega}(\text{poly}(n, d))$	Any d	(S)GD global convergence
[13]	$\tilde{\Omega}(n^8 2^{O(d)})$	Any d	(S)GD global convergence
[55]	$\tilde{\Omega}(n^8 d^1 2)$	Any d	(S)GD global convergence
[27]	$\tilde{\Omega}(n)$ (Training last layer)	Any d	(S)GD global convergence
[42]	$\tilde{\Omega}(n^{\frac{3}{2}})$ (Training all layers)	1	(S)GD global convergence
[8]	$\tilde{\Omega}(n)$ (Training all layers)	Any d	(S)GD global convergence

Table: Summary of results on overparametrization. Minimum number of parameters required as a function of data size n and depth d. The result is classified either as *Existence* i.e., there exists a neural network achieving zero error on the data, or *(S)GD global convergence* i.e., (S)GD converges to zero training error, a much stronger condition.

Stochastic adaptive first-order methods

Adaptive methods

Stochastic adaptive methods converge without knowing the smoothness constant.

They do so by making use of the information from stochastic gradients and their norms.

Variable metric stochastic gradient descent algorithm

Variable metric stochastic gradient descent algorithm
1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point and $\mathbf{H}_0 \succ 0$. **2**. For $k = 0, 1, \cdots,$ perform: $$\begin{cases} \mathbf{d}^k & := -\mathbf{H}_k^{-1}\mathbf{g}^k, \\ \mathbf{x}^{k+1} & := \mathbf{x}^k + \alpha_k \mathbf{d}^k, \end{cases}$$ where $\alpha_k \in (0, 1]$ is a given step size. **3**. Update $\mathbf{H}_{k+1} \succ 0$ if necessary.

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3. Update $\mathbf{H}_{k+1} \succ 0$ if necessary.

Common choices of the variable metric $\mathbf{H}_k$

- $\mathbf{H}_k := \lambda_k \mathbf{I}$ $\Longrightarrow$ stochastic gradient descent method.
- $\mathbf{H}_k := \mathbf{D}_k$ (a positive diagonal matrix) $\Longrightarrow$ stochastic adaptive gradient methods.

Adaptive gradient methods

Intuition

Adaptive gradient methods adapt locally by setting $\mathbf{H}_k$ as a function of past stochastic gradient information.

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- Roughly speaking, $\mathbf{H}_k = \text{function}(\mathbf{g}^1, \mathbf{g}^2, \cdots, \mathbf{g}^k)$
- Some well-known examples:

AdaGrad [15]

$$\mathbf{H}_k = \sqrt{\sum_{t=1}^{k} \mathbf{g}^k {\mathbf{g}^k}^\top}$$

RmsProp [44]

$$\mathbf{H}_k = \sqrt{\beta \mathbf{H}_{k-1} + (1-\beta)\text{diag}(\mathbf{g}^k)^2}$$

ADAM [29]

$$\hat{\mathbf{H}}_k = \beta \hat{\mathbf{H}}_{k-1} + (1-\beta)\text{diag}(\mathbf{g}^k)^2$$
$$\mathbf{H}_k = \sqrt{\hat{\mathbf{H}}_k / (1-\beta^k)}$$

AdaGrad - Adaptive gradient method with $\mathbf{H}_k = \lambda_k \mathbf{I}$

- If $\mathbf{H}_k = \lambda_k \mathbf{I}$, it becomes stochastic gradient descent method with adaptive step-size $\frac{\alpha_k}{\lambda_k}$.

How step-size adapts?

If the stochastic gradient $\|\mathbf{g}^k\|$ is large/small $\rightarrow$ AdaGrad adjusts step-size α_k/λ_k smaller/larger

Adaptive gradient descent (AdaGrad with $\mathbf{H}_k = \lambda_k \mathbf{I}$) [31]

1. Set $Q^0 = 0$.
2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} Q^k &= Q^{k-1} + \|\mathbf{g}^k\|^2 \\ \mathbf{H}_k &= \sqrt{Q^k} I \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1} \mathbf{g}^k \end{cases}$$

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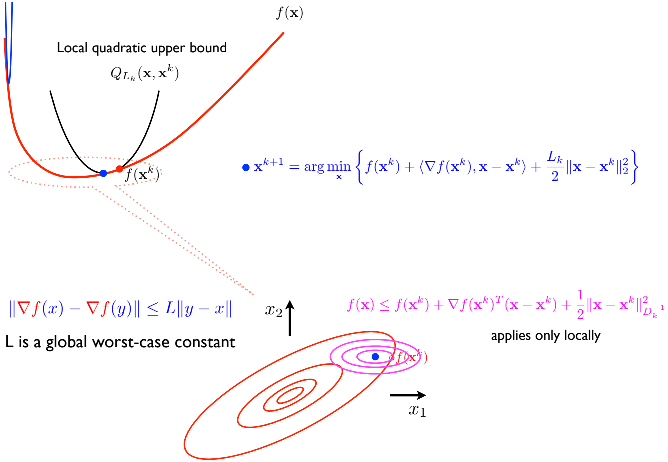
Adaptation through first-order information

- When $H_k = \lambda_k I$, AdaGrad estimates local geometry through stochastic gradient norms.
- Akin to estimating a local quadratic upper bound (majorization / minimization) using gradient history.

AdaGrad - Adaptive gradient method with $\mathbf{H}_k = \mathbf{D}_k$

Adaptation strategy with a positive diagonal matrix $\mathbf{D}_k$

Adaptive step-size + coordinate-wise extension = adaptive step-size for each coordinate



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- Suppose $\mathbf{H}_k$ is diagonal,

$$\mathbf{H}_k := \begin{bmatrix} \lambda_{k,1} & & 0 \\ & \ddots & \\ 0 & & \lambda_{k,d} \end{bmatrix},$$

- For each coordinate i, we have different step-size $\frac{\alpha_k}{\lambda_{k,i}}$ is the step-size.

Adaptive gradient descent(AdaGrad with $\mathbf{H}_k = \mathbf{D}_k$)

1. Set $\mathbf{Q}^0$ =0.
2. For $k = 0, 1, \ldots,$ iterate

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Adaptation across each coordinate

- When $\mathbf{H}_k = \mathbf{D}_k$, we adapt across each coordinate individually.
- Essentially, we have a finer treatment of the function we want to optimize.

RMSProp - Adaptive gradient method with $\mathbf{H}_k = \mathbf{D}_k$

What could be improved over AdaGrad?

1. Stochastic gradients have equal weights in step size.
2. Consider a *steep* function, flat around minimum $\rightarrow$ slow convergence at flat region.

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RMSProp

1. Set $\mathbf{Q}_0 = 0$.
2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \mathbf{Q}^k &= \beta\mathbf{Q}^{k-1} + (1-\beta)\mathrm{diag}(\mathbf{g}^k)^2 \\ \mathbf{H}_k &= \sqrt{\mathbf{Q}^k} \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1}\mathbf{g}^k \end{cases}$$

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- RMSProp uses weighted averaging with constant β
- Recent gradients have greater importance

AcceleGrad - Adaptive gradient + Accelerated gradient [32]

Motivation behind AcceleGrad

Is it possible to achieve acceleration when f is L-smooth, without knowing the Lipschitz constant?

AcceleGrad (Accelerated Adaptive Gradient Method)

Input : $\mathbf{x}^0 \in \mathcal{K}$, diameter D, weights $\{\alpha_k\}_{k\in\mathbb{N}}$, learning rate $\{\eta_k\}_{k\in\mathbb{N}}$

1. Set $\mathbf{y}^0 = \mathbf{z}^0 = \mathbf{x}^0$
2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \tau_k & := 1/\alpha_k \\ \mathbf{x}^{k+1} & = \tau_k \mathbf{z}^k + (1-\tau_k)\mathbf{y}^k, \text{define } \mathbf{g}_k := \nabla f(\mathbf{x}^{k+1}) \\ \mathbf{z}^{k+1} & = \Pi_{\mathcal{K}}(\mathbf{z}^k - \alpha_k \eta_k \mathbf{g}_k) \\ \mathbf{y}^{k+1} & = \mathbf{x}^{k+1} - \eta_k \mathbf{g}_k \end{cases}$$

Output : $\overline{\mathbf{y}}^k \propto \sum_{i=0}^{k-1} \alpha_i \mathbf{y}^{i+1}$

where $\Pi_{\mathcal{K}}(\mathbf{y}) = \arg\min_{\mathbf{x}\in\mathcal{K}} \langle \mathbf{x}-\mathbf{y}, \mathbf{x}-\mathbf{y}\rangle$ (projection onto $\mathcal{K}$).

***Remark:** ◦ This is essentially the **MD + GD** scheme [3], with an adaptive step size!

AcceleGrad - Properties and convergence

Learning rate and weight computation

Assume that function f has uniformly bounded gradient norms $\|\mathbf{g}^k\|^2 \leq G^2$, i.e., f is G-Lipschitz continuous. AcceleGrad uses the following weights and learning rate:

$$\alpha_k = \frac{k+1}{4}, \quad \eta_k = \frac{2D}{\sqrt{G^2 + \sum_{\tau=0}^{k} \alpha_\tau^2 \|\mathbf{g}^{\tau+1}\|^2}}$$

- Similar to RmsProp, AcceleGrad assignes greater weights to recent gradients.

Convergence rate of AcceleGrad

Assume that f is convex and L-smooth. Let $\mathcal{K}$ be a convex set with bounded diameter D, and assume $\mathbf{x}^\star \in \mathcal{K}$. Define $\bar{\mathbf{y}}^k = (\sum_{i=0}^{k-1} \alpha_i \mathbf{y}^{i+1})/(\sum_{i=0}^{k-1} \alpha_i)$. Then,

$$f(\overline{\mathbf{y}}^k) - f^\star \leq O\left(\frac{DG + LD^2 \log(LD/G)}{k^2}\right)$$

If f is only convex and G-Lipschitz, then

$$f(\overline{\mathbf{y}}^k) - f^\star \leq O\left(GD\sqrt{\log k}/\sqrt{k}\right)$$

ADAM - Adaptive moment estimation

Over-simplified idea of ADAM

RMSProp + 2nd order moment estimation = ADAM

ADAM - Adaptive moment estimation

Over-simplified idea of ADAM

RMSProp $+$ 2nd order moment estimation $=$ ADAM

ADAM
Input. Step size α, exponential decay rates $\beta_1, \beta_2 \in [0,1)$
1. Set $\mathbf{m}_0, \mathbf{v}_0 = 0$ **2.** For $k = 0, 1, \ldots,$ iterate $$\begin{cases} \mathbf{g}_k &= \nabla f(\mathbf{x}^{k-1}) \\ \mathbf{m}_k &= \beta_1 \mathbf{m}_{k-1} + (1-\beta_1)\mathbf{g}_k \leftarrow \text{1st order estimate} \\ \mathbf{v}_k &= \beta_2 \mathbf{v}_{k-1} + (1-\beta_2)\mathbf{g}_k^{.2} \leftarrow \text{2nd order estimate} \\ \hat{\mathbf{m}}_k &= \mathbf{m}_k/(1-\beta_1^k) \leftarrow \text{Bias correction} \\ \hat{\mathbf{v}}_k &= \mathbf{v}_k/(1-\beta_2^k) \leftarrow \text{Bias correction} \\ \mathbf{H}_k &= \sqrt{\hat{\mathbf{v}}_k} + \epsilon \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha \hat{\mathbf{m}}_k./\mathbf{H}_k \end{cases}$$
Output : $\mathbf{x}^k$

(Every vector operation is an element-wise operation)

Non-convergence of ADAM and a new method: AmsGrad

- It has been shown that ADAM may not converge for *some* objective functions [50].
- An ADAM alternative is proposed that is proved to be convergent [40].

AmsGrad
Input. Step size $\{\gamma_k\}_{k\in\mathbb{N}}$, exponential decay rates $\{\beta_{1,k}\}_{k\in\mathbb{N}}$, $\beta_2 \in [0,1)$
1. Set $\mathbf{m}_0 = 0, \mathbf{v}_0 = 0$ and $\hat{\mathbf{v}}_0 > 0$ **2.** For $k = 1, 2, \ldots,$ iterate $\begin{cases} \mathbf{g}_k &= G(\mathbf{x}^k, \theta) \\ \mathbf{m}_k &= \beta_{1,k}\mathbf{m}_{k-1} + (1-\beta_{1,k})\mathbf{g}_k \leftarrow \text{1st order estimate} \\ \mathbf{v}_k &= \beta_2\mathbf{v}_{k-1} + (1-\beta_2)\mathbf{g}_k^{.2} \leftarrow \text{2nd order estimate} \\ \hat{\mathbf{v}}_k &= \max\{\hat{\mathbf{v}}_{k-1}, \mathbf{v}_k\} \text{ and } \hat{\mathbf{V}}_k = \text{diag}(\hat{\mathbf{v}}_k) \\ \mathbf{H}_k &= \sqrt{\hat{\mathbf{v}}_k} \\ \mathbf{x}^{k+1} &= \Pi_{\mathcal{X}}^{\sqrt{\hat{\mathbf{V}}_k}}(\mathbf{x}^k - \gamma_k \hat{\mathbf{m}}_k./\mathbf{H}_k) \end{cases}$
Output : $\mathbf{x}^k$

where $\Pi_{\mathcal{K}}^{\mathbf{A}}(\mathbf{y}) = \arg\min_{\mathbf{x}\in\mathcal{K}} \langle(\mathbf{x}-\mathbf{y}), \mathbf{A}(\mathbf{x}-\mathbf{y})\rangle$ (weighted projection onto $\mathcal{K}$).
(Every vector operation is an element-wise operation)

AdaGrad & AmsGrad for non-convex optimization

Theorem (AdaGrad convergence rate: stochastic, non-convex [46])

Assume f is non-convex and L-smooth, such that $\|\nabla f(\mathbf{x})\|^2 \leq G^2$ and $f^\star = \inf_{\mathbf{x}} f(\mathbf{x}) > \infty$. Also consider bounded variance for unbiased gradient estimates, i.e., $\mathbb{E}\left[\|G(\mathbf{x},\theta) - \nabla f(\mathbf{x})\|^2|\mathbf{x}\right] \leq \sigma^2$. Then with probability $1-\delta$,

$$\min_{i\in\{1,..,k-1\}} \|\nabla f(\mathbf{x}^i)\|^2 = \tilde{\mathcal{O}}\left(\frac{\sigma}{\delta^{3/2}\sqrt{k}}\right)$$

◦ **Note:** As $1-\delta \to 1$, the rate deteriorates by a factor of $\delta^{-3/2}$.

Theorem (AmsGrad convergence rate 1: stochastic, non-convex [10])

Let $\mathbf{g}_k = G(\mathbf{x}^k, \theta)$. Assume $\|\mathbf{g}_k\| \leq G$. Consider a non-increasing sequence $\beta_{1,k}$ and $\beta_{1,k} \leq \beta_1 \in [0,1)$. Set $\gamma_k = 1/\sqrt{k}$. Then,

$$\min_{i\in\{1,..,k-1\}} \mathbb{E}\left[\|\nabla f(\mathbf{x}^i)\|^2\right] = O\left(\frac{\log k}{\sqrt{k}}\right).$$

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Theorem (AdaGrad convergence rate: stochastic, non-convex [46])

Assume f is non-convex and L-smooth, such that $\|\nabla f(\mathbf{x})\|^2 \leq G^2$ and $f^\star = \inf_{\mathbf{x}} f(\mathbf{x}) > \infty$. Also consider bounded variance for unbiased gradient estimates, i.e., $\mathbb{E}\left[\|G(\mathbf{x},\theta) - \nabla f(\mathbf{x})\|^2 | \mathbf{x}\right] \leq \sigma^2$. Then with probability $1-\delta$,

$$\min_{i \in \{1,..,k-1\}} \|\nabla f(\mathbf{x}^i)\|^2 = \tilde{\mathcal{O}}\left(\frac{\sigma}{\delta^{3/2}\sqrt{k}}\right)$$

◦ **Note:** As $1-\delta \to 1$, the rate deteriorates by a factor of $\delta^{-3/2}$.

Theorem (AmsGrad convergence rate 2: stochastic, non-convex [52, 9])

Consider $f : \mathbb{R}^p \to \mathbb{R}$ to be non-convex and L-smooth. Assume $\|G(\mathbf{x},\theta)\|_\infty \leq G_\infty$ and set $\gamma_k = 1/\sqrt{pT}$. Also define $\mathbf{x}_{out} = \mathbf{x}^k$, for $k = 1,\ldots,T$ with probability $\gamma_k / \sum_{i=1}^T \gamma_i$. Then,

$$\mathbb{E}\left[\|\nabla f(\mathbf{x}_{out})\|^2\right] = \mathcal{O}\left(\sqrt{\frac{p}{T}}\right).$$

Adam variants without large batch sizes

Guarantees of Adam-variants [1]

By using one subgradient each iteration, with the same setup as before, AMSGrad converges for $\min_{\mathbf{x}\in\mathcal{X}} f(\mathbf{x})$

$$\mathbb{E}\|G_\lambda(\mathbf{x}_{\text{out}})\|^2 \leq \tilde{\mathcal{O}}\left(\sqrt{\frac{1}{T}}\right), \tag{2}$$

on the gradient mapping $G_\lambda(\mathbf{x}) = \frac{\mathbf{H}_k^{1/2}}{\lambda}\left(\mathbf{x} - P_{\mathcal{X}}^{\mathbf{H}_k}(\mathbf{x} - \lambda\mathbf{H}_k^{-1}\nabla f(\mathbf{x}))\right)$, where $\mathbf{x}_{\text{out}}$ is chosen uniformly at random from the iterates.

A comparison of adaptive algorithms

	GD/SGD	Accelerated GD/SGD	AdaGrad	AcceleGrad/UniXgrad	Adam/AMSGrad
Convex, stochastic	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ [1]	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ [1]	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ [2]	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ [3,4]	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ [5]
Convex, deterministic, L-smooth	$\mathcal{O}\left(\frac{1}{k}\right)$ [1]	$\mathcal{O}\left(\frac{1}{k^2}\right)$ [1]	$\mathcal{O}\left(\frac{1}{k}\right)$ [3]	$\mathcal{O}\left(\frac{1}{k^2}\right)$ [3,4]	$\mathcal{O}\left(\frac{1}{k}\right)$ [6]
Nonconvex, stochastic, L-smooth	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ [1]	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ [1]	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ [7]	?	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ [8]
Nonconvex, deterministic, L-smooth	$\mathcal{O}\left(\frac{1}{k}\right)$ [1]	$\mathcal{O}\left(\frac{1}{k}\right)$ [1]	$\mathcal{O}\left(\frac{1}{k}\right)$ [7]	?	$\mathcal{O}\left(\frac{1}{k}\right)$ [6]

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Example: ADAM vs. AcceleGrad

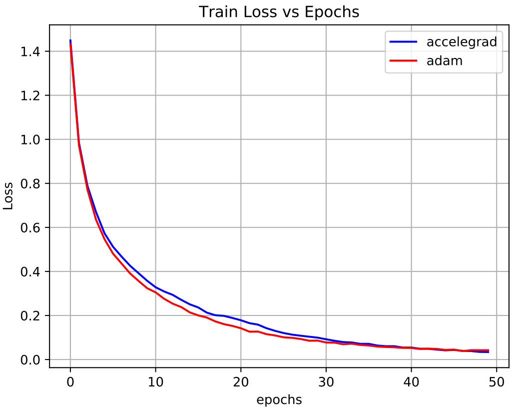

Figure: Resnet classifier optimization (train loss)

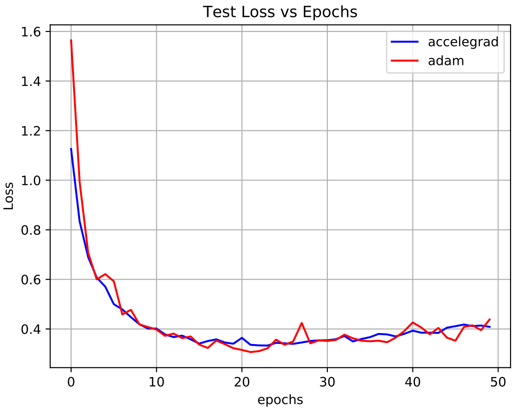

Figure: Resnet classifier optimization (test loss)

Example: Least squares with synthetic data

Setting:

- $f(x) = \| Ax - b \|^2$
- $A \in \mathbb{R}^{n \times d}$, $A \sim N(\mu, \sigma^2 I)$
- $n = 1000$, $d = 1000$

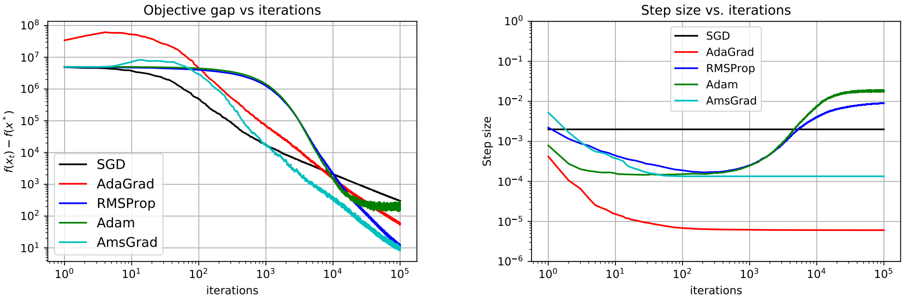

Figure: Comparison of convergence rate and stepsize evolution. Mini-batch stochastic gradients with a batch size of 20

Performance of optimization algorithms (nonconvex)

◦ Assuming only L-smoothness, SGD, Adagrad, RmsProp, ADAM & AmsGrad and Accelegrad has $\frac{1}{\sqrt{k}}$-rate

◦ Additional assumptions help improve this rate

- Polyak-Lojasiewicz (PL)[9]
- (Strong) growth condition (SGC)[10]
- Averaged L-smoothness [16]
- Interpolation (IP) [37]

[9] J. Bolte, T. P. Nguyen, J. Peypouquet, and B. W. Suter. "From error bounds to the complexity of first-order descent methods for convex functions."

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Performance of optimization algorithms (nonconvex)

◦ Assuming only L-smoothness, SGD, Adagrad, RmsProp, ADAM & AmsGrad and Accelegrad has $\frac{1}{\sqrt{k}}$-rate

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◦ A non-exhaustive comparison:

Assumptions on f	Algorithm	Convergence rate	Iteration complexity
L-smooth	Basically all first order methods	Sublinear $(1/\sqrt{k})$	One stochastic gradient
Averaged L-smooth	STORM [11] & STORM+ [33]	Sublinear $(1/k^{2/3})$	Two stochastic gradients
L-smooth + SGC	SGD	Sublinear $(1/k)$[45]	One stochastic gradient
L-smooth + SGC + PL	SGD	Linear (ρ^k) [45]	One stochastic gradient
$f(\mathbf{x}) := \frac{1}{n}\sum_{i=1}^{n} f_i(\mathbf{x})$ f_i are β-smooth f is L-smooth + IP + PL	(mini-batch) SGD	Linear (ρ^k) [4]	m stochastic gradients $m \in \mathbb{N}$

[9] J. Bolte, T. P. Nguyen, J. Peypouquet, and B. W. Suter. "From error bounds to the complexity of first-order descent methods for convex functions."

[10] V. Cevher and B. C. Vu. "On the linear convergence of the stochastic gradient method with constant step-size."

Implicit regularization of adaptive methods may overfit

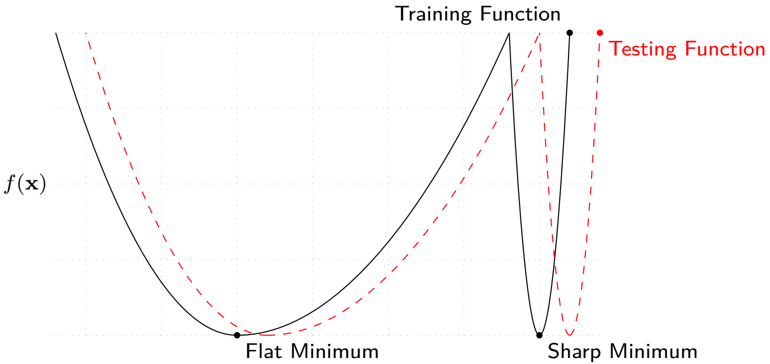

Figure: Sharp Minima vs Flat Minima [28]

- Intuition suggests flat minima has better generalization property than sharp minima
- Empirically, adaptive methods finds sharper minima than ones found by SGD
- The relationship between sharpness of minima and their generalization is open [12, 17]

ϵ-stability: a first approach to sharpness aware optimization

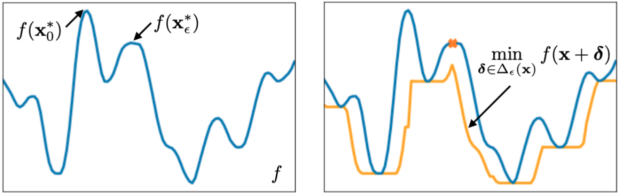

Figure: Smoothing effect of ϵ-stable loss characterization [7]

ϵ-stability [7]

[7] defines an ϵ-stable point $\mathbf{x}_\epsilon^*$ $(\epsilon > 0)$ for zero-th order global function *maximization* as follows:

$$\mathbf{x}_\epsilon^* \in \arg\max_{\mathbf{x}} \min_{\delta:\|\delta\|\leq\epsilon} f(\mathbf{x}+\delta)$$

Remarks:

- Consider finding the (global) maximum of a function.
- We want to avoid sharp maxima and identify a flat, stable (local) optimum.
- This formulation favors broad peaks, rather than sharp maxima with lesser regard to its value.

Explicit regularization through ϵ-stability

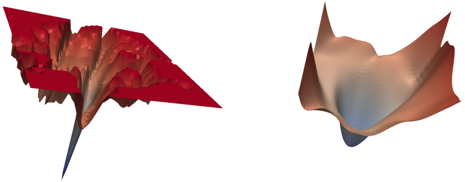

Figure: Loss lanscape of ResNet and ResNet with an approximation of SAM formulation [18].

Sharpness-aware minimization (SAM) [18]

[18] reuses the ϵ-stable point $\mathbf{x}_\epsilon^*$ for firsth order function *minimization* as follows:

$$\min_{\mathbf{x}} \max_{\|\epsilon\| \le \rho} f(\mathbf{x} + \epsilon).$$

Remarks:

- ◦ [18] argues that this objective approximates the function $\min_{\mathbf{x}} f(\mathbf{x} + \tau \nabla f(\mathbf{x}))$.
- ◦ There is interest in understanding their heuristic algorithm.

Example: Generalization performance

◦ Adaptive learning methods may converge fast but generalize worse

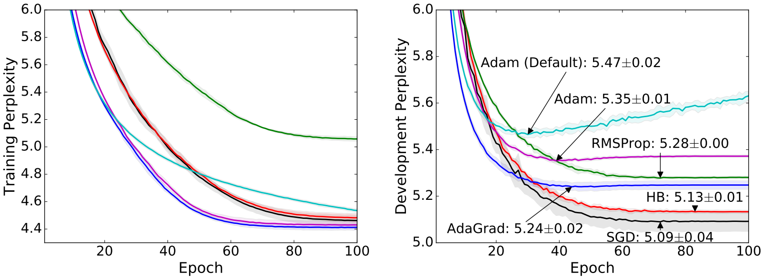

Figure: Performance of different optimizers in training and development set of a language modeling problem. The training and test perplexity are the exponential values of training and test losses.[48]

Neural Network Architectures

- Deeper and more complicated models correlates with better performance
- No universal optimizers other than slow and steady SGD
- A long way to go (makes it exciting)...

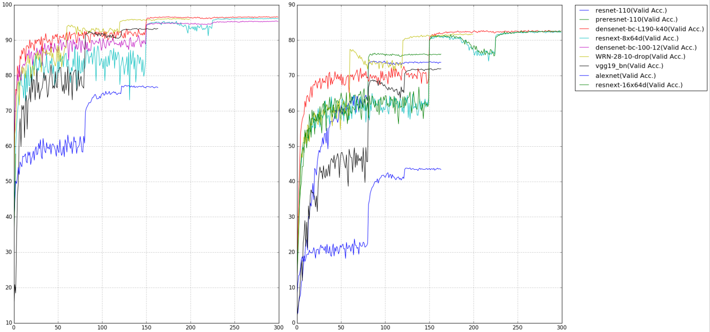

Figure: Performance of popular architectures on test set in CIFAR10 (left) and CIFAR100 (right). [11]

[11] Credit to: https://github.com/bearpaw/pytorch-classification

Wrap up!

- Deep learning recitation on Friday!

*Perturbed SGD escapes saddle points

Theorem (Convergence of PSGD [19])

Suppose that f has the following properties

- f *is an* $(\alpha, \gamma, \epsilon, \delta)$*-strict saddle,*
- f *is* β*-smooth.*
- *its Hessian is* ρ*-Lipschitz. i.e.* $\| \nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y}) \| \leq \rho \| \mathbf{x} - \mathbf{y} \|$.

Then there exists a threshold $\alpha_{\max}$ *such that by choosing*

- $\alpha \leq \alpha_{\max} / \max\{1, \log(1/\zeta)\}$
- $T = O(\alpha^{-2} \log(1/\zeta))$.

the algorithm ***Perturbed SGD*** *outputs with probability at least* $1 - \zeta$ *a point* $\mathbf{x}_T$ *that is* $O(\sqrt{\alpha \log(1/\alpha\zeta)})$ *close to some local minimum* $\mathbf{x}^\star$.

*Convergence of SGD in non-convex problems with small step-size

Assumptions

1. Function f is lower bounded: $\exists f^\star$ s.t. $\forall \mathbf{x} \in \mathcal{X}, f(\mathbf{x}) \geq f^\star$
2. Function f has Lipschitz continuous gradient:

$$\|\nabla f(\mathbf{x}_1) - \nabla f(\mathbf{x}_2)\|_2 \leq L\|\mathbf{x}_1 - \mathbf{x}_2\|_2 \tag{3}$$

3. The stochastic gradient $\hat{\mathbf{g}}_{\mathbf{x}}$ is unbiased and has bounded variance:

$$\mathbb{E}(\hat{\mathbf{g}}) = \mathbf{g}, \quad \mathbb{E}(\|\hat{\mathbf{g}} - \mathbf{g}\|_2^2) \leq \sigma^2 \tag{4}$$

Theorem (Convergence of SGD in non-convex problems [6])

For SGD with assumptions above, N iterations and stepsize $\gamma_t = \frac{1}{L\sqrt{N}}$, we have

$$\mathbb{E}\left[\frac{1}{N}\sum_{t=0}^{N-1}\|\mathbf{g}^t\|_2^2\right] \sim \mathcal{O}\left(\frac{1}{\sqrt{N}}\right), \tag{5}$$

where the convergence is captured by the gradient norm.

*Convergence of SGD

Proof

Take the assumption 2 and algorithmic update policy $\mathbf{x}^{t+1} = \mathbf{x}^t - \gamma\hat{\mathbf{g}}^t$

$$\begin{aligned} f(\mathbf{x}_{t+1}) - f(\mathbf{x}_t) &\leq (\mathbf{x}_{t+1} - \mathbf{x}_t)^T \mathbf{g}^t + \frac{L}{2}\|\mathbf{x}_{t+1} - \mathbf{x}_t\|_2^2 \\ &= -\gamma_t(\hat{\mathbf{g}}^t)^T \mathbf{g}^t + \frac{\gamma_t^2 L}{2}\|\hat{\mathbf{g}}^t\|_2^2 \end{aligned} \tag{6}$$

Take the expectation and use the assumption 3

$$\mathbb{E}[f(\mathbf{x}_{t+1}) - f(\mathbf{x}_t)] = -\gamma_t\|\mathbf{g}^t\|_2^2 + \frac{\gamma_t^2 L}{2}(\|\mathbf{g}^t\|_2^2 + \sigma^2) \tag{7}$$

Set the learning rate $\gamma_t = \frac{1}{L\sqrt{N}}$

$$\begin{aligned} \mathbb{E}[f(\mathbf{x}_{t+1}) - f(\mathbf{x}_t)] &= -\frac{1}{L\sqrt{N}}\|\mathbf{g}^t\|_2^2 + \frac{1}{2LN}(\|\mathbf{g}^t\|_2^2 + \sigma^2) \\ &\leq -\frac{1}{2L\sqrt{N}}\|\mathbf{g}^t\|_2^2 + \frac{\sigma^2}{2LN} \end{aligned} \tag{8}$$

*Convergence of SGD

Proof (Cont'd).

Sum the inequality of N steps together and use assumption 1

$$
\begin{aligned}
f(\mathbf{x}_0) - f^\star \geq f(\mathbf{x}_0) - \mathbb{E}[f(\mathbf{x}_N)] \\
= \mathbb{E}\left[\sum_{t=0}^{N-1} (f(\mathbf{x}_t) - f(\mathbf{x}_{t+1}))\right] \\
\geq \frac{1}{2L}\mathbb{E}\left[\sum_{t=0}^{N-1} (\frac{\|\mathbf{g}^t\|_2^2}{\sqrt{N}} - \frac{\sigma^2}{N})\right]
\end{aligned}
\tag{9}
$$

Rearrange the inequality, we have the following

$$
\mathbb{E}\left[\frac{1}{N}\sum_{t=0}^{N-1} \|\mathbf{g}^t\|_2^2\right] \leq \frac{1}{\sqrt{N}}[2L(f(\mathbf{x}_0) - f^\star + \sigma^2)] \tag{10}
$$

The right hand side vanishes as $N \to \infty$, so $\mathbb{E}\left[\frac{1}{N}\sum_{t=0}^{N-1} \|\mathbf{g}^t\|_2^2\right]$ vanishes also. This indicates the model converges to a critical point. □

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