

Large-scale Machine Learning and Optimization

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Why Optimization in Machine Learning?

Many problems in ML can be written as

$$\min_{x \in \mathcal{W}} \sum_{i=1}^N \frac{1}{2} \|a_i^\top x - y_i\|_2^2 + \mu \|x\|_1 \quad \text{linear regression}$$

$$\min_{x \in \mathcal{W}} \frac{1}{N} \sum_{i=1}^N \log(1 + \exp(-y_i a_i^\top x)) + \mu \|x\|_1 \quad \text{logistic regression}$$

$$\min_{x \in \mathcal{W}} \sum_{i=1}^N \ell(h(x, a_i), y_i) + \mu \varphi(x) \quad \text{general formulation}$$

- The pairs (a_i, y_i) are given data, y_i is the label of the data point a_i
- $\ell(\cdot)$: measures how model fit for data points (avoids under-fitting)
- $\varphi(x)$: regularization term (avoids over-fitting)
- $h(x, a)$: linear function or models constructed from deep neural networks

Sparse Logistic Regression

The ℓ_1 logistic regression problem.

$$\min_{x \in \mathbb{R}^n} \frac{1}{N} \sum_{i=1}^N \log(1 + \exp(-y_i a_i^T x)) + \mu \|x\|_1.$$

- The data pair $\{a_i, y_i\} \in \mathbb{R}^n \times \{-1, 1\}, i \in [N]$,

Data Set	# data N	# features n	sparsity(%)
cina	16,033	132	70.49
a9a	32,561	123	88.72
ijcnn1	49,990	22	40.91
covtype	581,012	54	77.88
url	2,396,130	3,231,961	99.99
susy	5,000,000	18	1.18
higgs	11,000,000	28	7.89
news20	19,996	1,355,191	99.97
rcv1	20,242	47,236	99.84
kdda	8,407,752	20,216,830	99.99

Deep Learning

The objective function is the CrossEntropy function plus ℓ_1 term:

$$\min_x \frac{1}{N} \sum_{i=1}^N -\log \left(\frac{\exp(h(x, a_i)[y_i])}{\sum_j \exp(h(x, a_i)[j])} \right) + \mu \|x\|_1$$

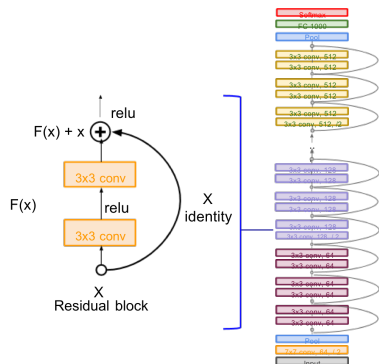
where $h(x, a_i)$ is output from network, and (a_i, y_i) are data points.

	Cifar-10	Cifar-100
# num_class	10	100
# number per class (training set)	5,000	500
# number per class (testing set)	1,000	100
# Total parameters of VGG-16	15,253,578	15,299,748
# Total parameters of ResNet-18	11,173,962	11,220,132

Table: A description of datasets used in the neural network experiments

ResNet Architecture

- Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun, Cited by **25911 since 2015** at Google scholar
- Stack residual blocks. Every residual block has two 3x3 conv layers.
- Make networks from shallow to deep.
- Fancy network architecture. Many Applications.
- High-computationally-cost !
- ResNet-50 on ImageNet, **29 hours using 8 Tesla P100 GPUs**



- 1 Problem Description
- 2 Subgradient Methods
 - The gradient and subgradient methods
 - Stochastic subgradient methods
- 3 Stochastic Gradient Descent
 - Gradient Descent
 - Stochastic Gradient methods
- 4 Variance Reduction
 - SAG method and SAGA method
 - SVRG method
- 5 Stochastic Algorithms in Deeplearning

Machine Learning Model

Machine learning model:

- $(x, y) \sim \mathcal{P}$, \mathcal{P} is a underlying distribution.
- Given a dataset $\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$. $(x_i, y_i) \sim \mathcal{P}$ i.i.d.
- Our goal is to find a hypothesis h_s with the smallest expected risk, i.e.,

$$\min_{h_s \in \mathcal{H}} R[h_s] := \mathbb{E}[\ell(h_s(x), y)] \quad (1)$$

where \mathcal{H} is hypothesis class.

Machine Learning Model

- In practice, we don not know the exact form of the underlying distribution \mathcal{P} .
- Empirical Risk Minimization (ERM)

$$\min_{h_S \in \mathcal{H}} \hat{R}_n[h_S] := \frac{1}{n} \sum_{i=1}^n \ell(h_S(x_i), y_i) \quad (2)$$

- We care about two questions on ERM:
 - When does the ERM concentrate around the true risk?
 - How does the hypothesis class affect the ERM?

Machine Learning Model

- Empirical risk minimizer $\hat{h}_n^* \in \operatorname{argmin}_{h \in \mathcal{H}} \hat{R}_n[h]$
- Expected risk minimizer $h^* \in \operatorname{argmin}_{h \in \mathcal{H}} R[h]$
- The concentration means that for any $\epsilon > 0, 0 < \delta < 1$, if n is larger enough, we have

$$\mathbb{P}(|R[\hat{h}_n^*] - R[h^*]| \leq \epsilon) > 1 - \delta \quad (3)$$

- It just means that $R[\hat{h}_n^*]$ converges to $R[h^*]$ in probability.
- The concentration will fail in some cases

Hoeffding Inequality

Let X_1, X_2, \dots be a sequence of i.i.d. random variables and assume that for all i , $E(X_i) = \mu$ and $\mathbb{P}(a \leq X_i \leq b) = 1$. Then for any $\epsilon > 0$

$$\mathbb{P}\left(\left|\frac{1}{n} \sum_{i=1}^n X_i - \mu\right| \geq \epsilon\right) \leq 2 \exp\left(-\frac{2n\epsilon^2}{(b-a)^2}\right) \quad (4)$$

- The Hoeffding Inequality describes the asymptotic property that sampling mean converges to expectation.
- Azuma-Hoeffding inequality is a martingale version. Let X_1, X_2, \dots be a martingale difference sequence with $|X_i| \leq B$ for all $i = 1, 2, \dots$. Then

$$\mathbb{P}\left(\sum_{i=1}^n X_i \geq t\right) \leq \exp\left(-\frac{2t^2}{nB^2}\right) \quad (5)$$

$$\mathbb{P}\left(\sum_{i=1}^n X_i \leq -t\right) \leq \exp\left(-\frac{2t^2}{nB^2}\right) \quad (6)$$

- To make the exposition simpler, we assume that our loss function, $0 \leq \ell(a, b) \leq 1, \forall a, b$.
- By Hoeffding Inequality, fixed h

$$\mathbb{P}(|\hat{R}_n[h] - R[h]| \geq \epsilon) \leq 2e^{-2n\epsilon^2} \quad (7)$$

- Union Bound

$$\mathbb{P}\left(\bigcup_{h \in \mathcal{H}} \{|\hat{R}_n[h] - R[h]| \geq \epsilon\}\right) \leq 2|\mathcal{H}|e^{-2n\epsilon^2} \quad (8)$$

- If we want to bound $\mathbb{P}\left(\bigcup_{h \in \mathcal{H}} \{|\hat{R}_n[h] - R[h]| \geq \epsilon\}\right) \leq \delta$, we need the size of sample

$$n \geq \frac{1}{2\epsilon^2} \log\left(\frac{2|\mathcal{H}|}{\delta}\right) = O\left(\frac{\log|\mathcal{H}| + \log(\delta^{-1})}{\epsilon^2}\right) \quad (9)$$

- What if $|\mathcal{H}| = \infty$? This bound doesn't work

- If n is large enough, with a probability $1 - \delta$, we have

$$\begin{aligned} R[\hat{h}_n^*] - R[h^*] &= (R[\hat{h}_n^*] - \hat{R}_n[\hat{h}_n^*]) + (\hat{R}_n[\hat{h}_n^*] - \hat{R}_n[h^*]) \\ &\quad + (\hat{R}_n[h^*] - R[h^*]). \\ &\leq \epsilon + 0 + \epsilon. \end{aligned}$$

- For a two label classification problem, with a probability $1 - \delta$, we have

$$\sup_{h \in \mathcal{H}} |\hat{R}_n[h] - R[h]| \leq O \left(\sqrt{\frac{VC[\mathcal{H}] \log\left(\frac{n}{VC[\mathcal{H}]}\right) + \log\left(\frac{1}{\delta}\right)}{n}} \right) \quad (10)$$

where $VC[\mathcal{H}]$ is a VC dimension of \mathcal{H} .

- Finite VC dimension is sufficient and necessary condition of empirical risk concentration for two label classification.

VC dimension

- VC dimension of a set-family: Let H be a set family (a set of sets) and C a set. Their intersection is defined as the following set-family:

$$H \cap C := \{h \cap C \mid h \in H\}$$

We say that a set C is shattered by H if $H \cap C = 2^C$.

The **VC dimension** of H is the largest integer D such that there exists a set C with cardinality D that is shattered by H .

- A classification model f with some parameter vector θ is said to shatter a set of data points (x_1, x_2, \dots, x_n) if, for all assignments of labels to those points, there exists a θ such that the model f makes no errors when evaluating that set of data points.

The **VC dimension** of a model f is the maximum number of points that can be arranged so that f shatters them. More formally, it is the maximum cardinal D such that some data point set of cardinality D can be shattered by f .

VC dimension

- example:
 - If $\forall n$ and $\{(x_1, y_1), \dots, (x_n, y_n)\}$, there exists $h \in \mathcal{H}$ s.t. $h(x_i) = y_i$, then $VC[\mathcal{H}] = \infty$
 - For a neural network whose activation functions are all sign functions, then $VC[\mathcal{H}] \leq O(w \log(w))$, where w is the number of parameters.
- We must use prior knowledge and choose a proper hypothesis class.
- Suppose a is the true model

$$R[\hat{h}_n^*] - R[a] = \underbrace{(R[\hat{h}_n^*] - R[h^*])}_A + \underbrace{(R[h^*] - R[a])}_B$$

- If the hypothesis class is too large, B will be small but A will be large. (overfitting)
- If the hypothesis class is too small, A will be small but B will be large. (underfitting)

Outline

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The gradient and subgradient methods

- Consider the problem

$$\min_{x \in \mathbb{R}^n} f(x) \quad (11)$$

- **gradient methods**

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k) \quad (12)$$

- **subgradient methods**

$$x_{k+1} = x_k - \alpha_k g_k, g_k \in \partial f(x_k) \quad (13)$$

- the update is equal to

$$x_{k+1} = \arg \min_x f(x_k) + \langle g_k, x - x_k \rangle + \frac{1}{2\alpha_k} \|x - x_k\|_2^2 \quad (14)$$

Convergence guarantees

Assumption

- There is at least one minimizing point $x^* \in \arg \min_x f(x)$ with $f(x^*) > -\infty$
- The subgradients are bounded: $\|g\|_2 \leq M < \infty$ for all x and all $g \in \partial f(x)$.

Theorem 1: Convergence of subgradient

Let $\alpha_k \geq 0$ be any non-negative sequence of stepsizes and the preceding assumptions hold. Let x_k be generated by the subgradient iteration. Then for all $K \geq 1$,

$$\sum_{k=1}^K \alpha_k [f(x_k) - f(x^*)] \leq \frac{1}{2} \|x_1 - x^*\|_2^2 + \frac{1}{2} \sum_{k=1}^K \alpha_k^2 M^2. \quad (15)$$

Proof of Theorem 1

- By convexity

$$\langle g_k, x^* - x_k \rangle \leq f(x^*) - f(x_k)$$



$$\begin{aligned} \frac{1}{2} \|x_{k+1} - x^*\|_2^2 &= \frac{1}{2} \|x_k - \alpha_k g_k - x^*\|_2^2 \\ &= \frac{1}{2} \|x_k - x^*\|_2^2 + \alpha_k \langle g_k, x^* - x_k \rangle + \frac{\alpha_k^2}{2} \|g_k\|_2^2 \\ &\leq \frac{1}{2} \|x_k - x^*\|_2^2 - \alpha_k (f(x_k) - f(x^*)) + \frac{\alpha_k^2}{2} M^2 \end{aligned}$$



$$\alpha_k (f(x_k) - f(x^*)) \leq \frac{1}{2} \|x_k - x^*\|_2^2 - \frac{1}{2} \|x_{k+1} - x^*\|_2^2 + \frac{\alpha_k^2}{2} M^2$$

Convergence guarantees

Corollary

Let $A_k = \sum_{i=1}^K \alpha_i$ and define $\bar{x}_K = \frac{1}{A_K} \sum_{k=1}^K \alpha_k x_k$

$$f(\bar{x}_k) - f(x^*) \leq \frac{\|x_1 - x^*\|_2^2 + \sum_{k=1}^K \alpha_k^2 M^2}{2 \sum_{k=1}^K \alpha_k}. \quad (16)$$

- Convergence: $\sum_{k=1}^{\infty} \alpha_k = \infty$ and $\frac{\sum_{k=1}^K \alpha_k^2}{\sum_{k=1}^K \alpha_k} \rightarrow 0$
- Let $\|x_1 - x^*\| \leq R$. For a fixed stepsize $\alpha_k = \alpha$:

$$f(\bar{x}_K) - f(x^*) \leq \frac{R^2}{2K\alpha} + \frac{\alpha M^2}{2}$$

- For a given K , take $\alpha = \frac{R}{M\sqrt{K}}$:

$$f(\bar{x}_K) - f(x^*) \leq \frac{RM}{\sqrt{K}}$$

Projected subgradient methods

- Consider the problem

$$\min_{x \in C} f(x) \quad (17)$$

- **subgradient methods**

$$x_{k+1} = \pi_C(x_k - \alpha_k g_k), g_k \in \partial f(x_k) \quad (18)$$

- projection: $\pi_C(x) = \arg \min_{y \in C} \|x - y\|_2^2$

- the update is equal to

$$x_{k+1} = \arg \min_{x \in C} f(x_k) + \langle g_k, x - x_k \rangle + \frac{1}{2\alpha_k} \|x - x_k\|_2^2 \quad (19)$$

Convergence guarantees

Assumption

- The set $C \subset \mathbb{R}^n$ is compact and convex, and $\|x - x^*\|_2 \leq R < \infty$ for all $x \in C$.
- The subgradients are bounded: $\|g\|_2 \leq M \leq \infty$ for all x and all $g \in \partial f(x)$.

Theorem 2: Convergence of projected subgradient method

Let $\alpha_k \geq 0$ be any non-negative sequence of stepsizes and the preceding assumptions hold. Let x_k be generated by the projected subgradient iteration. Then for all $K \geq 1$,

$$\sum_{k=1}^K \alpha_k [f(x_k) - f(x^*)] \leq \frac{1}{2} \|x_1 - x^*\|_2^2 + \frac{1}{2} \sum_{k=1}^K \alpha_k^2 M^2. \quad (20)$$

Proof of Theorem 2

- By non-expansiveness of $\pi_C(x)$

$$\|x_{k+1} - x^*\|_2^2 = \|\pi_C(x_k - \alpha g_k) - x^*\|_2^2 \leq \|x_k - \alpha g_k - x^*\|_2^2$$



$$\begin{aligned} \frac{1}{2} \|x_{k+1} - x^*\|_2^2 &\leq \frac{1}{2} \|x_k - \alpha g_k - x^*\|_2^2 \\ &= \frac{1}{2} \|x_k - x^*\|_2^2 + \alpha_k \langle g_k, x^* - x_k \rangle + \frac{\alpha_k^2}{2} \|g_k\|_2^2 \\ &\leq \frac{1}{2} \|x_k - x^*\|_2^2 - \alpha_k (f(x_k) - f(x^*)) + \frac{\alpha_k^2}{2} M^2 \end{aligned}$$



$$\alpha_k (f(x_k) - f(x^*)) \leq \frac{1}{2} \|x_k - x^*\|_2^2 - \frac{1}{2} \|x_{k+1} - x^*\|_2^2 + \frac{\alpha_k^2}{2} M^2$$

Convergence guarantees

Corollary

Let $A_k = \sum_{i=1}^k \alpha_i$ and define $\bar{x}_K = \frac{1}{A_K} \sum_{k=1}^K \alpha_k x_k$

$$f(\bar{x}_K) - f(x^*) \leq \frac{\|x_1 - x^*\|_2^2 + \sum_{k=1}^K \alpha_k^2 M^2}{2 \sum_{k=1}^K \alpha_k}. \quad (21)$$

- Convergence: $\sum_{k=1}^{\infty} \alpha_k = \infty$ and $\frac{\sum_{k=1}^K \alpha_k^2}{\sum_{k=1}^K \alpha_k} \rightarrow 0$
- a fixed stepsize $\alpha_k = \alpha$:

$$f(\bar{x}_K) - f(x^*) \leq \frac{R^2}{2K\alpha} + \frac{\alpha M^2}{2}$$

- Take $\alpha = \frac{R}{M\sqrt{K}}$:

$$f(\bar{x}_K) - f(x^*) \leq \frac{RM}{\sqrt{K}}$$

Stochastic subgradient methods

- the stochastic optimization problem

$$\min_{x \in C} f(x) := \mathbb{E}_{\mathbf{P}}[F(x; S)] \quad (22)$$

- S is a random space is a random variable on the space \mathcal{S} with distribution \mathbf{P} .
- for each s , $x \rightarrow F(x; s)$ is convex.
- The subgradient $\mathbb{E}_{\mathbf{P}}[g(x; S)] \in \partial f(x)$, where $g(x; s) \in \partial F(x; s)$.
-

$$\begin{aligned} f(y) &= \mathbb{E}_{\mathbf{P}}[F(y; S)] \geq \mathbb{E}_{\mathbf{P}}[F(x; S) + \langle g(x, S), y - x \rangle] \\ &= f(x) + \langle \mathbb{E}_{\mathbf{P}}[g(x; S)], y - x \rangle \end{aligned}$$

Stochastic subgradient methods

- the deterministic optimization problem

$$\min_{x \in C} f(x) := \frac{1}{m} \sum_{i=1}^m F(x; s_i) \quad (23)$$

- Why Stochastic?

- $\mathbb{E}_{\mathcal{P}}[F(x; S)]$ is generally intractable to compute
- Small complexity: only one subgradient $g(x; s) \in \partial F(x; s)$ needs to be computed in one iteration.
- More possible to get global solution for non-convex case.

- stochastic subgradient method

$$x_{k+1} = \pi_C(x_k - \alpha_k g_k), \quad \mathbb{E}[g_k | x_k] \in \partial f(x_k)$$

Convergence guarantees

Assumption

- The set $C \subset \mathbb{R}^n$ is compact and convex, and $\|x - x^*\|_2 \leq R < \infty$ for all $x \in C$.
- The variance are bounded: $\mathbb{E}\|g(x, S)\|_2^2 \leq M^2 \leq \infty$ for all x .

Theorem 3: Convergence of stochastic subgradient method

Let $\alpha_k \geq 0$ be any non-negative sequence of stepsizes and the preceding assumptions hold. Let x_k be generated by the stochastic subgradient iteration. Then for all $K \geq 1$,

$$\sum_{k=1}^K \alpha_k \mathbb{E}(f(x_k) - f(x^*)) \leq \frac{1}{2} \mathbb{E}\|x_1 - x^*\|_2^2 + \frac{\sum_{k=1}^K \alpha_k^2 M^2}{2} \quad (24)$$

Proof of Theorem 2

- Let $f'(x_k) = E[g_k|x_k]$ and $\xi_k = g_k - f'(x_k)$,

$$\begin{aligned} & \frac{1}{2} \|x_{k+1} - x^*\|_2^2 \leq \frac{1}{2} \|x_k - \alpha_k g_k - x^*\|_2^2 \\ &= \frac{1}{2} \|x_k - x^*\|_2^2 + \alpha_k \langle g_k, x^* - x_k \rangle + \frac{\alpha_k^2}{2} \|g_k\|_2^2 \\ &= \frac{1}{2} \|x_k - x^*\|_2^2 + \alpha_k \langle f'(x_k), x^* - x_k \rangle + \frac{\alpha_k^2}{2} \|g_k\|_2^2 + \alpha_k \langle \xi_k, x^* - x_k \rangle \\ &\leq \frac{1}{2} \|x_k - x^*\|_2^2 - \alpha_k (f(x_k) - f(x^*)) + \frac{\alpha_k^2}{2} \|g_k\|_2^2 + \alpha_k \langle \xi_k, x^* - x_k \rangle \end{aligned}$$



$$\mathbb{E}[\langle \xi_k, x^* - x_k \rangle] = \mathbb{E}[\mathbb{E}[\langle \xi_k, x^* - x_k \rangle | x_k]] = 0.$$



$$\alpha_k \mathbb{E}(f(x_k) - f(x^*)) \leq \frac{1}{2} \mathbb{E} \|x_k - x^*\|_2^2 - \frac{1}{2} \mathbb{E} \|x_{k+1} - x^*\|_2^2 + \frac{\alpha_k^2}{2} M^2$$

Convergence guarantees

Corollary

Let $A_k = \sum_{i=1}^k \alpha_i$ and define $\bar{x}_K = \frac{1}{A_K} \sum_{k=1}^K \alpha_k x_k$

$$\mathbb{E}[f(\bar{x}_K) - f(x^*)] \leq \frac{R^2 + \sum_{k=1}^K \alpha_k^2 M^2}{2 \sum_{k=1}^K \alpha_k}. \quad (25)$$

- Convergence: $\sum_{k=1}^{\infty} \alpha_k = \infty$ and $\frac{\sum_{k=1}^K \alpha_k^2}{\sum_{k=1}^K \alpha_k} \rightarrow 0$
- a fixed stepsize $\alpha_k = \alpha$:

$$\mathbb{E}(f(\bar{x}_K) - f(x^*)) \leq \frac{R^2}{2K\alpha} + \frac{\alpha M^2}{2}$$

- Take $\alpha = \frac{R}{M\sqrt{K}}$:

$$\mathbb{E}(f(\bar{x}_K) - f(x^*)) \leq \frac{RM}{\sqrt{K}}$$

Theorem 5: Convergence of stochastic subgradient method

Let $\alpha_k > 0$ be non-increasing sequence of stepsizes and the preceding assumptions hold. Let $\bar{x} = \frac{1}{K} \sum_{k=1}^K x_k$. Then,

$$\mathbb{E}[f(\bar{x}_K) - f(x^*)] \leq \frac{R^2}{2K\alpha_K} + \frac{1}{2K} \sum_{k=1}^K \alpha_k M^2. \quad (26)$$



$$\alpha_k \mathbb{E}(f(x_k) - f(x^*)) \leq \frac{1}{2} \mathbb{E} \|x_k - x^*\|_2^2 - \frac{1}{2} \mathbb{E} \|x_{k+1} - x^*\|_2^2 + \frac{\alpha_k^2}{2} M^2$$



$$\mathbb{E}(f(x_k) - f(x^*)) \leq \frac{1}{2\alpha_k} \mathbb{E} \|x_k - x^*\|_2^2 - \frac{1}{2\alpha_k} \mathbb{E} \|x_{k+1} - x^*\|_2^2 + \frac{\alpha_k}{2} M^2$$

Corollary

Let the conditions of Theorem 5 hold, and let $\alpha_k = \frac{R}{M\sqrt{k}}$ for each k . Then,

$$\mathbb{E}[f(\bar{x}_K) - f(x^*)] \leq \frac{3RM}{2\sqrt{K}}. \quad (27)$$

- proof

$$\sum_{k=1}^K \frac{1}{\sqrt{k}} \leq \int_0^K \frac{1}{\sqrt{t}} dt = 2\sqrt{K}.$$

Corollary

Let α_k be chosen such that $\mathbb{E}[f(\bar{x}_K) - f(x^*)] \rightarrow 0$. Then $f(\bar{x}_K) - f(x^*) \xrightarrow{P} 0$ as $K \rightarrow \infty$, that is, for all $\epsilon > 0$ we have

$$\limsup_{k \rightarrow \infty} \mathbb{P}(f(\bar{x}_K) - f(x^*) \geq \epsilon) = 0. \quad (28)$$

- By markov inequality: $P(X \geq \alpha) \leq \frac{EX}{\alpha}$ if $X \geq 0$ and $\alpha > 0$

$$P(f(\bar{x}_K) - f(x^*) \geq \epsilon) \leq \frac{1}{\epsilon} \mathbb{E}[f(\bar{x}_K) - f(x^*)] \rightarrow 0$$

Theorem 6: Convergence of stochastic subgradient method

In addition to the conditions of Theorem 5, assume that $\|g\|_2 \leq M$ for all stochastic subgradients g , Then for anything $\epsilon > 0$,

$$f(\bar{x}_K) - f(x^*) \leq \frac{R^2}{2K\alpha_K} + \frac{1}{2K} \sum_{k=1}^K \alpha_k M^2 + \frac{RM}{\sqrt{K}} \epsilon. \quad (29)$$

with probability at least $1 - e^{-\frac{1}{2}\epsilon^2}$

- Taking $\alpha_k = \frac{R}{\sqrt{kM}}$ and setting $\delta = e^{-\frac{1}{2}\epsilon^2}$

$$f(\bar{x}_K) - f(x^*) \leq \frac{3RM}{2\sqrt{K}} + \frac{RM\sqrt{2 \log \frac{1}{\delta}}}{\sqrt{K}}.$$

with probability at least $1 - \delta$

Azuma-Hoeffding Inequality

- **martingale:** A sequence X_1, X_2, \dots of random vectors is a martingale if there is a sequence of random vectors Z_1, Z_2, \dots such that for each n ,
 - X_n is a function of Z_n ,
 - Z_{n-1} is a function of Z_n ,
 - we have the conditional expectation condition

$$\mathbb{E}[X_n | Z_{n-1}] = X_{n-1}.$$

- **martingale difference sequence** X_1, X_2, \dots is a martingale difference sequence if $S_n = \sum_{i=1}^n X_i$ is a martingale or, equivalently

$$\mathbb{E}[X_n | Z_{n-1}] = 0.$$

- **example** X_1, X_2, \dots independent and $E(X_i) = 0$, $Z_i = (X_1, \dots, X_i)$.

Azuma-Hoeffding Inequality

Let X_1, X_2, \dots be a martingale difference sequence with $|X_i| \leq B$ for all $i = 1, 2, \dots$. Then

$$\mathbb{P}\left(\sum_{i=1}^n X_i \geq t\right) \leq \exp\left(-\frac{2t^2}{nB^2}\right) \quad (30)$$

$$\mathbb{P}\left(\sum_{i=1}^n X_i \leq -t\right) \leq \exp\left(-\frac{2t^2}{nB^2}\right) \quad (31)$$

- Let $\delta = \frac{t}{n}$

$$\mathbb{P}\left(\frac{1}{n} \sum_{i=1}^m X_i \geq \delta\right) \leq \exp\left(-\frac{2n\delta^2}{B^2}\right)$$

- X_1, X_2, \dots i.i.d, $EX_i = \mu$

$$\mathbb{P}\left(\left|\frac{1}{n} \sum_{i=1}^m X_i - \mu\right| \geq \delta\right) \leq 2 \exp\left(-\frac{2n\delta^2}{B^2}\right)$$

Azuma-Hoeffding Inequality

Theorem 5: Convergence of stochastic subgradient method

Let $\alpha_k > 0$ be non-increasing sequence of stepsizes and the preceding assumptions hold. Let $\bar{x} = \frac{1}{K} \sum_{k=1}^K x_k$. Then,

$$\mathbb{E}[f(\bar{x}_K) - f(x^*)] \leq \frac{R^2}{2K\alpha_K} + \frac{1}{2K} \sum_{k=1}^K \alpha_k M^2. \quad (32)$$

Theorem 6: Convergence of stochastic subgradient method

In addition to the conditions of Theorem 5, assume that $\|g\|_2 \leq M$ for all stochastic subgradients g , Then for anything $\epsilon > 0$,

$$f(\bar{x}_K) - f(x^*) \leq \frac{R^2}{2K\alpha_K} + \frac{1}{2K} \sum_{k=1}^K \alpha_k M^2 + \frac{RM}{\sqrt{K}} \epsilon. \quad (33)$$

with probability at least $1 - e^{-\frac{1}{2}\epsilon^2}$

Proof of Theorem 6

- Let $f'(x_k) = E[g_k|x_k]$ and $\xi_k = g_k - f'(x_k)$,

$$\begin{aligned} \frac{1}{2} \|x_{k+1} - x^*\|_2^2 &= \frac{1}{2} \|x_k - \alpha_k g_k - x^*\|_2^2 \\ &= \frac{1}{2} \|x_k - x^*\|_2^2 + \alpha_k \langle g_k, x^* - x_k \rangle + \frac{\alpha_k^2}{2} \|g_k\|_2^2 \\ &= \frac{1}{2} \|x_k - x^*\|_2^2 + \alpha_k \langle f'(x_k), x^* - x_k \rangle + \frac{\alpha_k^2}{2} \|g_k\|_2^2 + \alpha_k \langle \xi_k, x^* - x_k \rangle \\ &\leq \frac{1}{2} \|x_k - x^*\|_2^2 - \alpha_k (f(x_k) - f(x^*)) + \frac{\alpha_k^2}{2} \|g_k\|_2^2 + \alpha_k \langle \xi_k, x^* - x_k \rangle \end{aligned}$$



$$f(x_k) - f(x^*) \leq \frac{1}{2\alpha_k} \|x_k - x^*\|_2^2 - \frac{1}{2\alpha_k} \|x_{k+1} - x^*\|_2^2 + \frac{\alpha_k}{2} \|g_k\|_2^2 + \langle \xi_k, x^* - x_k \rangle$$

Proof of Theorem 6



$$\begin{aligned} f(\bar{x}_K) - f(x) &\leq \frac{1}{K} \sum_{k=1}^K f(x_k) - f(x^*) \\ &\leq \frac{1}{2K\alpha_K} \|x_1 - x^*\|_2^2 + \frac{1}{2K} \sum_{k=1}^K \alpha_k \|g_k\|_2^2 + \frac{1}{K} \sum_{i=1}^K \langle \xi_k, x^* - x_k \rangle \\ &\leq \frac{1}{2K\alpha_K} \|x_1 - x^*\|_2^2 + \frac{1}{2K} \sum_{k=1}^K \alpha_k M^2 + \frac{1}{K} \sum_{i=1}^K \langle \xi_k, x^* - x_k \rangle \end{aligned}$$

• Let $\omega = \frac{1}{2K\alpha_K} \|x_1 - x^*\|_2^2 + \frac{1}{2K} \sum_{k=1}^K \alpha_k M^2$

$$\mathbb{P}(f(\bar{x}_K) - f(x) - \omega \geq t) \leq \mathbb{P}\left(\frac{1}{K} \sum_{i=1}^K \langle \xi_k, x^* - x_k \rangle \geq t\right),$$

Proof of Theorem 6

- $\langle \xi_k, x^* - x_k \rangle$ is a bounded difference martingale sequence

- $Z_k = (x_1, \dots, x_{k+1})$

- Since $\mathbb{E}[\xi_k | Z_{k-1}] = 0$ and $\mathbb{E}[x_k | Z_{k-1}] = x_k$.

$$\mathbb{E} \langle \xi_k, x^* - x_k \rangle = 0.$$

- Since $\|\xi_k\|_2 = \|g_k - f'(x_k)\| \leq 2M$

$$|\langle \xi_k, x^* - x_k \rangle| \leq \|\xi_k\|_2 \|x^* - x_k\|_2 \leq 2MR$$

- By Azuma-Hoeffding Inequality,

$$\mathbb{P}\left(\sum_{i=1}^K \langle \xi_k, x^* - x_k \rangle \geq t\right) \leq \exp\left(-\frac{t^2}{2KM^2R^2}\right).$$

- Substituting $t = MR\sqrt{K}\epsilon$

$$\mathbb{P}\left(\frac{1}{K} \sum_{i=1}^K \langle \xi_k, x^* - x_k \rangle \geq \frac{MR\epsilon}{\sqrt{K}}\right) \leq \exp\left(-\frac{\epsilon^2}{2}\right).$$

Adaptive stepsizes

- choose an appropriate metric and associated distance-generating function h .
- it may be advantageous to adapt the metric being used, or at least the stepsizes, to achieve faster convergence guarantees.
- a simple scheme

$$h(x) = \frac{1}{2}x^T Ax$$

where A may change depending on information observed during solution of the problem.

Adaptive stepsizes

- Recall the bounds

$$\mathbb{E}[f(\bar{x}_K) - f(x^*)] \leq \mathbb{E}\left[\frac{R^2}{K\alpha_k} + \frac{1}{2K} \sum_{k=1}^K \alpha_k \|g_k\|^2\right]. \quad (34)$$

- Taking $\alpha_k = R/\sqrt{\sum_{i=1}^k \|g\|^2}$,

$$\mathbb{E}[f(\bar{x}_K) - f(x^*)] \leq 2\frac{R}{K}\mathbb{E}\left[\left(\sum_{k=1}^K \|g_k\|^2\right)^{\frac{1}{2}}\right]. \quad (35)$$

- if $\mathbb{E}[\|g_k\|^2] \leq M^2$ for all k , then

$$\mathbb{E}\left[\left(\sum_{k=1}^K \|g_k\|^2\right)^{\frac{1}{2}}\right] \leq \left[\mathbb{E}\left[\sum_{k=1}^K \|g_k\|^2\right]\right]^{\frac{1}{2}} \leq \sqrt{M^2 K} = M\sqrt{K} \quad (36)$$

- **Variable metric methods**

$$x_{k+1} = \arg \min_{x \in C} \left\{ \langle g_k, x \rangle + \frac{1}{2} \langle x - x_k, H_k(x - x_k) \rangle \right\}$$

- **Projected subgradient method:** $H_k = \alpha_k I$,

- **Newton method:** $H_k = \nabla^2 f(x_k)$,

- **AdaGrad:** $H_k = \frac{1}{\alpha} \text{diag}(\sum_{i=1}^k g_i \cdot * g_i)^{\frac{1}{2}}$

Variable metric methods

Theorem 9: Convergence of Variable metric methods

Let $H_k > 0$ be a sequence of positive definite matrices, where H_k is a function of g_1, \dots, g_k . Let g_k be stochastic subgradient with $\mathbb{E}[g_k | x_k] \in \partial f(x_k)$. Then

$$\begin{aligned} \mathbb{E}\left[\sum_{k=1}^K (f(x_k) - f(x^*))\right] &\leq \frac{1}{2} \mathbb{E}\left[\sum_{k=2}^K (\|x_k - x^*\|_{H_k}^2 - \|x_k - x^*\|_{H_{k-1}}^2)\right] \\ &\quad + \frac{1}{2} \mathbb{E}\left[\|x_1 - x^*\|_{H_1}^2 + \sum_{k=1}^K \|g_k\|_{H_k}^2\right]. \end{aligned}$$

$$\mathbb{E}[f(x_k) - f(x^*)] \leq \frac{1}{2} \mathbb{E}[\|x_k - x^*\|_{H_k}^2 - \|x_{k+1} - x^*\|_{H_k}^2 + \|g_k\|_{H_k}^2]$$

Proof of Theorem 9

- By non-expansiveness of $\pi_C(x)$ under $\|x\|_{H_k}^2 = \langle x, H_k x \rangle$

$$\|x_{k+1} - x^*\|_{H_k}^2 \leq \|x_k - H_k^{-1}g_k - x^*\|_{H_k}^2$$

- Define $\xi_k = g_k - f'(x_k)$

$$\begin{aligned} & \frac{1}{2} \|x_{k+1} - x^*\|_{H_k}^2 \\ & \leq \frac{1}{2} \|x_k - x^*\|_{H_k}^2 + \langle g_k, x^* - x_k \rangle + \frac{1}{2} \|g_k\|_{H_k^{-1}}^2 \\ & = \frac{1}{2} \|x_k - x^*\|_{H_k}^2 + \langle f'(x_k), x^* - x_k \rangle + \frac{1}{2} \|g_k\|_{H_k^{-1}}^2 + \langle \xi_k, x^* - x_k \rangle \\ & \leq \frac{1}{2} \|x_k - x^*\|_{H_k}^2 - (f(x_k) - f(x^*)) + \frac{1}{2} \|g_k\|_{H_k^{-1}}^2 + \langle \xi_k, x^* - x_k \rangle \end{aligned}$$



$$\mathbb{E}[f(x_k) - f(x^*)] \leq \frac{1}{2} \mathbb{E}[\|x_k - x^*\|_{H_k}^2 - \|x_{k+1} - x^*\|_{H_k}^2 + \|g_k\|_{H_k^{-1}}^2]$$

Variable metric methods

Assume $H_k = H$ for all k . Then

$$\mathbb{E} \left[\sum_{k=1}^K (f(x_k) - f(x^*)) \right] \leq \frac{1}{2} \mathbb{E} \left[\|x_1 - x^*\|_{H_1}^2 + \sum_{k=1}^K \|g_k\|_{H^{-1}}^2 \right]$$

Minimize the error by considering:

$$\begin{aligned} \min \quad & \sum_{t=1}^K \|g_t\|_{H^{-1}}^2 \\ \text{s.t.} \quad & H \succeq 0 \\ & \text{tr}(H) \leq c \end{aligned} \quad H = \begin{pmatrix} s_1 & 0 & \cdots & 0 \\ 0 & s_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & s_d \end{pmatrix}$$

It is equivalent to

$$\min_s \sum_{i=1}^d \frac{\sum_{t=1}^K g_{t,i}^2}{s_i}, \quad \text{s.t.} \quad \mathbf{1}^\top s \leq c, \quad s \geq 0.$$

Variable metric methods

The Lagrangian function of the problem is:

$$L(s, \lambda, \theta) = \sum_{i=1}^d \frac{\|g_{1:K,i}\|_2^2}{s_i} - \lambda^\top s + \theta(1^\top s - c).$$

The complementarity condition gives $\lambda_i s_i = 0$. Then we obtain

$$\frac{\partial L}{\partial s_i} = -\frac{\|g_{1:K,i}\|_2^2}{s_i^2} - \lambda_i + \theta = 0,$$

which yields: $0 = -\|g_{1:K,i}\|_2^2 - \lambda_i s_i^2 + \theta s_i^2 = -\|g_{1:K,i}\|_2^2 + \theta s_i^2$. Hence, we have

$$s_i = \frac{c \|g_{1:K,i}\|_2}{\sum_{i=1}^d \|g_{1:K,i}\|_2}$$

Taking $c = \sum_{i=1}^d \|g_{1:K,i}\|_2$ gives $s_i = \|g_{1:K,i}\|_2$.

Variable metric methods

Corollary: Convergence of AdaGrad

Let $R_\infty = \sup_{x \in C} \|x - x^*\|_\infty$ and let the conditions of Theorem 9 hold. Then we have

$$\mathbb{E}\left[\sum_{k=1}^K (f(x_k) - f(x^*))\right] \leq \frac{1}{2\alpha} R_\infty^2 \mathbb{E}[\text{tr}(M_K)] + \alpha \mathbb{E}[\text{tr}(M_K)]$$

where $M_k = \text{diag}(\sum_{i=1}^k g_{i \cdot} * g_{i \cdot})^{\frac{1}{2}}$ and $H_k = \frac{1}{\alpha} M_k$

- Let $\alpha = R_\infty$, Then

$$\mathbb{E}[f(\bar{x}_K) - f(x^*)] \leq \frac{3}{2K} R_\infty \mathbb{E}[\text{tr}(M_K)] = \frac{3}{2K} R_\infty \sum_{j=1}^n \mathbb{E}\left[\left(\sum_{k=1}^K g_{k,j}^2\right)^{\frac{1}{2}}\right] \quad (37)$$

- If $C = \{x : \|x\| \leq 1\}$, the bound is lower than the one of adaptive stepsize.

Proof of Corolory

- Aim: $\|x_k - x^*\|_{H_k}^2 - \|x_k - x^*\|_{H_{k-1}}^2 \leq \|x_k - x^*\|_\infty^2 \text{tr}(H_k - H_{k-1})$
Let $z = x - x^*$

$$\begin{aligned} & \|z\|_{H_k}^2 - \|z\|_{H_{k-1}}^2 \\ &= \sum_{j=1}^n H_{k,j} z_j^2 - \sum_{j=1}^n H_{k-1,j} z_j^2 \\ &= \sum_{j=1}^n (H_{k,j} - H_{k-1,j}) z_j^2 \\ &\leq \|z\|_\infty^2 \sum_{j=1}^n (H_{k,j} - H_{k-1,j}) \\ &= \|z\|_\infty^2 \text{tr}(H_k - H_{k-1}) \end{aligned}$$

Proof of Corolory

- Assume $a = (a_1, a_2, \dots, a_T)$, a simple inequality(prove by induction),

$$\sum_{t=1}^T \frac{a_t^2}{\sqrt{a_1^2 + \dots + a_t^2}} \leq 2\sqrt{a_1^2 + \dots + a_T^2}$$

- Aim: $\sum_{k=1}^K \|g_k\|_{H_k^{-1}} \leq 2\alpha \text{tr}(M_K)$.

$$\begin{aligned} & \sum_{k=1}^K \|g_k\|_{H_k^{-1}}^2 \\ &= \alpha \sum_{k=1}^K \sum_{j=1}^n \frac{g_{k,j}^2}{M_{k,j}} = \alpha \sum_{j=1}^n \sum_{k=1}^K \frac{g_{k,j}^2}{\sqrt{\sum_{i=1}^k g_{i,j}^2}} \\ &\leq 2\alpha \sum_{j=1}^n \sqrt{\sum_{i=1}^K g_{i,j}^2} = 2\alpha \text{tr}(M_K) \end{aligned} \tag{38}$$

Summary

- expectation

$$\mathbb{E}[f(\bar{x}_K) - f(x^*)] \leq \frac{3RM}{2\sqrt{K}}$$

- convergence in probability

$$f(\bar{x}_K) - f(x^*) \leq \frac{3RM}{2\sqrt{K}} + \frac{RM\sqrt{2\log\frac{1}{\delta}}}{\sqrt{K}}.$$

with probability at least $1 - \delta$

- Using proper metric and adapted strategy can improve the convergence: Mirror Descent method and Adagrad.

Outline

- 1 Problem Description
- 2 Subgradient Methods
 - The gradient and subgradient methods
 - Stochastic subgradient methods
- 3 Stochastic Gradient Descent**
 - Gradient Descent**
 - Stochastic Gradient methods**
- 4 Variance Reduction
 - SAG method and SAGA method
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Gradient methods

- Rewrite the ERM problem

$$\min_{x \in \mathbb{R}^n} f(x) := \frac{1}{n} \sum_{i=1}^n f_i(x) \quad (39)$$

- **gradient methods**

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k) \quad (40)$$

- the update is equal to

$$x_{k+1} = \arg \min_x f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2\alpha_k} \|x - x_k\|_2^2 \quad (41)$$

Basic Properties

- We only consider the convex differentiable functions.
- **convex functions:**

$$f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y), \forall \lambda \in [0, 1], x, y$$

- **M -Lipschitz functions:**

$$|f(x) - f(y)| \leq M\|x - y\|_2$$

- **L -smooth functions:**

$$\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|_2$$

- **μ -strongly convex functions:**

$$f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y) - \frac{\mu}{2}\lambda(1 - \lambda)\|x - y\|_2^2, \forall \lambda \in [0, 1], x, y$$

Some useful results

- **convex functions:**

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle$$

- **M -Lipschitz functions:**

$$\|\nabla f(x)\|_2 \leq M$$

- **L -smooth functions:** $\frac{L}{2}x^T x - f(x)$ is convex

$$f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2}\|x - y\|_2^2$$

$$\frac{1}{2L}\|\nabla f(x)\|_2^2 \leq f(x) - f(x^*) \leq \frac{L}{2}\|x - x^*\|_2^2$$

- **μ -strongly convex functions:** $f(x) - \frac{\mu}{2}x^T x$ is convex

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2}\|x - y\|_2^2$$

Co-coercivity of gradient

if f is convex with $\text{dom } f = \mathbf{R}^n$ and $(L/2)x^\top x - f(x)$ is convex then

$$(\nabla f(x) - \nabla f(y))^\top (x - y) \geq \frac{1}{L} \|\nabla f(x) - \nabla f(y)\|_2^2 \quad \forall x, y$$

proof: define convex functions f_x, f_y with domain \mathbf{R}^n :

$$f_x(z) = f(z) - \nabla f(x)^\top z, \quad f_y(z) = f(z) - \nabla f(y)^\top z$$

the functions $(L/2)z^\top z - f_x(z)$ and $(L/2)z^\top z - f_y(z)$ are convex

- $z = x$ minimizes $f_x(z)$; from the left-hand inequality,

$$\begin{aligned} f(y) - f(x) - \nabla f(x)^\top (y - x) &= f_x(y) - f_x(x) \\ &\geq \frac{1}{2L} \|\nabla f_x(y)\|_2^2 = \frac{1}{2L} \|\nabla f(y) - \nabla f(x)\|_2^2 \end{aligned}$$

- similarly, $z = y$ minimizes $f_y(z)$; therefore

$$f(x) - f(y) - \nabla f(y)^\top (x - y) \geq \frac{1}{2L} \|\nabla f(y) - \nabla f(x)\|_2^2$$

combining the two inequalities shows co-coercivity

Extension of co-coercivity

if f is strongly convex and ∇f is Lipschitz continuous, then

$$g(x) = f(x) - \frac{\mu}{2} \|x\|_2^2$$

is convex and ∇g is Lipschitz continuous with parameter $L - \mu$.

co-coercivity of g gives

$$\begin{aligned} & (\nabla f(x) - \nabla f(y))^\top (x - y) \\ & \geq \frac{\mu L}{\mu + L} \|x - y\|_2^2 + \frac{1}{\mu + L} \|\nabla f(x) - \nabla f(y)\|_2^2 \end{aligned}$$

for all $x, y \in \mathbf{dom} f$

Convergence guarantees

Assumption

- f is L -smooth and μ -strongly convex.

lemma: Coercivity of gradients

$$\langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \frac{L\mu}{L + \mu} \|x - y\|^2 + \frac{1}{L + \mu} \|\nabla f(x) - \nabla f(y)\|^2 \quad (42)$$

Theorem: Convergence rates of GD

Let $\alpha_k = \frac{2}{L + \mu}$ and let $\kappa = \frac{L}{\mu}$. Define $\Delta_k = \|x_k - x^*\|$. Then we get,

$$f(x_{T+1}) - f(x^*) \leq \frac{L\Delta_1^2}{2} \exp\left(-\frac{4T}{\kappa + 1}\right). \quad (43)$$

Proof of Theorem



$$\begin{aligned}\Delta_{k+1}^2 &= \|x_{k+1} - x^*\|_2^2 = \|x_k - \alpha_k \nabla f(x_k) - x^*\|_2^2 \\ &= \|x_k - x^*\|_2^2 - 2\alpha_k \langle \nabla f(x_k), x_k - x^* \rangle + \alpha_k^2 \|\nabla f(x_k)\|_2^2 \\ &= \Delta_k^2 - 2\alpha_k \langle \nabla f(x_k), x_k - x^* \rangle + \alpha_k^2 \|\nabla f(x_k)\|_2^2\end{aligned}$$

• By the lemma

$$\begin{aligned}\Delta_{k+1}^2 &\leq \Delta_k^2 - 2\alpha_k \left(\frac{L\mu}{L+\mu} \Delta_k^2 + \frac{1}{L+\mu} \|\nabla f(x_k)\|_2^2 \right) + \alpha_k^2 \|\nabla f(x_k)\|_2^2 \\ &= \left(1 - 2\alpha_k \frac{L\mu}{L+\mu} \right) \Delta_k^2 + \left(-\frac{2\alpha_k}{L+\mu} + \alpha_k^2 \right) \|\nabla f(x_k)\|_2^2 \\ &\leq \left(1 - 2\alpha_k \frac{L\mu}{L+\mu} \right) \Delta_k^2 + \left(-\frac{2\alpha_k}{L+\mu} + \alpha_k^2 \right) L^2 \Delta_k^2\end{aligned}\tag{44}$$

Proof of Theorem

- $\alpha_k = \frac{2}{L+\mu}$

$$\begin{aligned}\Delta_{k+1}^2 &\leq \left(1 - \frac{4L\mu}{(L+\mu)^2}\right)\Delta_k^2 \\ &= \left(\frac{L-\mu}{L+\mu}\right)^2\Delta_k^2 = \left(\frac{\kappa-1}{\kappa+1}\right)^2\Delta_k^2\end{aligned}$$

-

$$\begin{aligned}\Delta_{T+1}^2 &\leq \left(\frac{\kappa-1}{\kappa+1}\right)^{2T}\Delta_1^2 \\ &= \Delta_1^2 \exp\left(2T \log\left(1 - \frac{2}{\kappa+1}\right)\right) \\ &\leq \Delta_1^2 \exp\left(-\frac{4T}{\kappa+1}\right)\end{aligned}$$

-

$$f(x_{T+1}) - f(x^*) \leq \frac{L}{2}\Delta_{T+1}^2 \leq \frac{L\Delta_1^2}{2} \exp\left(-\frac{4T}{\kappa+1}\right)$$

Stochastic Gradient methods

- ERM problem

$$\min_{x \in \mathbb{R}^n} f(x) := \frac{1}{n} \sum_{i=1}^n f_i(x) \quad (45)$$

- gradient descent**

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k) \quad (46)$$

- stochastic gradient descent**

$$x_{k+1} = x_k - \alpha_k \nabla f_{s_k}(x_k), \quad (47)$$

where s_k is uniformly sampled from $\{1, \dots, n\}$

Convergence guarantees

Assumption

- $f(x)$ is L -smooth: $\|\nabla f(x) - \nabla f(y)\|_2^2 \leq L\|x - y\|_2^2$
- $f(x)$ is μ -strongly convex: $\langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu\|x - y\|_2^2$
- $\mathbb{E}_s[\nabla f_s(x)] = \nabla f(x)$
- $\mathbb{E}_s\|\nabla f_s(x)\|^2 \leq M^2$

Theorem: Convergence rates of SGD

Define $\Delta_k = \|x_k - x^*\|$. For a fixed Stepsize $\alpha_k = \alpha$, $0 < \alpha < \frac{1}{2\mu}$ we have,

$$\mathbb{E}[f(x_{T+1}) - f(x^*)] \leq \frac{L}{2}\mathbb{E}[\Delta_{T+1}^2] \leq \frac{L}{2}[(1 - 2\alpha\mu)^T \Delta_1^2 + \frac{\alpha M^2}{2\mu}]. \quad (48)$$

Proof of Theorem



$$\begin{aligned}\Delta_{k+1}^2 &= \|x_{k+1} - x^*\|_2^2 = \|x_k - \alpha_k \nabla f_{s_k}(x_k) - x^*\|_2^2 \\ &= \|x_k - x^*\|_2^2 - 2\alpha_k \langle \nabla f_{s_k}(x_k), x_k - x^* \rangle + \alpha_k^2 \|\nabla f_{s_k}(x_k)\|_2^2 \\ &= \Delta_k^2 - 2\alpha_k \langle \nabla f_{s_k}(x_k), x_k - x^* \rangle + \alpha_k^2 \|\nabla f_{s_k}(x_k)\|_2^2\end{aligned}$$

- Using $E[X] = E[E[X|Y]]$:

$$\begin{aligned}\mathbb{E}_{s_1, \dots, s_k} [\langle \nabla f_{s_k}(x_k), x_k - x^* \rangle] &= \mathbb{E}_{s_1, \dots, s_{k-1}} [\mathbb{E}_{s_k} [\langle \nabla f_{s_k}(x_k), x_k - x^* \rangle]] \\ &= \mathbb{E}_{s_1, \dots, s_{k-1}} [\langle \mathbb{E}_{s_k} [\nabla f_{s_k}(x_k)], x_k - x^* \rangle] \\ &= \mathbb{E}_{s_1, \dots, s_{k-1}} [\langle \nabla f(x_k), x_k - x^* \rangle] \\ &= \mathbb{E}_{s_1, \dots, s_k} [\langle \nabla f(x_k), x_k - x^* \rangle]\end{aligned}$$

- By the strongly convexity

$$\mathbb{E}_{s_1, \dots, s_k} (\Delta_{k+1}^2) \leq (1 - 2\alpha\mu) \mathbb{E}_{s_1, \dots, s_k} (\Delta_k^2) + \alpha^2 M^2 \quad (49)$$

Proof of Theorem

- Taking induction from $k = 1$ to $k = T$, we have

$$\mathbb{E}_{s_1, \dots, s_T}(\Delta_{T+1}^2) \leq (1 - 2\alpha\mu)^T \Delta_1^2 + \sum_{i=0}^{T-1} (1 - 2\alpha\mu)^i \alpha^2 M^2 \quad (50)$$

- under the assumption that $0 \leq 2\alpha\mu \leq 1$, we have

$$\sum_{i=0}^{\infty} (1 - 2\alpha\mu)^i = \frac{1}{2\alpha\mu}$$

- Then

$$\mathbb{E}_{s_1, \dots, s_T}(\Delta_{T+1}^2) \leq (1 - 2\alpha\mu)^T \Delta_1^2 + \frac{\alpha M^2}{2\mu} \quad (51)$$

Convergence guarantees

- For fixed stepsize, we don't have the convergence
- For diminishing stepsize, the order of convergence is $O(\frac{1}{T})$

Theorem: Convergence rates of SGD

Define $\Delta_k = \|x_k - x^*\|$. For a diminishing stepsize

$$\alpha_k = \frac{\beta}{k + \gamma} \text{ for some } \beta > \frac{1}{2\mu} \text{ and } \gamma > 0 \text{ such that } \alpha_1 \leq \frac{1}{2\mu}.$$

Then we have, for any $T \geq 1$

$$\mathbb{E}[f(x_T) - f(x^*)] \leq \frac{L}{2} \mathbb{E}[\Delta_T^2] \leq \frac{L}{2} \frac{v}{\gamma + T}, \quad (52)$$

where $v = \max(\frac{\beta^2 M^2}{2\beta\mu - 1}, (\gamma + 1)\Delta_1^2)$

Proof of Theorem

- Recall the bounds

$$\mathbb{E}_{s_1, \dots, s_k}(\Delta_{k+1}^2) \leq (1 - 2\alpha\mu)\mathbb{E}_{s_1, \dots, s_k}(\Delta_k^2) + \alpha^2 M^2 \quad (53)$$

- We prove it by induction. Firstly, the definition of v ensures that it holds for $k = 1$.
- Assume the conclusion holds for some k , it follows that

$$\begin{aligned} \mathbb{E}(\Delta_{k+1}^2) &\leq \left(1 - \frac{2\beta\mu}{\hat{k}}\right) \frac{v}{\hat{k}} + \frac{\beta^2 M^2}{\hat{k}^2} \quad (\text{with } \hat{k} := \gamma + k) \\ &= \left(\frac{\hat{k} - 2\beta\mu}{\hat{k}^2}\right) v + \frac{\beta^2 M^2}{\hat{k}^2} \\ &= \frac{\hat{k} - 1}{\hat{k}^2} v \boxed{-\frac{2\beta\mu - 1}{\hat{k}^2} v + \frac{\beta^2 M^2}{\hat{k}^2}} \\ &\leq \frac{v}{\hat{k} + 1} \end{aligned}$$

stochastic optimization

- stochastic subgradient descent: $O(1/\epsilon^2)$
- stochastic gradient descent with strong convexity $O(1/\epsilon)$
- stochastic gradient descent with strong convexity and smoothness $O(1/\epsilon)$

deterministic optimization

- subgradient descent: $O(n/\epsilon^2)$
- gradient descent with strong convexity $O(n/\epsilon)$
- gradient descent with strong convexity and smoothness $O(n \log(1/\epsilon))$

The complexity refers to the times of computation of component (sub)gradients. We need to compute n gradients in every iterations of GD and one gradient in SGD.

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Variance Reduction

Assumption

- $f(x)$ is L -smooth: $\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2$
- $f(x)$ is μ -strongly convex: $\langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu\|x - y\|_2^2$
- $\mathbb{E}_s[\nabla f_s(x)] = \nabla f(x)$
- $\mathbb{E}_s\|\nabla f_s(x)\|^2 \leq M^2$
- GD: linear convergence $O(n \log(1/\epsilon))$
- SGD: sublinear convergence $O(1/\epsilon)$

What is the essential difference between SGD and GD?

Variance Reduction

- **GD**

$$\begin{aligned}\Delta_{k+1}^2 &= \|x_{k+1} - x^*\|_2^2 = \|x_k - \alpha \nabla f(x_k) - x^*\|_2^2 \\ &= \Delta_k^2 - 2\alpha \langle \nabla f(x_k), x_k - x^* \rangle + \alpha^2 \|\nabla f(x_k)\|_2^2 \\ &\leq (1 - 2\alpha\mu)\Delta_k^2 + \alpha^2 \|\nabla f(x_k)\|_2^2 \quad (\mu - \text{strongly convex}) \\ &\leq (1 - 2\alpha\mu + \alpha^2 L^2)\Delta_k^2 \quad (L - \text{smooth})\end{aligned}$$

- **SGD**

$$\begin{aligned}\mathbb{E}\Delta_{k+1}^2 &= \mathbb{E}\|x_{k+1} - x^*\|_2^2 = \mathbb{E}\|x_k - \alpha \nabla f_{s_k}(x_k) - x^*\|_2^2 \\ &= \mathbb{E}\Delta_k^2 - 2\alpha \mathbb{E} \langle \nabla f_{s_k}(x_k), x_k - x^* \rangle + \alpha^2 \mathbb{E}\|\nabla f_{s_k}(x_k)\|_2^2 \\ &= \mathbb{E}\Delta_k^2 - 2\alpha \mathbb{E} \langle \nabla f(x_k), x_k - x^* \rangle + \alpha^2 \mathbb{E}\|\nabla f_{s_k}(x_k)\|_2^2 \\ &\leq (1 - 2\alpha\mu)\mathbb{E}\Delta_k^2 + \alpha^2 \mathbb{E}\|\nabla f_{s_k}(x_k)\|_2^2 \quad (\mu - \text{strongly convex}) \\ &\leq (1 - 2\alpha\mu)\mathbb{E}\Delta_k^2 + \alpha^2 \mathbb{E}\|\nabla f_{s_k}(x_k) - \nabla f(x_k) + \nabla f(x_k)\|_2^2 \\ &\leq (1 - 2\alpha\mu + 2\alpha^2 L^2)\mathbb{E}\Delta_k^2 + \boxed{2\alpha^2 \mathbb{E}\|\nabla f_{s_k}(x_k) - \nabla f(x_k)\|_2^2}\end{aligned}$$

Variance Reduction

$$\mathbb{E}\Delta_{k+1}^2 \leq \underbrace{(1 - 2\alpha\mu + 2\alpha^2L^2)\mathbb{E}\Delta_k^2}_A + \underbrace{2\alpha^2\mathbb{E}\|\nabla f_{s_k}(x_k) - \nabla f(x_k)\|_2^2}_B \quad (54)$$

- a worst case convergence rate of $\sim 1/T$ for SGD
- In practice, the actual convergence rate may be somewhat better than this bound.
- Initially, $B \ll A$ and we observe the linear rate regime, once $B > A$ we observe $1/T$ rate.
- How to reduce variance term B to speed up SGD?
 - SAG (Stochastic average gradient)
 - SAGA
 - SVRG (Stochastic variance reduced gradient)

SAG method

- SAG method (Le Roux, Schmidt, Bach 2012)

$$x_{k+1} = x_k - \frac{\alpha_k}{n} \sum_{i=1}^n g_k^i = x_k - \alpha_k \left(\frac{1}{n} (\nabla f_{s_k}(x_k) - g_{k-1}^{s_k}) + \frac{1}{n} \sum_{i=1}^n g_{k-1}^i \right) \quad (55)$$

where

$$g_k^i = \begin{cases} \nabla f_i(x_k) & \text{if } i = s_k, \\ \nabla g_{k-1}^i & \text{o.w.}, \end{cases} \quad (56)$$

and s_k is uniformly sampled from $\{1, \dots, n\}$

- complexity (# component gradient evaluations):
 $O(\max\{n, \frac{L}{\mu}\} \log(1/\epsilon))$
- need to store most recent gradient of each component.
- SAGA(Defazio, Bach, Julien 2014) is unbiased revision of SAG

$$x_{k+1} = x_k - \alpha_k (\nabla f_{i_k}(x_k) - g_{k-1}^{i_k} + \frac{1}{n} \sum_{i=1}^n g_{k-1}^i) \quad (57)$$

SVRG method

- SVRG method (Johnson and Zhang 2013)

$$\begin{aligned}v_k &= \nabla f_{s_k}(x_k) - \nabla f_{s_k}(y) + \nabla f(y) \\x_{k+1} &= x_k - \alpha_k v_k\end{aligned}$$

where and s_k is uniformly sampled from $\{1, \dots, n\}$

- v_k is unbiased estimation of gradient $\nabla f(x_k)$

$$\mathbb{E}v_k = \nabla f(x_k) + \nabla f(y) - \nabla f(y) = \nabla f(x_k). \quad (58)$$

- Recall the bound

$$\mathbb{E}\Delta_{k+1}^2 \leq (1 - 2\alpha\mu)\mathbb{E}\Delta_k^2 + \alpha^2\mathbb{E}\|v_k\|_2^2 \quad (59)$$

SVRG method

- Additional assumption: L – smoothness for component functions

$$\|\nabla f_i(x) - \nabla f_i(y)\|_2 \leq L\|x - y\|_2 \quad (60)$$

- Let's analyze the "variance"

$$\begin{aligned} & \mathbb{E}\|v_k\|_2^2 \\ = & \mathbb{E}\|\nabla f_{s_k}(x_k) - \nabla f_{s_k}(y) + \nabla f(y)\|_2^2 \\ = & \mathbb{E}\|\nabla f_{s_k}(x_k) - \nabla f_{s_k}(y) + \nabla f(y) + \nabla f_{s_k}(x^*) - \nabla f_{s_k}(x^*)\|_2^2 \\ \leq & 2\mathbb{E}\|\nabla f_{s_k}(x_k) - \nabla f_{s_k}(x^*)\|_2^2 + 2\mathbb{E}\|\nabla f_{s_k}(y) - \nabla f(y) - \nabla f_{s_k}(x^*)\|_2^2 \\ \leq & 2L^2\mathbb{E}\Delta_k^2 + 2\mathbb{E}\|\nabla f_{s_k}(y) - \nabla f_{s_k}(x^*)\|_2^2 \\ \leq & 2L^2\mathbb{E}\Delta_k^2 + 2L^2\mathbb{E}\|y - x^*\|^2 \end{aligned}$$

- if x_k and y is close to x^* , the variance is small.

SVRG method

- We only need to choose a current point as y .
- picking a fresh y more often should decrease the variance, however doing this too often involves computing too many full gradients
- Let's set $y = x_1$,

$$\mathbb{E}\Delta_{k+1}^2 \leq (1 - 2\alpha\mu + 2\alpha^2L^2)\mathbb{E}\Delta_k^2 + 2\alpha^2L^2\mathbb{E}\Delta_1^2 \quad (61)$$

- Unrolling this:

$$\begin{aligned} & \mathbb{E}\Delta_{k+1}^2 \\ & \leq (1 - 2\alpha\mu + 2\alpha^2L^2)\mathbb{E}\Delta_1^2 + \sum_{i=0}^{k-1} (1 - 2\alpha\mu + 2\alpha^2L^2)^i 2\alpha^2L^2\mathbb{E}\Delta_1^2 \\ & \leq (1 - 2\alpha\mu + 2\alpha^2L^2)^k\mathbb{E}\Delta_1^2 + 2k\alpha^2L^2\mathbb{E}\Delta_1^2 \end{aligned} \quad (62)$$

SVRG method

- Unrolling this:

$$\mathbb{E}\Delta_{k+1}^2 \leq (1 - 2\alpha\mu + 2\alpha^2L^2)^k \mathbb{E}\Delta_1^2 + 2k\alpha^2L^2\mathbb{E}\Delta_1^2 \quad (63)$$

- Suppose we would like this to be $\leq 0.5E\Delta_1$ after T iterations.
- We pick $\alpha = O(1)\frac{\mu}{L^2}$, then it turns out that we can set $T = O(1)\frac{L^2}{\mu^2}$.
- In fact, we can improve it to $T = O(1)\frac{L}{\mu}$.
- condition number $\kappa = \frac{L}{\mu}$

SVRG method

Algorithm 2: SVRG method

Input: \tilde{x}_0, α, m

for $e = 1 : E$ **do**

- ▶ $y \leftarrow \tilde{x}_{e-1}, x_1 \leftarrow \tilde{x}_{e-1}.$
- ▶ $g \leftarrow \nabla f(y)$ (full gradient)
- ▶ **for** $k = 1 : m$ **do**
 - pick $s_k \in \{1, \dots, n\}$ uniformly at random.
 - $v_k = \nabla f_{s_k}(x_k) - \nabla f_{s_k}(y) + \nabla f(y)$
 - $x_{k+1} = x_k - \alpha v_k$

▶ **end for**

▶
$$\tilde{x}_e \leftarrow \frac{1}{m} \sum_{k=1}^m x_k$$

end for

SVRG method

Convergence of SVRG method

Suppose $0 < \alpha \leq \frac{1}{2L}$ and m sufficiently large such that

$$\rho = \frac{1}{\mu\alpha(1-2L\alpha)m} + \frac{2L\alpha}{1-2L\alpha} < 1 \quad (64)$$

then we have linear convergence in expectation

$$Ef(\tilde{x}_s) - f(x^*) \leq \rho^s [f(\tilde{x}_0) - f(x^*)] \quad (65)$$

- if $\alpha = \frac{\theta}{L}$, then

$$\rho = \frac{L/\mu}{\theta(1-2\theta)m} + \frac{2\theta}{1-2\theta} \quad (66)$$

choosing $\theta = 0.1$ and $m = 50(L/\mu)$ results in $\rho = 0.5$

- overall complexity: $O\left(\left(\frac{L}{\mu} + n\right) \log(1/\epsilon)\right)$

proof of theorem



$$\begin{aligned}\mathbb{E}\Delta_{k+1}^2 &= \mathbb{E}\|x_{k+1} - x^*\|_2^2 = \mathbb{E}\|x_k - \alpha v_k - x^*\|_2^2 \\ &= \mathbb{E}\Delta_k^2 - 2\alpha\mathbb{E}\langle v_k, x_k - x^* \rangle + \alpha^2\mathbb{E}\|v_k\|_2^2 \\ &= \mathbb{E}\Delta_k^2 - 2\alpha\mathbb{E}\langle \nabla f(x_k), x_k - x^* \rangle + \alpha^2\mathbb{E}\|v_k\|_2^2 \\ &\leq \mathbb{E}\Delta_k^2 - 2\alpha\mathbb{E}(f(x_{k-1}) - f(x^*)) + \alpha^2 \boxed{\mathbb{E}\|v_k\|_2^2}\end{aligned}$$

- By smoothness of $f_i(x)$

$$\|\nabla f_i(x) - \nabla f_i(x^*)\|^2 \leq 2L[f_i(x) - f_i(x^*) - \nabla f_i(x^*)^T(x - x^*)] \quad (67)$$

- summing above inequalities over $1, 2, \dots, n$ and using $\nabla f(x^*) = 0$

$$\frac{1}{n} \sum_{i=1}^n \|\nabla f_i(x) - \nabla f_i(x^*)\|^2 \leq 2L[f(x) - f(x^*)] \quad (68)$$

proof of theorem

- Using $E[(X - E[X])^2] \leq E[X^2]$, we obtain the bound

$$\begin{aligned} & \mathbb{E}_s \|v_k\|_2^2 \\ = & \mathbb{E} \|\nabla f_{s_k}(x_k) - \nabla f_{s_k}(y) + \nabla f(y) + \nabla f_{s_k}(x^*) - \nabla f_{s_k}(x^*)\|_2^2 \\ \leq & 2\mathbb{E} \|\nabla f_{s_k}(x_k) - \nabla f_{s_k}(x^*)\|_2^2 + 2\mathbb{E} \|\nabla f_{s_k}(y) - \nabla f(y) - \nabla f_{s_k}(x^*)\|_2^2 \\ = & 2\mathbb{E} \|\nabla f_{s_k}(x_k) - \nabla f_{s_k}(x^*)\|_2^2 \\ & + 2\mathbb{E} \|\nabla f_{s_k}(y) - \nabla f_{s_k}(x^*) - \mathbb{E}[\nabla f_{s_k}(y) - \nabla f_{s_k}(x^*)]\|_2^2 \\ \leq & 2\mathbb{E} \|\nabla f_{s_k}(x_k) - \nabla f_{s_k}(x^*)\|_2^2 + 2\mathbb{E} \|\nabla f(y) - \nabla f(x^*)\|_2^2 \\ \leq & 4L[f(x_k) - f(x^*) + f(y) - f(x^*)] \end{aligned}$$

- now continue the derivation

$$\begin{aligned} \mathbb{E} \Delta_{k+1}^2 & \leq \mathbb{E} \Delta_k^2 - 2\alpha \mathbb{E}(f(x_k) - f(x^*)) + \alpha^2 \mathbb{E} \|v_k\|_2^2 \\ & \leq \mathbb{E} \Delta_k^2 - 2\alpha(1 - 2\alpha L) \mathbb{E}(f(x_k) - f(x^*)) + 4L\alpha^2 [f(y) - f(x^*)] \end{aligned}$$

proof of theorem

- summing over $k = 1, \dots, m$ (note that $y = \tilde{x}_{e-1}$ and $\tilde{x}_e = \frac{1}{m} \sum_{k=1}^m x_k$)

$$\begin{aligned} & \mathbb{E} \Delta_{k+1}^2 + 2\alpha(1 - 2\alpha L) \sum_{k=1}^m \mathbb{E}(f(x_k) - f(x^*)) \\ & \leq \mathbb{E} \|\tilde{x}_{e-1} - x^*\|^2 + 4L\alpha^2 m \mathbb{E}[f(\tilde{x}_{e-1}) - f(x^*)] \\ & \leq \frac{2}{\mu} \mathbb{E}[f(\tilde{x}_{e-1}) - f(x^*)] + 4L\alpha^2 m \mathbb{E}[f(\tilde{x}_{e-1}) - f(x^*)] \end{aligned}$$

- therefore, for each stage s

$$\begin{aligned} & \mathbb{E}[f(\tilde{x}_e) - f(x^*)] \\ & \leq \frac{1}{m} \sum_{k=1}^m \mathbb{E}(f(x_k) - f(x^*)) \\ & \leq \frac{1}{2\alpha(1 - 2\alpha L)m} \left(\frac{2}{\mu} + 4mL\alpha^2 \right) \mathbb{E}[f(\tilde{x}_{e-1}) - f(x^*)] \quad (69) \end{aligned}$$

Summary

- condition number: $\kappa = \frac{L}{\mu}$
- **SVRG**: $E \sim \log(\frac{1}{\epsilon})$ so the complexity is $O((n + \kappa) \log(\frac{1}{\epsilon}))$
- **GD**: $T \sim \kappa \log(\frac{1}{\epsilon})$ so the complexity is $O(n\kappa \log(\frac{1}{\epsilon}))$
- **SGD**: $T \sim \frac{\kappa}{\epsilon}$ so the complexity is $O(\frac{\kappa}{\epsilon})$
- even though we are allowing ourselves a few gradient computations here, we don't really pay too much in terms of complexity.

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Stochastic Algorithms in Deeplearning

Consider problem $\min_{x \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n f_i(x)$

References: chapter 8 in

<http://www.deeplearningbook.org/>

- Gradient descent

$$x^{t+1} = x^t - \frac{\alpha^t}{n} \sum_{i=1}^n \nabla f_i(x^t)$$

- Stochastic gradient descent

$$x^{k+1} = x^t - \alpha^t \nabla f_i(x^t)$$

- SGD with momentum

$$v^{t+1} = \mu^t v^t - \alpha^t \nabla f_i(x^t)$$

$$x^{t+1} = x^t + v^{t+1}$$

Stochastic Algorithms in Deeplearning

- Nesterov accelerated gradient (original version)

$$\begin{aligned}v^{t+1} &= (1 + \mu^t)x^t - \mu^t x^{t-1} \\x^{t+1} &= v^{t+1} - \alpha^t \nabla f_i(v^{t+1})\end{aligned}$$

here $\mu^t = \frac{t+2}{t+5}$ and α^t fixed or determined by line search (inverse of Lipschitz constant).

- Nesterov accelerated gradient (momentum version)

$$\begin{aligned}v^{t+1} &= \mu^t v^t - \alpha^t \nabla f_i(x^t + \mu^t v^t) \\x^{t+1} &= x^t + v^{t+1}\end{aligned}$$

here $\mu^t = \frac{t+2}{t+5}$ and α^t fixed or determined by line search.

Stochastic Algorithms in Deeplearning

- Adaptive Subgradient Methods (Adagrad): let $g_t = \nabla f_i(x^t)$, $g_t^2 = \text{diag}[g_t g_t^T] \in \mathbb{R}^d$, and initial $G_1 = g_1^2$. At step t

$$x^{t+1} = x^t - \frac{\alpha^t}{\sqrt{G^t + \epsilon \mathbf{1}_d}} \nabla f_i(x^t)$$
$$G^{t+1} = G^t + g_{t+1}^2$$

in the upper and the following iterations we use element-wise vector-vector multiplication.

Stochastic Algorithms in Deeplearning

- Adadelta: denote exponentially decaying average

$E[g^2]_t = \rho E[g^2]_{t-1} + (1 - \rho)g_t^2$, $\text{RMS}[g]_t = \sqrt{E[g^2]_t + \epsilon \mathbf{1}_d} \in \mathbb{R}^d$, and

$E[\Delta x^2]_t = \rho E[\Delta x^2]_{t-1} + (1 - \rho)\Delta x_t^2$,

$\text{RMS}[\Delta x]_t = \sqrt{E[\Delta x^2]_t + \epsilon \mathbf{1}_d} \in \mathbb{R}^d$. Initial parameter: x^1 ,

$E[g^2]_0 = 0$, $E[\Delta x^2]_0 = 0$, decay rate ρ , constant ϵ . At step t ,

compute $g_t = \nabla f_i(x^t)$ and

$$E[g^2]_t = \rho E[g^2]_{t-1} + (1 - \rho)g_t^2$$

$$\Delta x_t = -\frac{\text{RMS}[\Delta x]_{t-1}}{\text{RMS}[g]_t} g_t$$

$$E[\Delta x^2]_t = \rho E[\Delta x^2]_{t-1} + (1 - \rho)\Delta x_t^2$$

$$x^{t+1} = x^t + \Delta x_t$$

Stochastic Algorithms in Deeplearning

- RMSprop: initial $E[g^2]_0 = 0$. At step t ,

$$E[g^2]_t = \rho E[g^2]_{t-1} + (1 - \rho)g_t^2$$
$$x^{t+1} = x^t - \frac{\alpha^t}{\sqrt{E[g^2]_t + \epsilon \mathbf{1}_d}} \nabla f_i(x^t)$$

here $\rho \equiv 0.9$, $\alpha^t \equiv 0.001$ is a good choice.

Stochastic Algorithms in Deeplearning

- Adam: initial $E[g^2]_0 = 0$, $E[g]_0 = 0$. At step t ,

$$\begin{aligned}E[g]_t &= \mu E[g]_{t-1} + (1 - \mu)g_t \\E[g^2]_t &= \rho E[g^2]_{t-1} + (1 - \rho)g_t^2 \\ \widehat{E}[g]_t &= \frac{E[g]_t}{1 - \mu^t} \\ \widehat{E}[g^2]_t &= \frac{E[g^2]_t}{1 - \rho^t} \\ x^{t+1} &= x^t - \frac{\alpha}{\sqrt{\widehat{E}[g^2]_t + \epsilon \mathbf{1}_d}} \widehat{E}[g]_t\end{aligned}$$

here ρ , μ are decay rates, α is learning rate.

Optimization algorithms in Deep learning

随机梯度类算法

- pytorch/caffe2 里实现的算法有 adadelat, adagrad, adam, nesterov, rmsprop, YellowFin

<https://github.com/pytorch/pytorch/tree/master/caffe2/sgd>

- pytorch/torch 里有 : sgd, asgd, adagrad, rmsprop, adadelat, adam, adamax

<https://github.com/pytorch/pytorch/tree/master/torch/optim>

- tensorflow 实现的算法有 : Adadelat, AdagradDA, Adagrad, ProximalAdagrad, Ftrl, Momentum, adam, Momentum, CenteredRMSProp

具体实现:

https://github.com/tensorflow/tensorflow/blob/master/tensorflow/core/kernels/training_ops.cc

数值例子：逻辑回归

给定数据集 $\{(a_i, b_i)_{i=1}^N\}$ ，逻辑回归对应的优化问题可以写成如下形式

$$\min_{x \in \mathbb{R}^n} f(x) = \frac{1}{N} \sum_{i=1}^N f_i(x) = \frac{1}{N} \sum_{i=1}^N \log(1 + \exp(-b_i \cdot a_i^\top x)) + \lambda \|x\|_2^2,$$

每步我们随机取一个数据 i_k 对应的梯度 $\nabla f_{i_k}(x^k)$ 作随机梯度下降，其迭代格式可以写成

$$x^{k+1} = x^k - \tau_k \nabla f_{i_k}(x^k) = x^k - \tau_k \frac{1}{N} \left(\frac{-\exp(-b_{i_k} \cdot a_{i_k}^\top x^k) b_{i_k} a_{i_k}}{1 + \exp(-b_{i_k} \cdot a_{i_k}^\top x^k)} + 2\lambda x^k \right),$$

其中 i_k 为从 $\{1, \dots, N\}$ 随机抽取的一个样本， τ_k 为步长。采用 LIBSVM 网站的数据集，并令 $\lambda = 10^{-4}$ 。分别测试不同随机算法在数据集 CINA 和 a9a 上的表现。我们采用网格搜索方法来确定随机算法中的参数值，对每个参数重复 5 次数值实验并取其平均表现。数值稳定参数均设置为 $\epsilon = 10^{-7}$ 。

