CMPT 409/981: Optimization for Machine Learning

Lecture 10

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For smooth, strongly-convex functions, SGD with an O(1/k) decreasing step-size converges to the minimizer at an $\Theta(1/\tau)$ rate (we will prove this later today).

Similar to the convex setting, using SGD with a constant step-size results in convergence to the neighbourhood that depends on the noise in the stochastic gradients.

Claim: For *L*-smooth, μ -strongly convex functions, T iterations of SGD with $\eta_k = \eta = \frac{1}{L}$ returns iterate w_T such that,

$$\mathbb{E}[\|w_T - w^*\|^2] \le \exp\left(\frac{-T}{\kappa}\right) \|w_0 - w^*\|^2 + \frac{\sigma^2}{\mu L}$$

Hence, SGD results in an exponential convergence to the neighbourhood of the minimizer.

Unlike the convex case for which we proved a guarantee on the average iterate \bar{w}_T , here we have a guarantee for the last iterate w_T .

Proof: Following a proof similar to the convex case,

$$||w_{k+1} - w^*||^2 = ||w_k - \eta_k \nabla f_{ik}(w_k) - w^*||^2$$

= $||w_k - w^*||^2 - 2\eta_k \langle \nabla f_{ik}(w_k), w_k - w^* \rangle + \eta_k^2 ||\nabla f_{ik}(w_k)||^2$

Taking expectation w.r.t i_k on both sides,

$$\mathbb{E}[\|w_{k+1} - w^*\|^2] = \|w_k - w^*\|^2 - 2\mathbb{E}\left[\eta_k \langle \nabla f_{ik}(w_k), w_k - w^* \rangle\right] + \mathbb{E}\left[\eta_k^2 \|\nabla f_{ik}(w_k)\|^2\right]$$

$$\implies \mathbb{E}[\|w_{k+1} - w^*\|^2] = \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + \eta_k^2 \mathbb{E}\left[\|\nabla f_{ik}(w_k)\|^2\right]$$
(Assuming η_k is independent of i_k and Unbiasedness)

Recall that
$$\mathbb{E}[\|w_{k+1} - w^*\|^2] = \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + \eta_k^2 \mathbb{E} \left[\|\nabla f_{ik}(w_k)\|^2 \right].$$

$$\mathbb{E}[\|w_{k+1} - w^*\|^2]$$

$$= \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + \eta_k^2 \mathbb{E} \left[\|\nabla f_{ik}(w_k) - \nabla f(w_k) + \nabla f(w_k)\|^2 \right]$$

$$\leq \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + \eta_k^2 \mathbb{E} \left[\|\nabla f(w_k)\|^2 \right] + \eta_k^2 \sigma^2$$
(Using the bounded variance assumption)

Using
$$\mu$$
-strong convexity, $f(y) \ge f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} \|y - x\|^2$ with $y = w^*$ and $x = w_k$,

$$< \|w_k - w^*\|^2 - 2n_k [f(w_k) - f(w^*)] - \mu n_k \|w_k - w^*\|^2 + n_k^2 \mathbb{E} \left[\|\nabla f(w_k)\|^2 \right] + n_k^2 \sigma^2$$

$$\leq \|w_{k} - w^{*}\|^{2} - 2\eta_{k}[f(w_{k}) - f(w^{*})] - \mu\eta_{k} \|w_{k} - w^{*}\|^{2} + \eta_{k}^{2} \mathbb{E}\left[\|\nabla f(w_{k})\|^{2}\right] + \eta_{k}^{2} \sigma^{2}$$
(Eq. (1))

$$\Rightarrow \mathbb{E}[\|w_{k+1} - w^*\|^2] \\ \leq (1 - \mu \eta_k) \|w_k - w^*\|^2 - 2\eta_k [f(w_k) - f(w^*)] + 2L \, \eta_k^2 \, \mathbb{E}[f(w_k) - f(w^*)] + \eta_k^2 \, \sigma^2$$
(Using *L*-smoothness of *f*)

$$\mathbb{E}[\|w_{k+1} - w^*\|^2] \le (1 - \mu \eta_k) \|w_k - w^*\|^2 - 2\eta_k [f(w_k) - f(w^*)] + 2L \eta_k^2 \mathbb{E}[f(w_k) - f(w^*)] + \eta_k^2 \sigma^2.$$
Setting $\eta_k = \eta = \frac{1}{L}$

$$\mathbb{E}[\|w_{k+1} - w^*\|^2] \le \left(1 - \frac{\mu}{L}\right) \|w_k - w^*\|^2 + \frac{\sigma^2}{L^2}$$

Since the above inequality is true for all k, using it for k = T - 1,

$$\mathbb{E}[\|w_{T} - w^{*}\|^{2}] \le \left(1 - \frac{\mu}{L}\right) \|w_{T-1} - w^{*}\|^{2} + \frac{\sigma^{2}}{L^{2}}$$

Taking expectation w.r.t the randomness from iterations k = 0 to T - 1,

$$\implies \mathbb{E}[\|w_T - w^*\|^2] \le \rho \, \mathbb{E} \|w_{T-1} - w^*\|^2 + \frac{\sigma^2}{I^2} \qquad \qquad \text{(Denoting } \rho := 1 - \mu/L)$$

Recall that $\mathbb{E}[\|w_T - w^*\|^2] \leq \rho \mathbb{E} \|w_{T-1} - w^*\|^2 + \frac{\sigma^2}{I^2}$. Unrolling the recursion until k = 0,

$$\mathbb{E}[\|w_{T} - w^{*}\|^{2}] \leq \rho^{T} \|w_{0} - w^{*}\|^{2} + \frac{\sigma^{2}}{L^{2}} \sum_{k=0}^{T-1} \rho^{k} \leq \rho^{T} \|w_{0} - w^{*}\|^{2} + \frac{\sigma^{2}}{L^{2}} \sum_{k=0}^{\infty} \rho^{k}$$

$$\leq \rho^{T} \|w_{0} - w^{*}\|^{2} + \frac{\sigma^{2}}{L^{2}} \frac{1}{1 - \rho} \qquad \text{(Infinite geometric series)}$$

$$= \left(1 - \frac{\mu}{L}\right)^{T} \|w_{0} - w^{*}\|^{2} + \frac{\sigma^{2}}{\mu L}$$

$$\leq \exp\left(\frac{-T}{\kappa}\right) \|w_{0} - w^{*}\|^{2} + \frac{\sigma^{2}}{\mu L} \qquad (1 - x \leq \exp(-x))$$

$$\implies \mathbb{E}[\|w_{T} - w^{*}\|^{2}] \leq \exp\left(\frac{-T}{\kappa}\right) \|w_{0} - w^{*}\|^{2} + \underbrace{\frac{\sigma^{2}}{\mu L}}_{\text{neighbourhood}}$$



Let us prove that SGD with an O(1/k) step-size results in O(1/T) convergence to the minimizer.

Claim: For *L*-smooth, μ -strongly convex functions, T iterations of SGD (for $T \ge 2\kappa$) with $\eta_k = \frac{1}{\mu(k+1)}$ returns iterate $\bar{w}_T = \frac{\sum_{k=0}^{T-1} w_k}{T}$ such that,

$$\mathbb{E}[\|\bar{w}_{\mathcal{T}} - w^*\|^2] \leq \frac{\sigma^2 \left[1 + \log(\mathcal{T})\right]}{\mu \, \mathcal{T}}$$

Three problems – the above result (i) requires knowledge of μ , (ii) the guarantee only holds for $T \geq 2\kappa$, (iii) the guarantee only holds for the average iterate and not the last iterate.

Instead of bounded variance, [LJSB12] assume that $\mathbb{E}[\|\nabla f_i(w)\|^2] \leq G$. Solves (ii) (not (i) and (iii)) and requires additional assumptions about the boundedness of iterates.

[GLQ $^+$ 19, Theorem 3.2] uses a constant, then O(1/k) step-size. Solves (iii) (not (i) and (ii))

[LZO21, VDTB21] use an $O\left((^1/\tau)^{k/T}\right)$ step-size and solves all three problems. Also prove a noise-adaptive $O\left(\exp\left(\frac{-T}{\kappa}\right)+\frac{\sigma^2}{T}\right)$ rate, but requires knowledge of T.

Proof: Following the previous proof, we can recover (Eq. (1) on Slide 3),

$$\Longrightarrow \mathbb{E}[f(w_k) - f(w^*)] \leq \frac{\left[\|w_k - w^*\|^2 \left(1 - \mu \eta_k\right) - \mathbb{E} \|w_{k+1} - w^*\|^2\right]}{\eta_k} + \eta_k \sigma^2$$

Taking expectation w.r.t the randomness from iterations k = 0 to T - 1,

$$\mathbb{E}[f(w_k) - f(w^*)] \le \frac{\mathbb{E}\left[\|w_k - w^*\|^2 (1 - \mu \eta_k) - \|w_{k+1} - w^*\|^2\right]}{\eta_k} + \eta_k \sigma^2$$

Recall that $\mathbb{E}[f(w_k) - f(w^*)] \le \frac{\mathbb{E}[\|w_k - w^*\|^2 (1 - \mu \eta_k) - \|w_{k+1} - w^*\|^2]}{\eta_k} + \eta_k \sigma^2$. Summing from k = 0 to T - 1,

$$\sum_{k=0}^{T-1} \mathbb{E}[f(w_k) - f(w^*)] \leq \sum_{k=0}^{T-1} \frac{\mathbb{E}\left[\|w_k - w^*\|^2 (1 - \mu \eta_k) - \|w_{k+1} - w^*\|^2\right]}{\eta_k} + \sigma^2 \sum_{k=0}^{T-1} \eta_k$$

$$= \sum_{k=0}^{T-1} \frac{\mathbb{E}\left[\|w_k - w^*\|^2 (1 - \mu \eta_k) - \|w_{k+1} - w^*\|^2\right]}{\eta_k} + \sigma^2 \sum_{k=0}^{T-1} \frac{1}{\mu(k+1)}$$

$$\leq \sum_{k=0}^{T-1} \frac{\mathbb{E}\left[\|w_k - w^*\|^2 (1 - \mu \eta_k) - \|w_{k+1} - w^*\|^2\right]}{\eta_k} + \frac{\sigma^2 [1 + \log(T)]}{\mu}$$

Dividing by T, using Jensen's inequality for the LHS, and by definition of \bar{w}_T ,

$$\mathbb{E}[f(\bar{w}_{\mathcal{T}}) - f(w^*)] \leq \frac{1}{T} \sum_{k=0}^{T-1} \frac{\mathbb{E}\left[\left\|w_k - w^*\right\|^2 (1 - \mu \eta_k) - \left\|w_{k+1} - w^*\right\|^2\right]}{\eta_k} + \frac{\sigma^2 \left[1 + \log(T)\right]}{\mu T}$$

Recall that
$$\mathbb{E}[f(\bar{w}_T) - f(w^*)] \leq \frac{1}{T} \sum_{k=0}^{T-1} \frac{\mathbb{E}[\|w_k - w^*\|^2 (1 - \mu \eta_k) - \|w_{k+1} - w^*\|^2]}{\eta_k} + \frac{\sigma^2 [1 + \log(T)]}{\mu T}.$$

$$\sum_{k=0}^{T-1} \frac{\mathbb{E}[\|w_k - w^*\|^2 (1 - \mu \eta_k) - \|w_{k+1} - w^*\|^2]}{\eta_k}$$

$$= \mathbb{E}\sum_{k=1}^{T-1} \left[\|w_k - w^*\|^2 \left(\frac{1}{\eta_k} - \frac{1}{\eta_{k-1}} - \mu\right)\right] + \|w_0 - w^*\|^2 \left(\frac{1}{\eta_0} - \mu\right) - \frac{\|w_T - w^*\|^2}{\eta_{T-1}}$$

$$\leq \mathbb{E}\sum_{k=1}^{T-1} \left[\|w_k - w^*\|^2 (\mu(k+1) - \mu k - \mu)\right] + \|w_0 - w^*\|^2 (\mu - \mu) = 0$$

Putting everything together,

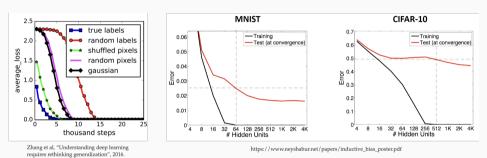
$$\mathbb{E}[f(\bar{w}_T) - f(w^*)] \leq \frac{\sigma^2 \left[1 + \log(T)\right]}{\mu T}$$

Since we used the fact that $\eta_k \leq \frac{1}{2L}$ for all k, it implies that $\frac{1}{\mu T} \leq \frac{1}{2L} \implies T \geq 2\kappa$.



Interpolation for over-parameterized models

Interpolation: Over-parameterized models (such as deep neural networks) are capable of exactly fitting the training dataset.



Loss vs Training steps on CIFAR-10 dataset

Error vs Network size

Formally, when minimizing $f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$, interpolation means that if $\|\nabla f(w)\| = 0$, then $\|\nabla f_i(w)\| = 0$ for all $i \in [n]$ i.e. the variance in the stochastic gradients becomes zero at a stationary point.

SGD under Interpolation

Recall that SGD needs to decrease the step-size to counteract the noise (variance).

Idea: Under interpolation, since the noise is zero at the optimum, SGD does not need to decrease the step-size and can converge to the minimizer by using a *constant* step-size.

If f is strongly-convex and the model is expressive enough such that interpolation is satisfied (for example, when using kernels or least squares with d > n), constant step-size SGD can converge to the minimizer at an $O(\exp(-T/\kappa))$ rate.

In this setting, SGD matches the rate of deterministic (full-batch) GD, but compared to GD, each iteration is cheap.

Moreover, empirical results (and theoretical results on "benign overfitting") suggest that interpolating the training dataset does not adversely affect the generalization error!

Minimizing smooth, strongly-convex functions using SGD under interpolation

Claim: When minimizing $f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ such that (i) f is μ -strongly convex, (ii) each f_i is convex and L-smooth, (iii) interpolation is exactly satisfied i.e. $\|\nabla f_i(w^*)\| = 0$, T iterations of SGD with $\eta_k = \eta = \frac{1}{2L}$ returns iterate w_T such that,

$$\mathbb{E}[\|w_T - w^*\|^2] \le \exp\left(\frac{-T}{\kappa}\right) \|w_0 - w^*\|^2$$

Before analyzing the convergence of SGD, let us first study the effect of interpolation on $\sigma^2(w)$.

$$\begin{split} \sigma^2(w) &:= \mathbb{E}_i \left\| \nabla f(w) - \nabla f_i(w) \right\|^2 = \left\| \nabla f(w) \right\|^2 + \mathbb{E}_i \left\| \nabla f_i(w) \right\|^2 - 2\mathbb{E} \left[\left\langle \nabla f(w), \nabla f_i(w) \right\rangle \right] \\ &= \mathbb{E}_i \left\| \nabla f_i(w) \right\|^2 + \left\| \nabla f(w) \right\|^2 - 2\left\| \nabla f(w) \right\|^2 \qquad \qquad \text{(Unbiasedness)} \\ &\leq \mathbb{E}_i \left\| \nabla f_i(w) \right\|^2 \leq \mathbb{E}_i \left[2L \left[f_i(w) - f_i(w^*) \right] \right] \\ &\qquad \qquad \text{(Using L-smoothness, convexity of f_i and $\nabla f_i(w^*) = 0$)} \end{split}$$

As w gets closer to the solution (in terms of the function values), the variance decreases becoming zero at w^* . Hence, under interpolation, we do not need to decrease the step-size.

 $\implies \sigma^2(w) < 2L[f(w) - f(w^*)]$

(Unbiasedness)

Minimizing smooth, strongly-convex functions using SGD under interpolation

Proof: Following the same proof as before, we get that,

$$\mathbb{E}[\|w_{k+1} - w^*\|^2] = \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + \eta_k^2 \mathbb{E}\left[\|\nabla f_{ik}(w_k)\|^2\right]$$

$$\leq \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + \eta_k^2 \mathbb{E}_i \left[2L \left[f_{ik}(w_k) - f_{ik}(w^*)\right]\right]$$
(Using *L*-smoothness, convexity of f_i and $\nabla f_i(w^*) = 0$)
$$= \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + 2L \eta_k^2 \mathbb{E}\left[f(w_k) - f(w^*)\right]$$
(Unbiasedness)
$$= \|w_k - w^*\|^2 (1 - \mu \eta_k) - 2\eta_k \left[f(w_k) - f(w^*)\right] + 2L \eta_k^2 \mathbb{E}\left[f(w_k) - f(w^*)\right]$$
(Strong-convexity)
$$= \left(1 - \frac{\mu}{2L}\right) \|w_k - w^*\|^2$$
(Since $\eta_k = \eta = \frac{1}{2L}$)

Taking expectation w.r.t the randomness from iterations k=0 to $\mathcal{T}-1$ and recursing,

$$\mathbb{E}[\|w_T - w^*\|^2] \le \left(1 - \frac{\mu}{2L}\right)^T \|w_0 - w^*\|^2 \le \exp\left(\frac{-T}{\kappa}\right) \|w_0 - w^*\|^2$$

Minimizing smooth, strongly-convex functions using SGD under interpolation

We can modify the proof in order to get an $O\left(\exp\left(\frac{-T}{\kappa}\right) + \zeta^2\right)$ where $\zeta^2 \propto \mathbb{E}_i \|\nabla f_i(w^*)\|^2$.

Moreover, as before, if we use a mini-batch of size b, the effective noise is $\zeta_b^2 \propto \frac{\mathbb{E}_l \|\nabla f_l(w^*)\|^2}{b}$. Hence, if the model is sufficiently over-parameterized so that it *almost* interpolates the data, and we are using a large batch-size, then ζ_b^2 is small, and constant step-size works well.

When minimizing convex functions under (exact) interpolation, constant step-size SGD results in O(1/T) convergence, matching deterministic GD, but with much smaller per-iteration cost (Need to prove this in Assignment 3!)



Minimizing smooth, non-convex functions using SGD under interpolation

When minimizing non-convex functions, interpolation is not enough to guarantee a fast (matching the deterministic) O(1/T) rate for SGD.

Can achieve this rate under the strong growth condition (SGC) on the stochastic gradients. Formally, there exists a constant $\rho > 1$ such that for all w,

$$\mathbb{E}_{i} \left\| \nabla f_{i}(w) \right\|^{2} \leq \rho \left\| \nabla f(w) \right\|^{2}$$

Hence, SGC implies that $\|\nabla f_i(w^*)\|^2 = 0$ for all i and hence interpolation.

As before, let us study the effect of SGC on the variance $\sigma^2(w)$.

$$\sigma^{2}(w) := \mathbb{E}_{i} \left\| \nabla f_{i}(w) - \nabla f(w) \right\|^{2} \leq \mathbb{E}_{i} \left\| \nabla f_{i}(w) \right\|^{2} - \left\| \nabla f(w) \right\|^{2} \qquad \text{(Unbiasedness)}$$

$$\implies \sigma^{2}(w) \leq (\rho - 1) \left\| \nabla f(w) \right\|^{2} \qquad \text{(SGC)}$$

Hence, SGC implies that as w gets closer to a stationary point (in terms of the gradient norm), the variance decreases and constant step-size SGD converges to a stationary point.

Minimizing smooth, non-convex functions using SGD under interpolation

Claim: For (i) *L*-smooth functions lower-bounded by f^* , (ii) under ρ -SGC, T iterations of SGD with $\eta_k = \frac{1}{\rho L}$ returns an iterate \hat{w} such that,

$$\mathbb{E}[\|\nabla f(\hat{w})\|^2] \leq \frac{2\rho L\left[f(w_0) - f^*\right]}{T}$$

Proof: Similar to the proof in Lecture 8, using the *L*-smoothness of *f* with $x = w_k$ and $y = w_{k+1} = w_k - \eta_k \nabla f_{ik}(w_k)$,

$$f(w_{k+1}) \leq f(w_k) + \langle \nabla f(w_k), -\eta_k \nabla f_{ik}(w_k) \rangle + \frac{L}{2} \eta_k^2 \| \nabla f_{ik}(w_k) \|^2$$

Taking expectation w.r.t i_k on both sides and using that η_k is independent of i_k

$$\mathbb{E}[f(w_{k+1})] \leq f(w_k) - \eta_k \mathbb{E}\left[\langle \nabla f(w_k), \nabla f_{ik}(w_k) \rangle\right] + \frac{L\eta_k^2}{2} \mathbb{E}\left[\|\nabla f_{ik}(w_k)\|^2\right]$$

$$\mathbb{E}[f(w_{k+1})] \leq f(w_k) - \eta_k \|\nabla f(w_k)\|^2 + \frac{L\eta_k^2}{2} \mathbb{E}\left[\|\nabla f_{ik}(w_k)\|^2\right] \qquad \text{(Unbiasedness)}$$

Minimizing smooth, non-convex functions using SGD under interpolation

Recall
$$\mathbb{E}[f(w_{k+1})] \le f(w_k) - \eta_k \|\nabla f(w_k)\|^2 + \frac{L\eta_k^2}{2} \mathbb{E}\left[\|\nabla f_{ik}(w_k)\|^2\right]$$
. Using ρ -SGC,
$$\mathbb{E}[f(w_{k+1})] \le f(w_k) - \eta_k \|\nabla f(w_k)\|^2 + \frac{L\rho\eta_k^2}{2} \|\nabla f(w_k)\|^2$$

$$\mathbb{E}[f(w_{k+1})] \le f(w_k) - \frac{1}{2\rho I} \|\nabla f(w_k)\|^2 \qquad \qquad \text{(Using } \eta_k = \eta = \frac{1}{\rho L}\text{)}$$

Taking expectation w.r.t the randomness from iterations i = 0 to k - 1, and summing

$$\sum_{k=0}^{T-1} \mathbb{E}[\|\nabla f(w_k)\|^2] \le 2\rho L \sum_{k=0}^{T-1} \mathbb{E}[f(w_k) - f(w_{k+1})] \implies \frac{\sum_{k=0}^{T-1} \mathbb{E}[\|\nabla f(w_k)\|^2]}{T} \le \frac{2\rho L \mathbb{E}[f(w_0) - f^*]}{T}$$
(Dividing by T)

Defining $\hat{w} := \arg\min_{k \in \{0,1,\dots,T-1\}} \mathbb{E}[\|\nabla f(w_k)\|^2]$,

$$\mathbb{E}[\|\nabla f(\hat{w})\|^2] \leq \frac{2\rho L\left[f(w_0) - f^*\right]}{T}$$



References

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