# Distributed Optimization for Machine Learning

Lecture 8 - Stochastic Gradient Methods

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### Revisit model training

Let's make our price predictor more realistic by adding more features.

Size (sq. ft.)	# Bedrooms	Age (years)	Price (\$k)
1200	3	10	250
2000	4	5	350
800	2	25	150

Our goal is to find the best parameter x of model  $h_x(a)$  by minimizing

$$f(\mathbf{x}) = \frac{1}{2n} \sum_{i=1}^{n} (h_{\mathbf{x}}(\mathbf{a}^{(i)}) - y^{(i)})^{2}$$

Given previous discussion about f(x), what is unique about this objective?



# Empirical risk minimization - a "machine learning" name

Let  $\{\mathbf{a}_i, y_i\}_{i=1}^n$  be n random samples, and consider

$$\min_{\mathbf{x}} F(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^{n} f(\mathbf{x}; \{\mathbf{a}_i, y_i\})$$
empirical risk

e.g., quadratic loss  $f(\mathbf{x}; \{\mathbf{a}_i, y_i\}) = (\mathbf{a}_i^{\top} \mathbf{x} - y_i)^2$ . If one draws index

 $j \sim \mathsf{Unif}(1,\ldots,n)$  uniformly at random, then

$$F(\mathbf{x}) = \mathbb{E}_j[f(\mathbf{x}; \{\mathbf{a}_j, y_j\})]$$



### Stochastic programming - an "optimization" name

We view both the model training and testing problems as

$$\min_{\mathbf{x}} \underbrace{F(\mathbf{x}) = \mathbb{E}[f(\mathbf{x}; \xi)]}_{\text{expected risk, popular risk, ...}}$$

- $\bullet$   $\xi$ : randomness in problem
- suppose  $f(\cdot; \xi)$  is convex for every  $\xi$  (and hence  $F(\cdot)$  is convex)



# Connecting the two views: Goal vs. Reality

We ideally want a model x that performs well on all future data  $\mathcal{D}$ :

$$\min_{\mathbf{x}} \ \mathbb{E}_{(\mathbf{a},y) \sim \mathcal{D}}[f(\mathbf{x}; \{\mathbf{a},y\})]$$

We can't compute this because we don't have access to all data.



We use our *finite training sample average* as a **proxy** for the true  $\mathcal{D}$ :

$$\frac{1}{n}\sum_{i=1}^{n}f(\mathbf{x};\{\mathbf{a}_{i},y_{i}\})\approx\mathbb{E}_{(\mathbf{a},y)\sim\mathcal{D}}[f(\mathbf{x};\{\mathbf{a},y\})]$$



#### A natural solution

Under "mild" technical conditions, if we run the gradient descent method from previous lectures, we have

$$\mathbf{x}^{t+1} = \mathbf{x}^{t} - \eta_{t} \nabla F(\mathbf{x}^{t})$$

$$= \mathbf{x}^{t} - \eta_{t} \nabla \mathbb{E}[f(\mathbf{x}^{t}; \xi)]$$

$$= \mathbf{x}^{t} - \eta_{t} \mathbb{E}[\nabla_{\mathbf{x}} f(\mathbf{x}^{t}; \xi)]$$

#### Issues:

- **testing setting** distribution of  $\xi$  may be unknown
- training setting even if it is known, evaluating is expensive



### Why is expectation expensive?

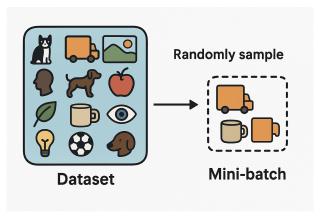
■ The expectation is over the entire data distribution:

$$\nabla F(\mathbf{x}) = \mathbb{E}_{\xi}[\nabla f(\mathbf{x}; \xi)]$$

- In practice, this means averaging gradients over all samples
- Example: ImageNet has > 1 million samples one full gradient step would require computing 1,000,000+ gradients!
- Takeaway: Exact expectation is computationally infeasible; motivates stochastic approximations.



#### What should we do?



Generated by GPT 5 with prompt "generate one cartoon for samping"



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Stochastic gradient descent (SGD)

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# Stochastic gradient descent (SGD)

#### Stochastic gradient descent (SGD)

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \eta_t g(\mathbf{x}^t; \xi^t) \tag{1}$$

where  $g(\mathbf{x}^t; \xi^t)$  is an *unbiased estimate* of  $\nabla F(\mathbf{x}^t)$ , i.e.

$$\mathbb{E}[g(\mathbf{x}^t; \xi^t)] = \nabla F(\mathbf{x}^t)$$

— Robbins, Monro '51



# Stochastic gradient descent (SGD)



Herbert Robbins

# Stochastic approximation / Stochastic gradient descent (SGD)

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \eta_t g(\mathbf{x}^t; \xi^t) \tag{1}$$

- **a** a stochastic algorithm for finding a critical point  $\mathbf{x}$  obeying  $\nabla F(\mathbf{x}) = 0$
- more generally, a stochastic algorithm for finding the roots of  $G(\mathbf{x}) := \mathbb{E}[g(\mathbf{x}; \xi)]$
- **x** does not necessarily obey  $g(\mathbf{x}; \xi) = 0$

— Robbins, Monro '51



### Example: SGD for empirical risk minimization

$$\min_{\mathbf{x}} F(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^{n} f(\mathbf{x}; \{\mathbf{a}_i, y_i\})$$

for t = 0, 1, ...

- choose  $i_t$  uniformly at random, and compute  $\nabla_{\mathbf{x}} f_{i_t}(\mathbf{x}^t; \{\mathbf{a}_{i_t}, y_{i_t}\})$
- run the gradient descent update

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \eta_t \nabla_{\mathbf{x}} f_{i_t}(\mathbf{x}^t; \{\mathbf{a}_{i_t}, y_{i_t}\})$$

end for



### Compare GD and SGD trajectories

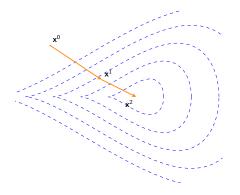


Figure: Example trajectory of Stochastic Gradient Descent (SGD) on a 2D loss landscape. The path is more erratic due to the noisy gradient estimates.



### Example: SGD for empirical risk minimization

Benefits: SGD exploits information more efficiently than batch methods

- practical data usually involve lots of redundancy; using all data simultaneously in each iteration might be inefficient
- SGD is particularly efficient at the very beginning, as it achieves fast initial improvement with low per-iteration cost



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### Strongly convex and smooth problems

$$\min_{\mathbf{x}} F(\mathbf{x}) := \mathbb{E}[f(\mathbf{x}; \xi)]$$

#### **Assumptions:**

- F:  $\mu$ -strongly convex, L-smooth
- $g(\mathbf{x}^t; \xi^t)$ : an unbiased estimate of  $\nabla F(\mathbf{x}^t)$  given  $\{\xi^0, \dots, \xi^{t-1}\}$
- $\mathbf{g}(\mathbf{x}^t; \xi^t)$  has bounded variance: for all  $\mathbf{x}$ ,

$$\mathbb{E}[||g(\mathbf{x};\xi)||_2^2] \le \sigma_g^2 + c_g||\nabla F(\mathbf{x})||_2^2$$
 (2)

Why having unbiasedness and bounded variance?



### Mini-batch gradients: Variance reduction

Instead of using a single sample  $\xi^t$ , we can use a **mini-batch** of B i.i.d. samples  $\{\xi_1^t,\ldots,\xi_B^t\}$  to form a better gradient estimate:

$$g_B(\mathbf{x}^t) := \frac{1}{B} \sum_{i=1}^B g(\mathbf{x}^t; \xi_i^t)$$

■ Unbiasedness: The mini-batch estimate is still unbiased.

$$\mathbb{E}[g_B(\mathbf{x}^t)] = \frac{1}{B} \sum_{i=1}^B \mathbb{E}[g(\mathbf{x}^t; \xi_i^t)] = \frac{1}{B} \sum_{i=1}^B \nabla F(\mathbf{x}^t) = \nabla F(\mathbf{x}^t)$$

**Reduced variance:** The variance  $\sigma_g^2$  is reduced by a factor of B:

$$\mathbb{E}[||g_B(\mathbf{x};\xi)||_2^2] \leq \underbrace{\frac{\sigma_g^2}{B}}_{\mathsf{Reduced!}} + \underbrace{\left(1 + \frac{c_g - 1}{B}\right)}_{c_B} ||\nabla F(\mathbf{x})||_2^2$$



#### Proof: Variance reduction

Let's expand the squared Euclidean norm of the mini-batch gradient:

$$\begin{aligned} \|g_{B}(\mathbf{x})\|_{2}^{2} &= \left\|\frac{1}{B}\sum_{i=1}^{B}g(\mathbf{x};\xi_{i})\right\|_{2}^{2} \\ &= \frac{1}{B^{2}}\left\|\sum_{i=1}^{B}g(\mathbf{x};\xi_{i})\right\|_{2}^{2} \\ &= \frac{1}{B^{2}}\left(\sum_{i=1}^{B}\|g(\mathbf{x};\xi_{i})\|_{2}^{2} + \sum_{i\neq j}g(\mathbf{x};\xi_{i})^{\top}g(\mathbf{x};\xi_{j})\right) \end{aligned}$$

Now, we take the expectation. By linearity of expectation:

$$\mathbb{E}[\|g_{\mathcal{B}}(\mathbf{x})\|_2^2] = \frac{1}{B^2} \left( \sum_{i=1}^B \mathbb{E}[\|g(\mathbf{x}; \xi_i)\|_2^2] + \sum_{i \neq j} \mathbb{E}[g(\mathbf{x}; \xi_i)^\top g(\mathbf{x}; \xi_j)] \right)$$



#### Proof: Variance reduction

1. Sum of squared norms: Using i.i.d. and the individual variance:

$$\sum_{i=1}^{B} \mathbb{E}[\|g(\mathbf{x}; \xi_i)\|_2^2] \le B(\sigma_g^2 + c_g \|\nabla F(\mathbf{x})\|_2^2)$$

2. Cross-terms: For  $i \neq j$ ,  $\mathbb{E}[g(\mathbf{x}; \xi_i)^{\top} g(\mathbf{x}; \xi_j)] = \|\nabla F(\mathbf{x})\|_2^2$ There are B(B-1) such cross-terms.

$$\sum_{i\neq j} \mathbb{E}[g(\mathbf{x};\xi_i)^\top g(\mathbf{x};\xi_j)] = B(B-1) \|\nabla F(\mathbf{x})\|_2^2$$

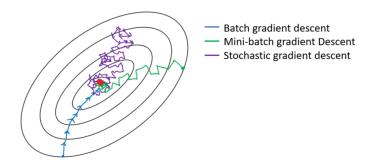
Substitute these back into the expectation:

$$\mathbb{E}[\|g_{B}(\mathbf{x})\|_{2}^{2}] \leq \frac{1}{B^{2}} \left(B(\sigma_{g}^{2} + c_{g}\|\nabla F(\mathbf{x})\|_{2}^{2}) + B(B-1)\|\nabla F(\mathbf{x})\|_{2}^{2}\right)$$

$$= \frac{B\sigma_{g}^{2}}{B^{2}} + \frac{Bc_{g}\|\nabla F(\mathbf{x})\|_{2}^{2}}{B^{2}} + \frac{(B^{2} - B)\|\nabla F(\mathbf{x})\|_{2}^{2}}{B^{2}}$$

$$= \frac{\sigma_{g}^{2}}{B} + \left(1 + \frac{c_{g} - 1}{B}\right)\|\nabla F(\mathbf{x})\|_{2}^{2}$$
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# Compare GD, SGD and mini-batch SGD trajectories





### Convergence: fixed stepsizes

#### Theorem 1 (Strong convexity and fixed stepsizes)

Under the assumptions in previous slide, if  $\eta_t \equiv \eta \leq \frac{1}{Lc_g}$ , then SGD (1) achieves

$$\mathbb{E}[F(\mathbf{x}^t) - F(\mathbf{x}^*)] \leq \frac{\eta L \sigma_g^2}{2\mu} + (1 - \eta \mu)^t (F(\mathbf{x}^0) - F(\mathbf{x}^*))$$

• check Bottou, Curtis, Nocedal '18 (Theorem 4.6) for the proof

"Optimization methods for large-scale machine learning," Bottou, Curtis, Noceda, arXiv, 2018.



### Implications: SGD with fixed stepsizes

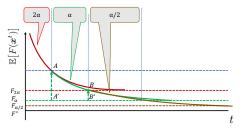
$$\mathbb{E}[F(\mathbf{x}^t) - F(\mathbf{x}^*)] \leq \frac{\eta L \sigma_g^2}{2\mu} + (1 - \eta \mu)^t (F(\mathbf{x}^0) - F(\mathbf{x}^*))$$

- fast (linear) convergence at the very beginning
- converges to some neighborhood of x\* variation in gradient computation prevents further progress
- when gradient computation is noiseless (i.e.  $\sigma_g=0$ ), it converges linearly to optimal points
- lacktriangleright smaller stepsizes  $\eta$  yield better converging points



### One practical strategy

Run SGD with fixed stepsizes; whenever progress stalls, reduce stepsizes and continue SGD.



Bottou, Curtis, Nocedal '18

whenever progress stalls, we half the stepsizes and repeat



### Convergence with diminishing stepsizes

#### Theorem 2 (Strong convexity and diminishing stepsizes)

Suppose F is  $\mu$ -strongly convex, and (2) holds with  $c_g=0$ . If  $\eta_t=\frac{\theta}{t+1}$  for some  $\theta>\frac{1}{2\mu}$ , then SGD (1) achieves

$$\mathbb{E}[||\mathbf{x}^t - \mathbf{x}^*||_2^2] \leq \frac{c_\theta}{t+1}$$

where 
$$c_{\theta} = \max\left\{ rac{2 heta^2\sigma_{g}^2}{2\mu heta - 1}, ||\mathbf{x}_0 - \mathbf{x}^*||_2^2 
ight\}.$$

lacksquare convergence rate  $\mathcal{O}(1/t)$  with diminishing stepsize  $\eta_t pprox 1/t$ 



#### Proof of Theorem 2

Using the SGD update rule, we have (compare with GD proof steps)

$$\begin{aligned} ||\mathbf{x}^{t+1} - \mathbf{x}^*||_2^2 &= ||\mathbf{x}^t - \eta_t g(\mathbf{x}^t; \xi^t) - \mathbf{x}^*||_2^2 \\ &= ||\mathbf{x}^t - \mathbf{x}^*||_2^2 - 2\eta_t (\mathbf{x}^t - \mathbf{x}^*)^\top g(\mathbf{x}^t; \xi^t) + \eta_t^2 ||g(\mathbf{x}^t; \xi^t)||_2^2 \; (\star) \end{aligned}$$

Since  $\mathbf{x}^t$  is independent of  $\xi_t$ , apply the law of total expectation to obtain

$$\mathbb{E}[(\mathbf{x}^{t} - \mathbf{x}^{*})^{\top} g(\mathbf{x}^{t}; \xi^{t})] = \mathbb{E}[\mathbb{E}[(\mathbf{x}^{t} - \mathbf{x}^{*})^{\top} g(\mathbf{x}^{t}; \xi^{t}) | \xi_{1}, \dots, \xi_{t-1}]]$$

$$= \mathbb{E}[(\mathbf{x}^{t} - \mathbf{x}^{*})^{\top} \mathbb{E}[g(\mathbf{x}^{t}; \xi^{t}) | \xi_{1}, \dots, \xi_{t-1}]]$$

$$= \mathbb{E}[(\mathbf{x}^{t} - \mathbf{x}^{*})^{\top} \nabla F(\mathbf{x}^{t})] \qquad (\diamond)$$



# Proof of Theorem 2 (cont.)

Furthermore, strong convexity gives

$$\begin{split} \langle \nabla F(\mathbf{x}^t), \mathbf{x}^t - \mathbf{x}^* \rangle &= \langle \nabla F(\mathbf{x}^t) - \underbrace{\nabla F(\mathbf{x}^*)}_{\mathbf{0}}, \mathbf{x}^t - \mathbf{x}^* \rangle \geq \mu ||\mathbf{x}^t - \mathbf{x}^*||_2^2 \\ \implies \mathbb{E}[\langle \nabla F(\mathbf{x}^t), \mathbf{x}^t - \mathbf{x}^* \rangle] \geq \mu \mathbb{E}[||\mathbf{x}^t - \mathbf{x}^*||_2^2] \end{split}$$

Combine the above inequalities and (2) (with  $c_g = 0$ ) to obtain

$$\mathbb{E}[||\mathbf{x}^{t+1} - \mathbf{x}^*||_2^2] \leq (1 - 2\mu\eta_t)\mathbb{E}[||\mathbf{x}^t - \mathbf{x}^*||_2^2] + \underbrace{\eta_t^2\sigma_g^2}_{\text{does not vanish unless the property of the p$$

does not vanish unless  $\eta_t{\to}0$ 

Take  $\eta_t = \frac{\theta}{t+1}$  and use induction to conclude the proof (exercise!)



# Optimality\*

- Nemirovski, Yudin '83, Agarwal et al. '11, Raginsky, Rakhlin '11
- Informally, when minimizing strongly convex functions, no algorithm performing t queries to noisy first-order oracles can achieve an accuracy better than the order of 1/t.
  - $\Rightarrow$  SGD with stepsizes  $\eta_t \approx 1/t$  is optimal.



# Optimality\*

— Nemirovski, Yudin '83

More precisely, consider a class of problems in which f is  $\mu$ -strongly convex and L-smooth, and  $Var(||g(\mathbf{x}^t; \xi^t)||_2) \leq \sigma^2$ . Then the worst-case iteration complexity for (stochastic) first-order methods:

$$\sqrt{\frac{L}{\mu}}\log\left(\frac{L||\mathbf{x}_0-\mathbf{x}^*||_2^2}{\epsilon}\right) + \frac{\sigma^2}{\mu\epsilon}$$

• for deterministic cases:  $\sigma = 0$ , and hence the lower bound is

$$\sqrt{\frac{L}{\mu}}\log\left(\frac{L||\mathbf{x}_0-\mathbf{x}^*||_2^2}{\epsilon}\right)$$

(achievable by Nesterov's method)



# Optimality\*

- Nemirovski, Yudin '83

More precisely, consider a class of problems in which f is  $\mu$ -strongly convex and L-smooth, and  $Var(||g(\mathbf{x}^t; \xi^t)||_2) \leq \sigma^2$ . Then the worst-case iteration complexity for (stochastic) first-order methods:

$$\sqrt{\frac{L}{\mu}}\log\left(\frac{L||\mathbf{x}_0-\mathbf{x}^*||_2^2}{\epsilon}\right) + \frac{\sigma^2}{\mu\epsilon}$$

• for noisy cases with large  $\sigma$ , the lower bound is dominated by

$$\frac{\sigma^2}{\mu} \cdot \frac{1}{\epsilon}$$



### Comparisons with batch GD

Empirical risk minimization with n samples:

	iteration complexity	per-iteration cost	total comput. cost
batch GD	$\log rac{1}{\epsilon}$	n	$n\log \frac{1}{\epsilon}$
SGD	$rac{1}{\epsilon}$	1	$rac{1}{\epsilon}$

SGD is more appealing for large n and moderate accuracy  $\epsilon$  (in which case  $\frac{1}{\epsilon} < n \log \frac{1}{\epsilon}$ )

⇒ which often arises in the *big data* regime!



### Convex problems

What if we lose strong convexity?

$$\min_{\mathbf{x}} F(\mathbf{x}) := \mathbb{E}[f(\mathbf{x}; \xi)]$$

#### **Assumptions:**

- F: convex
- $\blacksquare \mathbb{E}[||g(\mathbf{x};\xi)||_2^2] \leq \sigma_g^2 \text{ for all } \mathbf{x}$
- $g(\mathbf{x}^t; \xi^t)$  is an unbiased estimate of  $\nabla F(\mathbf{x}^t)$  given  $\{\xi^0, \dots, \xi^{t-1}\}$



# Convex problems

Suppose we return a weighted average

$$\tilde{\mathbf{x}}^t := \sum_{k=0}^t \frac{\eta_k}{\sum_{j=0}^t \eta_j} \mathbf{x}^k$$

**Theorem 3** Under the assumptions in the previous slide, then

$$\mathbb{E}[F(\tilde{\mathbf{x}}^t) - F(\mathbf{x}^*)] \le \frac{\frac{1}{2}\mathbb{E}[||\mathbf{x}^0 - \mathbf{x}^*||_2^2] + \frac{1}{2}\sigma_g^2 \sum_{k=0}^t \eta_k^2}{\sum_{k=0}^t \eta_k}$$

• if  $\eta_t \approx 1/\sqrt{t}$ , then

$$\mathbb{E}[F(\tilde{\mathbf{x}}^t) - F(\mathbf{x}^*)] \le \frac{\log t}{\sqrt{t}}$$



#### Proof of Theorem 3

By convexity of  $F(\mathbf{x})$ , we have  $F(\mathbf{x}) \geq F(\mathbf{x}^t) + (\mathbf{x} - \mathbf{x}^t)^\top \nabla F(\mathbf{x}^t)$ 

$$\implies \mathbb{E}[(\mathbf{x}^t - \mathbf{x}^*)^\top \nabla F(\mathbf{x}^t)] \ge \mathbb{E}[F(\mathbf{x}^t) - F(\mathbf{x}^*)]$$

This together with  $(\star)$  and  $(\diamond)$  in Proof of Theorem 2 implies

$$2\eta_k \mathbb{E}[F(\mathbf{x}^k) - F(\mathbf{x}^*)] \le \mathbb{E}[||\mathbf{x}^k - \mathbf{x}^*||_2^2] - \mathbb{E}[||\mathbf{x}^{k+1} - \mathbf{x}^*||_2^2] + \eta_k^2 \sigma_g^2$$

Sum over  $k = 0, \ldots, t$  to obtain

$$\sum_{k=0}^{t} 2\eta_{k} \mathbb{E}[F(\mathbf{x}^{k}) - F(\mathbf{x}^{*})] \leq \mathbb{E}[||\mathbf{x}^{0} - \mathbf{x}^{*}||_{2}^{2}] - \mathbb{E}[||\mathbf{x}^{t+1} - \mathbf{x}^{*}||_{2}^{2}] + \sigma_{g}^{2} \sum_{k=0}^{t} \eta_{k}^{2}$$

$$\leq \mathbb{E}[||\mathbf{x}^{0} - \mathbf{x}^{*}||_{2}^{2}] + \sigma_{g}^{2} \sum_{k=0}^{t} \eta_{k}^{2}$$



# Proof of Theorem 3 (cont.)

Setting  $v_t = \frac{\eta_t}{\sum_{k=0}^t \eta_k}$  yields

$$\sum_{k=0}^{t} v_k \mathbb{E}[F(\mathbf{x}^k) - F(\mathbf{x}^*)] \le \frac{\frac{1}{2} \mathbb{E}[||\mathbf{x}^0 - \mathbf{x}^*||_2^2] + \frac{1}{2} \sigma_g^2 \sum_{k=0}^{t} \eta_k^2}{\sum_{k=0}^{t} \eta_k}$$

By convexity of  $F(\mathbf{x})$ , we arrive at

$$\mathbb{E}[F(\tilde{\mathbf{x}}^{t}) - F(\mathbf{x}^{*})] \leq \sum_{k=0}^{t} v_{k} \mathbb{E}[F(\mathbf{x}^{k}) - F(\mathbf{x}^{*})]$$

$$\leq \frac{\frac{1}{2} \mathbb{E}[||\mathbf{x}^{0} - \mathbf{x}^{*}||_{2}^{2}] + \frac{1}{2} \sigma_{g}^{2} \sum_{k=0}^{t} \eta_{k}^{2}}{\sum_{k=0}^{t} \eta_{k}}$$



### Recap and fine-tuning

- What we have talked about today?
  - ⇒ Why we need SGD and how it works?
  - ⇒ What is its convergence properties?



Welcome anonymous survey!



#### Reference

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