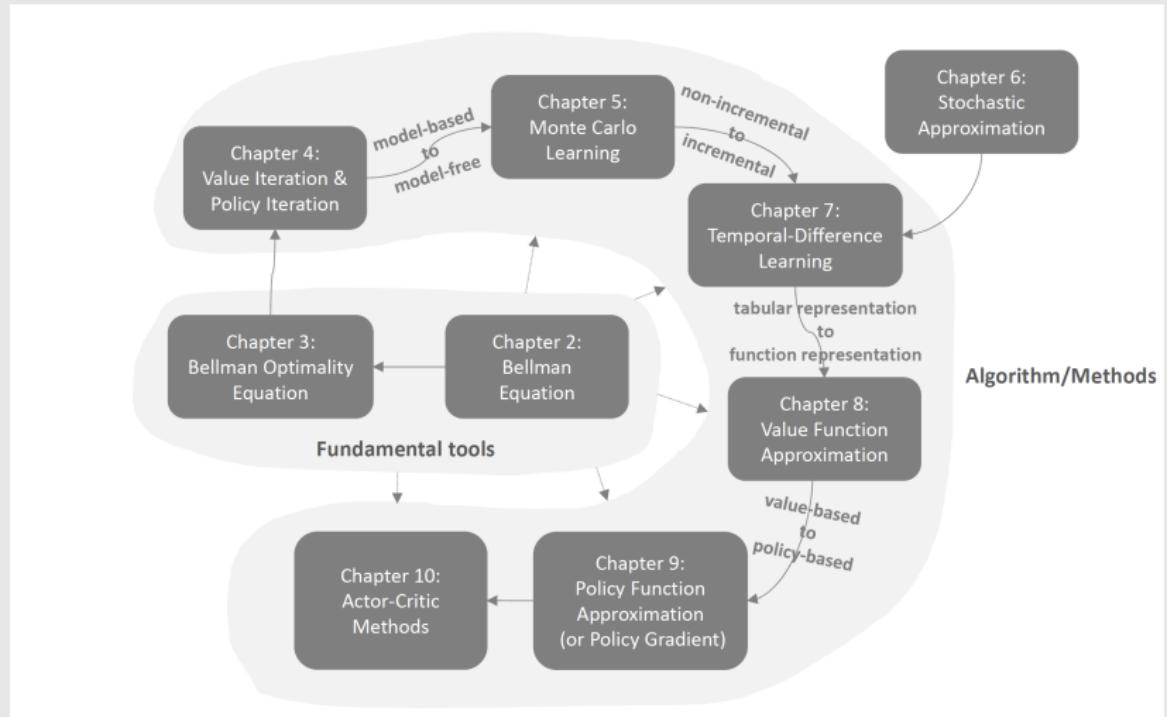


Lecture 6:  
Stochastic Approximation  
and  
Stochastic Gradient Descent

Shiyu Zhao

# Outline



# Introduction

- In the last lecture, we introduced Monte-Carlo learning.
- In the next lecture, we will introduce temporal-difference (TD) learning.
- In this lecture, we press the pause button to get us better prepared.

Why?

- The ideas and expressions of TD algorithms are very different from the algorithms we studied so far.
- Many students who see the TD algorithms the first time many wonder why these algorithms were designed in the first place and why they work effectively.
- There is a knowledge gap!

# Introduction

In this lecture,

- We fill the knowledge gap between the previous and upcoming lectures by introducing basic stochastic approximation (SA) algorithms.
- We will see in the next lecture that the temporal-difference algorithms are special SA algorithms. As a result, it will be much easier to understand these algorithms.

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# Motivating example: mean estimation, again

## Revisit the mean estimation problem:

- Consider a random variable  $X$ .
- Our aim is to estimate  $\mathbb{E}[X]$ .
- Suppose that we collected a sequence of iid samples  $\{x_i\}_{i=1}^N$ .
- The expectation of  $X$  can be approximated by

$$\mathbb{E}[X] \approx \bar{x} := \frac{1}{N} \sum_{i=1}^N x_i.$$

## We already know from the last lecture:

- This approximation is the basic idea of Monte Carlo estimation.
- We know that  $\bar{x} \rightarrow \mathbb{E}[X]$  as  $N \rightarrow \infty$ .

## Why do we care about mean estimation so much?

- Many values in RL such as state/action values are defined as means.

# Motivating example: mean estimation

**New question:** how to calculate the mean  $\bar{x}$ ?

$$\mathbb{E}[X] \approx \bar{x} := \frac{1}{N} \sum_{i=1}^N x_i.$$

We have two ways.

- **The first way**, which is trivial, is to collect all the samples then calculate the average.
- The **drawback** of such way is that, if the samples are collected one by one over a period of time, we have to wait until all the samples to be collected.
- **The second way** can avoid this drawback because it calculates the average in an **incremental** and **iterative** manner.

# Motivating example: mean estimation

In particular, suppose

$$w_{k+1} = \frac{1}{k} \sum_{i=1}^k x_i, \quad k = 1, 2, \dots$$

and hence

$$w_k = \frac{1}{k-1} \sum_{i=1}^{k-1} x_i, \quad k = 2, 3, \dots$$

Then,  $w_{k+1}$  can be expressed in terms of  $w_k$  as

$$\begin{aligned} w_{k+1} &= \frac{1}{k} \sum_{i=1}^k x_i = \frac{1}{k} \left( \sum_{i=1}^{k-1} x_i + x_k \right) \\ &= \frac{1}{k} ((k-1)w_k + x_k) = w_k - \frac{1}{k}(w_k - x_k). \end{aligned}$$

Therefore, we obtain the following iterative algorithm:

$$w_{k+1} = w_k - \frac{1}{k}(w_k - x_k).$$

## Motivating example: mean estimation

We can use

$$w_{k+1} = w_k - \frac{1}{k}(w_k - x_k).$$

to calculate the mean  $\bar{x}$  incrementally:

$$w_1 = x_1,$$

$$w_2 = w_1 - \frac{1}{1}(w_1 - x_1) = x_1,$$

$$w_3 = w_2 - \frac{1}{2}(w_2 - x_2) = x_1 - \frac{1}{2}(x_1 - x_2) = \frac{1}{2}(x_1 + x_2),$$

$$w_4 = w_3 - \frac{1}{3}(w_3 - x_3) = \frac{1}{3}(x_1 + x_2 + x_3),$$

⋮

$$w_{k+1} = \frac{1}{k} \sum_{i=1}^k x_i.$$

# Motivating example: mean estimation

Remarks about this algorithm:

$$w_{k+1} = w_k - \frac{1}{k}(w_k - x_k).$$

- An advantage of this algorithm is that a mean estimate can be obtained immediately once a sample is received. Then, the mean estimate can be used for other purposes immediately.
- The mean estimate is not accurate in the beginning due to insufficient samples (that is  $w_k \neq \mathbb{E}[X]$ ). However, it is better than nothing. As more samples are obtained, the estimate can be improved gradually (that is  $w_k \rightarrow \mathbb{E}[X]$  as  $k \rightarrow \infty$ ).

## Motivating example: mean estimation

Furthermore, consider an algorithm with a more general expression:

$$w_{k+1} = w_k - \alpha_k (w_k - x_k),$$

where  $1/k$  is replaced by  $\alpha_k > 0$ .

- Does this algorithm still converge to the mean  $\mathbb{E}[X]$ ? We will show that the answer is yes if  $\{\alpha_k\}$  satisfy some mild conditions.
- We will also show that this algorithm is a special **SA algorithm** and also a special **stochastic gradient descent algorithm**.
- In the next lecture, we will see that the temporal-difference algorithms have similar (but more complex) expressions.

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# Robbins-Monro algorithm

Stochastic approximation (SA):

- SA refers to a broad class of stochastic iterative algorithms solving root finding or optimization problems.
- Compared to many other root-finding algorithms such as gradient-based methods, SA is powerful in the sense that it does not require to know the expression of the objective function nor its derivative.

Robbins-Monro (RM) algorithm:

- The is a pioneering work in the field of stochastic approximation.
- The famous stochastic gradient descent algorithm is a special form of the RM algorithm.
- It can be used to analyze the mean estimation algorithms introduced in the beginning.

## Robbins-Monro algorithm – Problem statement

**Problem statement:** Suppose we would like to find the root of the equation

$$g(w) = 0,$$

where  $w \in \mathbb{R}$  is the variable to be solved and  $g : \mathbb{R} \rightarrow \mathbb{R}$  is a function.

- Many problems can be eventually converted to this root finding problem. For example, suppose  $J(w)$  is an objective function to be minimized. Then, the optimization problem can be converged to

$$g(w) = \nabla_w J(w) = 0$$

- Note that an equation like  $g(w) = c$  with  $c$  as a constant can also be converted to the above equation by rewriting  $g(w) - c$  as a new function.

# Robbins-Monro algorithm – Problem statement

**How to calculate the root of  $g(w) = 0$ ?**

- If the expression of  $g$  or its derivative is known, there are many numerical algorithms that can solve this problem.
- What if the expression of the function  $g$  is unknown? For example, the function is represented by an artificial neuron network.

# Robbins-Monro algorithm – The algorithm

The Robbins-Monro (RM) algorithm can solve this problem:

$$w_{k+1} = w_k - a_k \tilde{g}(w_k, \eta_k), \quad k = 1, 2, 3, \dots$$

where

- $w_k$  is the  $k$ th estimate of the root
- $\tilde{g}(w_k, \eta_k) = g(w_k) + \eta_k$  is the  $k$ th noisy observation
- $a_k$  is a positive coefficient.

The function  $g(w)$  is a **black box!** This algorithm relies on data:

- Input sequence:  $\{w_k\}$
- Noisy output sequence:  $\{\tilde{g}(w_k, \eta_k)\}$

**Philosophy:** without model, we need data!

- Here, the model refers to the expression of the function.

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# Robbins-Monro algorithm – Illustrative examples

**Excise:** manually solve  $g(w) = w - 10$  using the RM algorithm.

**Set:**  $w_1 = 20$ ,  $a_k \equiv 0.5$ ,  $\eta_k = 0$  (i.e., no observation error)

$$w_1 = 20 \implies g(w_1) = 10$$

$$w_2 = w_1 - a_1 g(w_1) = 20 - 0.5 * 10 = 15 \implies g(w_2) = 5$$

$$w_3 = w_2 - a_2 g(w_2) = 15 - 0.5 * 5 = 12.5 \implies g(w_3) = 2.5$$

⋮

$$w_k \rightarrow 10$$

Excises:

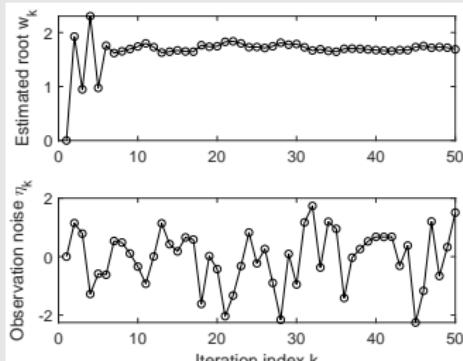
- What if  $a_k = 1$ ?
- What if  $a_k = 2$ ?

# Robbins-Monro algorithm – Illustrative examples

Another example: solve  $g(w) = w^3 - 5$  using the RM algorithm.

- The true root is  $5^{1/3} \approx 1.71$ .
- We only know is  $\tilde{g}(w) = g(w) + \eta$ .
- Suppose  $\eta_k$  is iid and obeys a standard normal distribution with a mean of zero and standard deviation of 1.
- The initial guess is  $w_1 = 0$  and  $a_k$  is selected to be  $a_k = 1/k$ .

The evolution of  $w_k$  is shown in the figure. As can be seen, the estimate  $w_k$  can converge to the true root.



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## Robbins-Monro algorithm – Convergence properties

Why can the RM algorithm find the root of  $g(w) = 0$ ?

- First present an illustrative example.
- Second give the rigorous convergence analysis.

# Robbins-Monro algorithm – Convergence properties

An illustrative example:

- $g(w) = \tanh(w - 1)$
- The true root of  $g(w) = 0$  is  $w^* = 1$ .
- Parameters:  $w_1 = 3$ ,  $a_k = 1/k$ ,  $\eta_k \equiv 0$  (no noise for the sake of simplicity)

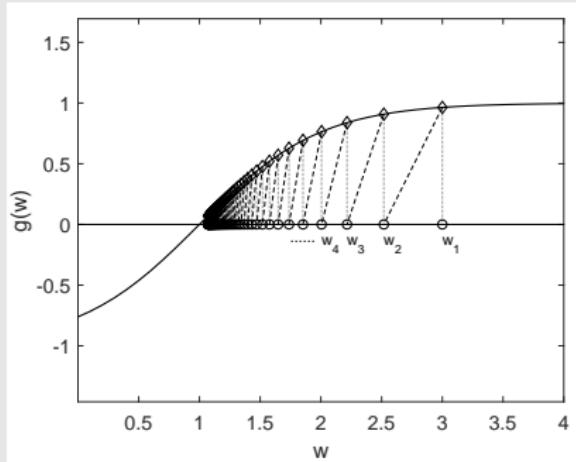
The RM algorithm in this case is

$$w_{k+1} = w_k - a_k g(w_k)$$

since  $\tilde{g}(w_k, \eta_k) = g(w_k)$  when  $\eta_k = 0$ .

# Robbins-Monro algorithm – Convergence properties

Simulation result:  $w_k$  converges to the true root  $w^* = 1$ .



Intuition:  $w_{k+1}$  is closer to  $w^*$  than  $w_k$ .

- When  $w_k > w^*$ , we have  $g(w_k) > 0$ . Then,

$$w_{k+1} = w_k - a_k g(w_k) < w_k \text{ and hence } w_{k+1} \text{ is closer to } w^* \text{ than } w_k.$$

- When  $w_k < w^*$ , we have  $g(w_k) < 0$ . Then,

$$w_{k+1} = w_k - a_k g(w_k) > w_k \text{ and } w_{k+1} \text{ is closer to } w^* \text{ than } w_k.$$

# Robbins-Monro algorithm – Convergence properties

The above analysis is intuitive, but not rigorous. A rigorous convergence result is given below.

## Theorem (Robbins-Monro Theorem)

*In the Robbins-Monro algorithm, if*

- 1)  $0 < c_1 \leq \nabla_w g(w) \leq c_2$  for all  $w$ ;
- 2)  $\sum_{k=1}^{\infty} a_k = \infty$  and  $\sum_{k=1}^{\infty} a_k^2 < \infty$ ;
- 3)  $\mathbb{E}[\eta_k | \mathcal{H}_k] = 0$  and  $\mathbb{E}[\eta_k^2 | \mathcal{H}_k] < \infty$ ;

*where  $\mathcal{H}_k = \{w_k, w_{k-1}, \dots\}$ , then  $w_k$  converges with probability 1 (w.p.1) to the root  $w^*$  satisfying  $g(w^*) = 0$ .*

# Robbins-Monro algorithm – Convergence properties

Explanation of the three conditions:

- $0 < c_1 \leq \nabla_w g(w) \leq c_2$  for all  $w$

This condition indicates

- $g$  to be monotonically increasing, which ensures that the root of  $g(w) = 0$  exists and is unique
- The gradient is bounded from the above.
- $\sum_{k=1}^{\infty} a_k = \infty$  and  $\sum_{k=1}^{\infty} a_k^2 < \infty$
- The condition of  $\sum_{k=1}^{\infty} a_k^2 < \infty$  ensures that  $a_k$  converges to zero as  $k \rightarrow \infty$ .
- The condition of  $\sum_{k=1}^{\infty} a_k = \infty$  ensures that  $a_k$  do not converge to zero too fast.
- $\mathbb{E}[\eta_k | \mathcal{H}_k] = 0$  and  $\mathbb{E}[\eta_k^2 | \mathcal{H}_k] < \infty$ 
  - A special yet common case is that  $\{\eta_k\}$  is an iid stochastic sequence satisfying  $\mathbb{E}[\eta_k] = 0$  and  $\mathbb{E}[\eta_k^2] < \infty$ . The observation error  $\eta_k$  is not required to be Gaussian.

# Robbins-Monro algorithm – Convergence properties

Examine the second condition more closely:

$$\sum_{k=1}^{\infty} a_k^2 < \infty \quad \sum_{k=1}^{\infty} a_k = \infty$$

- First,  $\sum_{k=1}^{\infty} a_k^2 < \infty$  indicates that  $a_k \rightarrow 0$  as  $k \rightarrow \infty$ .
- **Why is this condition important?**

Since

$$w_{k+1} - w_k = -a_k \tilde{g}(w_k, \eta_k),$$

- If  $a_k \rightarrow 0$ , then  $a_k \tilde{g}(w_k, \eta_k) \rightarrow 0$  and hence  $w_{k+1} - w_k \rightarrow 0$ .
- We need the fact that  $w_{k+1} - w_k \rightarrow 0$  if  $w_k$  converges eventually.
- If  $w_k \rightarrow w^*$ ,  $g(w_k) \rightarrow 0$  and  $\tilde{g}(w_k, \eta_k)$  is dominant by  $\eta_k$ .

# Robbins-Monro algorithm – Convergence properties

Examine the second condition more closely:

$$\sum_{k=1}^{\infty} a_k^2 < \infty \quad \sum_{k=1}^{\infty} a_k = \infty$$

- Second,  $\sum_{k=1}^{\infty} a_k = \infty$  indicates that  $a_k$  should not converge to zero too fast.
- **Why is this condition important?**

Summarizing  $w_2 = w_1 - a_1 \tilde{g}(w_1, \eta_1)$ ,  $w_3 = w_2 - a_2 \tilde{g}(w_2, \eta_2)$ ,  $\dots$ ,  $w_{k+1} = w_k - a_k \tilde{g}(w_k, \eta_k)$  leads to

$$w_1 - w_{\infty} = \sum_{k=1}^{\infty} a_k \tilde{g}(w_k, \eta_k).$$

Suppose  $w_{\infty} = w^*$ . If  $\sum_{k=1}^{\infty} a_k < \infty$ , then  $\sum_{k=1}^{\infty} a_k \tilde{g}(w_k, \eta_k)$  may be bounded. Then, if the initial guess  $w_1$  is chosen arbitrarily far away from  $w^*$ , then the above equality would be invalid.

# Robbins-Monro algorithm – Convergence properties

What  $\{a_k\}$  satisfies the two conditions?  $\sum_{k=1}^{\infty} a_k^2 < \infty$ ,  $\sum_{k=1}^{\infty} a_k = \infty$

One typical sequence is

$$a_k = \frac{1}{k}$$

- It holds that

$$\lim_{n \rightarrow \infty} \left( \sum_{k=1}^n \frac{1}{k} - \ln n \right) = \kappa,$$

where  $\kappa \approx 0.577$  is called the Euler-Mascheroni constant (also called Euler's constant).

- It is notable that

$$\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6} < \infty.$$

The limit  $\sum_{k=1}^{\infty} 1/k^2$  also has a specific name in the number theory:  
Basel problem.

# Robbins-Monro algorithm – Convergence properties

If the three conditions are not satisfied, the algorithm may not work.

- For example,  $g(w) = w^3 - 5$  does not satisfy the first condition on gradient boundedness. If the initial guess is good, the algorithm can converge (locally). Otherwise, it will diverge.

We will see that  $a_k$  is often selected as a **sufficiently small constant** in many RL algorithms. Although the second condition is not satisfied in this case, the algorithm can still work effectively.

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# Robbins-Monro algorithm – Apply to mean estimation

Recall that

$$w_{k+1} = w_k + \alpha_k(x_k - w_k).$$

is the mean estimation algorithm.

We know that

- If  $\alpha_k = 1/k$ , then  $w_{k+1} = 1/k \sum_{i=1}^k x_i$ .
- If  $\alpha_k$  is not  $1/k$ , the convergence was not analyzed.

Next, we show that this algorithm is a special case of the RM algorithm.

Then, its convergence naturally follows.

# Robbins-Monro algorithm – Apply to mean estimation

1) Consider a function:

$$g(w) \doteq w - \mathbb{E}[X].$$

Our aim is to solve  $g(w) = 0$ . If we can do that, then we can obtain  $\mathbb{E}[X]$ .

2) The observation we can get is

$$\tilde{g}(w, x) \doteq w - x,$$

because we can only obtain samples of  $X$ . Note that

$$\begin{aligned}\tilde{g}(w, \eta) &= w - x = w - x + \mathbb{E}[X] - \mathbb{E}[X] \\ &= (w - \mathbb{E}[X]) + (\mathbb{E}[X] - x) \doteq g(w) + \eta,\end{aligned}$$

3) The RM algorithm for solving  $g(x) = 0$  is

$$w_{k+1} = w_k - \alpha_k \tilde{g}(w_k, \eta_k) = w_k - \alpha_k (w_k - x_k),$$

which is exactly the mean estimation algorithm.

The convergence naturally follows.

# Dvoretzky's convergence theorem (optional)

## Theorem (Dvoretzky's Theorem)

Consider a stochastic process

$$w_{k+1} = (1 - \alpha_k)w_k + \beta_k \eta_k,$$

where  $\{\alpha_k\}_{k=1}^{\infty}$ ,  $\{\beta_k\}_{k=1}^{\infty}$ ,  $\{\eta_k\}_{k=1}^{\infty}$  are stochastic sequences. Here  $\alpha_k \geq 0$ ,  $\beta_k \geq 0$  for all  $k$ . Then,  $w_k$  would converge to zero with probability 1 if the following conditions are satisfied:

- 1)  $\sum_{k=1}^{\infty} \alpha_k = \infty$ ,  $\sum_{k=1}^{\infty} \alpha_k^2 < \infty$ ;  $\sum_{k=1}^{\infty} \beta_k^2 < \infty$  uniformly w.p.1;
- 2)  $\mathbb{E}[\eta_k | \mathcal{H}_k] = 0$  and  $\mathbb{E}[\eta_k^2 | \mathcal{H}_k] \leq C$  w.p.1;

where  $\mathcal{H}_k = \{w_k, w_{k-1}, \dots, \eta_{k-1}, \dots, \alpha_{k-1}, \dots, \beta_{k-1}, \dots\}$ .

- A more general result than the RM theorem. It can be used to prove the RM theorem
- It can also directly analyze the mean estimation problem.
- An extension of it can be used to analyze Q-learning and TD learning algorithms.

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# Stochastic gradient descent

Next, we introduce stochastic gradient descent (SGD) algorithms:

- SGD is widely used in the field of machine learning and also in RL.
- SGD is a special RM algorithm.
- The mean estimation algorithm is a special SGD algorithm.

Suppose we aim to solve the following optimization problem:

$$\min_w J(w) = \mathbb{E}[f(w, X)]$$

- $w$  is the parameter to be optimized.
- $X$  is a random variable. The expectation is with respect to  $X$ .
- $w$  and  $X$  can be either scalars or vectors. The function  $f(\cdot)$  is a scalar.

# Stochastic gradient descent

## Method 1: gradient descent (GD)

$$w_{k+1} = w_k - \alpha_k \nabla_w \mathbb{E}[f(w_k, X)] = w_k - \alpha_k \mathbb{E}[\nabla_w f(w_k, X)]$$

Drawback: the expected value is difficult to obtain.

## Method 2: batch gradient descent (BGD)

$$\mathbb{E}[\nabla_w f(w_k, X)] \approx \frac{1}{n} \sum_{i=1}^n \nabla_w f(w_k, x_i).$$

$$w_{k+1} = w_k - \alpha_k \frac{1}{n} \sum_{i=1}^n \nabla_w f(w_k, x_i).$$

Drawback: it requires many samples in each iteration for each  $w_k$ .

# Stochastic gradient descent – Algorithm

## Method 3: stochastic gradient descent (SGD)

$$w_{k+1} = w_k - \alpha_k \nabla_w f(w_k, x_k),$$

- Compared to the gradient descent method: Replace the **true gradient**  $\mathbb{E}[\nabla_w f(w_k, X)]$  by the **stochastic gradient**  $\nabla_w f(w_k, x_k)$ .
- Compared to the batch gradient descent method: let  $n = 1$ .

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# Stochastic gradient descent – Example and application

We next consider an example:

$$\min_w \quad J(w) = \mathbb{E}[f(w, X)] = \mathbb{E} \left[ \frac{1}{2} \|w - X\|^2 \right],$$

where

$$f(w, X) = \|w - X\|^2 / 2 \quad \nabla_w f(w, X) = w - X$$

**Excises:**

- Excise 1: Show that the optimal solution is  $w^* = \mathbb{E}[X]$ .
- Excise 2: Write out the GD algorithm for solving this problem.
- Excise 3: Write out the SGD algorithm for solving this problem.

# Stochastic gradient descent – Example and application

## Answer:

- The GD algorithm for solving the above problem is

$$\begin{aligned}w_{k+1} &= w_k - \alpha_k \nabla_w J(w_k) \\&= w_k - \alpha_k \mathbb{E}[\nabla_w f(w_k, X)] \\&= w_k - \alpha_k \mathbb{E}[w_k - X].\end{aligned}$$

- The SGD algorithm for solving the above problem is

$$w_{k+1} = w_k - \alpha_k \nabla_w f(w_k, x_k) = w_k - \alpha_k (w_k - x_k)$$

- Note:

- It is the same as the mean estimation algorithm we presented before.
- That mean estimation algorithm is a special SGD algorithm.

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# Stochastic gradient descent – Convergence

From GD to SGD:

$$w_{k+1} = w_k - \alpha_k \mathbb{E}[\nabla_w f(w_k, X)]$$



$$w_{k+1} = w_k - \alpha_k \nabla_w f(w_k, x_k)$$

$\nabla_w f(w_k, x_k)$  can be viewed as a noisy measurement of  $\mathbb{E}[\nabla_w f(w, X)]$ :

$$\nabla_w f(w_k, x_k) = \mathbb{E}[\nabla_w f(w, X)] + \underbrace{\nabla_w f(w_k, x_k) - \mathbb{E}[\nabla_w f(w, X)]}_{\eta}.$$

Since

$$\nabla_w f(w_k, x_k) \neq \mathbb{E}[\nabla_w f(w, X)]$$

whether  $w_k \rightarrow w^*$  as  $k \rightarrow \infty$  by SGD?

# Stochastic gradient descent – Convergence

We next show that SGD is a special RM algorithm. Then, the convergence naturally follows.

The aim of SGD is to minimize

$$J(w) = \mathbb{E}[f(w, X)]$$

This problem can be converted to a root-finding problem:

$$\nabla_w J(w) = \mathbb{E}[\nabla_w f(w, X)] = 0$$

Let

$$g(w) = \nabla_w J(w) = \mathbb{E}[\nabla_w f(w, X)].$$

Then, the aim of SGD is to find the root of  $g(w) = 0$ .

# Stochastic gradient descent – Convergence

What we can measure is

$$\begin{aligned}\tilde{g}(w, \eta) &= \nabla_w f(w, x) \\ &= \underbrace{\mathbb{E}[\nabla_w f(w, X)]}_{g(w)} + \underbrace{\nabla_w f(w, x) - \mathbb{E}[\nabla_w f(w, X)]}_{\eta}.\end{aligned}$$

Then, the RM algorithm for solving  $g(w) = 0$  is

$$w_{k+1} = w_k - a_k \tilde{g}(w_k, \eta_k) = w_k - a_k \nabla_w f(w_k, x_k).$$

- It is exactly the SGD algorithm.
- Therefore, SGD is a special RM algorithm.

# Stochastic gradient descent – Convergence

Since SGD is a special RM algorithm, its convergence naturally follows.

## Theorem (Convergence of SGD)

*In the SGD algorithm, if*

- 1)  $0 < c_1 \leq \nabla_w^2 f(w, X) \leq c_2$ ;
- 2)  $\sum_{k=1}^{\infty} a_k = \infty$  and  $\sum_{k=1}^{\infty} a_k^2 < \infty$ ;
- 3)  $\{x_k\}_{k=1}^{\infty}$  is iid;

*then  $w_k$  converges to the root of  $\nabla_w \mathbb{E}[f(w, X)] = 0$  with probability 1.*

For the proof see the book.

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# Stochastic gradient descent – Convergence pattern

**Question:** Since the stochastic gradient is random and hence the approximation is inaccurate, whether the convergence of SGD is slow or random?

To answer this question, we consider the **relative error** between the stochastic and batch gradients:

$$\delta_k \doteq \frac{|\nabla_w f(w_k, x_k) - \mathbb{E}[\nabla_w f(w_k, X)]|}{|\mathbb{E}[\nabla_w f(w_k, X)]|}.$$

Since  $\mathbb{E}[\nabla_w f(w^*, X)] = 0$ , we further have

$$\delta_k = \frac{|\nabla_w f(w_k, x_k) - \mathbb{E}[\nabla_w f(w_k, X)]|}{|\mathbb{E}[\nabla_w f(w_k, X)] - \mathbb{E}[\nabla_w f(w^*, X)]|} = \frac{|\nabla_w f(w_k, x_k) - \mathbb{E}[\nabla_w f(w_k, X)]|}{|\mathbb{E}[\nabla_w^2 f(\tilde{w}_k, X)(w_k - w^*)]|}.$$

where the last equality is due to the mean value theorem and  
 $\tilde{w}_k \in [w_k, w^*]$ .

# Stochastic gradient descent – Convergence pattern

Suppose  $f$  is strictly convex such that

$$\nabla_w^2 f \geq c > 0$$

for all  $w, X$ , where  $c$  is a positive bound.

Then, the denominator of  $\delta_k$  becomes

$$\begin{aligned} |\mathbb{E}[\nabla_w^2 f(\tilde{w}_k, X)(w_k - w^*)]| &= |\mathbb{E}[\nabla_w^2 f(\tilde{w}_k, X)](w_k - w^*)| \\ &= |\mathbb{E}[\nabla_w^2 f(\tilde{w}_k, X)]| |(w_k - w^*)| \geq c|w_k - w^*|. \end{aligned}$$

Substituting the above inequality to  $\delta_k$  gives

$$\delta_k \leq \frac{|\nabla_w f(w_k, x_k) - \mathbb{E}[\nabla_w f(w_k, X)]|}{c|w_k - w^*|}.$$

# Stochastic gradient descent – Convergence pattern

Note that

$$\delta_k \leq \frac{\left| \overbrace{\nabla_w f(w_k, x_k)}^{\text{stochastic gradient}} - \overbrace{\mathbb{E}[\nabla_w f(w_k, X)]}^{\text{true gradient}} \right|}{\underbrace{c|w_k - w^*|}_{\text{distance to the optimal solution}}}.$$

The above equation suggests an interesting convergence pattern of SGD.

- The relative error  $\delta_k$  is inversely proportional to  $|w_k - w^*|$ .
- When  $|w_k - w^*|$  is large,  $\delta_k$  is small and SGD behaves like GD.
- When  $w_k$  is close to  $w^*$ , the relative error may be large and the convergence exhibits more randomness in the neighborhood of  $w^*$ .

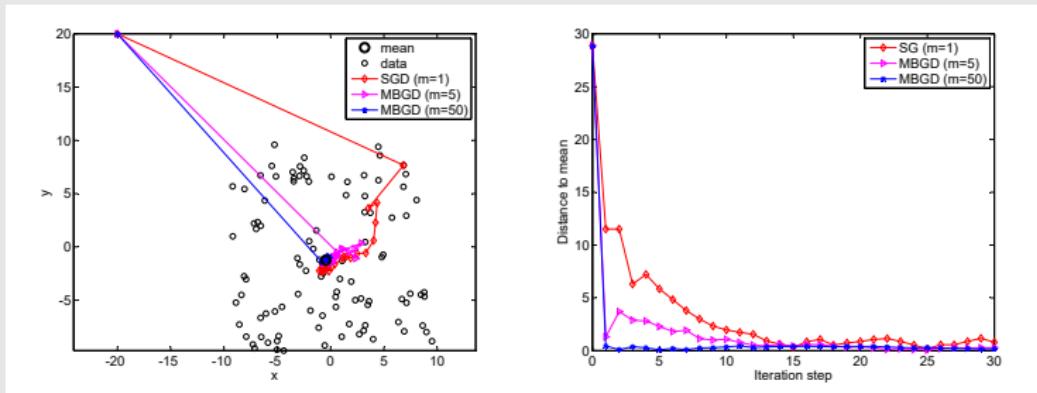
# Stochastic gradient descent – Convergence pattern

Consider an illustrative example:

**Setup:**  $X \in \mathbb{R}^2$  represents a random position in the plane. Its distribution is uniform in the square area centered at the origin with the side length as 20. The true mean is  $\mathbb{E}[X] = 0$ . The mean estimation is based on 100 iid samples  $\{x_i\}_{i=1}^{100}$ .

# Stochastic gradient descent – Convergence pattern

## Result:



- Although the initial guess of the mean is far away from the true value, the SGD estimate can approach the neighborhood of the true value fast.
- When the estimate is close to the true value, it exhibits certain randomness but still approaches the true value gradually.

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# Stochastic gradient descent – A deterministic formulation

- The formulation of SGD we introduced above involves random variables and expectation.
- One may often encounter a **deterministic** formulation of SGD without involving any random variables.

Consider the optimization problem:

$$\min_w J(w) = \frac{1}{n} \sum_{i=1}^n f(w, x_i),$$

- $f(w, x_i)$  is a parameterized function.
- $w$  is the parameter to be optimized.
- a set of real numbers  $\{x_i\}_{i=1}^n$ , where  $x_i$  does not have to be a sample of any random variable.

# Stochastic gradient descent – A deterministic formulation

The gradient descent algorithm for solving this problem is

$$w_{k+1} = w_k - \alpha_k \nabla_w J(w_k) = w_k - \alpha_k \frac{1}{n} \sum_{i=1}^n \nabla_w f(w_k, x_i).$$

Suppose the set is large and we can only fetch a single number every time. In this case, we can use the following iterative algorithm:

$$w_{k+1} = w_k - \alpha_k \nabla_w f(w_k, x_k).$$

## Questions:

- Is this algorithm SGD? It does not involve any random variables or expected values.
- How should we use the finite set of numbers  $\{x_i\}_{i=1}^n$ ? Should we sort these numbers in a certain order and then use them one by one? Or should we randomly sample a number from the set?

# Stochastic gradient descent – A deterministic formulation

A quick answer to the above questions is that we can introduce a random variable manually and convert the *deterministic formulation* to the *stochastic formulation* of SGD.

In particular, suppose  $X$  is a random variable defined on the set  $\{x_i\}_{i=1}^n$ . Suppose its probability distribution is uniform such that

$$p(X = x_i) = 1/n$$

Then, the deterministic optimization problem becomes a stochastic one:

$$\min_w J(w) = \frac{1}{n} \sum_{i=1}^n f(w, x_i) = \mathbb{E}[f(w, X)].$$

- The last equality in the above equation is strict instead of approximate. Therefore, the algorithm is SGD.
- The estimate converges if  $x_k$  is *uniformly* and independently sampled from  $\{x_i\}_{i=1}^n$ .  $x_k$  may repeatedly take the same number in  $\{x_i\}_{i=1}^n$  since it is sampled randomly.

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# BGD, MBGD, and SGD

Suppose we would like to minimize  $J(w) = \mathbb{E}[f(w, X)]$  given a set of random samples  $\{x_i\}_{i=1}^n$  of  $X$ . The BGD, SGD, MBGD algorithms solving this problem are, respectively,

$$w_{k+1} = w_k - \alpha_k \frac{1}{n} \sum_{i=1}^n \nabla_w f(w_k, x_i), \quad (\text{BGD})$$

$$w_{k+1} = w_k - \alpha_k \frac{1}{m} \sum_{j \in \mathcal{I}_k} \nabla_w f(w_k, x_j), \quad (\text{MBGD})$$

$$w_{k+1} = w_k - \alpha_k \nabla_w f(w_k, x_k). \quad (\text{SGD})$$

- **In the BGD algorithm**, all the samples are used in every iteration. When  $n$  is large,  $(1/n) \sum_{i=1}^n \nabla_w f(w_k, x_i)$  is close to the true gradient  $\mathbb{E}[\nabla_w f(w_k, X)]$ .
- **In the MBGD algorithm**,  $\mathcal{I}_k$  is a subset of  $\{1, \dots, n\}$  with the size as  $|\mathcal{I}_k| = m$ . The set  $\mathcal{I}_k$  is obtained by  $m$  times iid samplings.
- **In the SGD algorithm**,  $x_k$  is randomly sampled from  $\{x_i\}_{i=1}^n$  at time  $k$ .

# BGD, MBGD, and SGD

Compare MBGD with BGD and SGD:

- Compared to SGD, MBGD has less randomness because it uses more samples instead of just one as in SGD.
- Compared to BGD, MBGD does not require to use all the samples in every iteration, making it more flexible and efficient.
- If  $m = 1$ , MBGD becomes SGD.
- If  $m = n$ , MBGD does NOT become BGD strictly speaking because MBGD uses randomly fetched  $n$  samples whereas BGD uses all  $n$  numbers. In particular, MBGD may use a value in  $\{x_i\}_{i=1}^n$  multiple times whereas BGD uses each number once.

# BGD, MBGD, and SGD – Illustrative examples

Given some numbers  $\{x_i\}_{i=1}^n$ , our aim is to calculate the mean  $\bar{x} = \sum_{i=1}^n x_i/n$ . This problem can be equivalently stated as the following optimization problem:

$$\min_w J(w) = \frac{1}{2n} \sum_{i=1}^n \|w - x_i\|^2$$

The three algorithms for solving this problem are, respectively,

$$w_{k+1} = w_k - \alpha_k \frac{1}{n} \sum_{i=1}^n (w_k - x_i) = w_k - \alpha_k (w_k - \bar{x}), \quad (\text{BGD})$$

$$w_{k+1} = w_k - \alpha_k \frac{1}{m} \sum_{j \in \mathcal{I}_k} (w_k - x_j) = w_k - \alpha_k \left( w_k - \bar{x}_k^{(m)} \right), \quad (\text{MBGD})$$

$$w_{k+1} = w_k - \alpha_k (w_k - x_k), \quad (\text{SGD})$$

where  $\bar{x}_k^{(m)} = \sum_{j \in \mathcal{I}_k} x_j / m$ .

## BGD, MBGD, and SGD

Furthermore, if  $\alpha_k = 1/k$ , the above equation can be solved as

$$w_{k+1} = \frac{1}{k} \sum_{j=1}^k \bar{x} = \bar{x}, \quad (\text{BGD})$$

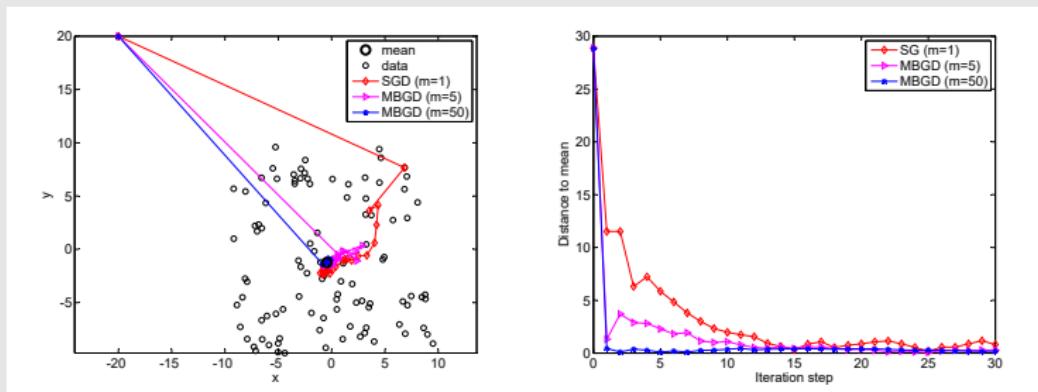
$$w_{k+1} = \frac{1}{k} \sum_{j=1}^k \bar{x}_j^{(m)}, \quad (\text{MBGD})$$

$$w_{k+1} = \frac{1}{k} \sum_{j=1}^k x_j. \quad (\text{SGD})$$

- The estimate of BGD at each step is exactly the optimal solution  
 $w^* = \bar{x}$ .
- The estimate of MBGD approaches the mean faster than SGD because  $\bar{x}_k^{(m)}$  is already an average.

# BGD, MBGD, and SGD

Let  $\alpha_k = 1/k$ . Given 100 points, using different mini-batch sizes leads to different convergence speed.



**Figure:** An illustrative example for mean estimation by different GD algorithms.

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# Summary

- Mean estimation: compute  $\mathbb{E}[X]$  using  $\{x_k\}$

$$w_{k+1} = w_k - \frac{1}{k}(w_k - x_k).$$

- RM algorithm: solve  $g(w) = 0$  using  $\{\tilde{g}(w_k, \eta_k)\}$

$$w_{k+1} = w_k - a_k \tilde{g}(w_k, \eta_k)$$

- SGD algorithm: minimize  $J(w) = \mathbb{E}[f(w, X)]$  using  $\{\nabla_w f(w_k, x_k)\}$

$$w_{k+1} = w_k - \alpha_k \nabla_w f(w_k, x_k),$$

These results are useful:

- We will see in the next chapter that the temporal-difference learning algorithms can be viewed as stochastic approximation algorithms and hence have similar expressions.
- They are important optimization techniques that can be applied to many other fields.