Lecture 6:
Stochastic Approximation
and
Stochastic Gradient Descent

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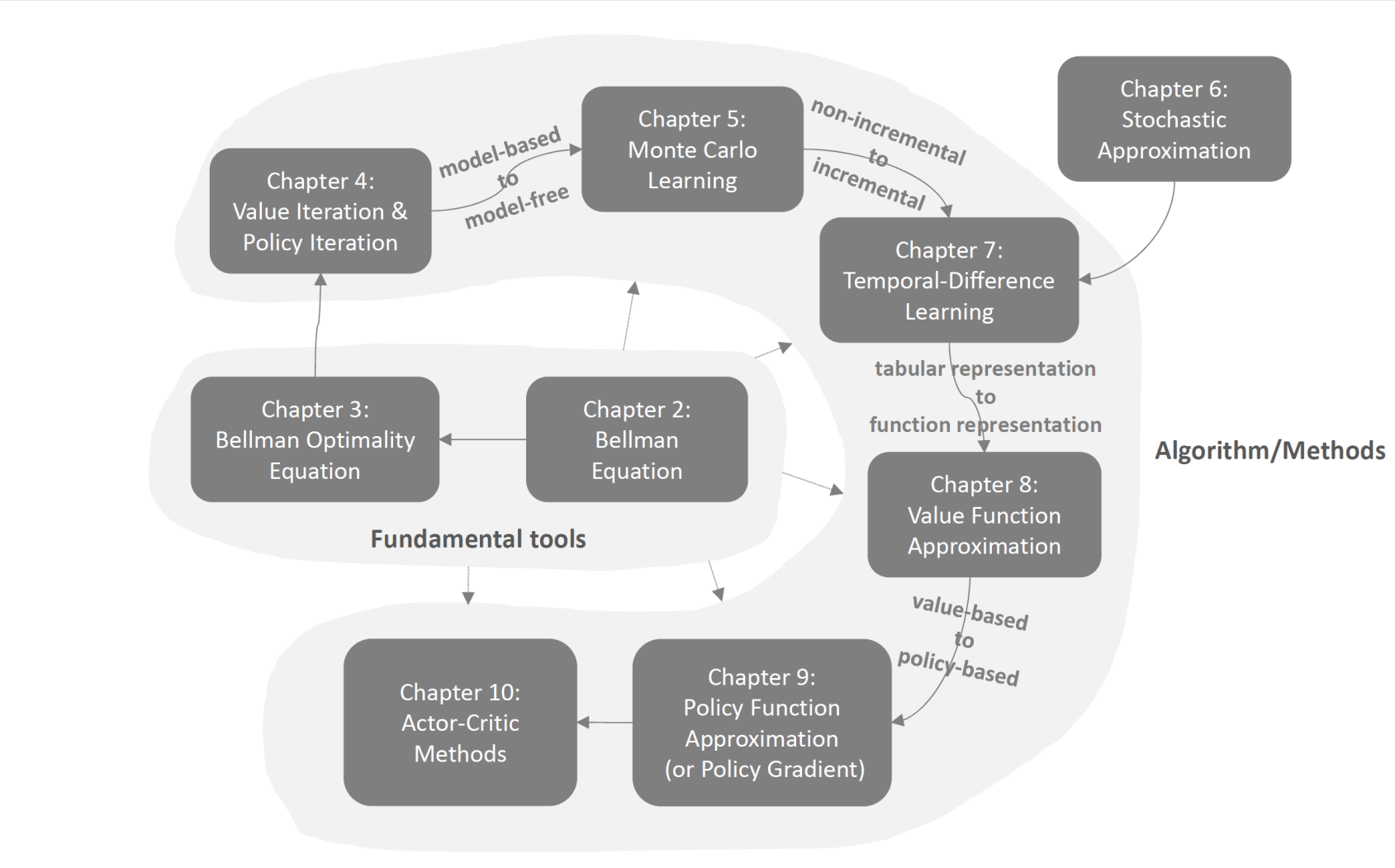
Outline


Chapter 4:
Value Iteration &
Policy Iteration
model-based
to
model-free
Chapter 5:
Monte Carlo
Learning
non-incremental
to
incremental
Chapter 6:
Stochastic
Approximation
Chapter 7:
Temporal-Difference
Learning
tabular representation
to
function representation
Chapter 3:
Bellman Optimality
Equation
Chapter 2:
Bellman
Equation
Fundamental tools
Chapter 8:
Value Function
Approximation
Algorithm/Methods
value-based
to
policy-based
Chapter 10:
Actor-Critic
Methods
Chapter 9:
Policy Function
Approximation
(or Policy Gradient)

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.

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
3. Stochastic gradient descent
   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
   - A deterministic formulation
4. BGD, MBGD, and SGD
5. Summary

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
3. Stochastic gradient descent
   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
   - A deterministic formulation
4. BGD, MBGD, and SGD
5. Summary

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 $\bar{x} \to \mathbb{E}[X]$ as $N \to \infty$.

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

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

and hence

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

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:

$$\begin{aligned}
w_1 &= x_1, \\
w_2 &= w_1 - \frac{1}{1}(w_1 - x_1) = x_1, \\
w_3 &= w_2 - \frac{1}{2}(w_2 - x_2) = x_1 - \frac{1}{2}(x_1 - x_2) = \frac{1}{2}(x_1 + x_2), \\
w_4 &= w_3 - \frac{1}{3}(w_3 - x_3) = \frac{1}{3}(x_1 + x_2 + x_3), \\
&\vdots \\
w_{k+1} &= \frac{1}{k}\sum_{i=1}^{k} x_i.
\end{aligned}$$

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 $w_k \to \mathbb{E}[X]$ as $k \to \infty$).

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.

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
3. Stochastic gradient descent
   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
   - A deterministic formulation
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5. Summary

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
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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 $g : \mathbb{R} \to \mathbb{R}$ 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:

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

where

- w_k is the kth estimate of the root
- $\tilde{g}(w_k, \eta_k) = g(w_k) + \eta_k$ is the kth 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)

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

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

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

$$\vdots$$

$$w_k \to 10$$

Excises:

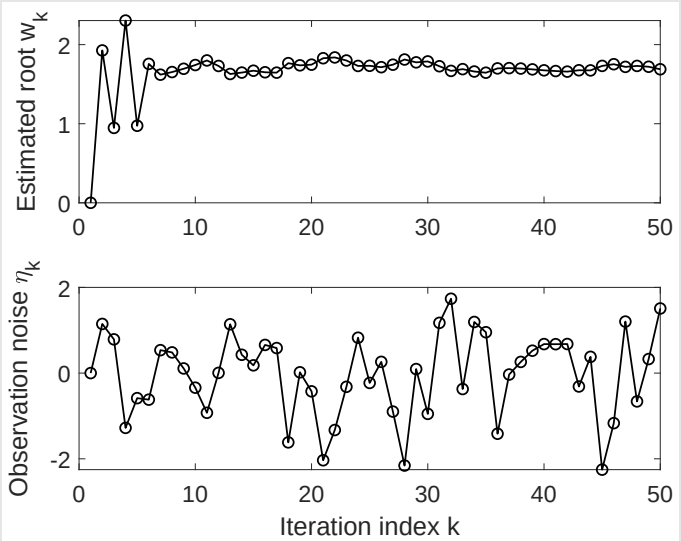
- What if $a_k = 1$?
- What if $a_k = 2$?

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 η_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.



Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
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   - Algorithm description
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5. Summary

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)

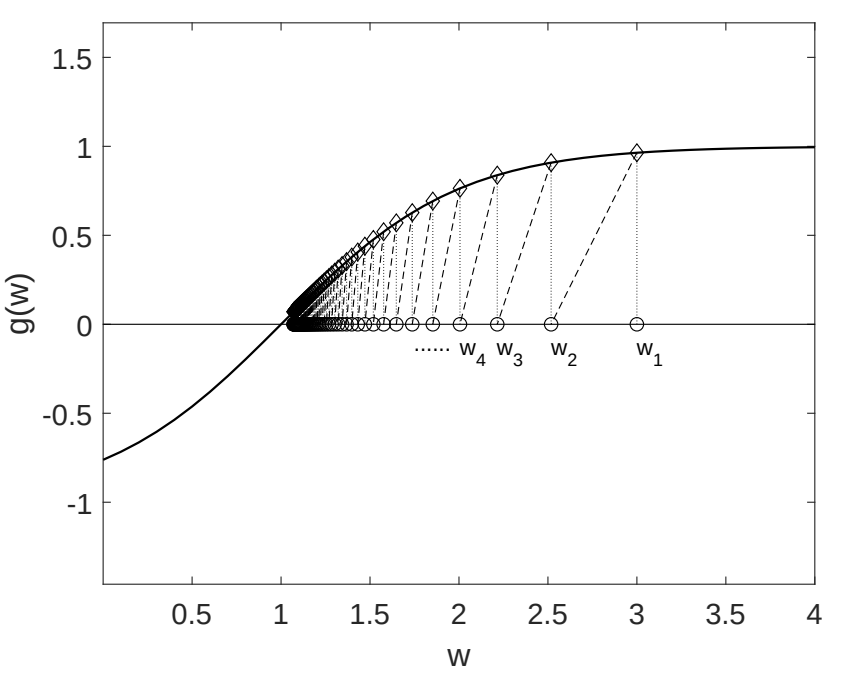
The RM algorithm in this case is

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

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,

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

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

  $w_{k+1} = w_k - a_k g(w_k) > w_k$ and w_{k+1} is closer to w^* 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 $k \to \infty$.
  - 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 η_k is not required to be Gaussian.

Robbins-Monro algorithm – Convergence properties

Examine the second condition more closely:

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

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

  Since

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

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

Robbins-Monro algorithm – Convergence properties

Examine the second condition more closely:

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

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

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

  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.

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
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   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
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4. BGD, MBGD, and SGD
5. Summary

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 α_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.

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

- 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.

Outline

1. Motivating examples
2. Robbins-Monro algorithm
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3. Stochastic gradient descent
   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
   - A deterministic formulation
4. BGD, MBGD, and SGD
5. Summary

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
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   - Convergence pattern
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5. Summary

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:

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

- 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 $n = 1$.

Outline

1. Motivating examples
2. Robbins-Monro algorithm
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3. Stochastic gradient descent
   - Algorithm description
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   - Convergence analysis
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5. Summary

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

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

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.

Outline

1. Motivating examples
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   - Application to mean estimation
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   - Algorithm description
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5. Summary

Stochastic gradient descent – Convergence

From GD to SGD:

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

$$\Downarrow$$

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

$\nabla_w f(w_k, x_k)$ 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 $w_k \to w^*$ as $k \to \infty$ 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.

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
3. Stochastic gradient descent
   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
   - A deterministic formulation
4. BGD, MBGD, and SGD
5. Summary

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 δ_k becomes

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

Substituting the above inequality to δ_k gives

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

Stochastic gradient descent – Convergence pattern

Note that

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

The above equation suggests an interesting convergence pattern of SGD.

- The relative error δ_k is inversely proportional to $|w_k - w^*|$.
- When $|w_k - w^*|$ is large, δ_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^*.

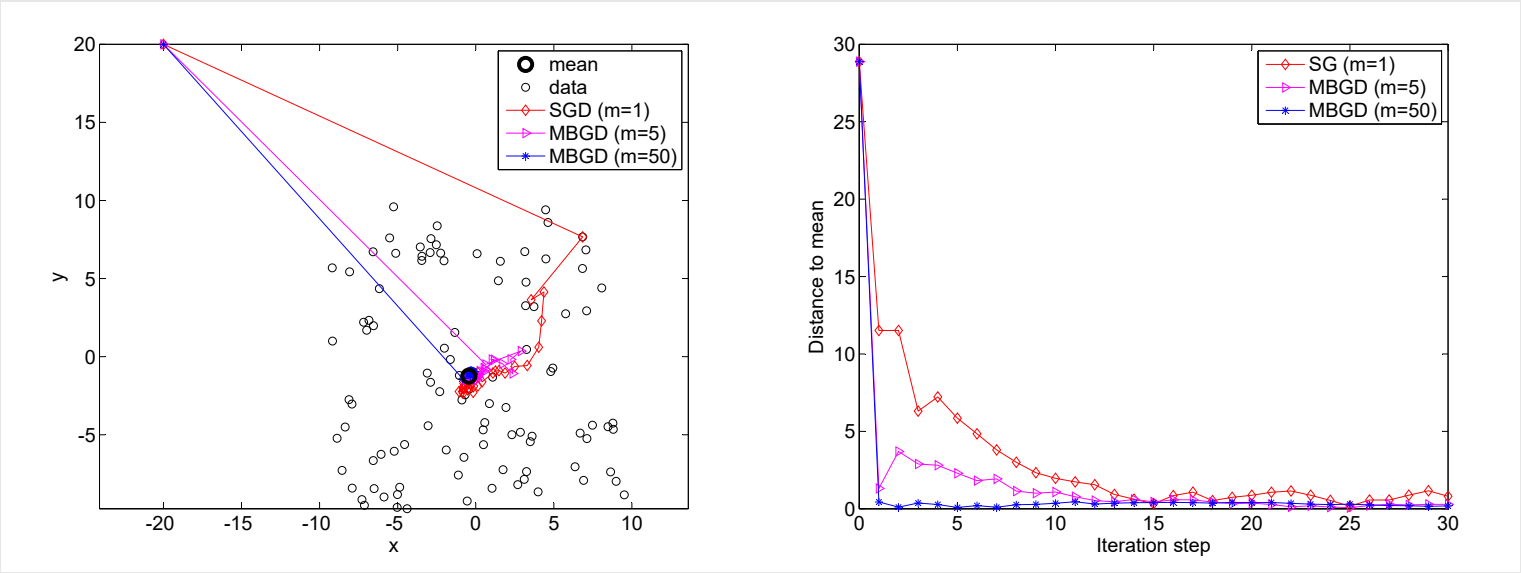
Stochastic gradient descent – Convergence pattern

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.

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
3. Stochastic gradient descent
   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
   - A deterministic formulation
4. BGD, MBGD, and SGD
5. Summary

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:

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

- $f(w, x_i)$ 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:

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

- 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.

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
3. Stochastic gradient descent
   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
   - A deterministic formulation
4. BGD, MBGD, and SGD
5. Summary

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,

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

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

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

- **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 $\{1, \ldots, n\}$ with the size as $|\mathcal{I}_k| = m$. The set $\mathcal{I}_k$ is obtained by m times idd 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:

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

The three algorithms for solving this problem are, respectively,

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

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

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

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

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

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

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

- 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.

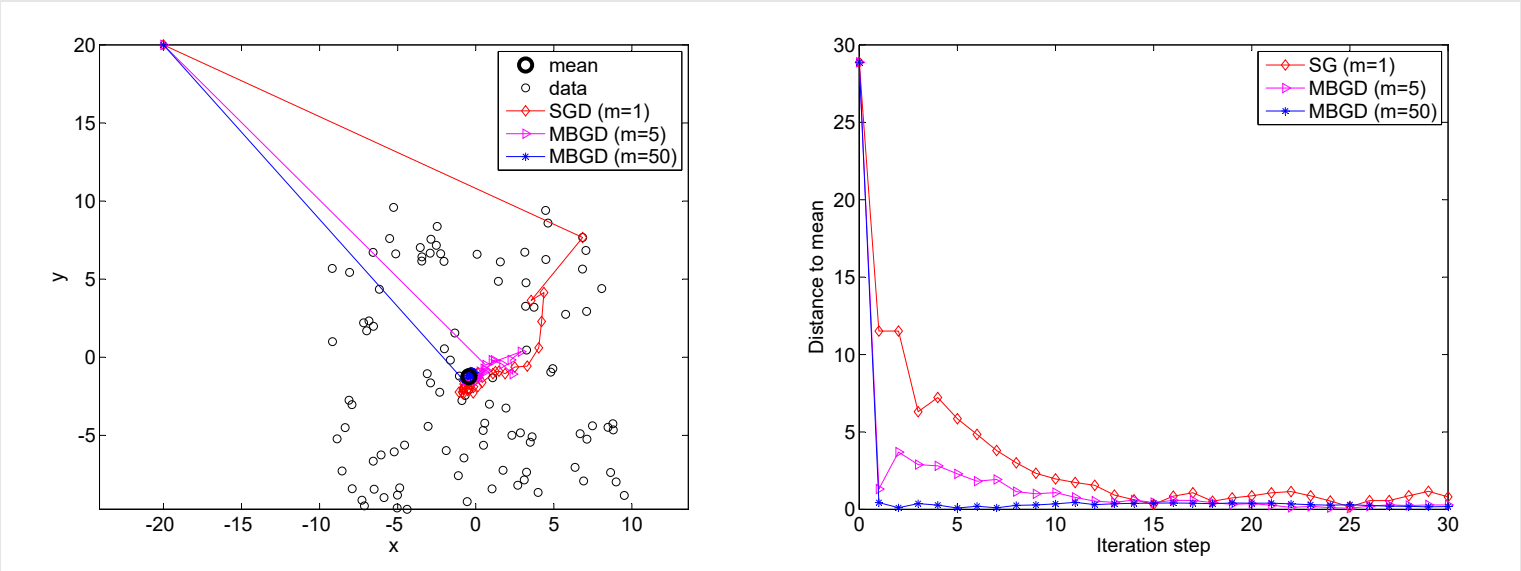


Figure: An illustrative example for mean estimation by different GD algorithms.

Outline

1. Motivating examples
2. Robbins-Monro algorithm
   - Algorithm description
   - Illustrative examples
   - Convergence analysis
   - Application to mean estimation
3. Stochastic gradient descent
   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
   - A deterministic formulation
4. BGD, MBGD, and SGD
5. Summary

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.