Lecture 6: Stochastic Approximation and Stochastic Gradient Descent

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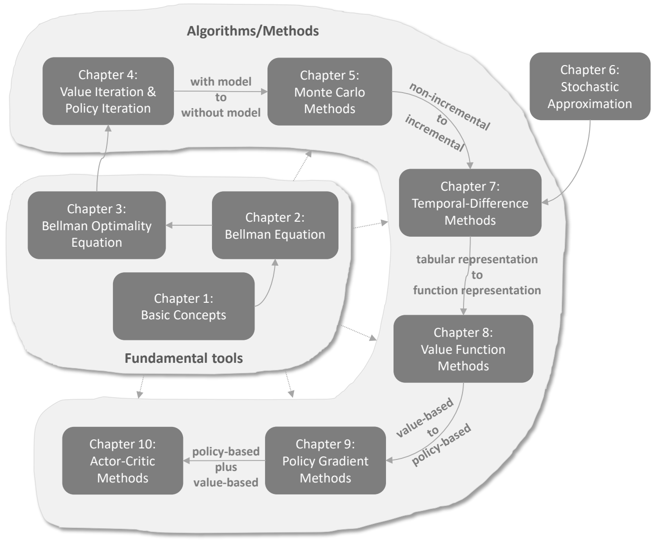
Outline



Algorithms/Methods
Chapter 4: Value Iteration & Policy Iteration
with model to without model
Chapter 5: Monte Carlo Methods
non-incremental to incremental
Chapter 6: Stochastic Approximation
Chapter 7: Temporal-Difference Methods
tabular representation to function representation
Chapter 8: Value Function Methods
value-based to policy-based
Chapter 9: Policy Gradient Methods
policy-based plus value-based
Chapter 10: Actor-Critic Methods
Chapter 3: Bellman Optimality Equation
Chapter 2: Bellman Equation
Chapter 1: Basic Concepts
Fundamental tools

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.
- We will also understand the important algorithm of stochastic gradient descent (SGD).

Outline

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

产生
一种特殊情况

3. Stochastic gradient descent
   - Algorithm description
   - Examples and application
   - Convergence analysis
   - Convergence pattern
   - BGD, MBGD, and SGD
4. Summary

Outline

Motivating example: mean estimation, again

Revisit the mean estimation problem:

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

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

蒙特卡洛方法/大数定律

- 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 quantities in RL such as action values and gradients are defined as expectations!

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:

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

不需要把前面所有的x再加一遍

Motivating example: mean estimation

Verification: 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 it is incremental. 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 $k \to \infty$).

把 k 换成其它满足某种条件的参数 a_k，w 仍然会收敛到 E[X]

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. Stochastic Approximation
- 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

Outline

是一类随机的迭代algorithms，用于方程求解/优化问题
不需要知道目标函数的expresion

梯度下降/上升方法 need the expression

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.

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

  优化J(w)到minimum (eg. cost function)

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

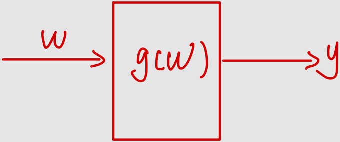
- Note that an equation like $g(w) = c$ with c as a constant can also be converted to the above equation by rewriting $g(w) - c$ as a new function.

Robbins-Monro algorithm – Problem statement

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

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

神经网络是一个黑箱



有点像 mean estimation 的增量式:

$$W_{k+1} = W_k - \frac{1}{k}(W_k - X_k)$$

The Robbins-Monro (RM) algorithm that can solve this problem is as follows:

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

$g(W_k)$ 加上噪音

where

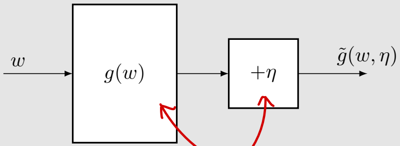
- w_k is the kth estimate of the root
- $\tilde{g}(w_k, \eta_k) = g(w_k) + \eta_k$ is the kth noisy observation
  - Why noise here? For example, consider a random sampling x of X.
- a_k is a positive coefficient.

通过带噪声的观测，找到一个方程的根

Robbins-Monro algorithm – The algorithm

This algorithm relies on data instead of model:

- Input sequence: $\{w_k\}$
- Output sequence (noisy): $\{\tilde{g}(w_k, \eta_k)\}$



都不知道 (Black Box)

Philosophy: without model, we need data!

- The function $g(w)$ is viewed as a black box.
- The model here refers to the expression of the function.

Outline

$w_1 \longrightarrow g(w_1)$

$w_2 \longrightarrow g(w_2)$

$w_3 \quad \cdots\cdots \quad w_k = 10 \longrightarrow g(w_k) = 0$

Toy example: 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)

$$
\begin{aligned}
w_1 &= 20 \Longrightarrow g(w_1) = 10 \\
w_2 &= w_1 - a_1 g(w_1) = 20 - 0.5 * 10 = 15 \Longrightarrow g(w_2) = 5 \\
w_3 &= w_2 - a_2 g(w_2) = 15 - 0.5 * 5 = 12.5 \Longrightarrow g(w_3) = 2.5 \\
&\vdots \\
w_k &\to 10
\end{aligned}
$$

Outline

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:

- $g(w) = \tanh(w-1)$ 求 $g(w)=0$ 的 w 值 .
- 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

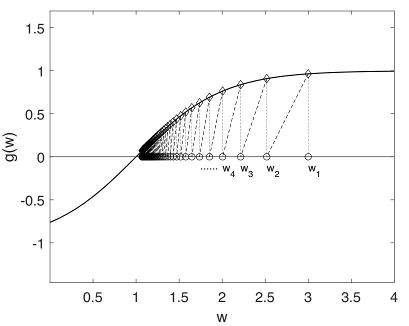
$$w_{k+1} = w_k - a_k g(w_k)$$

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 $w^* = 1$.

目标是让 w_k 靠近方程的根 w^*



如果函数有多个根，每次只会收敛到一个根.

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.

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* $g(w^*) = 0$.

Wk是随机变量（采样），所以是概率意义的收敛

g(w)的导数是单调递增的
且gradient是有界的

Explanation of the three conditions:

- **Condition 1:** $0 < c_1 \leq \nabla_w g(w) \leq c_2$ for all w
  - g should be monotonically increasing, which ensures that the root of $g(w) = 0$ exists and is unique
  - The gradient is bounded from the above.
  - This condition is not strict. Consider the example $g(w) = \nabla_w J(w) = 0$. This condition requires that $g(w)$ is convex.
- **Condition 2:** $\sum_{k=1}^{\infty} a_k = \infty$ and $\sum_{k=1}^{\infty} a_k^2 < \infty$
  - $\sum_{k=1}^{\infty} a_k^2 < \infty$ ensures that a_k converges to zero as $k \to \infty$.
  - $\sum_{k=1}^{\infty} a_k = \infty$ ensures that a_k do not converge to zero too fast.
- **Condition 3:** $\mathbb{E}[\eta_k|\mathcal{H}_k] = 0$ 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.

独立同分布

noises的mean = 0

variance有界限

Examine Condition 2 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.

w_k 最后收敛到 w^*，$g(w_k) \to 0$，但有波动（noises 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.

如果 $\sum_{k=1}^{\infty} a_k < \infty$，则 a_k 很快收敛到 0，则下面这个函数的绝对值会有界。当 w_1 和 w^* 相差比较大时，w_k 可能最终无法收敛到 $w_\infty = w^*$

- **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.

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

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

在实际应用时，当data非常多，$\frac{1}{k}$会导致后面的data没有作用。会用 $a_k = \frac{1}{2}$ 等常数，即使不满足 condition 2.

- 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.

Outline

$W_k = \frac{1}{k-1} \sum_{k=1}^{k-1} x_k$

增量式求和 $W_{k+1} = \frac{1}{k}[(k-1)W_k + x_k]$

$= W_k - \frac{1}{k}W_k + \frac{1}{k}x_k$

$= W_k + \frac{1}{k}(x_k - W_k)$

Recall that

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

is the mean estimation algorithm introduced at the beginning of this lecture.

- 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.

RM算法为：

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

$g(w_k) + \eta_k$

 单调递增

想寻找 $w^* = E(X)$，则设方程 $g(w) = w - E(x)$，求根

1) Consider a function:

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

则为 $w_{k+1} = w_k - \alpha_k g(w_k)$

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

- Mean estimation (i.e., finding $\mathbb{E}[X]$) is formulated as a root-finding problem (i.e., solving $g(w) = 0$).
- **Question:** Do we know the expression of $g(w)$ here?

2) The observation we can get is

设的变量　每次增加的数

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

because we can only obtain samples of X. Note that

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

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

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

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

RM算法

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 be used to analyze the mean estimation problem.
  - An extension of it can be used to analyze Q-learning and TD learning algorithms.

Outline

RM algorithm $\xrightarrow{\text{特殊情况}}$ SGD $\xrightarrow{\text{特殊情况}}$ mean estimation

Outline

Stochastic gradient descent

w：一个参数或变量

X：一个随机变量，是输入的数据

E(f(w,x))：以 x 为变量的期望值

$\min_w J(w)$：求让 f(w,x) 的期望值最小的 w.

Problem setup: 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

沿负梯度 步长 J(w) 的梯度

Method 1: gradient descent (GD)

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

Drawback: Calculating the expectation requires the distribution of X.

对

Method 2: batch gradient descent (BGD) ⟵ 用数据求 J(w,X) 的导数

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

Hence

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

Drawback: it requires <u>many samples in each iteration for each w_k.</u>

每次 update k 时，需要采样 n 次

精确度：GD > BGD > SGD

Method 3: stochastic gradient descent (SGD)

大写

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

和 GD 相比：
- GD 对模型用求导，得出 true gradient $E[\nabla_w f(w_k, X)]$
- SGD 没有模型参数，用一个 stochastic gradiant $\nabla_w f(w_k, x_k)$ 来近似

和 BGD 相比：
- BGD 也是近似 gradient，但用 n 个 x，大数定律，来近似。
- SGD 只用了 1 个 x (n=1)

1. GD（经典数学意义）只有一个样本

假设我们只有一个确定的函数，比如 $X = 3$：

$$f(w) = \tfrac{1}{2}(w-3)^2$$

- 梯度：

$$\nabla f(w) = w - 3$$

- 更新：

$$w \leftarrow w - \eta(w-3)$$

- **特点**：直接知道函数表达式，直接算梯度。

2. BGD（批量梯度下降）有多个样本，但因为noises，不知道真实样本分布

机器学习场景下，损失是所有样本的平均：

假设样本集合 $\{X_1, X_2, \ldots, X_N\}$，则目标函数是：

$$J(w) = \frac{1}{N}\sum_{i=1}^{N} \tfrac{1}{2}(w - X_i)^2$$

- 梯度：

$$\nabla J(w) = \frac{1}{N}\sum_{i=1}^{N}(w - X_i) = w - \frac{1}{N}\sum_{i=1}^{N} X_i$$

其实就是：w 与 **所有样本的均值** 的差。

- 更新：

$$w \leftarrow w - \eta\Big(w - \bar{X}\Big), \quad \bar{X} = \frac{1}{N}\sum_{i=1}^{N} X_i$$

- **特点**：每次迭代都要用全体数据。

3. SGD（随机梯度下降）

同样目标函数 $J(w)$，但 SGD 每次只抽一个样本近似梯度。

- 取样本 X_i，梯度：

$$g(w; X_i) = (w - X_i)$$

- 更新：

$$w \leftarrow w - \eta(w - X_i)$$

- **特点**：每次迭代只用一个样本，更新路径有噪声，但期望方向与真实梯度一致。

Outline

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

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

Exercises:

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

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

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

- **Exercise 1:** Show that the optimal solution is $w^* = \mathbb{E}[X]$.

求 J(W) 的最小值 (J(W)为凸函数)，即求 $\nabla J(W)=0$

$$\nabla J(W) = \nabla E\left[\frac{1}{2}\|W-X\|^2\right] = E[W-X] = W-E(X)=0$$

$$W^* = E(X)$$

求 $\min_W J(W)$ 的最小值，即求 $\nabla J(W) = W - E(X) = 0$ 时的 W

Therefore, we formulate the mean estimation problem (i.e., finding $\mathbb{E}[X]$) as an optimization problem (i.e., optimizing $J(w)$).

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

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

- **Exercise 2:** Write out the GD algorithm for solving this problem.
- **Answer to exercise 2:** The GD algorithm for solving the above problem is

用GD求 $\nabla_w J(w_k)=0$
的 root w^*

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

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

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

- **Exercise 3:** Write out the SGD algorithm for solving this problem.
- **Answer to exercise 3:** The SGD algorithm for solving the above problem is

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

近似于 $\nabla J(w)$

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

Outline

Idea of SGD:

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

$$\Downarrow$$

GD中

SGD中

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

where the true gradient $\mathbb{E}[\nabla_w f(w_k, X)]$ is replaced by the stochastic gradient $\nabla_w f(w_k, X)$.

Question: 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?

Observation: The stochastic gradient is a noisy measurement of the true gradient:

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

where η is the noise.

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 $g(w) = 0$.

这和RM算法一样，在不知道的g(w)表达式的情况下，求g(w)=0的根

$g(w)$ 表达式不知道，有一些有噪音的数据：$g(w) = \tilde{g}(w,\eta)$

What we can measure is

所有data的期望梯度

1个数据的梯度.

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

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.

每次迭代用的数据 x 不一样

Stochastic gradient descent – Convergence

$\nabla^2_w f(w,x)$ 是二阶导数，即 $0 < c_1 \le \nabla g(w,x) \le c_2$，$g(w,x)$ 是单调增

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

Theorem (Convergence of SGD)

In the SGD algorithm, if

1) $0 < c_1 \leq \nabla^2_w f(w, X) \leq c_2$; ← 严格凸函数
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.*

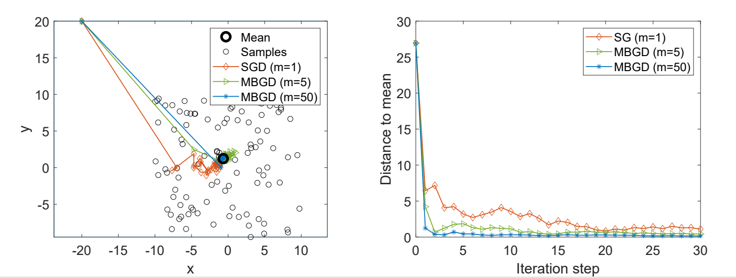
For the proof see the book.

Outline

GD中的true gradiant被SGD的stochastic gradient代替

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

Example: $X \in \mathbb{R}^2$ 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 $\{x_i\}_{i=1}^{100}$.



Observations:

- When the estimate (e.g., the initial guess) 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.

stochastic gradient

Question: Why such a pattern?

Answer: We answer this question by considering the relative error between the stochastic and batch gradients:

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

true gradient

It can be proven that

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

The proof is given in the next slide. The proof is optional.

Stochastic gradient descent – Convergence pattern (optional)

最优解

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

拉格朗日中值定理

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

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

Suppose f is strictly convex such that

$$\nabla^2_w f \geq c > 0$$

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

Then, the denominator of δ_k becomes

$w_k - w^*$ 没有 random variable，可以提出

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

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

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

The above equation suggests an interesting convergence pattern of SGD.

- The upper bound is inversely proportional to $|w_k - w^*|$.
  - When $|w_k - w^*|$ is large, the relative error δ_k is small and SGD behaves like GD.
  - When $|w_k - w^*|$ is small, the relative error δ_k may be large (the upper bound may not be tight). Then, SGD exhibits more randomness in the neighborhood of w^*.

Outline

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,

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

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

一共有n个数据

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

- **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 $|\mathcal{I}_k| = m$. $(m<n)$ The set $\mathcal{I}_k$ is obtained by m times idd samplings. 随机从n中抽取m个数据.
- **In the SGD algorithm**, x_k is randomly sampled from $\{x_i\}_{i=1}^n$ at time k.

随机采一个 x_i

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.

从n个数据中抽n个，可能有的数据多次被抽到

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

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

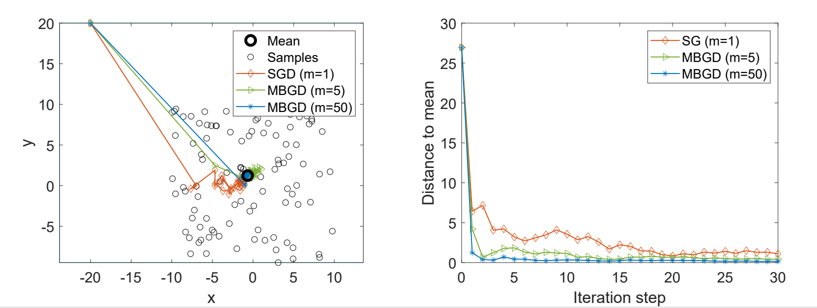


Figure: An illustrative example for mean estimation by different GD algorithms.

Outline

Summary

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

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

增量式求和

- 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.