Introduction to Neural Networks and Deep Learning

Optimization in Deep Learning

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Outline

1. Introduction
   - A Problematic View
   - Review of Gradient Descent
   - The Problems of Gradient Descent with Large Data Sets
   - Convergence of gradient descent with fixed step size
   - Convergence Rate
   - Accelerating the Gradient Descent
   - Even with such Speeds

2. Accelerating Gradient Descent
   - Robbins-Monro Theorem
   - Robbins-Monro Scheme for Minimum-Square Error
   - Convergence

3. Improving and Measuring Stochastic Gradient Descent
   - Example of SGD Vs BGD
   - Using The Expected Value, The Mini-Batch
   - Adaptive Learning Step

4. Derived and New Methods
   - The Stochastic Gradient Descent
   - Stochastic Gradient Descent with Momentum
   - The Least-Mean Squares Adaptive Algorithm
   - Adaptive Gradient Algorithm (AdaGrad)
   - AdaDelta, an extension of AdaGrad
   - Adaptive Moment Estimation, The ADAM Algorithm
   - Conclusions

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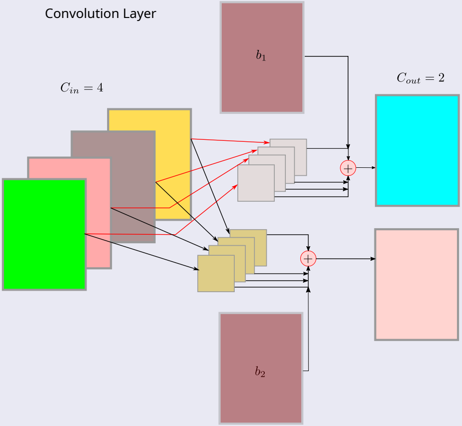
Beyond Simple Optimization [2]

As always Optimization is a Problem in Deep Learning

- We have a huge composition of linear and non-linear functions [1]



Thus

It is not possible to talk about

- That classic optimization theory [3, 4, 5] can explain totally the complexities on those deep architectures.

For example, we have

- The well-known "exploding/vanishing" gradient.

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Actually, we have

The following Issues

$$\text{Opt Problems} \begin{cases} \text{Local} & \Rightarrow \begin{cases} \text{Convergence Issue} & \Rightarrow \text{Vanishing/Exploding Gradient} \\ \text{Convergence Speed Issue} & \Rightarrow \text{As always problematic} \end{cases} \\ \text{Global} & \Rightarrow \text{Bad Local Minima, Plateaus, etc} \end{cases}$$

We have a data set

We have the following

- Data points $x_i \in \mathbb{R}^{d_x}$ and labels $y_i \in \mathbb{R}^{d_y}$ for $i = 1 \ldots n$

Thus, we want the architecture to predict y_i based on x_i

$$f_\theta = W^L \phi \left[W^{L-1} \cdots \phi \left[W^2 \phi \left[W^1 x_i + b_1 \right] + b_2 \right] + b_{L-1} \right] + b_L$$

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This is “trained”

By the use of Backpropagation

- With Gradient Descent, Stochastic Gradient Descent, ADAM, etc

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Gradient Descent [6, 7, 5, 4]

The basic procedure is as follow

1. Start with a random weight vector $\boldsymbol{w}_0$.
2. Compute the gradient vector $\nabla J(\boldsymbol{w}_0) = \sum_{i=1}^{N} l(\boldsymbol{w}_0, x_i, y_i)$.
3. Obtain value w_1 by moving from w_0 in the direction of the steepest descent:

$$\boldsymbol{w}_{n+1} = \boldsymbol{w}_n - \eta_n \nabla J(\boldsymbol{w}_n) \quad (1)$$

η_n is a positive scale factor or learning rate!!!

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We can derive it from the First Taylor Approximation

By using a step $\boldsymbol{w} + \boldsymbol{\epsilon}$

$$
\begin{aligned}
f\left(\boldsymbol{w}+\boldsymbol{\epsilon}\right) &\approx f\left(\boldsymbol{w}\right) + \nabla^T f\left(\boldsymbol{w}\right)\left(\boldsymbol{w}+\boldsymbol{\epsilon}-\boldsymbol{w}\right) \\
&\approx f\left(\boldsymbol{w}\right) + \nabla^T f\left(\boldsymbol{w}\right)\boldsymbol{\epsilon}
\end{aligned}
$$

Now, we choose $\boldsymbol{\epsilon} = -\eta \nabla f\left(\boldsymbol{w}\right)$

- Therefore, we have $f\left(\boldsymbol{w} - \eta \nabla f\left(\boldsymbol{w}\right)\right) \approx f\left(\boldsymbol{w}\right) - \eta \nabla^T f\left(\boldsymbol{w}\right) \nabla f\left(\boldsymbol{w}\right) = f\left(\boldsymbol{w}\right) - \eta \left\|\nabla f\left(\boldsymbol{w}\right)\right\|^2 \lesssim f\left(\boldsymbol{w}\right)$

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$$\begin{aligned} f\left(\boldsymbol{w}+\boldsymbol{\epsilon}\right) &\approx f\left(\boldsymbol{w}\right)+\nabla^{T} f\left(\boldsymbol{w}\right)\left(\boldsymbol{w}+\boldsymbol{\epsilon}-\boldsymbol{w}\right) \\ &\approx f\left(\boldsymbol{w}\right)+\nabla^{T} f\left(\boldsymbol{w}\right)\boldsymbol{\epsilon} \end{aligned}$$

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- Therefore, we have $f\left(\boldsymbol{w}-\eta\nabla f\left(\boldsymbol{w}\right)\right) \approx f\left(\boldsymbol{w}\right)-\eta\nabla^{T} f\left(\boldsymbol{w}\right)\nabla f\left(\boldsymbol{w}\right)=f\left(\boldsymbol{w}\right)-\eta\left\|\nabla f\left(\boldsymbol{w}\right)\right\|^{2} \lessapprox f\left(\boldsymbol{w}\right)$

Therefore, we get the following properties

The gradient descent $\boldsymbol{w} - \eta \nabla f(\boldsymbol{w})$

- Always minimize the previous value of $f(\boldsymbol{w})$

Second

- It is the direction on largest increase

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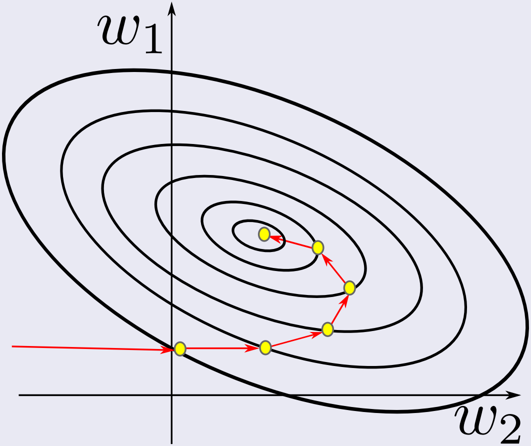
Geometrically

We have the following



$$\boldsymbol{w}(k+1) = \boldsymbol{w}(k) - \eta(k)\nabla J(\boldsymbol{w}(k))$$

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The Problems of Gradient Descent with Large Data Sets

It is possible to prove

- That the gradient direction gives the greatest increase direction!!!

We have a problem in cost functions like in Deep Neural Networks

$$J(w) = \sum_{i=1}^{N} (y_i - f(w, x_i))^2$$

- Where, we have that $f(w, x_i) = f_1 \circ f_2 \circ f_3 \circ \cdots \circ f_T(w, x_i)$

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Even though

Gradient Descent could be discarded easily

- For the Deep Learning Architectures

It is good to analyze some of its properties

- Given how they apply to other optimization algorithms for Deep Learning

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Thus, we need to talk about

Convergence Rate

- Important for Speed Ups
  - After all you want to avoid slow algorithms

Convex Functions

- The most basic stuff
  - A unique minima

Attempts to Accelerate Gradient Descent

- To obtain better performances
  - Momentum, Nesterov... and Stochatic Gradient Descent

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Do you remember the problem of the η step size?

Gradient Descent with fixed step size

$$\boldsymbol{w}_{n+1} = \boldsymbol{w}_n - \eta \nabla J\left(\boldsymbol{w}_n\right)$$

Why to worry about this?

- Because, we want to know how fast Gradient Descent will find the answer...

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Lipschitz Continuous [8]

- Lipschitz continuity, named after Rudolf Lipschitz, is a strong form of uniform continuity for functions.

Uniform continuity

- The function $f : A \rightarrow \mathbb{R}$ is said to be uniformly continuous on A iff for every $\epsilon > 0$, $\exists \delta > 0$ such that $|x - y| < \delta$ implies $|f(x) - f(y)| < \epsilon$.

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Lipschitz Continuous

Definition

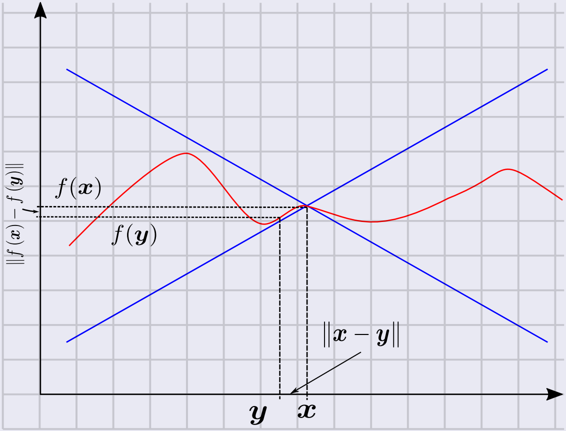
- A function $f : S \subset \mathbb{R}^n \to \mathbb{R}$ satisfies the Lipschitz Continuous at $\boldsymbol{x} \in S$, if there is a such constant $L > 0$ such that

$$\|f(\boldsymbol{x}) - f(\boldsymbol{y})\| \leq L \|\boldsymbol{x} - \boldsymbol{y}\|$$

for all $\boldsymbol{y} \in S$ sufficiently near to $\boldsymbol{x}$. **Lipschitz continuity can be seen as a refinement of continuity.**

Example when you see L as the slope

Here the function $f : \mathbb{R} \to \mathbb{R}$



An interesting property of such setup

The derivative of the function cannot exceed L (Example, $f : \mathbb{R} \to \mathbb{R}$)

$$f'(x) = \lim_{\delta \to \infty} \frac{f(x+\delta) - f(x)}{\delta}$$

Then, we have that

$$f'(x) = \lim_{\delta \to \infty} \frac{f(x) - f(y)}{x - y} \leq \lim_{\delta \to \infty} \frac{|f(x) - f(y)|}{|x - y|} \leq L$$

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Lipschitz Continuity implies

$$\left|f'(x)\right| < L$$

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Convergence Idea

Definition (Big O - Upper Bound) [9]

For a given function $g(n)$:

$$O(g(n)) = \{f(n) | \text{ There exists } c > 0 \text{ and } n_0 > 0 \text{ s.t. } 0 \leq f(n) \leq cg(n) \; \forall n \geq n_0\}$$

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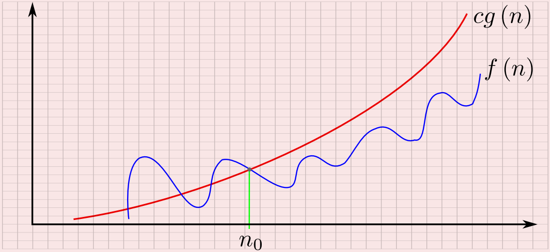

What are the implications?

Definition [8]

- Suppose that the sequence $\{x_n\}$ converges to the number L:

We say that this sequence converges linearly to L, if there exists a number $r \in (0,1)$ such that

$$\lim_{k \longrightarrow \infty} \frac{|x_{k+1} - L|}{|x_k - L|} = r$$

Thus, Gradient Descent has a linear convergence speed

- If you do a comparison with quadratic convergence...

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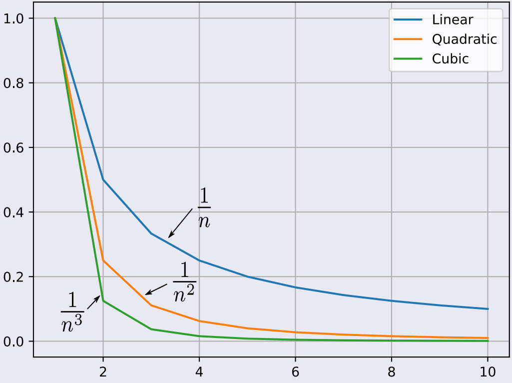
Example

As you can see the quadratic is faster than linear in convergence



Why the importance of Convex Functions? [4, 5, 3]

There is an interest on the rates of convergence for many optimization algorithms

- And they are affected by the different cost function that can be used:
  - Lipschitz-continuity, convexity, strong convexity, and smoothness

There are different rates of convergence for the Gradient Descent

- For example, when a function is strongly convex with $\alpha > 0$

$$\nabla^2 f(x) \succeq \alpha I \iff \nabla^2 f(x) - \alpha I \succeq 0 \text{ (Matrix greater)}$$

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Actually

You have $\nabla^2 f(x)$ is a squared symmetric matrix

- Thus, it is positive semi-definite

This means that

- The curvature of $f(x)$ is not very close to zero, making possible to accelerate the convergence

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Convex Sets

Definition

- For a convex set X, for any two points $\boldsymbol{x}$ and $\boldsymbol{y}$ such that $\boldsymbol{x}, \boldsymbol{y} \in X$, the line between them lies within the set

$$\boldsymbol{z} = \lambda \boldsymbol{x} + (1-\lambda)\, \boldsymbol{y},\ \forall \theta \in (0,1) \text{ then } \boldsymbol{z} \in X$$

  - The sum $\lambda \boldsymbol{x} + (1-\lambda)\, \boldsymbol{y}$ is termed as convex linear combination.

Convex Functions

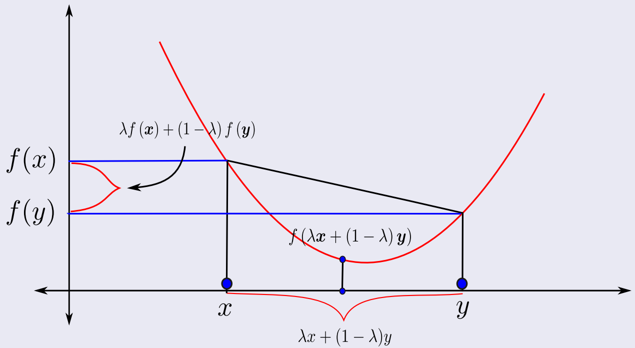
Definition

- . A function $f(\boldsymbol{x})$ is convex if the following holds:
  1. The Domain of f is convex
  2. $\forall \boldsymbol{x}, \boldsymbol{y}$ in the Domain of f and $\lambda \in (0,1)$

$$f(\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}) \leq \lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y})$$

Graphically

We have the following



Convergence of gradient descent with **fixed step size**

Theorem

- Suppose the function $f : \mathbb{R}^d \to \mathbb{R}$ is convex and differentiable, and we have that $\left\|\nabla f\left(\boldsymbol{x}\right) - \nabla f\left(\boldsymbol{y}\right)\right\| \leq L \left\|\boldsymbol{x} - \boldsymbol{y}\right\|$ (Lipschitz Continuous Gradient) for any $\boldsymbol{x}, \boldsymbol{y}$ and $L > 0$.

We have that

- Then, if we run the **gradient descent** for n iterations with a fixed step size $\eta \leq \frac{1}{L}$, it will yield a solution f_n which satisfies

$$f\left(x_n\right) - f\left(x^*\right) \leq \frac{\left\|x_{(0)} - x^*\right\|_2^2}{2\eta n}$$

where $f\left(x^*\right)$ is the optimal value and $\eta < \frac{1}{L}$

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Proof

First, consider the following function

$$g(x) = \frac{L}{2} x^T x - f(x)$$

We apply the Lemma of the monotonicity of gradient

- A differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if

$$[\nabla f(y) - \nabla f(x)]^T (y - x) \geq 0$$

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Proof

To use the Lemma, we first notice the following

$$[\nabla f(y) - \nabla f(x)]^T (y - x) = \left[\sqrt{\langle \nabla f(y) - \nabla f(x), y - x \rangle}\right]^2$$

We have the following situation because Cauchy-Schwarz inequality

$$\left[\sqrt{\langle \nabla f(y) - \nabla f(x), y - x \rangle}\right]^2 \leq \|\nabla f(y) - \nabla f(x)\| \, \|y - x\|$$

Then, we have

$$\|\nabla f(y) - \nabla f(x)\| \, \|y - x\| \leq L \|x - y\|^2$$

Proof

To use the Lemma, we first notice the following

$$[\nabla f(y) - \nabla f(x)]^T (y - x) = \left[\sqrt{\langle \nabla f(y) - \nabla f(x), y - x \rangle}\right]^2$$

We have the following situation because Cauchy–Schwarz inequality

$$\left[\sqrt{\langle \nabla f(y) - \nabla f(x), y - x \rangle}\right]^2 \leq \|\nabla f(y) - \nabla f(x)\| \, \|y - x\|$$

Then, we have

$$\|\nabla f(y) - \nabla f(x)\| \, \|y - x\| \leq L \, \|x - y\|^2$$

Proof

To use the Lemma, we first notice the following

$$\left[\nabla f\left(y\right)-\nabla f\left(x\right)\right]^{T}\left(y-x\right)=\left[\sqrt{\left\langle \nabla f\left(y\right)-\nabla f\left(x\right),y-x\right\rangle }\right]^{2}$$

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$$\left[\sqrt{\left\langle \nabla f\left(y\right)-\nabla f\left(x\right),y-x\right\rangle }\right]^{2}\leq\left\Vert \nabla f\left(y\right)-\nabla f\left(x\right)\right\Vert \left\Vert y-x\right\Vert$$

Then, we have

$$\left\Vert \nabla f\left(y\right)-\nabla f\left(x\right)\right\Vert \left\Vert y-x\right\Vert \leq L\left\Vert \boldsymbol{x}-\boldsymbol{y}\right\Vert ^{2}$$

Proof

And f is Lipschitz Continuous Gradient

$$
\begin{aligned}
\left[\nabla g\left(y\right)-\nabla g\left(x\right)\right]^{T}\left[y-x\right] =& \left[Ly-Lx+\nabla f\left(x\right)-\nabla f\left(y\right)\right]^{T}\left(y-x\right)\\
=& L\left\Vert y-x\right\Vert ^{2}-\left(\nabla f\left(x\right)-\nabla f\left(y\right)\right)^{T}\left(y-x\right)\\
\geq& 0
\end{aligned}
$$

Therefore $g(x)$ is convex

We have for the first condition of convexity, we have

$$f(y) \geq f(x) + \nabla f(x)^T (y - x)$$

We have that $g(x) = \frac{L}{2} x^T x - f(x)$

$$\begin{aligned} \frac{L}{2} y^T y - f(y) \geq & g(x) + \nabla g(x)^T (y - x) \\ \geq & \frac{L}{2} x^T x - f(x) + (Lx - \nabla f(x))^T (y - x) \end{aligned}$$

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Proof

$f(x)$ is Lipschitz continuous with constant L implies

$$f(y) \leq f(x) + \nabla f(x)^T (y - x) + \frac{L}{2}\left[y^T y - 2x^t y + x^t x\right]$$

Proof

Now, if we apply the Gradient update $\boldsymbol{y} = \boldsymbol{x}^+ = \boldsymbol{x} - \eta \nabla f(\boldsymbol{x})$

$$
\begin{aligned}
f\left(\boldsymbol{x}^+\right) &\leq f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T \left(\boldsymbol{x}^+ - \boldsymbol{x}\right) + \frac{1}{2} L \left\|\boldsymbol{x}^+ - \boldsymbol{x}\right\|^2 \\
&= f(\boldsymbol{x}) - \eta \left\|\nabla f(\boldsymbol{x})\right\|^2 + \frac{1}{2} L \eta^2 \left\|\nabla f(\boldsymbol{x})\right\|^2 \\
&= f(\boldsymbol{x}) - \left(1 - \frac{1}{2} L \eta\right) \eta \left\|\nabla f(\boldsymbol{x})\right\|^2
\end{aligned}
$$

Using $\eta \leq \frac{1}{L}$

$$
-\left(1 - \frac{1}{2} L \eta\right) \leq -\frac{1}{2}
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Implying that

- This inequality implies that the objective function value strictly decreases until it reaches the optimal value

This only holds when η is small enough

- This explains why we observe in practice that gradient descent diverges when the step size is too large.

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We can write

$$f\left(\boldsymbol{x}^{*}\right) \geq f\left(\boldsymbol{x}\right)+\nabla f\left(\boldsymbol{x}\right)^{T}\left(\boldsymbol{x}^{*}-\boldsymbol{x}\right)$$
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Therefore

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Therefore

$$f\left(\boldsymbol{x}^{+}\right) - f\left(\boldsymbol{x}^{*}\right) \leq \frac{1}{2\eta}\left[\left\Vert \boldsymbol{x} - \boldsymbol{x}^{*}\right\Vert^{2} - \left\Vert \boldsymbol{x} - \eta\nabla f\left(\boldsymbol{x}\right) - \boldsymbol{x}^{*}\right\Vert^{2}\right]$$

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This inequality holds x^{+} for on every iteration of gradient descent

Summing over all iterations and the telescopic sum in the right side

$$\sum_{i=1}^{n}\left[f\left(\boldsymbol{x}_{i}\right)-f\left(\boldsymbol{x}^{*}\right)\right]\leq\frac{1}{2\eta}\left[\left\|\boldsymbol{x}_{0}-\boldsymbol{x}^{*}\right\|^{2}\right]$$

Finally, using the fact that f decreases on every iteration

$$f\left(\boldsymbol{x}_{n}\right)-f\left(\boldsymbol{x}^{*}\right)\leq\frac{1}{n}\sum_{i=1}^{n}\left[f\left(\boldsymbol{x}_{i}\right)-f\left(\boldsymbol{x}^{*}\right)\right]\leq\frac{1}{2\eta n}\left[\left\|\boldsymbol{x}_{0}-\boldsymbol{x}^{*}\right\|^{2}\right]=O\left(\frac{1}{n}\right)$$

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Therefore

It converges with rate

$$O\left(\frac{1}{n}\right)$$

Outline

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- A Problematic View
- Review of Gradient Descent
- The Problems of Gradient Descent with Large Data Sets
- Convergence of gradient descent with fixed step size
- Convergence Rate
- Accelerating the Gradient Descent
- Even with such Speeds

2. Accelerating Gradient Descent
- Robbins-Monro Theorem
- Robbins-Monro Scheme for Minimum-Square Error
- Convergence

3. Improving and Measuring Stochastic Gradient Descent
- Example of SGD Vs BGD
- Using The Expected Value, The Mini-Batch
- Adaptive Learning Step

4. Derived and New Methods
- The Stochastic Gradient Descent
- Stochastic Gradient Descent with Momentum
- The Least-Mean Squares Adaptive Algorithm
- Adaptive Gradient Algorithm (AdaGrad)
- AdaDelta, an extension of AdaGrad
- Adaptive Moment Estimation, The ADAM Algorithm
- Conclusions

Accelerating the Gradient Descent

It is possible to modify the Batch Gradient Descent

- In order to accelerate it several modifications have been proposed

Possible Methods

- Polyak's Momentum Method or Heavy-Ball Method (1964) [10]
- Nesterov's Proposal (1983) [11]
- Stochastic Gradient Descent (1951) [12]

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Polyak's Momentum Method

Polyak's Step Size

- He Proposed that the step size could be modified to

$$\boldsymbol{w}_{n+1} = \boldsymbol{w}_n - \alpha \nabla f(\boldsymbol{w}_n) + \mu (\boldsymbol{w}_n - \boldsymbol{w}_{n-1}) \text{ with } \mu \in [0,1], \alpha > 0$$

Basically, the method uses the previous gradient information through the step difference $(\boldsymbol{w}_n - \boldsymbol{w}_{n-1})$

- By the discretization of the second order ODE

$$\ddot{\boldsymbol{w}} + a\dot{\boldsymbol{w}} + b\nabla f(\boldsymbol{w}) = 0$$

  - **which models the motion of a body in a potential field given by f with friction.**

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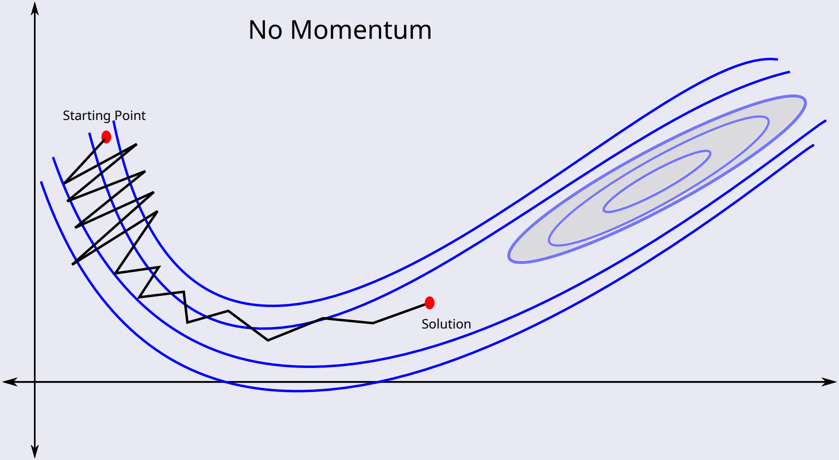
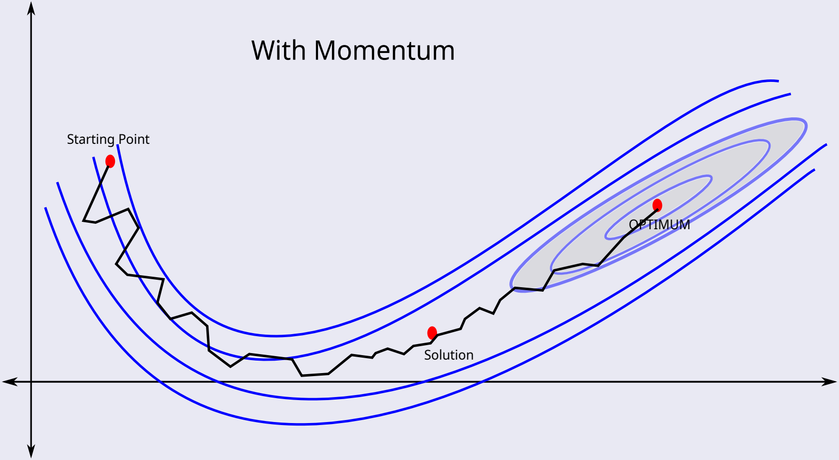
The Momentum helps to stabilize the GD

If we do not have Momentum



Then, with Momentum

If we have Momentum



Problem

It has been proved that the method has problems

- L. Lessard, B. Recht, and A. Packard. Analysis and Design of Optimization Algorithms via Integral Quadratic Constraints. ArXiv e-prints, Aug. 2014.

Under the function

$$\nabla f(x) = \begin{cases} 25x & \text{if } x < 1 \\ x + 24 & \text{if } 1 \leq x \leq 2 \\ 25x - 24 & \text{if otherwise} \end{cases}$$

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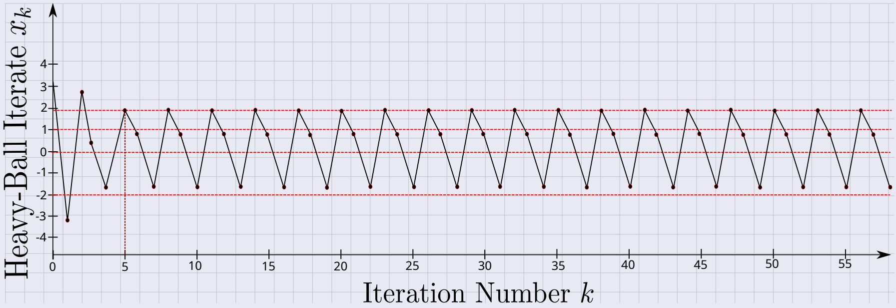
In Lessard et al.

We have a non-convergence (Original Lessard et al.) [13]



Nesterov's Proposal to solve the issue

He proposed a Quasi-Convex Combination

- Instead to use

$$\boldsymbol{w}_{n+1} = \boldsymbol{w}_n - \alpha \nabla f\left(\boldsymbol{w}_n\right) + \mu\left(\boldsymbol{w}_n - \boldsymbol{w}_{n-1}\right)$$

Have an intermediate step to update $\boldsymbol{w}_{n+1}$

$$\boldsymbol{w}_{n+1} = \left(1 - \gamma_n\right) \boldsymbol{y}_{n+1} + \gamma_n \boldsymbol{y}_n$$

This allow to weight the actual original gradient change

- with the previous gradient change... making possible to avoid the original problem by Polyak... Which is based in Lyapunov Analysis

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Nesterov's Accelerated Gradient Descent (A Quasi-Convex Modification)

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Nesterov Accelerated Gradient

Input: Training Time T, Learning Rate β, an initialization $\boldsymbol{w}_0$

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6. $\quad \lambda_{n+1} = \frac{1+\sqrt{1+4\lambda_n^2}}{2}$
7. $\quad \gamma_n = \frac{1-\lambda_n}{\lambda_{n+1}}$
8. $\quad \boldsymbol{w}_{n+1} = \left(1 - \gamma_n\right)\boldsymbol{y}_{n+1} + \gamma_n \boldsymbol{y}_n$

With the following complexity

Theorem (Nesterov 1983)

- Let f be a convex and β-smooth function (∇f is β-Lipschitz continous), then Nesterov's Accelerated Gradient Descent satisfies:

$$f\left(\boldsymbol{y}_{n+1}\right) - f\left(\boldsymbol{w}^{*}\right) \leq \frac{2\beta \left\|\boldsymbol{w}_1 - \boldsymbol{w}^{*}\right\|^2}{n^2}$$

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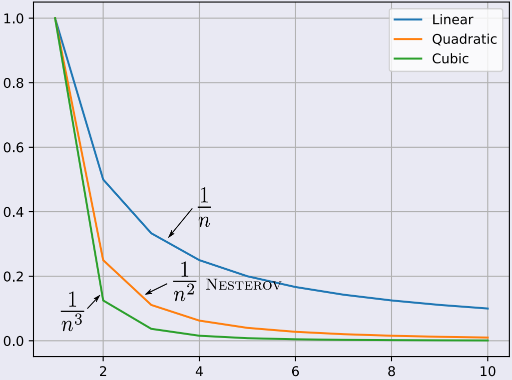
Example

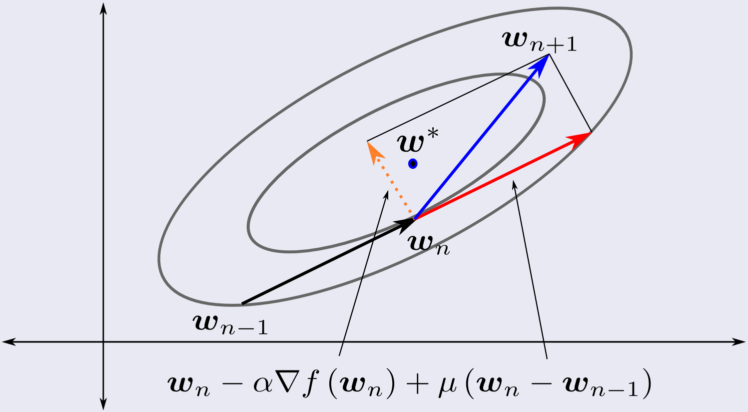
As you can see Nesterov is faster...



Remark, Polyak vs Nesterov

We have a remarkable difference

- The gradient descent step (orange arrow) is perpendicular to the level set before applying momentum to $\boldsymbol{w}_1$ (red arrow) in Polyak's algorithm



In the case of Nesterov

If we rewrite the equations

$$\boldsymbol{w}_{n+1} = (1-\gamma_n)\left[\boldsymbol{w}_n - \frac{1}{\beta}\nabla J\left(\boldsymbol{w}_n\right)\right] + \gamma_n \boldsymbol{y}_n$$

$$= \boldsymbol{w}_n - \gamma_n \boldsymbol{w}_n - \frac{1}{\beta}\nabla J\left(\boldsymbol{w}_n\right) + \frac{\gamma_n}{\beta}\nabla J\left(\boldsymbol{w}_n\right) + \gamma_n \boldsymbol{w}_{n-1} - \frac{\gamma_n}{\beta}\nabla J\left(\boldsymbol{w}_{n-1}\right)$$

$$= \boldsymbol{w}_n - \gamma_n\left(\boldsymbol{w}_n - \boldsymbol{w}_{n-1}\right) - \frac{1}{\beta}\left[\nabla J\left(\boldsymbol{w}_n\right) + \gamma_n \nabla J\left(\boldsymbol{w}_n\right) - \gamma_n \nabla J\left(\boldsymbol{w}_{n-1}\right)\right]$$

$$= \boldsymbol{w}_n - \gamma_n\left(\boldsymbol{w}_n - \boldsymbol{w}_{n-1}\right) - \frac{1}{\beta}\left[\nabla J\left(\boldsymbol{w}_n + \gamma_n\left[\boldsymbol{w}_n - \boldsymbol{w}_{n-1}\right]\right)\right]$$

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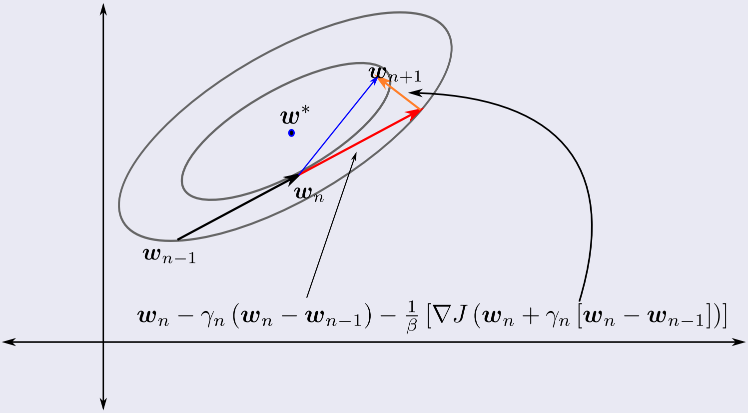

Basically

Nesterov new Momemtum

- It tries to move towards the optimum because the dampening term $\gamma_n \left(\boldsymbol{w}_n - \boldsymbol{w}_{n-1} \right)$

Even with these attempts

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There is a dependence with respect with different properties of f

In this table, we can see upper bounds for the convergences $D = \|x_1 - x^*\|_2$ and λ regularization term [3]

Properties of the Objective Function	Upper Bound for Gradient Descent
convex and L-Lipschitz	$\frac{D_1 L}{\sqrt{n}}$
convex and β-smooth	$\frac{\beta D_1^2}{n}$
α-strongly convex and L-Lipschitz	$\frac{L^2}{\alpha n}$
α-strongly convex and β-smooth	$\beta D_1^2 \exp\left(-\frac{4n}{\beta/\lambda}\right)$

A Hierarchy can be established (Black Box Model)

Based on the following idea

- A black box model assumes that the algorithm does not know the objective function f being minimized.

Not only that

- Information about the objective function can only be accessed by querying an oracle.

Remarks

- The oracle serves as a bridge between the unknown objective function and the optimizer.

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Zeroth Order Methods [14, 15, 16]

- These methods only require the value of function f at the current guess x.
  - The Bisection, Genetic Algorithms, Simulated Annealing and Metropolis-Hastings methods

First Order Methods

- These methods can inquire the value of the function f and its first derivative [5, 10, 11].
  - Gradient descent, Nesterov's and and Polyak's

Second Order Methods

- These methods require the value of the function f, its first derivative ∇f, and its second derivative $\nabla^2 f$ [5, 17, 3, 11].
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- The methods we mentioned until this point assume that all dimensions of a vector-valued variable have a common set of hyperparameters.

Adaptive methods relax this assumption

- They allow for every variable to have its own set of hyper-parameters.

Some popular methods under this paradigm

- AdaGrad, AdaDelta and ADAM

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Lower Bounds

- Lower bounds are useful because they tell us what's the best possible rate of convergence we can have given a category of optimizer.

Something Notable

- Without lower bounds, an unnecessary amount of research energy would be spent in designing better optimizers
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However, if we prove that each procedure has a lower bounded rate of convergence

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However

Please, take a look

- Convex Optimization: Algorithms and Complexity by Sébastien Bubeck - Theory Group, Microsoft Research [3]

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   - A Problematic View
   - Review of Gradient Descent
   - The Problems of Gradient Descent with Large Data Sets
   - Convergence of gradient descent with fixed step size
   - Convergence Rate
   - Accelerating the Gradient Descent
   - Even with such Speeds

2. Accelerating Gradient Descent
   - Robbins-Monro Theorem
   - Robbins-Monro Scheme for Minimum-Square Error
   - Convergence

3. Improving and Measuring Stochastic Gradient Descent
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   - Conclusions

In our classic Convex Scenario [7]

Least Square Problem locking to minimize the average of the LSE

$$\min_{\boldsymbol{x}\in\mathbb{R}^d} f\left(\boldsymbol{x}\right) = \min_{\boldsymbol{x}\in\mathbb{R}^d} \frac{1}{2M}\sum_{m=1}^{M}\left(\boldsymbol{w}^T\boldsymbol{x}_m - y_m\right)^2 = \min_{\boldsymbol{x}\in\mathbb{R}^d} \frac{1}{2M}\left\|X\boldsymbol{w} - Y\right\|^2$$

Therefore

Calculating the Gradient

$$\nabla_{\boldsymbol{w}} f\left(\boldsymbol{x}\right) = \frac{1}{M}\sum_{i=1}^{M}\left(\boldsymbol{w}^{T}\boldsymbol{x}_{m} - y_{m}\right)\boldsymbol{x}_{m}$$

Observations

It is easy to verify that the complexity per iteration is $O(dM)$

- With M is for the sum and d is for $\boldsymbol{w}^T \boldsymbol{x}_m$.

Drawbacks

When the number of samples M is Large

- Even with a rate of linear convergence, Gradient Descent

Not only that but in the On-line Learning scenario

- The data (x_i, y_i) is coming one by one making the gradient not computable.

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Therefore

Thus, the need to look for something faster

- Two possibilities:
  - Accelerating Gradient Decent Using Stochastic Gradient Descent!!!
  - Accelerating Gradient Descent Using The Best of Both World, Min-Batch!!!

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We have that the Robbins-Monro Theorem[12]

The origins of such techniques are traced back to 1951

- When Robbins and Monro introduced the method of stochastic approximation
  - DARPA project!!!

Setup, given a function $M(w)$ and a constant α such that the equation

$$M(w) = \alpha$$

- It has a unique root $w = w^*$

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Goal

We want to compute the root, $\boldsymbol{w}$, of such equation

$$M\left(\boldsymbol{w}^{*}\right)=\alpha$$

Then, we want to generate values $\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_{n-1}$ thus, we generate $\boldsymbol{w}_n$ from

1. $M\left(\boldsymbol{w}_1\right), M\left(\boldsymbol{w}_2\right), \ldots, M\left(\boldsymbol{w}_{n-1}\right)$
2. and the possible derivatives $M'\left(\boldsymbol{w}_1\right), M'\left(\boldsymbol{w}_2\right), \ldots, M'\left(\boldsymbol{w}_{n-1}\right)$

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$$\lim_{n\rightarrow\infty}\boldsymbol{w}_n=\boldsymbol{w}^{*}$$

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Instead, we suppose that for each $\boldsymbol{w}$ corresponds a Random Variable $Y = Y(\boldsymbol{w})$

This Random Variable has a distribution function

$$Pr\left[Y(\boldsymbol{w}) \leq y\right] = H\left(y|\boldsymbol{w}\right)$$

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We Postulate

First a bound to the $M(\boldsymbol{w})$

$$|M(\boldsymbol{w})| \leq C < \infty, \quad \int_{-\infty}^{\infty} (y - M(\boldsymbol{w}))^2 \, dH(y|\boldsymbol{w}) \leq \sigma^2 < \infty$$

IMPORTANT

Neither the exact nature of $H(y|\boldsymbol{w})$ nor that of $M(\boldsymbol{w})$ is known

- But an important assumption is that

$$M(\boldsymbol{w}) - \alpha = 0$$

It has only one root

Here is we use the α value to generate the root by assuming

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$M(\boldsymbol{w})$ is strictly increasing if

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Now choose a sequence $\{\mu_i\}$

Such that

$$\sum_{i=1}^{\infty} \mu_i^2 = A < \infty \text{ and } \sum_{i=1}^{\infty} \mu_i = \infty$$

Now, we define a non-stationary Markov Chain $\{w_n\}$

$$w_{n+1} - w_n = \mu_n \left(\alpha - y_n\right)$$

Where y_n is a random variable such that

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Using the expected value!!!

Here, we define b_n

$$b_n = E\left[\boldsymbol{w}_n - \boldsymbol{w}^*\right]^2$$

We want conditions where this variance goes to zero

$$\lim_{n \to \infty} b_n = 0$$

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$$\boldsymbol{w}_{n+1} - \boldsymbol{w}_n = \mu_n \left(\alpha - y_n\right)$$

We have then

$$\begin{aligned}
b_{n+1} =& E\left[\boldsymbol{w}_{n+1} - \boldsymbol{w}^*\right]^2 = E\left[E\left[\boldsymbol{w}_{n+1} - \boldsymbol{w}^*\right]^2 | \boldsymbol{w}_n\right] \\
=& E\left[\int_{-\infty}^{\infty} \left[\boldsymbol{w}_n - \boldsymbol{w}^* - \mu_n \left(y - \alpha\right)^2\right] dH\left(y | \boldsymbol{w}_n\right)\right] \\
=& b_n + \mu_n E\left[\int_{-\infty}^{\infty} \left(y - \alpha\right)^2 dH\left(y | \boldsymbol{w}_n\right)\right] - 2\mu_n E\left[\left(\boldsymbol{w}_n - \boldsymbol{w}^*\right)\left(M\left(\boldsymbol{w}_n\right) - \alpha\right)\right] \\
=& b_n + \mu_n^2 e_n - 2\mu_n d_n
\end{aligned}$$

With Values

We have

$$d_n = E\left[\left(\boldsymbol{w}_n - \boldsymbol{w}^*\right)\left(M\left(\boldsymbol{w}_n\right) - \alpha\right)\right]$$

$$e_n = E\left[\int_{-\infty}^{\infty} \left(y - \alpha\right)^2 dH\left(y|\boldsymbol{w}_n\right)\right]$$

From $M(w) \leq \alpha$ for $w \leq w^*$ and $M(w) \geq \alpha$ for $w > w^*$

$$d_n \geq 0$$

With Values

We have

$$d_n = E\left[\left(\boldsymbol{w}_n - \boldsymbol{w}^*\right)\left(M\left(\boldsymbol{w}_n\right) - \alpha\right)\right]$$
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From $M\left(\boldsymbol{w}\right) \leq \alpha$ for $\boldsymbol{w} \leq \boldsymbol{w}^*$ and $M\left(\boldsymbol{w}\right) \geq \alpha$ for $\boldsymbol{w} > \boldsymbol{w}^*$

$$d_n \geq 0$$

Additionally

Now, assuming that exist C such that

$$Pr\left[|Y(\boldsymbol{w})| \leq C\right] = \int_{-C}^{C} dH\left(y|\boldsymbol{w}\right) = 1 \ \forall x$$

We can prove that

$$0 \leq e_n \leq \left[C + |\alpha|^2\right] < \infty$$

Now, given

$$\sum_{i=1}^{\infty} \mu_i^2 = A < \infty \text{ and } \sum_{i=1}^{\infty} \mu_i = \infty$$

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Therefore $\sum_{i=1}^{\infty} \mu_i^2 e_i$ converges

Then, summing over i we obtain

$$b_{n+1} = b_1 + \sum_{i=1}^{n} \mu_i^2 e_i - 2 \sum_{i=1}^{n} \mu_i d_i$$

Since $b_{n+1} \geq 0$

$$\sum_{i=1}^{n} \mu_i d_i \leq \frac{1}{2} \left[b_1 + \sum_{i=1}^{n} \mu_i^2 e_i \right] < \infty$$

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Hence the positive-term series

$$\sum_{i=1}^{\infty} \mu_i d_i \text{ converges}$$

Then, $\lim_{n\to\infty} b_n$ exists and...

$$\lim_{n\to\infty} b_n = b_1 + \sum_{i=1}^{\infty} \mu_i^2 c_i - 2\sum_{i=1}^{\infty} \mu_i d_i = b$$

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Therefore

If a sequence of $\{k_i\}$ of non-negative constants such that

$$d_i \geq k_i b_i, \; \sum_{i=1}^{\infty} \mu_i k_i = \infty$$

We want to prove that

$$\sum_{i=1}^{\infty} \mu_i k_i b_i < \infty$$

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$$k_i b_i \leq d_i \Rightarrow \mu_i k_i b_i \leq \mu_i d_i$$

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Finally

For any $\epsilon > 0$ there must be infinitely values i such that $b_i < \epsilon$

- Therefore given that $\lim_{n\to\infty} b_n = b$ then $b = 0$.

Robbins and Monro Theorem (Original)

If $\{\mu_n\}$ is of type $\frac{1}{n}$

- Given a family of conditional probabilities

$$\{H(y|\boldsymbol{w}) = Pr(Y(\boldsymbol{w}) \leq y|\boldsymbol{w})\}$$

We have the following Expected Risk

$$M(\boldsymbol{w}) = \int_{-\infty}^{\infty} y dH(y|\boldsymbol{w})$$

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If we additionally have that

$$Pr\left(\left|Y\left(\boldsymbol{w}\right)\right| \leq C\right) = \int_{-C}^{C} dH\left(y|\boldsymbol{w}\right) = 1 \tag{3}$$

Then under the following constraints

For some $\delta > 0$

$$
\begin{aligned}
M(\boldsymbol{w}) &\leq \alpha - \delta \text{ for } \boldsymbol{w} < \boldsymbol{w}^* \\
M(\boldsymbol{w}) &\geq \alpha + \delta \text{ for } \boldsymbol{w} > \boldsymbol{w}^*
\end{aligned} \tag{4}
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Or Else

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M(\boldsymbol{w}) &< \alpha \text{ for } \boldsymbol{w} < \boldsymbol{w}^* \\
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Furthermore

$$M\left(\boldsymbol{w}\right) \text{ is strictily increasing if } \left|\boldsymbol{w}-\boldsymbol{w}^{*}\right|<\delta \tag{6}$$

And

$$\inf_{\left|\boldsymbol{w}-\boldsymbol{w}^{*}\right|\geq\delta}\left|M\left(\boldsymbol{w}\right)-\alpha\right|>0 \tag{7}$$

And Let $\{\mu_i\}$ be a sequence of positive numbers such that

$$\sum_{n=1}^{\infty}\mu_n=\infty \text{ and } \sum_{n=1}^{\infty}\mu_n^2<\infty \tag{8}$$

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Then

Let x_1 an arbitrary number, then under the recursion

$$\boldsymbol{w}_{n+1} = \boldsymbol{w}_n + \mu_n \left(\alpha - y_n \right)$$

- Where $y_n \sim P\left(y | \boldsymbol{w}_n \right)$

Theorem

- If (3) and (8), either (4) or (5,6,7) hold, then w_n converges stochastically to w^* given that $b = 0$.

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- If (3) and (8), either (4) or (5,6,7) hold, then $\boldsymbol{w}_n$ converges stochastically to $\boldsymbol{w}^*$ given that $b = 0$.

Recap of Robbins-Monro Proposal

Given the following function

$$f(\boldsymbol{w}) = E\left[\phi(\boldsymbol{w}, \eta)\right], \; \boldsymbol{w} \in \mathbb{R}^{d+1}$$

Given a series of i.i.d. observations $x_0, x_1, \cdots$

- The following iterative procedure (Robbins-Monro Scheme)

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Robbins-Monro Proposal

Starting from an arbitrary initial condition, $\boldsymbol{w}_0$

- It converges to a root of $M(\boldsymbol{w}) = \alpha$

Under some general conditions about the step size

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Mean-Square Error [7]

Cost function for MSE

$$J(\boldsymbol{w}) = E\left[\mathcal{L}(\boldsymbol{w}, \boldsymbol{x}, y)\right]$$

- Also known as the expected risk or the expected loss.

Then, our objective is the reduction of the Expected Risk!!!

- Thus, the simple thing to do is to derive the function and make such gradient equal to zero.

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Therefore

We can get the Gradient of the Expected Cost Function

$$\nabla J(\boldsymbol{w}) = E\left[\nabla \mathcal{L}(\boldsymbol{w}, \boldsymbol{x}, y)\right]$$

- where the expectation is w.r.t. the pair $(\boldsymbol{x}, y)$

Therefore, everything depends on the form of the Loss function

$$\mathcal{L}_1(\boldsymbol{w}, \boldsymbol{x}, y) = \frac{1}{2}\left\|\boldsymbol{w}^T\boldsymbol{x} - y\right\|_2^2 \text{ (Least Squared Loss)}$$

$$\mathcal{L}_2(\boldsymbol{w}, \boldsymbol{x}, y) = \left[\frac{1}{1+\exp\{\boldsymbol{w}^T\boldsymbol{x}\}}\right]^{1-y}\left[\frac{\exp\{\boldsymbol{w}^T\boldsymbol{x}\}}{1+\exp\{\boldsymbol{w}^T\boldsymbol{x}\}}\right]^{y} \text{ (Logistic Loss)}$$

$$\mathcal{L}_3(\boldsymbol{w}, \boldsymbol{x}, y) = \sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk}\log\left(y_{nk}^{(l)}\right) \text{ (Cross-Entropy Loss)}$$

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We simply take $\alpha = 0$ then

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Then, we apply the Robbins-Monroe Schema to the function

$$f(\boldsymbol{w}) = \nabla J(\boldsymbol{w}) = 0$$

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Then

Given the sequence of observations $\{(\boldsymbol{x}_i, y_i)\}_{i=1,2,\ldots}$ and values $\{\mu_n\}_{n=1,2,\ldots}$

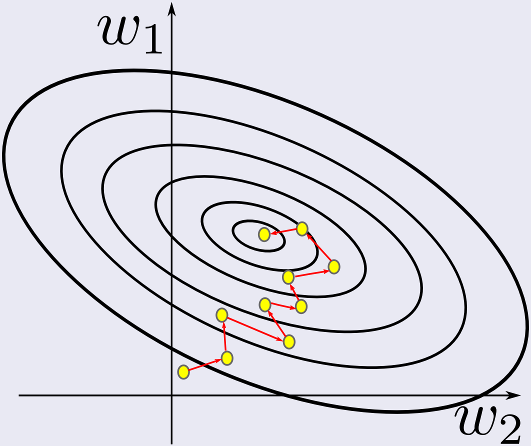
- We have that the iterative procedure becomes by picking randomly i:

$$\boldsymbol{w}_n = \boldsymbol{w}_{n-1} - \mu_n \nabla \mathcal{L}\left(\boldsymbol{w}_n, \boldsymbol{x}_i, y_i\right)$$

  - The Well known Vanilla Stochastic Gradient Descent (SGD)

Geometrically

We have the following



$$\boldsymbol{w}_n = \boldsymbol{w}_{n-1} - \mu_n \nabla \mathcal{L}\left(\boldsymbol{w}_n, \boldsymbol{x}_i, y_i\right)$$

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However, although the theorem is important

- it is not by itself enough.

One has to know something more concerning

- The rate of convergence of such a scheme.

It has been shown that

$$\mu_n = O\left(\frac{1}{n}\right)$$

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Additionally

Assuming that iterations have brought the estimate close to the optimal value

$$E\left(\boldsymbol{w}_n\right) = \boldsymbol{w}^* + \frac{1}{n}\boldsymbol{c}$$

And

$$Cov\left(w_n\right) = \frac{1}{n}V + O\left(\frac{1}{n^2}\right)$$

- Where c and V are constants that depend on the form of the expected risk.

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Therefore

- These formulas indicate that the parameter vector estimate fluctuates around the optimal value.

However

- Low complexity requirements makes this algorithmic family to be the one that is selected in a number of practical applications.
  - Given the problem with Batch Gradient Descent (BGD)

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Remarks Stochastic Gradient Descent

It has become the corner stone

- For the development of new methods of Optimization

As for Examples

- AdaGrad
- ADAM
- etc

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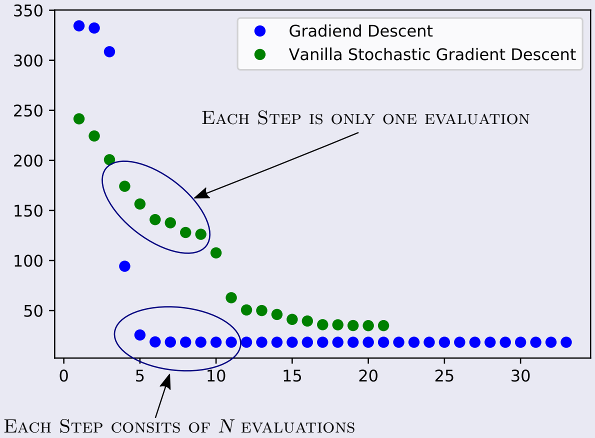
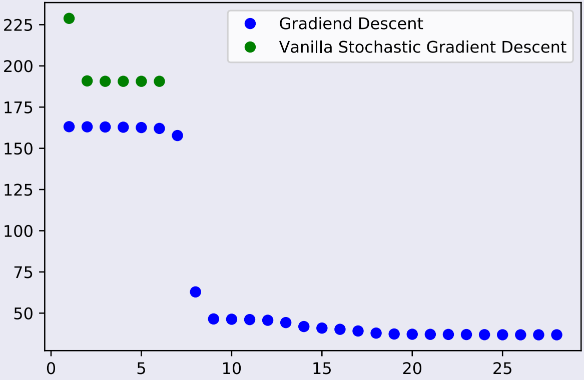
Example of SGD for, $\frac{1}{2}\sum_{i=1}^{N}\left(\boldsymbol{w}^{T}\boldsymbol{x}-\boldsymbol{y}\right)^{2}$

We can see how from the Vanilla SGD improves over the Batch GD with respect to Speed of Evaluation



Problems

However, we need to improve such Vanilla Stochastic Gradient Descent



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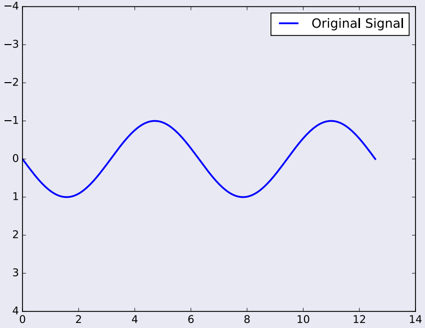
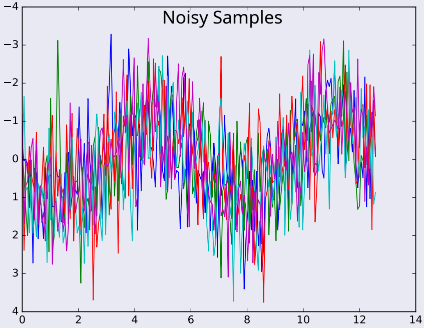
Do you Remember?

Imagine the following signal from $\sin(\theta)$





What if we know the noise?

Given a series of observed samples $\{\widehat{\boldsymbol{x}}_1, \widehat{\boldsymbol{x}}_2, ..., \widehat{\boldsymbol{x}}_N\}$ with noise $\epsilon \sim N(0,1)$

We could use our knowledge on the noise, for example additive:

$$\widehat{\boldsymbol{x}}_i = \boldsymbol{x}_i + \epsilon$$

We can use our knowledge of probability to remove such noise

$$E\left[\widehat{\boldsymbol{x}}_i\right] = E\left[\boldsymbol{x}_i + \epsilon\right] = E\left[\boldsymbol{x}_i\right] + E\left[\epsilon\right]$$

Then, because $E\left[\epsilon\right] = 0$

$$E\left[\boldsymbol{x}_i\right] = E\left[\widehat{\boldsymbol{x}}_i\right] \approx \frac{1}{N}\sum_{i=1}^{N} \widehat{\boldsymbol{x}}_i$$

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Given a series of observed samples $\{\widehat{\boldsymbol{x}}_1, \widehat{\boldsymbol{x}}_2, ..., \widehat{\boldsymbol{x}}_N\}$ with noise $\epsilon \sim N(0,1)$

We could use our knowledge on the noise, for example additive:

$$\widehat{\boldsymbol{x}}_i = \boldsymbol{x}_i + \epsilon$$

We can use our knowledge of probability to remove such noise

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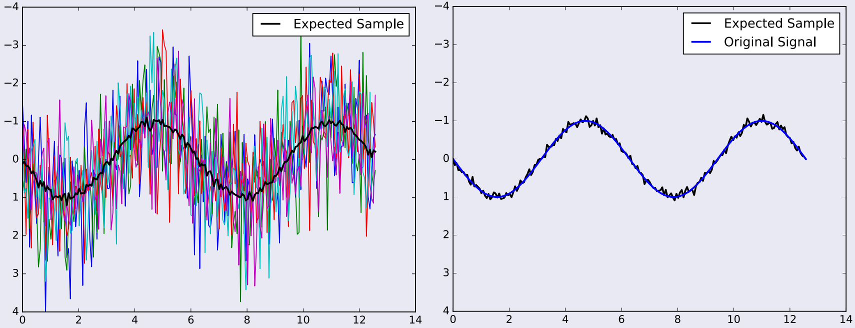
In our example

We have a nice result



Thus

Using a similar idea, you could use an average [18]

$$\nabla J\left(\boldsymbol{w}_{k-1}|\boldsymbol{x}_{i:i+m}, y_{i:i+m}\right) = \ldots$$
$$\frac{1}{m}\sum_{i=1}^{m}\nabla J\left(\boldsymbol{w}_{k-1}, \boldsymbol{x}_i, y_i\right)$$

This allows to reduce the variance of the original Stochastic Gradient

- It reduces the variance of the parameter updates, which can lead to more stable convergence.
- It can make use of highly optimized matrix optimizations common to state-of-the-art deep learning libraries that make computing the gradient w.r.t. a mini-batch very efficient.

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There are other more efficient options

We can update the $\boldsymbol{w}(k)$

- By Batches per epoch...

Therefore

1. for i in batch k

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Mini-batch gradient descent finally takes the best of both worlds

Min-Batch(X)

Input:

- Initialize $\boldsymbol{w}_0$, Set number of epochs, L, Set learning rate α

1. for $k = 1$ to L:
2. Randomly pick a mini batch of size m.
3. for $i = 1$ to m do:
4. Evaluate $g(k) = \nabla J(\boldsymbol{w}_{k-1}, \boldsymbol{x}_i, y_i)$
5. $\boldsymbol{w}_k = \boldsymbol{w}_{k-1} - \alpha g(k)$

Notes

Remark, for $\alpha = \frac{1}{m}$, the method is equivalent to average sample way

$$
\begin{aligned}
\boldsymbol{w}_k = & \boldsymbol{w}_{k-1} - \alpha \nabla J\left(\boldsymbol{w}_{k-1}, \boldsymbol{x}_i, y_i\right) - \ldots \\
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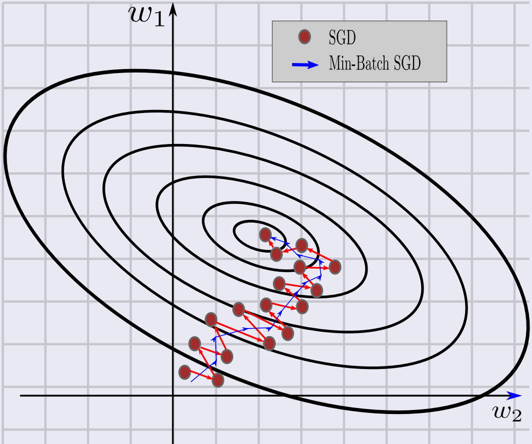
Notes

We have the following

- Common mini-batch sizes range between 50 and 256, but can vary for different applications.
- Mini-batch gradient descent is typically the algorithm of choice when training a neural network.

A Small Intuition

We have smoother version of the Stochastic Gradient Descent



$$\boldsymbol{w}_n = \boldsymbol{w}_{n-1} - \mu_n \nabla \mathcal{L}\left(\boldsymbol{w}_n, \boldsymbol{x}_n, y_n\right)$$

Drawbacks

Choosing a proper learning rate can be difficult

- A learning rate that is too small leads to painfully slow convergence,
- Too large can hinder convergence and cause the loss function to fluctuate around the minimum or even to diverge.

Learning Rate Schedules

- To adjust the learning rate during training by e.g. annealing
- These schedules and thresholds, however, have to be defined in advance not on-line

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- For example, neural networks, it is avoiding getting trapped in their numerous suboptimal local minima.

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Using Traditional Methods used in Gradient Descent

- Golden Ratio
- Bisection Method
- etc

Nevertheless

- Experiments with the Bisection Method has produced not so great results!!!

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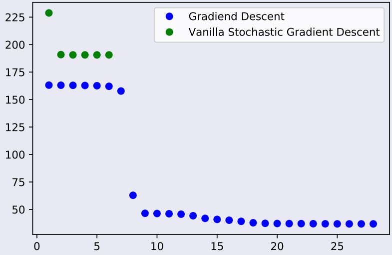

Adaptive Rate Speeds in SGD [19]

Structure of SGD with an adaptive learning rate

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\begin{aligned}
\boldsymbol{w}(t+1) &= \boldsymbol{w}(t) - \eta(t)\,\nabla L(\boldsymbol{w}(t)) \\
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First Order Methods

Gradient descent on the learning rate

- Given and estimator function $f : \mathbb{R} \to \mathbb{R}$ and $f(\eta(t)) = L(\boldsymbol{w}(t) - \eta(t)\nabla L(\boldsymbol{w}(t)))$,

This comes from thinking

- At time t using $\eta(t)$, we suffer a loss of $L(\boldsymbol{w}(t) - \eta \nabla L(\boldsymbol{w}(t)))$ in the next iteration:
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Therefore

The first order method is written as

$$\begin{aligned} \boldsymbol{w}(t) &= \boldsymbol{w}(t) - \eta(t)\nabla L(\boldsymbol{w}(t)) \\ \eta(t+1) &= \eta(t) - \alpha f'(\eta(t)) \end{aligned}$$

Remark

- This method introduces a new "meta" learning rate α.

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Actually

All These looks

- like a Bisection Method to find the minimal, but using the idea of linear search methods.
  - Take a look at chapter 8.1 on Bazaraa, Mokhtar S., Hanif D. Sherali, and Chitharanjan M. Shetty. Nonlinear programming: theory and algorithms. John wiley & sons, 20013

The final update is $f'(\eta(t))$

We have that $\forall \eta$

$$f'(\eta) = -\nabla L(\boldsymbol{w}(t))^T \cdot \nabla L(\boldsymbol{w}(t) - \eta \nabla L(\boldsymbol{w}(t)))$$

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If we continue in a similar direction

- We increase the learning rate, if we backtrack then we decrease it.

However

- The algorithm is not scale invariant anymore:

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Second Order Methods

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- The previous method presents the problem of choosing another meta-learning rate for optimizing the actual learning rate.

In order to avoid such problems

- We can use a second-order Newton-Raphson optimization method

$$w(t) = w(t) - \eta(t) \nabla L(w(t))$$

$$\eta(t+1) = \eta(t) - \frac{f'(\eta(t))}{f''(\eta(t))}$$

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Hessian Matrix

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$$f''(\eta) = -\nabla L(\boldsymbol{w}(t))^T H_L(\boldsymbol{w}(t) - \eta \nabla L(\boldsymbol{w}(t)))$$

Here, we can use an approximation

- "Deep learning via hessian-free optimization" by James Martens
  - They are actually know as finite Calculus ("Calculus of Finite Differences" by Charles Jordan)

$$f'(\eta + \epsilon) = \frac{f(\eta + 2\epsilon) - f(\eta)}{2\epsilon} \text{ (Forward Difference)}$$

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We have an approximation to the η hyper-parameter

$$\eta(t+1) = \eta(t) - 2\epsilon \frac{f(\eta+\epsilon) - f(\eta-\epsilon)}{f(\eta+2\epsilon) + f(\eta-2\epsilon) - 2f(\eta)}$$

Meaning

- When slightly increasing, the learning rate corresponds to a lower loss than slightly reducing it, then the numerator is negative.

In consequence

- The learning rate is raised at this update, as pushing in the ascending direction for the learning rate seems to help reducing the loss.

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Some Considerations

As you have notice in the second order method, we can have an underflow

1. If $f\left(\eta+2\epsilon\right)+f\left(\eta-2\epsilon\right)-2f\left(\eta\right)\approx 0$
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A typical value for δ is 10^{-6}

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At k Iteration,

we have a loss value $L^{(k)}$ and a learning rate value $\eta^{(k)}$

- At the $k+1$ step, we have the five loss values $f\left(\eta^{(k)}+\epsilon\right)$, $f\left(\eta^{(k)}-\epsilon\right)$, $f\left(\eta^{(k)}+2\epsilon\right)$, $f\left(\eta^{(k)}-2\epsilon\right)$ and $f\left(\eta^{(k)}\right)$
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Final Remark

Something Notable

- First-order and second-order updates of the learning rate do not guarantee positive learning rates

A simple way to avoid this problem is to use

$$\eta(k+1) = \max\{\eta(t+1), \delta\}$$

- With an appropriate smoothing δ value.

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We have that for a single sample

$$\mathcal{L}(w, y, x) = \frac{1}{2}\left(w^T x - y\right)^2$$

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Therefore

We know

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Remember Momentum

Polyak's

$$\boldsymbol{w}_{n+1} = \boldsymbol{w}_n - \alpha \nabla f\left(\boldsymbol{w}_n\right) + \mu\left(\boldsymbol{w}_n - \boldsymbol{w}_{n-1}\right) \text{ with } \mu \in [0,1], \alpha > 0$$

Then, the SGD...

SGD with momentum works as follows

- At n^{th} iteration, pick randomly an element $\{\boldsymbol{x}_i, y_i\}$ at the mini-batch

$$\boldsymbol{w}_{n+1} = \beta \boldsymbol{w}_n + (1-\beta) \nabla J(\theta_n, x_i, y_i)$$

Where, we have

$$\theta_{n+1} = \theta_n - \alpha_n w_n$$

Having a clear improvement

- As desired... and also we have the Nesterov's Momentum

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   - Convergence of gradient descent with fixed step size
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   - Even with such Speeds

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The Least-Mean Squares Adaptive Algorithm

We can improve the previous algorithm

- By using an adaptive step

Based in the error estimation given the n^{th} sample

$$e_n = \underbrace{y_n}_{label} - x_n^T \underbrace{w_{n-1}}_{\text{weight}}$$

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The stochastic gradient algorithm for MSE

- It converges to the optimal mean-square error solution provided that μ_n satisfies the two convergence conditions.

Once the algorithm has converged

- It "locks" at the obtained solution.

In a case where the statistics of the involved process changes

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if such changes occur, the error term

$$e_n = y_n - \boldsymbol{x}_n^T \boldsymbol{w}_{n-1}$$

- It will get larger values.

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Solution

This can be overcome if one sets the value of μ_n

- To a preselected fixed value, μ.

Least-Mean-Squares Algorithms

- Algorithm LMS
  1. $\boldsymbol{w}_{-1} = 0 \in \mathbb{R}^d$
  2. Select a value μ
  3. **for** $n = 0, 1, \dots$ **do**
  4. $\quad e_n = y_n - \boldsymbol{x}_n^T \boldsymbol{w}_{n-1}$
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Complexity

Something Notable

- The complexity of the algorithm amounts to $2d$ multiplications/additions (MADs) per time update.

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Given that μ has a constant value

- The algorithm has now the "agility" to update the estimates
  - In an attempt to "push" the error to lower values.

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- This small variation of the iterative scheme has important implications.

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- The resulting algorithm is no more a member of the Robbins–Monro stochastic approximation family.

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Now

We will look at the following algorithms

- Adaptive Gradient
- AdaDelta
- ADAM Algorithm
  - Nesterov-accelerated ADAM
- Natural Gradient Descent

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AdaGrad

Adaptive Gradient Algorithm (AdaGrad) [20]

- It is a variation of the SGD based on the subgradient idea

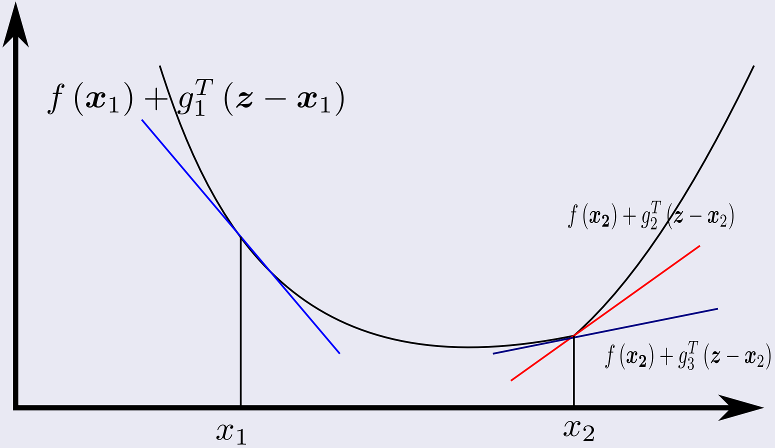
Definition (Subgradient) [4]

- A vector g is a subgradient of a function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ at a point $\boldsymbol{x} \in dom f$, if for all $\boldsymbol{z} \in dom f$

$$f(\boldsymbol{z}) \geq f(\boldsymbol{x}) + g^T (\boldsymbol{z} - \boldsymbol{x})$$

Then

Example



Standard Subgradient Algorithms

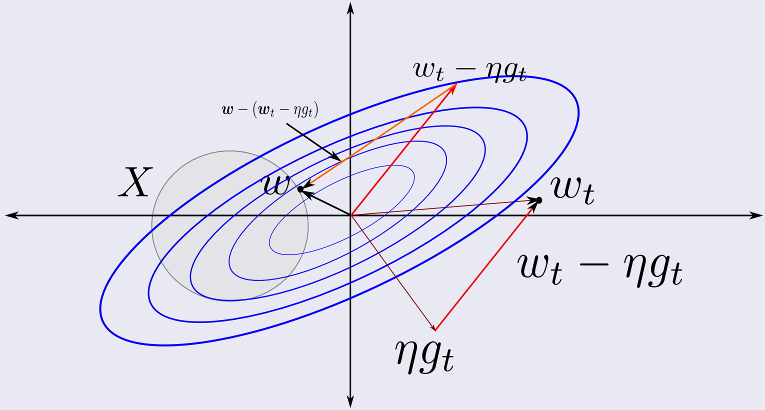
At Every Timestamp t, the learner gets the subgradient information $g_t \in \partial f_t(\boldsymbol{w}_t)$

- They move the predictor x_t in the opposite direction of g_t while projecting the gradient update is from the update $(\boldsymbol{w}_t - \eta g_t)$ to any $\boldsymbol{w}$

$$\boldsymbol{w}_{t+1} = \Pi_X(\boldsymbol{x}_t - \eta g_t) = \arg\min_{\boldsymbol{w} \in X} \|\boldsymbol{w} - (\boldsymbol{w}_t - \eta g_t)\|_2^2$$

Graphically

We have that we need to find the nearest $\boldsymbol{w} \in X$



However, we need something faster

It has a problem when searching for the best $\boldsymbol{w}$

- Then, we need to have something way better and simpler!!!

We can do that by accumulating the gradients and use them for mapping

$$G_{1:t} = \begin{bmatrix} g_1 & g_2 & \cdots & g_t \end{bmatrix}$$

- It is the the matrix obtained by concatenating the sub-gradient sequence in row format...

We denote the i^{th} row of this matrix

- The concatenation of the i^{th} component of each sub-gradient by $g_{1:t,i}$

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A First Approach

The Covariance matrix

$$G_t = \sum_{i=1}^{T} g_i g_i^T$$

It is an accumulation into the past of the previous gradients

- Therefore, the larger changes happen at the beginning of the updates
  - Not only that $g_1 g_1^T$ has rank 1

Therefore as we go into the building process of G_t

- We might add new dimensions if the g_t is not in the subspace of the G_{t-1}

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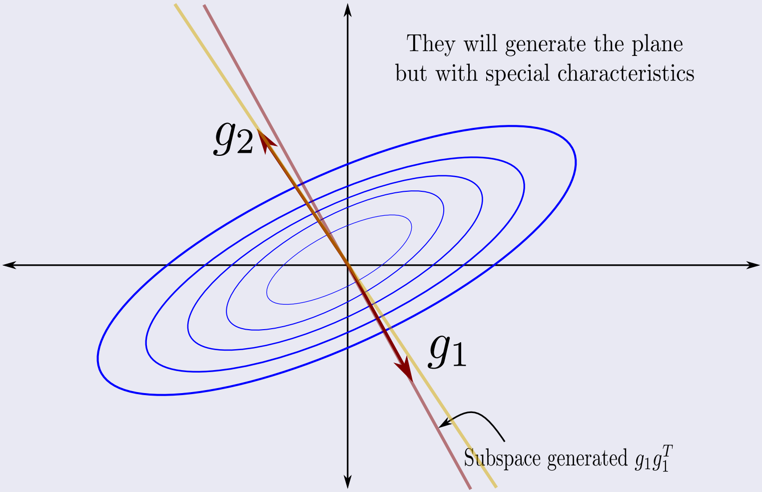
Graphically

The gradient descent iterations start building a possible space of projection



Mahalanobis Idea

If we think in the Mahalanobis Norm $\|\cdot\|_A = \sqrt{\langle \cdot, A \cdot \rangle}$

- Denoting the projection of a point y onto X according to A

$$\Pi^A_{\mathcal{X}}\left(\boldsymbol{y}\right) = \arg\min_{\boldsymbol{w}\in\mathcal{X}} \|\boldsymbol{w}-\boldsymbol{y}\|^2_A = \arg\min_{\boldsymbol{w}\in\boldsymbol{X}} \langle \boldsymbol{w}-\boldsymbol{y}, A\left(\boldsymbol{w}-\boldsymbol{y}\right)\rangle$$

In Mahalonobis, the A generate a subspace where you are mapping

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Using this, we can define

Therefore, we can use the inverse of such a covariance matrix

$$\boldsymbol{w}_{t+1} = \Pi_{\mathcal{X}}^{G_t^{1/2}} \left(\boldsymbol{w}_t - \eta G_t^{-\frac{1}{2}} g_t \right)$$

- $g_t = \nabla f \left(\boldsymbol{w}_t \right)$
- $G = \sum_{\tau=1}^{t} g_\tau g_\tau^T$

Remark

Actually, the inverse of the term G is related with the Hessian

- When you have a Gaussian $\boldsymbol{w}$ vector, we have that

$$H\left(\boldsymbol{w}^{*}\right)=\Sigma_{\theta}^{-1}$$

And given that $G=\sum_{\tau=1}^{t} g_{\tau} g_{\tau}^{T}$

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Given that $G_t^{-\frac{1}{2}}$ is computationally intensive $O\left(d^3\right)$

- And the diagonal has the necessary information!!! We can choose the information at the diagonal $O\left(d\right)$:

$$\boldsymbol{w}_{t+1} = \Pi_X^{diag(G)^{\frac{1}{2}}}\left[\boldsymbol{w}_t - \eta diag\left(G\right)^{-\frac{1}{2}} g_t\right]$$

Basically, it looks as a normalization

- G acts as memory for the variance of g_t

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Given that the diagonal elements $G_{j,j} = \sum_{\tau=1}^{t} g_{\tau,j}^2$, the parameters are updated

$$w_j^{t+1} = w_j^t - \frac{\eta}{\sqrt{G_{j,j}}} g_j$$

Something Notable

- Since the denominator in this factor, $\sqrt{G_{j,j}} = \sqrt{\sum_{\tau=1}^{t} g_{\tau,j}^2}$ is the $L2$ norm.

We have that

- Extreme parameter updates get dampened, while parameters that get few or small updates receive higher learning rates.

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Improving over AdaGrad

Becker and LecCun [17]

- They proposed a diagonal approximation to the Hessian.

An interesting thing

- This diagonal approximation can be computed with one additional forward and back-propagation through the model

They have the following update

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1. The continual decay of learning rates throughout training,
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- In the AdaGrad method the denominator accumulates the squared gradients from each iteration.

This accumulation is problematic

- It continues to grow throughout training

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Thus, the modification

Use a window instead of taking all time elements and compute

$$E\left[g^2\right]_t = \rho E\left[g^2\right]_{t-1} + (1-\rho)\, g_t^2$$

- where ρ is a decay constant similar to the one in the momentum method.

Since this require the square root, this become the Root Mean Square

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Idea 2: Correct Units with Hessian Approximation

When considering the parameter updates

- "If the parameter had some hypothetical units, the changes to the parameter should be changes in those units as well"

SGD and Momentum has the following problem

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$$\frac{\Delta \boldsymbol{w}}{\frac{\partial f}{\partial \boldsymbol{w}}} \approx \frac{RMS\left[\Delta \boldsymbol{w}\right]_{t-1}}{RMS\left[g\right]_{t}}$$

The final update is

Then for the new update, we have

$$\Delta \boldsymbol{w}_t \approx -\frac{RMS\left[\Delta \boldsymbol{w}\right]_{t-1}}{RMS\left[g\right]_t} g_t$$

Outline

1. Introduction
- A Problematic View
- Review of Gradient Descent
- The Problems of Gradient Descent with Large Data Sets
- Convergence of gradient descent with fixed step size
- Convergence Rate
- Accelerating the Gradient Descent
- Even with such Speeds

2. Accelerating Gradient Descent
- Robbins-Monro Theorem
- Robbins-Monro Scheme for Minimum-Square Error
- Convergence

3. Improving and Measuring Stochastic Gradient Descent
- Example of SGD Vs BGD
- Using The Expected Value, The Mini-Batch
- Adaptive Learning Step

4. Derived and New Methods
- The Stochastic Gradient Descent
- Stochastic Gradient Descent with Momentum
- The Least-Mean Squares Adaptive Algorithm
- Adaptive Gradient Algorithm (AdaGrad)
- AdaDelta, an extension of AdaGrad
- Adaptive Moment Estimation, The ADAM Algorithm
- Conclusions

As in MSE [22]

We are interested in minimizing the expected value of f

$$E\left[f\left(\boldsymbol{w}\right)\right]$$

Now, assuming $g_t = \nabla_{\boldsymbol{w}} f_t\left(\boldsymbol{w}\right)$

- The algorithm updates moving averages of the gradient m_t and the squared gradient v_t.

We can define the following terms

$$m_t = \sum_{t=1}^{n} \tau_n g_t \approx E\left[g_t\right] \text{ and } v_t = \sum_{t=1}^{n} \tau_n g_t^2 \approx E\left[\left(g_t - 0\right)^2\right]$$

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Thus we have

Using linear combinations with $\beta_1, \beta_2 \in [0, 1)$

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$$\widehat{m}_t = \frac{m_t}{(1 - \beta_1^t)} \text{ and } \widehat{v}_t = \frac{v_t}{(1 - \beta_2^t)}$$

The algorithm tries to control the step size Δ_t

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We have two upper bounds

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$$|\Delta_t| \leq \alpha \frac{(1 - \beta_1)}{\sqrt{1 - \beta_2}}$$

Otherwise

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Something Notable

- Since α sets (an upper bound of) the magnitude of steps in parameter space
  - We can often deduce the right order of magnitude of α for the problem at hand.

Furthermore, $\frac{\widehat{m}_t}{\left(\sqrt{\widehat{v}_t}\right)}$ can be seen as a Signal to Noise Ration (SNR)

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Leading to smaller effective steps in parameter space

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Adam Algorithm

Input: α step size, $\beta_1, \beta_2 \in [0, 1)$, $f(\boldsymbol{w})$ objective function, $\boldsymbol{w}_0$ Initial Parameter

$m_0 = 0$, $v_0 = 0$, 1st and 2nd moment vector respectively.
$t = 0$ initial time step
while w_t not converged **do**
    $t = t + 1$
    $g_t = \nabla f(w_{t-1})$ ←Get gradients w.r.t. stochastic objective at timestep t
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The adaptive method ADAM achieves

$$R(T) = O\left(\log d\sqrt{n}\right)$$

Compared with the Online Gradient Descent

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Looking into the past

If we look at the following equations

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Doing some Math work

We have that the last updating term look like when making $\epsilon = 0$

$$\sum_{k=1}^{t}\frac{\widehat{m}_k}{\left(\sqrt{\widehat{v}_k}\right)}=\sum_{k=1}^{t}\frac{\frac{m_k}{\left(1-\beta_1^k\right)}}{\left(\sqrt{\frac{v_k}{\left(1-\beta_2^k\right)}}\right)}=\sum_{k=1}^{t}\frac{\left(1-\beta_2^k\right)^{\frac{1}{2}}}{\left(1-\beta_1^k\right)}\times\frac{m_k}{\sqrt{v_k}}$$

Clearly

$$\left(1-\beta_2^k\right)^{\frac{1}{2}}\to 1 \text{ and } 1-\beta_1^k \to 1$$

But the second one faster than the first one

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- Therefore the steps modifications depend on the different values for the betas.

We have different cases

For Example, we could have

- $\beta_1 = 0.9$ and $\beta_2 = 0.9$
  - Making going to zero slower than when values are near to 0.
  - A more detailed analysis is needed!!!

However, if we assume that they cancel each other, and if v_k tend to zero at slower pace

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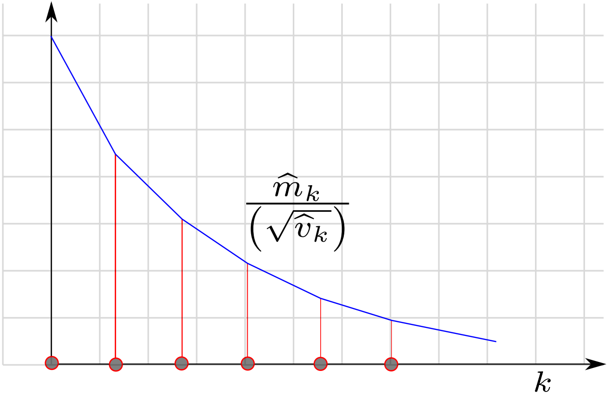
Actually we need to analyze the convergence

We could have something like



Simulated Annealing and Adam

Simulated_Annealing$(\omega, M_k, \epsilon_t, \epsilon, t_k, f)$

$\Delta E = \infty$

while $|\Delta E| > \epsilon$

  for $i = 0, 1, 2, ..., M_k$

    Randomly select ω' **in** $N(\omega)$

    $\Delta E = f(\omega') - f(\omega)$

    if $\Delta E \leq 0$

      $\omega = \omega'$

    if $\Delta E > 0$

      $\omega = \omega'$ **with probability** $Pr\{Accepted\} = \exp\left\{\frac{-\Delta E}{t_k}\right\}$

  $t_k = t_k - \epsilon_t$ **# We can also use** $t_k = \epsilon_t \cdot t_k$

In accordance with the Simulated Annealing part

This makes ADAMS adaptive

- But with a limitation on the change because you always take the step
  - Remember the step $\omega = \omega'$ **with probability** $Pr\left\{Accepted\right\} = \exp\left\{\frac{-\Delta E}{t_k}\right\}$

Making the past more important than the present

- When updating the values

Actually it is form of cooling as in Simulated Annealing by the term

$$\sum_{k=1}^{t} \frac{\left(1-\beta_2^k\right)^{\frac{1}{2}}}{\left(1-\beta_1^k\right)}$$

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You require more information from your surroundings optimization landscape

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A naive idea would be to substitute the term $\frac{\alpha}{\left(\sqrt{\widehat{v}_t}+\epsilon\right)}$ by the Fisher Information matrix [23]

$$w_t = w_{t-1} - E\left[\frac{\partial \log f\left(X|\theta\right)}{\partial\theta}|\theta\right]^{-1}\widehat{m}_t$$

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Remarks about ADAM

ADAM is favored in Deep Learning given that

1. Given the use of stochastic gradient update:
    1. It is Computationally Efficient
    2. It requires Little memory.
    3. It is suited for problems that are large in terms of data and/or parameters.
2. Invariant to diagonal rescale of the gradients.
3. Appropriate for non-stationary objectives.
4. Appropriate for problems with very noisy/or sparse gradients.

Finally and most important

- Hyper-parameters have intuitive interpretation and typically require little tuning.

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Outline

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- A Problematic View
- Review of Gradient Descent
- The Problems of Gradient Descent with Large Data Sets
- Convergence of gradient descent with fixed step size
- Convergence Rate
- Accelerating the Gradient Descent
- Even with such Speeds

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- Robbins-Monro Scheme for Minimum-Square Error
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3. Improving and Measuring Stochastic Gradient Descent
- Example of SGD Vs BGD
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- Adaptive Moment Estimation, The ADAM Algorithm
- Conclusions

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