Introduction to Machine Learning
Stochastic Gradient Descent

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Outline

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Gradient Descent [1, 2]

The basic procedure is as follow

1. Start with a random weight vector w_0.

2. Compute the gradient vector $\nabla J(w_0)$

3. Obtain value w_1 by moving from w_0 in the direction of the steepest descent.

$$w_{n+1} = w_n - \eta_n \nabla J(w_n) \tag{1}$$

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

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Geometrically

We have the following

Outline

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It is possible to prove

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

$$J\left(\boldsymbol{w}\right) = \sum_{i=1}^{N} \left(y_i - f\left(\boldsymbol{w}, \boldsymbol{x}_i\right)\right)^2$$

- Where, we have that $f\left(\boldsymbol{w}, \boldsymbol{x}_i\right) = f_1 \circ f_2 \circ f_3 \circ \cdots \circ f_T\left(\boldsymbol{w}, \boldsymbol{x}_i\right)$

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Do you remember the problem of the η step size?

Gradient Descent with fixed step size

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Why to worry about this?

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

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Lipschitz Continuous [3]

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

Uniform continuity

- The function $f : A \to \mathbb{R}$ 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 $f : S \subset \mathbb{R}^n \to \mathbb{R}^n$ 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

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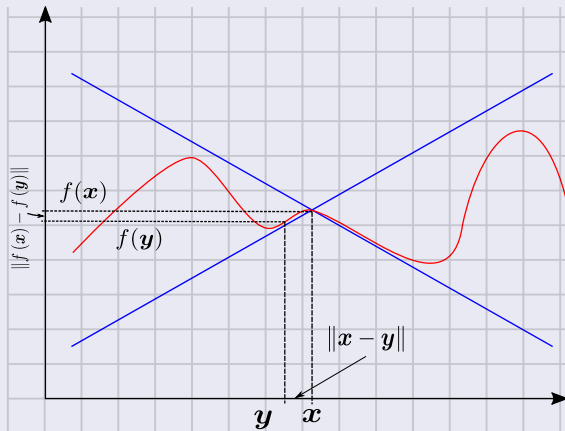
$$f'(x) = \lim_{\delta \to \infty} \frac{f(x) - f(y)}{x - y} \leq \lim_{\delta \to \infty} \frac{|f(x) - f(y)|}{|x - y|} \leq L$$

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

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

Therefore

> **Lipschitz Continuity implies**
>
> $$|f'(x)| < L$$

Outline

Convergence idea

Definition (Big O - Upper Bound) [4]

For a given function $g(n)$:

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

Example

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Example

What are the implications?

Definition [3]

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

We say that this sequence converges linearly to L, if there exists a number $\frac{1}{n} \in [0, 1)$ such that

$$\lim_{k \to \infty} \frac{|x_{n+1} - L|}{|x_n - L|} = \frac{1}{n}$$

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

Outline

Why the importance of Convex Functions?

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

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

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 x and y such that $x, y \in X$, the line between them lies within the set

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

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

Convex Functions

Definition

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

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

Graphically

This can further expanded to functions

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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 $\|\nabla f(\boldsymbol{x}) - \nabla f(\boldsymbol{y})\|_2 \leq L \|\boldsymbol{x} - \boldsymbol{y}\|$ (Lipschitz Continuous Gradient) for any $\boldsymbol{x}, \boldsymbol{y}$ and $L > 0$.

We have that

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

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

where $f(x^*)$ is the optimal value.

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Proof

$f(\boldsymbol{x})$ is Lipschitz continuous with constant L implies
$(\|\boldsymbol{y} - \boldsymbol{x}\|^2 = \|\boldsymbol{y} - \boldsymbol{x}\|_2^2)$

$\nabla^2 f(x) - LI$ as semi-definite matrix

We have the following inequality

$$f(y) = f(x) + \nabla f(x)^T (y - x) + \frac{1}{2} \nabla^2 f(x) \|y - x\|^2$$

$$\leq f(x) + \nabla f(x)^T (y - x) + \frac{1}{2} L \|y - x\|^2$$

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$$\leq f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T (\boldsymbol{y} - \boldsymbol{x}) + \frac{1}{2} L \|\boldsymbol{y} - \boldsymbol{x}\|^2$$

Proof

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

$$f\left(x^+\right) \le f\left(x\right) + \nabla f\left(x\right)^T \left(x^+ - x\right) + \frac{1}{2}L \left\|x^+ - x\right\|^2$$

$$= f\left(x\right) - \eta \left\|\nabla f\left(x\right)\right\|^2 + \frac{1}{2}L\eta^2 \left\|\nabla f\left(x\right)\right\|^2$$

$$= f\left(x\right) - \left(1 - \frac{1}{2}L\eta\right)\eta \left\|\nabla f\left(x\right)\right\|^2$$

Proof

$$f\left(\boldsymbol{x}^+\right) \leq f\left(\boldsymbol{x}\right) + \nabla f\left(\boldsymbol{x}\right)^T \left(\boldsymbol{x}^+ - \boldsymbol{x}\right) + \frac{1}{2} L \left\|\boldsymbol{x}^+ - \boldsymbol{x}\right\|^2$$

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

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

Proof

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\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 \\
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Therefore

We have that

$$f\left(\boldsymbol{x}^+\right) \leq f\left(\boldsymbol{x}\right) - \frac{1}{2}\eta \left\|\nabla f\left(\boldsymbol{x}\right)\right\|^2 \tag{2}$$

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.

Therefore

We have that

$$f\left(\boldsymbol{x}^{+}\right) \le f\left(\boldsymbol{x}\right) - \frac{1}{2}\eta\left\|\nabla f\left(\boldsymbol{x}\right)\right\|^{2} \tag{2}$$

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Since f is convex

We can write

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

This comes from the 'First order condition for convexity'

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Then

Plugging this in to (Equation 2)

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

Therefore

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

Then plugging this $x^+ = x - \eta\nabla f\left(x\right)$ into

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Then

Plugging this in to (Equation 2)

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

Therefore

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

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Then

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

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Therefore

It converges with rate

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

Outline

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)
- Nesterov's Proposal (1983)
- Stochastic Gradient Descent (1951)

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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

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

- 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

No Momentum

Starting Point

Solution
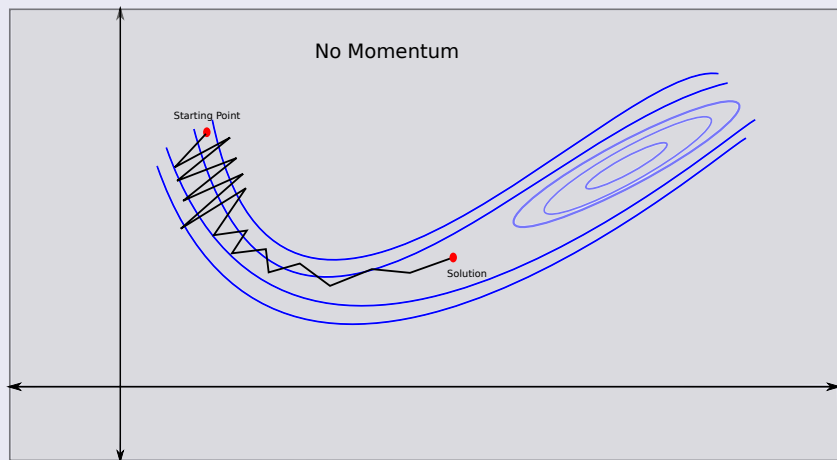
Then, with Momentum

If we have Momentum
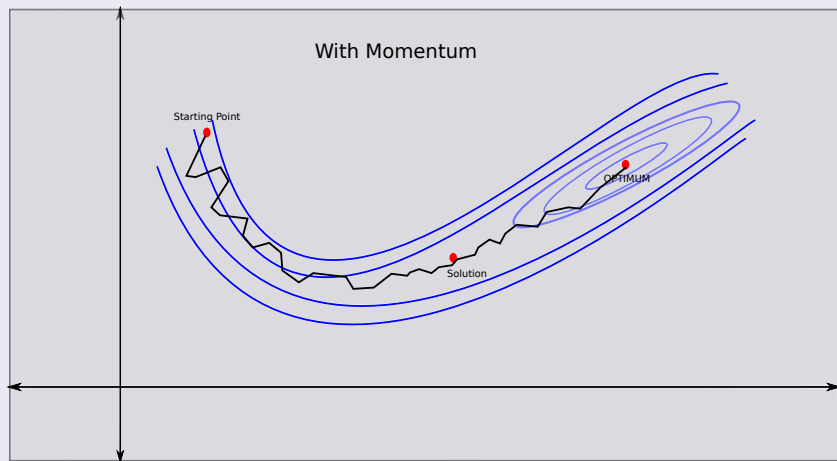
Problem

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.) [5]

Nesterov's Proposal

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 w_{n-1}

$$w_{n+1} = (1 - \gamma_n) y_{n+1} + \gamma_n y_n$$

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 Proposal [6]

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

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

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

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$$\lambda_0 = 0$$

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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...
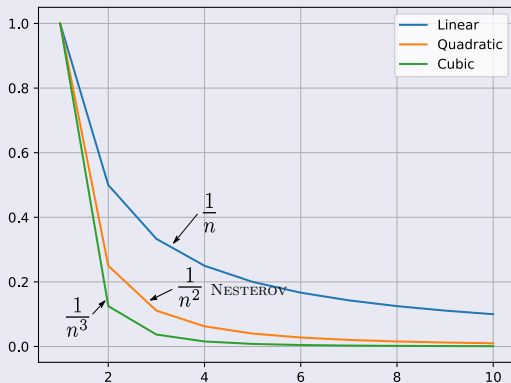
Remark, Polyak vs Nesterov

We have a remarkable difference

- The gradient descent step (orange arrow) is perpendicular to the level set before applying momentum to w_1 (red arrow) in Polyak's algorithm
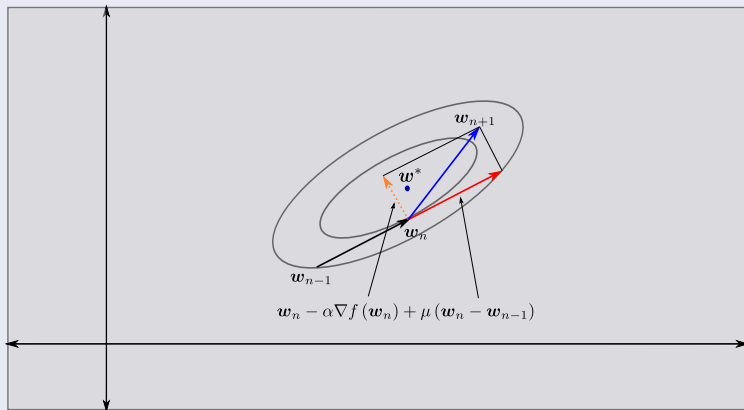
In the case of Nesterov

If we rewrite the equations

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- it is perpendicular to the level set after applying momentum to $\boldsymbol{w}_1$ in Nesterov's algorithm.

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

There is a dependence with respect with different properties of f

In this table, we can see upper bounds for the convergences
$D = \|\boldsymbol{x}_1 - \boldsymbol{x}^*\|_2$ and λ regularization term [7]

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	$\beta D_1^2 \exp\left(-\frac{4n}{\beta/\lambda}\right)$

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Based on the following idea

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

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At any given step, the optimizer queries the oracle with a guess x
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Then, we have

Zeroth Order Methods

- These methods only require the value of function f at the current guess $\boldsymbol{x}$.
  - 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.
  - Gradient descent, Nesterov's and and Polyak's

Second Order Methods

- These methods require the value of the function f, its first derivative (gradient), and its second derivative (Hessian).
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Adaptive Methods and Conjugate Gradients

- 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 hyperparameters.

Some popular methods under this paradigm

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Finally, but not less important

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

Please, take a look

- Convex Optimization: Algorithms and Complexity by Sébastien Bubeck - Theory Group, Microsoft Research [7]

Outline

In our classic Convex Scenario [2]

Least Square Problem locking to minimize the average of the LSE

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

Therefore

Calculating the Gradient

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

Observations

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

- 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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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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Outline

Using the Mean Squared Error (MSE)

It is used to measure how good our estimators are

- The average squared difference between the estimated values and what is estimated

We have the following equation

$$MSE = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2 = E\left[(y - \hat{y})^2\right]$$

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Then, we have that

This Measure is equal to (We know this as the Variance-Bias Trade-off)

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If the MSE is small

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Furthermore

What will happen if we can decrease the Variance at MSE

- In such a way that the bias does not produce a too simplistic $\widehat{y}$?

Then we want as the process MSE evolves over time

- $Var_D^{(t)}(\widehat{y}|x \in D) \to V > 0$ as $t \to \infty$ to avoid over-fitting
- $(E_D[\widehat{y} - y|x \in D])^2 \to B > 0$ as $t \to \infty$ to avoid over-fitting

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Therefore, if we think in the parameters $\boldsymbol{w}$ of a Linear Model

We have a function

$$L\left(\boldsymbol{w}\right) = \left(E_D\left[\boldsymbol{w}^T x - y | \boldsymbol{x} \in D\right]\right)^2$$

We can see that the optimal $\boldsymbol{w}^*$ as the root of the function ∇L, the minimal possible for L

$$\nabla_{\boldsymbol{w}} L\left(\boldsymbol{w}^*\right) = \nabla_{\boldsymbol{w}}\left(E_D\left[\boldsymbol{w}^T x - y | \boldsymbol{x} \in D\right]\right)^2 = 0 + \epsilon \text{ with } \epsilon \sim p\left(\epsilon | \theta\right)$$

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Outline

The MSE Linear Estimation, the Normal Equations

It was proved in slide set 2

- The optimal **Mean-Square Error estimate** of y given the value $X = \boldsymbol{x}$ is

$$E\left[y|\boldsymbol{x}\right] = \widehat{y}$$

  ▶ In general, a nonlinear function.

For Linear Estimators, in $(\boldsymbol{x}, y) \in \mathbb{R}^{d+1}$ joint distributed random variables of zero mean values

- Our goal is to obtain an estimate of $w \in \mathbb{R}^d$ (Our Unknown θ) in the linear estimator model

$$\widehat{y} = w^T x$$

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$$\widehat{y} = \boldsymbol{w}^T \boldsymbol{x}$$

Thus, using MSE as the Cost Equation

Cost Function

$$J\left(\boldsymbol{w}\right) = E\left[\left(y - \widehat{y}\right)^2\right]$$

Thus, we are looking for an estimator that minimize the variance of the error

$$\epsilon = y - \widehat{y}$$

We want to Minimize the cost function $J(w)$ by finding an optimal w^*

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We have

$$\nabla J\left(\boldsymbol{w}\right) = \nabla E\left[\left(y - \boldsymbol{w}^T\boldsymbol{x}\right)^2\right]$$

$$= \nabla E\left[\left(y - w^T x\right)\left(y - w^T x\right)\right]$$

$$= \nabla\left\{E\left[y^2\right] - 2w^T E\left[xy\right] + w^T E\left[xx^T\right]w^T\right\}$$

$$= -2p + 2\Sigma_x w = 0$$

Where, we have

$$p = \left[E\left[yx_1\right], E\left[yx_2\right], \ldots, E\left[yx_n\right]\right] = E\left[xy\right]$$

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=& -2\boldsymbol{p} + 2\Sigma_x \boldsymbol{w} = 0
\end{aligned}
$$

Where, we have

$$
\begin{aligned}
\boldsymbol{p} =& \left[E\left[yx_1\right], E\left[yx_2\right], ..., E\left[yx_d\right]\right] = E\left[\boldsymbol{x}y\right] \\
\Sigma_x =& E\left[\boldsymbol{x}\boldsymbol{x}^T\right]
\end{aligned}
$$

This generates what is know as

> **Then, we get the Normal Equations**
>
> $$\Sigma_x \boldsymbol{w}^* = \boldsymbol{p}$$

Outline

We can use our gradient method[2]

Therefore, we have

$$\boldsymbol{w}_{n+1} = \boldsymbol{w}_n - \mu\left[-\boldsymbol{p} + \Sigma_x \boldsymbol{w}_n\right]$$

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Then, the final idea is to find a μ

- Which allows for convergence!!!
- This is the first step in the idea of Stochastic Gradient Descent (SGD)
  - Given that SGD depends on specifics μ

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Outline

How can we do this?

$$c_n = \boldsymbol{w}_n - \boldsymbol{w}^*$$

Thus, we obtain

$$w_n - w^* = w_{n-1} + \mu \left[p - \Sigma_x w_{n-1} \right] - w^*$$

Then

$$c_n = c_{n-1} + \mu \left[p - \Sigma_x \left(c_{n-1} + w^* \right) \right]$$

How can we do this?

We can use our error to measure the convergence by μ

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Remembering $\Sigma_x \boldsymbol{w}^* = \boldsymbol{p}$

- We can try to guess the rate of convergence:

$$c_n = I c_{n-1} - \mu \left[\Sigma_x c_{n-1} \right] = \left[I - \mu \Sigma_x \right] c_{n-1}$$

Remember that

$\Sigma_x = Q \Lambda Q^T$ with $Q Q^T = I$

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We have

$$c_n = \left[QQ^T - \mu Q \Lambda Q^T \right] c_{n-1} = Q \left[I - \mu \Lambda \right] Q^T c_{n-1}$$

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Iterating over all the sequence

We have by using recursion

$$\boldsymbol{v}(i) = [I - \mu\Lambda]^i \boldsymbol{v}(0)$$

Thus, for each component

$$v_{ji} = (1 - \mu\lambda_j)^i v_{j0}$$

Now, we have that

$$|1 - \mu\lambda_j| < 1 \text{ for all } j = 1, 2, ..., d$$

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What about the Rate of Convergence?

As you can see the quadratic is faster than linear in convergence
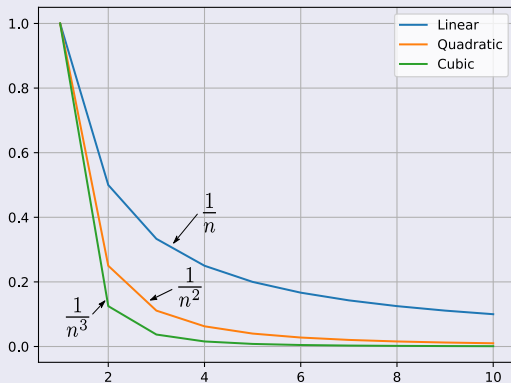
What about the Rate of Convergence?

Assume an ideal case for the evolution of v_{ji} as it converges

Given the evolution of this curve, $f(t)$

Then, we can assume $f(t) = \exp\{-t/\tau_j\}$

- We can try to guess the rate of convergence τ_i.

Then we have $t = iT$ and $t - 1 = iT$

- Assuming a step size of T

Then, using $v_i = [1 - \mu\lambda_j] v_{i-1}$

$$\exp\{-iT/\tau_j\} = [1 - \mu\lambda_j]\exp\{-(i-1)T/\tau_j\}$$

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Then, Solving the Equation

We have applying the function $\ln$

$$-\frac{iT}{\tau_j} = \ln\left[1 - \mu\lambda_j\right] - \frac{(i-1)T}{\tau_j}$$

Solving, we have

$$\tau_j = -\frac{1}{\ln\left(1 - \mu\lambda_j\right)}$$

The time constant results as

$$\tau_j \approx \frac{1}{\mu\lambda_j} \text{ for } \mu \ll 1$$

- The slowest rate of convergence is associated with the component that corresponds to the smallest eigenvalue.

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- **The slowest rate of convergence is associated with the component that corresponds to the smallest eigenvalue.**

However

However, this is only true for small enough values of μ

- Therefore, we need to consider something different

Therefore, we take two extreme vases

Let us consider as an example the case of μ taking a value

$$\mu \simeq \frac{2}{\lambda_{\max}}$$

The value of $|1 - \mu\lambda|$ corresponding to the maximum eigenvalue

- It will have an absolute value very close to one.

$$|1 - \mu\lambda_{\max}| = \left|1 - \frac{2}{\lambda_{\max}}\lambda_{\max}\right| = 1$$

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The Optimal Value

We can use the following cost function

$$\mu_0 = \arg \min_{\mu} \max_{j} |1 - \mu \lambda_j|$$

$$s.t. \ |1 - \mu \lambda_j| < 1 \ j = 1, 2, ..., d$$

This has the following solution

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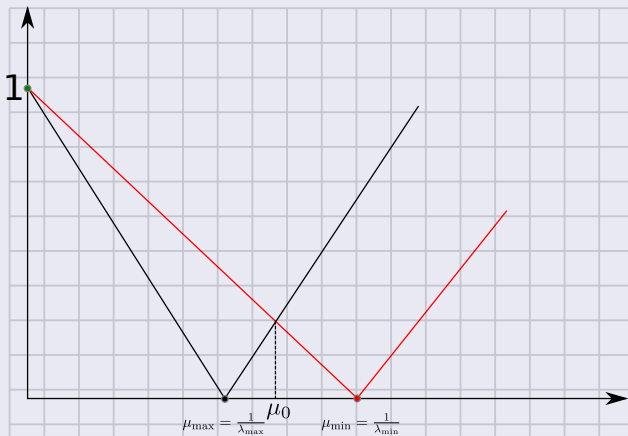
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> **This has the following solution**
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Outline

Focusing on the mean-square error.

> **Adding and Subtracting $\boldsymbol{w}^{*T}\Sigma_x\boldsymbol{w}^*$ and taking the definition**
>
> $$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} J\left(\boldsymbol{w}\right) \text{ and } \Sigma_x\boldsymbol{w}^* = \boldsymbol{p}$$

Therefore, we have

$$J\left(\boldsymbol{w}\right) = J\left(\boldsymbol{w}^*\right) + \left(\boldsymbol{w} - \boldsymbol{w}^*\right)^T \Sigma_x \left(\boldsymbol{w} - \boldsymbol{w}^*\right)$$

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Where we have that at the optimal

It is possible to see that

$$J\left(\boldsymbol{w}^*\right) = \sigma_y^2 - \boldsymbol{p}^T \Sigma_x^{-1} \boldsymbol{p} = \sigma_y^2 - \boldsymbol{w}^{*T} \Sigma_x^{-1} \boldsymbol{w}^* = \sigma_y^2 - \boldsymbol{p}\boldsymbol{w}^*$$

- The minimum at the optimal solution!!!

Taking the orthonormality of the eigenvectors

$$J\left(\boldsymbol{w}\right) = J\left(\boldsymbol{w}^*\right) + \sum_{j=1}^{d} \lambda_j \left|v_{ji}\right|^2$$

Therefore, we have

$$J\left(\boldsymbol{w}\right) = J\left(\boldsymbol{w}^*\right) + \sum_{j=1}^{d} \lambda_j \left(1 - \mu\lambda_j\right)^{2i} \left|v_{j0}\right|^2$$

Convergence

This converges to the minimum value $J(\boldsymbol{w}^*)$ asymptotically

- This convergence is monotonic, because $\lambda_j (1 - \mu\lambda_j)^2$ is positive.

The rates of convergence are finally

$$\tau_j = \frac{-1}{2\ln(1-\mu\lambda_j)} \approx \frac{1}{2\mu\lambda_j}$$

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We have a problem

The previous analysis cannot be carried out

- For the case of an iteration-dependent step-size.
  - But we have a card in the sleeve

It is possible to show in such cases

The Gradient Descent Algorithm convergences if

$$\mu_i \to 0, \text{ as } i \to \infty$$

$$\sum_{i=1}^{\infty} \mu_i = \infty$$

A classic which comply with both conditions

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

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Solving for the normal equations as well as using the gradient descent

There is a small problem

- You are required to have access to the analytical model.

Additionally

- You need to have access to the second order statistics of the involved variables
  - The Covariance Matrix Σ_x

$$\Sigma_x w^* = p$$

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We have that the Robbins-Monro Theorem[8]

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 a such that the equation

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

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

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

- It has a unique root $\boldsymbol{w} = \boldsymbol{w}^*$

Goal

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

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

Then, we want to generate values $w_1, w_2, ..., w_n$, thus, we generate w_n from

- $M\left(w_1\right), M\left(w_2\right), ..., M\left(w_{n-1}\right)$
- and the possible derivatives $M'\left(w_1\right), M'\left(w_2\right), ..., M'\left(w_{n-1}\right)$

Thus, we would love that

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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

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

Such that

$$M\left(w\right) = \int_{-\infty}^{\infty} ydH\left(y|w\right)$$

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We Postulate

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

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

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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Now, For a positive δ

$M\left(\boldsymbol{w}\right)$ 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 $\{w_n\}$

$$w_{n+1} = w_n + \mu_n (a - y_n)$$

Where y_n is a random variable such that

$$Pr[y_n \le y | w_n] = H(y | w_n)$$

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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

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

- No matter what is the initial value w_0.

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

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

$$= b_n + \mu_n^2 c_n - 2\mu_n d_n$$

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\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)\right.\right. \\
=& b_n + \mu_n^2 e_n - 2\mu_n d_n
\end{aligned}
$$

With Values

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

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

From $M(w) \leq 0$ for $w \leq w^*$ and $M(w) \geq 0$ for $w > w^*$

$$d_n \geq 0$$

With Values

We have

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

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

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

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

We can prove that

$$0 \leq r_n \leq \left[C + |a|^2\right] < \infty$$

Now, given

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

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Then, summing over i we obtain

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

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Then, summing over i we obtain

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

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

Then

Hence the positive-term series

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

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

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

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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Then, we have that

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

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

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

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Now

> **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 $\delta > 0$

$$M\left(\boldsymbol{w}\right) \leq \alpha - \delta \text{ for } \boldsymbol{w} < \boldsymbol{w}^*$$
$$M\left(\boldsymbol{w}\right) \geq \alpha + \delta \text{ for } \boldsymbol{w} > \boldsymbol{w}^* \tag{4}$$

Or Else

$$M\left(\boldsymbol{w}\right) < \alpha \text{ for } \boldsymbol{w} < \boldsymbol{w}^*$$
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And

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

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

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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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Recap of Robbins-Monro Proposal

Given the following function

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

Given a series of i.i.d. observations

- The following iterative procedure (Robbins-Monro Scheme)

$$w_n = w_{n-1} - \mu_n \phi\left(w_{n-1}, x_n\right)$$

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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

$$\sum_{i=0}^{\infty} \mu_i^2 < \infty$$

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Outline

Mean-Square Error [2]

Cost function for MSE

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

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

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

Therefore, everything depends on the form of the Loss function

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

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

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

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Therefore

We simply take $\alpha = 0$ then

$$\nabla J\left(\boldsymbol{w}\right) = E\left[\nabla \mathcal{L}\left(\boldsymbol{w}, \boldsymbol{x}, y\right)\right] = 0$$

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

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

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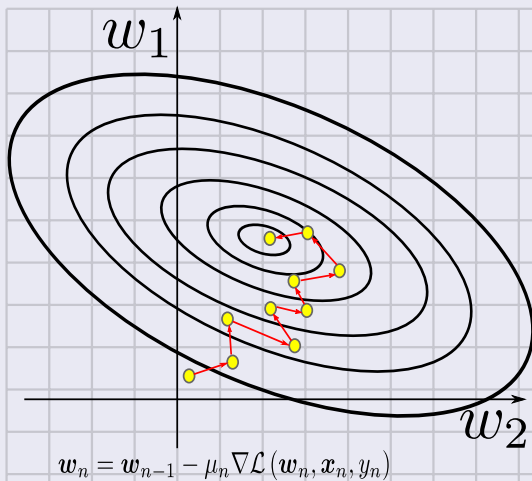Given the sequence of observations $\{(\boldsymbol{x}_i, y_i)\}_{i=1,2,\dots}$ and values $\{\mu_i\}_{i=1,2,\dots}$

- We have that the iterative procedure becomes:

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

  ▸ The Well known Vanilla Stochastic Gradient Descent (SGD)

Geometrically

We have the following

$$w_n = w_{n-1} - \mu_n \nabla \mathcal{L}(w_n, x_n, y_n)$$

Outline

Therefore

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

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

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

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- Low complexity requirements makes this algorithmic family to be the one that is selected in a number of practical applications.
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Outline

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
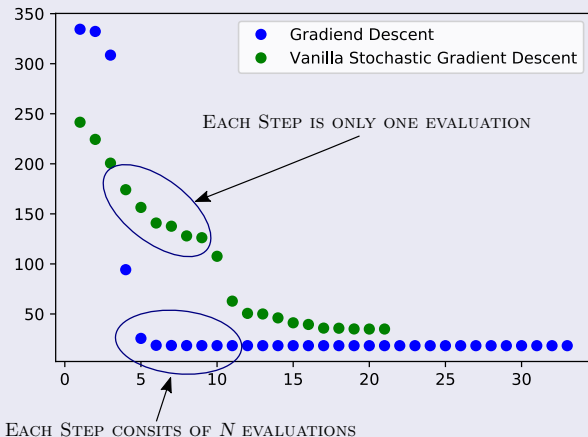
Problems

However, we need to improve such Vanilla Stochastic Gradient Descent

Outline

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

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

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

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

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In our example

We have a nice result
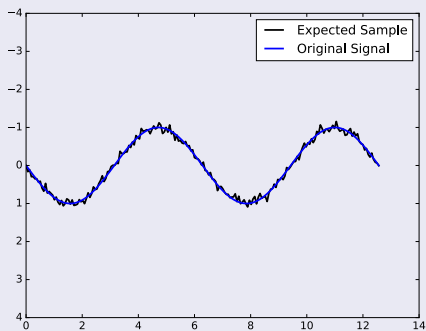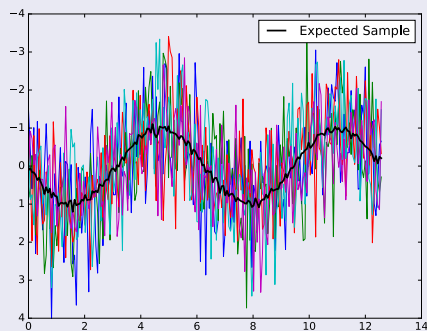
Thus

Using a similar idea, you could use an average [9]

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

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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 $\boldsymbol{w}\,(k)$
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Therefore

1. for i in batch k

$$\boldsymbol{w}_k = \boldsymbol{w}_{k-1} - \alpha \nabla J(\boldsymbol{w}_{k-1}, \boldsymbol{x}_i, y_i)$$

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

$$\boldsymbol{w}_k = \boldsymbol{w}_{k-1} - \alpha \nabla J \left(\boldsymbol{w}_{k-1}, \boldsymbol{x}_i, y_i \right) - ...$$
$$\alpha \nabla J \left(\boldsymbol{w}_{k-1}, \boldsymbol{x}_{i+1}, y_{i+1} \right) - ...$$
$$\alpha \nabla J \left(\boldsymbol{w}_{k-1}, \boldsymbol{x}_{i+m}, y_{i+m} \right)$$

$$= w_{k-1} - \frac{1}{m} \sum_{i=1}^{m} \nabla J \left(w_{k-1}, x_i, y_i \right)$$

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$$
\begin{aligned}
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& \alpha \nabla J\left(\boldsymbol{w}_{k-1}, \boldsymbol{x}_{i+1}, y_{i+1}\right) - ... \\
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=& \boldsymbol{w}_{k-1} - \frac{1}{m} \sum_{i=1}^{m} \nabla J\left(\boldsymbol{w}_{k-1}, \boldsymbol{x}_i, y_i\right)
\end{aligned}
$$

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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Outline

Observations

Using Traditional Methods used in Gradient Descent

- Golden Ratio
- Bisection Method
- etc

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

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Adaptive Rate Speeds in SGD [10]

Structure of SGD with an adaptive learning rate

$$\boldsymbol{w}\left(t+1\right) = \boldsymbol{w}\left(t\right) - \eta\left(t\right)g\left(t\right)$$
$$\eta\left(t\right) = h\left(t\right)$$

Where

- $g\left(t\right) = \nabla L\left(w\left(t\right)\right)$
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First Order Methods

Gradient descent on the learning rate

- Introducing the following function:

$$f : \mathbb{R}^n \to \mathbb{R}$$
$$\eta \to L\left(\boldsymbol{w}\left(t\right) - \eta g\left(t\right)\right)$$

This comes a simple intuition

- At time t using $\eta\left(t\right)$, we suffer a loss of $L\left(\boldsymbol{w}\left(t\right) - \eta g\left(t\right)\right)$ in the next iteration.
  - So f represents such loss in the future if we choose $\boldsymbol{w}\left(t+1\right) = \boldsymbol{w}\left(t\right) - \eta g\left(t\right)$

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Remark

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

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

We have that $\forall \eta$

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

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Intuition

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

  Different scales $L'(w) = \lambda L(w)$ different results

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Second Order Methods

Remark
- 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

$$w(t) = w(t) - \eta(t) g(t)$$

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Hessian Matrix

We have

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

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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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 $f(\eta + 2\epsilon) + f(\eta - 2\epsilon) - 2f(\eta) \approx 0$

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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 $f\left(\eta^{(k)}\right)$
  - Actually five passes over the function f

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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

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- With an appropriate smoothing δ value.

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Outline

Introduction

We have been able to accelerate the speed with SGD

- However, Is this enough?
  - ▶ After all, we are dealing with large data sets that are costly to train on them.

Therefore

- We introduce the concept of regret which is used in on-line learning.
  - ▶ After all SGD is a way of doing on-line learning!!!

What is regret?

- It measures how "sorry" the learning algorithm is, in retrospect, of not having followed the predictions of some hypothesis $h \in \mathcal{H}$.

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A Better Intuition

$$X_1, X_2, ..., X_t$$

Your task

- To guess X_{t+1} and an estimator of X, $\hat{X}$

Clearly, you have looses

- They could be exemplified by the square distance between $\left(\hat{X} - X_{t+1}\right)^2$

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Imagine you are playing a game where data is given to you

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Strategies to minimize the regret

In the case of least squared error

$$\hat{X} = \frac{1}{T} \sum_{t=i}^{T} X_t$$

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- This is actually a good estimate given, if we assume $X \sim \mathcal{N}\left(\mu, \sigma^2\right)$
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- **How well can I do using the information from my samples compared to how well I could have done had I known the distribution in advance?**

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$$Cost_T \left(Alg \right) - Cost \left(OPT \right)$$

Regret

Definition

- The sum of all the previous difference between the on-line prediction $f_i(\boldsymbol{w}_i)$ and the best optimal parameter $f_i(\boldsymbol{w}^*)$

$$R(T) = \sum_{i=1}^{N} [f_i(\boldsymbol{w}_i) - f_i(\boldsymbol{w}^*)] = f(T)$$

  ▸ Where $\boldsymbol{w}^* = \arg\min_{\boldsymbol{w} \in \mathcal{X}} \sum_{i=1}^{n} f_t(\boldsymbol{w})$

What do we want?

> ## We want $f(T) = o(T)$ (Little o) i.e.
> $$\frac{f(T)}{T} \to 0$$

Example

The Expert Advice Model

- On a sequence of rounds $t = 1, ..., T$ a player choose an action $i_t \in \{1, ..., n\}$
- The adversary chooses cost or loses for each action $l_t(1), ..., l_t(n) \in \{0, 1\}$

It looks like a Min-Max Play from Artificial Intelligence

- Theorem (Von Neumann Minimax Theorem)

$$\min_{y \in \Delta^n} \max_{x \in \Delta^m} y^t A x = V = \max_{x \in \Delta^m} \min_{y \in \Delta^n} y^t A x$$

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Then, the player pays $E[l_t(I)]$ observes l_t

- Updates $p_{t+1} \in \Delta_n$, where Δ_n is the probability simplex over the n actions.

The probability simplex is the $(n-1)$-dimensional simplex determined by the unit vectors $e_1, ..., e_n \in R^n$

- It is the set of vectors that satisfy $x \succeq 0$ with $1^T x = 1$

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Furthermore

$$Regret = \sum_{t=1}^{T} p_t l_t - \min_{i \in \{1,...,N\}} \sum_{t=1}^{T} l_t(i)$$

We now introduce the Weighted Majority Algorithm

- We define $L_t(i) = \sum_{s=1}^{t} l_s(i)$ to be the vector of cumulative losses of the experts at time t.

The algorithm chooses an expert at time t by distribution p_t where

- $w_t(i) = \exp\{-\eta L_t(i)\}$ Weight assigned to expert i at time t and $\eta > 0$ is a parameter of the algorithm.
- $p_t(i) = \frac{w_t(i)}{\sum_{j=1}^{N} w_t(i)}$ Probability of choosing expert i at time t.

Furthermore

This is typically called the "Expert" or "Hedge" setting with regret

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Randomized Weighted-Majority(n experts)

Algorithm

Input: **Penalty** $\beta \in \left[\frac{1}{2}, 1\right)$

1 **for** $i = 1$ **to** n

2 $\quad w_1(i) = 1$

3 $\quad p_1(i) = \frac{1}{N}$

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8.   **else** $w_{t+1}(i) = w_t(i)$
9. $W_{t+1} = \sum_{i=1}^{n} w_{t+1}(i)$
10.   **for** $i = 1$ **to** n
11. $p_{t+1}(i) = \frac{w_{t+1}(i)}{W_{t+1}}$

Randomized Weighted-Majority(n experts)

Algorithm

      Input: **Penalty** $\beta \in \left[\frac{1}{2}, 1\right)$

1. **for** $i = 1$ **to** n
2. $w_1(i) = 1$
3. $p_1(i) = \frac{1}{N}$
4. **for** $t = 1$ **to** T
5.   **for** $i = 1$ **to** n
6.   **if** $l_t(i) = 1$:
7. $w_{t+1}(i) = \beta w_t(i)$
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11. $p_{t+1}(i) = \frac{w_{t+1}(i)}{W_{t+1}}$
12. **return** w_{T+1}

Then

Theorem

- Then, for any $T \geq 1$, the expected cumulative loss of Randomized Weighted-Majority can be bounded as follows

$$\mathcal{L}_T \leq \frac{\log n}{1 - \beta} + (2 - \beta)\, \mathcal{L}_T^{\min}$$

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- with $\mathcal{L}_T = \sum_{t=1}^{T} p_t l_t$, $\mathcal{L}_T^{\min} = \min_{i \in \{1, \dots, N\}} \sum_{t=1}^{T} l_t(i)$

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- For $\beta = 1 - \frac{\sqrt{\log n}}{T}$ when $1 - \frac{\sqrt{\log n}}{T} \geq \frac{1}{2}$,

$$\mathcal{L}_T \leq \mathcal{L}_T^{\min} + 2\sqrt{T \log N}$$

Now, the proof

We define the following function

$$W_t = \sum_{i=1}^{n} w_t(i)$$

Where

We have that

$$W_{t+1} = \sum_{i:l_t(i)=0} w_t(i) + \beta \sum_{i:l_t(i)=1} w_t(i)$$

Then

$$W_{t+1} = \sum_{i:l_t(i)=0} w_t(i) + \sum_{i:l_t(i)=1} w_t(i) - \sum_{i:l_t(i)=1} w_t(i) + \beta \sum_{i:l_t(i)=1} w_t(i)$$

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We have

$$W_{t+1} = W_t + (\beta - 1) \sum_{i:l_t(i)=1} w_t(i) \times \frac{W_t}{W_t}$$

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Finally

$$W_{t+1} = W_t + (\beta - 1) W_t L_t = W_t (1 - (1 - \beta) L_t)$$

Then, we have an upper bound

We have by recursion

$$W_{T+1} = n \prod_{t=1}^{T} \left(1 - (1 - \beta) L_t\right)$$

- With $W_1 = \sum_{i=1}^{n} 1$ which correspond to the initialization of the algorithm

Now, we have a lower bound lower bound

$$W_{T+1} \geq \max_{i \in \{1,...,N\}} w_{T+1}(i) = \beta^{L_T^{min}}$$

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Using $\beta^{\mathcal{L}_T^{\min}} \le n \prod_{t=1}^{T} \left[1 - (1 - \beta) L_T\right]$

$$\mathcal{L}_T^{\min} \log \beta \le \log n + \sum_{t=1}^{T} \log \left[1 - (1 - \beta) L_T\right]$$

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Furthermore

$$\mathcal{L}_T^{\min} \log \beta \le \log n - (1 - \beta) \mathcal{L}_T$$

After a small math manipulation we have

$$\mathcal{L}_T \le \frac{\log n}{1 - \beta} - \frac{\log (1 - (1 - \beta))}{1 - \beta} \mathcal{L}_T^{\min}$$

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Finally

> We have that $\mathcal{L}_T^{\min} = \min_{i \in \{1,...,N\}} \sum_{t=1}^{T} l_t(i) \leq T$
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I leave this to you, please remember

- For For $\beta = 1 - \frac{\sqrt{\log n}}{t}$ when $1 - \frac{\sqrt{\log n}}{t} \geq \frac{1}{2}$,

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Outline

The Stochastic Gradient Descent

Imagine the follow

- We assume that the covariance matrix and the cross-correlation vector are unknown.

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

- The solution corresponds to the root of the gradient of the cost function:

$$\Sigma_x w - p = E\left[x\left(x^T w - y\right)\right] = 0$$

We have

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Outline

The Least-Mean Squares Adaptive Algorithm

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

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

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Solution

This can be overcome if one sets the value of μ_n

- To a preselected fixed value, μ.

The celebrated Least-Mean-Squares Algorithms

- Algorithm LMS
  1. $w_{-1} = 0 \in \mathbb{R}^d$
  2. Select a value μ
  3. for $n = 0, 1, \ldots,$ do
  4. $e_n = y_n - x_n^T w_{n-1}$
  5. $w_n = w_{n-1} + \mu e_n x_n$

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</div>

Complexity

Something Notable

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

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Thus

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Important

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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Outline

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AdaGrad

Adaptive Gradient Algorithm (AdaGrad) [11]

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

Definition (Subgradient) [12]

- A vector g is a subgradient of a function $f : \mathbb{R}^d \to \mathbb{R}$ 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

$f(\boldsymbol{x}_1) + g_1^T(\boldsymbol{z} - \boldsymbol{x}_1)$

$f(\boldsymbol{x_2}) + g_2^T(\boldsymbol{z} - \boldsymbol{x}_2)$

$f(\boldsymbol{x_2}) + g_3^T(\boldsymbol{z} - \boldsymbol{x}_2)$

x_1 x_2
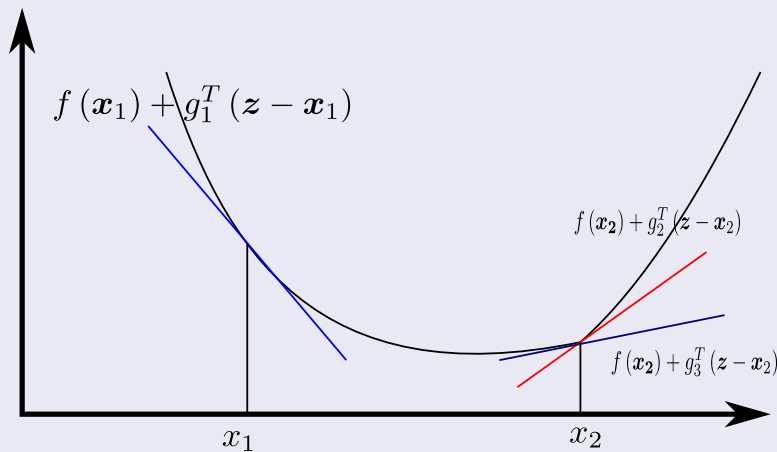
Standard Subgradient Algorithms

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

A Little Bit of Notation

First, the accumulation of gradients

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

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

We denote the ith row of this matrix

- The concatenation of the ith component of each subgradient by $g_{1:t,i}$

We also denote the outer product matrix

$$G_t = \sum_{t=1}^{t} g_\tau g_\tau^T$$

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A first approach

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

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

Therefore

$$w_{t+1} = \Pi_1^{G_t^{1/2}} \left(w_t - \eta G_t^{-\frac{1}{2}} g_t \right)$$

- $g_t = \nabla f(w_t)$
- $G = \sum_{\tau=1}^t g_\tau g_\tau^T$

A first approach

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

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Remarks

Given that $G_t^{-\frac{1}{2}}$ is computationally intensive

- And the diagonal has the necessary information!!! We can choose
$$\boldsymbol{w}_{t+1} = \Pi_X^{diag(G)^{\frac{1}{2}}} \left[\boldsymbol{w}_t - \eta \, diag\left(G\right)^{-\frac{1}{2}} g_t \right]$$

Basically, it looks as a normalization
- G acts as memory for the variance of η_t

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Remarks

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.

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

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Outline

As in MSE [13]

> **We are interested in minimizing the expected value of f**
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> $$E\left[f\left(\boldsymbol{w}\right)\right]$$

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.

Using combinations with $\alpha_1, \alpha_2 \in [0, 1]$

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Basically, they are the following quantities

You could thing on the following concepts

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

Therefore, given the decays by the following formulas

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

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Therefore

We have two upper bounds

- When $1 - \beta_1 > \sqrt{1 - \beta_2}$

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

Otherwise

$$|\Delta_t| \leq \alpha$$

Therefore

We have two upper bounds

- When $1 - \beta_1 > \sqrt{1 - \beta_2}$

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

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Something Notable

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Finally, ADAM Algorithm

Adam Algorithm

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

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

The adaptive method ADAM achieves

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

Compared with the Online Gradient Descent

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Outline

Looking into the past

> **If we look at the following equations**
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with the update

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

Now, we have

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We notice that the term $\sqrt{\widehat{v}_{t-1}} + \epsilon$

- It works as a variance that if $\nabla f(\boldsymbol{w}_{t-1}) \longrightarrow 0$ works as a dampener in the search

Then, the final recursion takes to the point 0

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Doing some Math work

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

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

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

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In accordance with the Simulated Annealing part

This makes ADAMS adaptive
- But with a limitation on the change because you always take the step

Making the past more important than the present
- When updating

Question
- Can we make the past less important or the memory more selective...?

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You require more information

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Making it quite light for methods as

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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.

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Conclusions

In Machine Learning

- We need to have the best speedups to handle the problem dealing with Big Data...

As we get more and more algorithms

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Take a look to

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