# 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 $\boldsymbol{w}_0$.
2. Compute the gradient vector $\nabla J(\boldsymbol{w}_0)$.
3. Obtain value $\boldsymbol{w}_1$ by moving from $\boldsymbol{w}_0$ in the direction of the steepest descent:

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

$\eta_n$ is a positive scale factor or learning rate!!!

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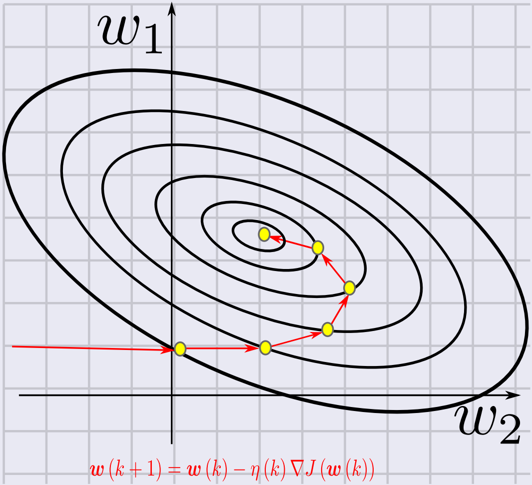
# Geometrically

## We have the following



# Outline

# Although

**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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# Do you remember the problem of the $\eta$ 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 [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**

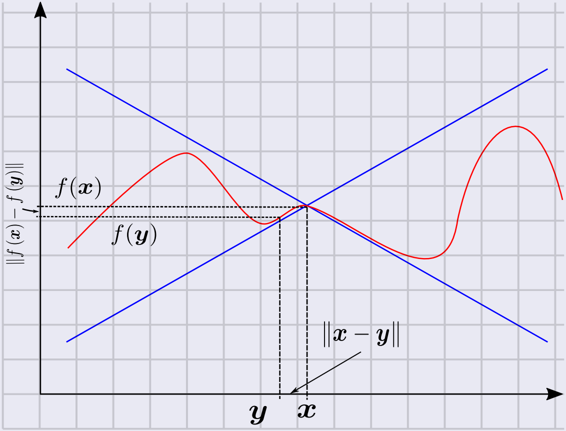
- A function $f : S \subset \mathbb{R}^n \to \mathbb{R}^n$ satisfies the Lipschitz Continuous at $\boldsymbol{x} \in S$, if there is a such constant $L > 0$ such that

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

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

# Example when you see $L$ as the slope

## Here the function $f : \mathbb{R} \rightarrow \mathbb{R}$



# 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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# Therefore

**Lipschitz Continuity implies**

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

# Outline

# Convergence idea

**Definition (Big $O$ - Upper Bound) [4]**

For a given function $g(n)$:

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

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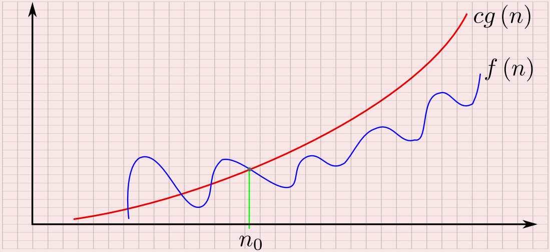
## Example



# 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

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

**Thus, Gradient Descent has a linear convergence speed**

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

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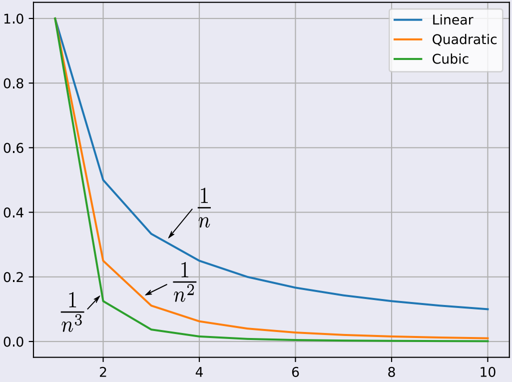
# Example

## 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 $\boldsymbol{x}$ 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 $\lambda \in (0,1)$

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

# Graphically

**This can further expanded to functions**

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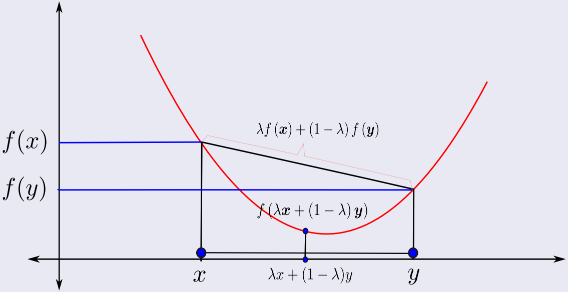

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# Convergence of gradient descent with **fixed step size**

## Theorem

- Suppose the function $f : \mathbb{R}^d \to \mathbb{R}$ is convex and differentiable, and we have that $\left\|\nabla f\left(\boldsymbol{x}\right) - \nabla f\left(\boldsymbol{y}\right)\right\|_2 \leq L \left\|\boldsymbol{x} - \boldsymbol{y}\right\|$ (Lipschitz Continuous Gradient) for any $\boldsymbol{x}, \boldsymbol{y}$ and $L > 0$.

## We have that

- Then, if we run the **gradient descent** for $k$ 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.

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# Proof

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

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

**We have the following inequality**

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\begin{aligned}
f(\boldsymbol{y}) &= f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T (\boldsymbol{y}-\boldsymbol{x}) + \frac{1}{2}\nabla^2 f(\boldsymbol{x}) \|\boldsymbol{y}-\boldsymbol{x}\|^2 \\
&\leq f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T (\boldsymbol{y}-\boldsymbol{x}) + \frac{1}{2} L \|\boldsymbol{y}-\boldsymbol{x}\|^2
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**Now, if we apply the Gradient update $\boldsymbol{y} = \boldsymbol{x}^{+} = \boldsymbol{x} - \eta \nabla f(\boldsymbol{x})$**

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

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

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

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

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**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 $\eta$ 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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# Since $f$ is convex

## We can write

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\begin{aligned}
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)
\end{aligned}
$$

## This comes from the "First order condition for convexity"

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**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**

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

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

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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**

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

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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 $(w_n - w_{n-1})$

- 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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## Polyak's Step Size

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

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

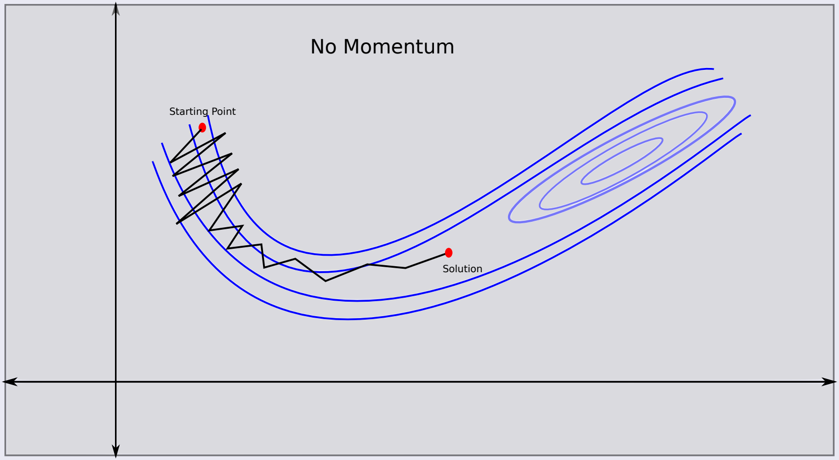
- By the discretization of the second order ODE

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

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

# The Momentum helps to stabilize the GD

## If we do not have Momentum



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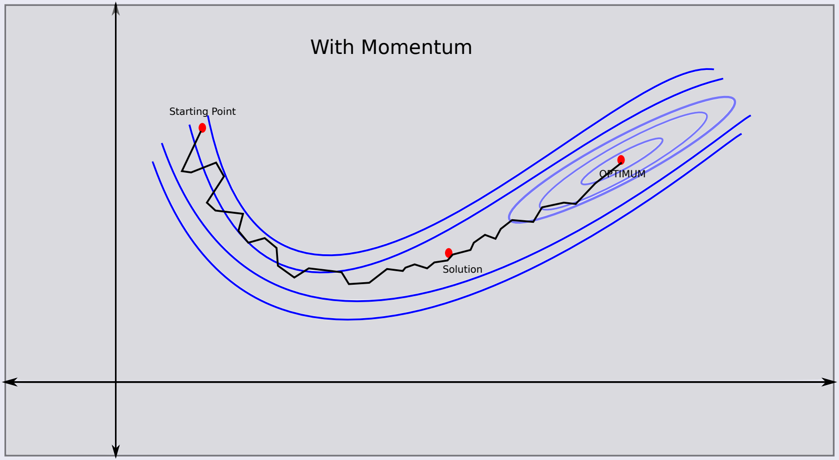

# Problem

**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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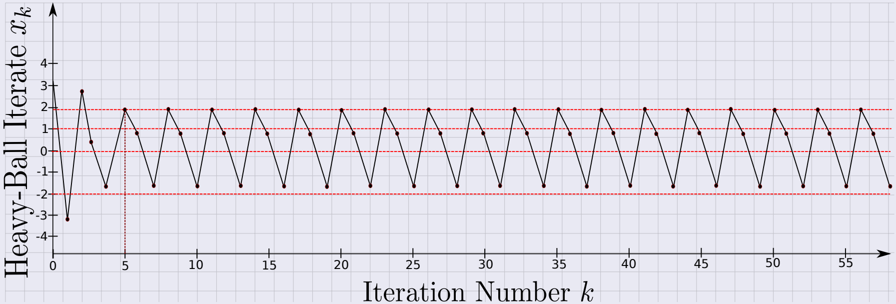
# In Lessard et al.

## 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 $\boldsymbol{w}_{n+1}$**

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

**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 Proposal [6]

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

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\boldsymbol{y}_{n+1} &= \boldsymbol{w}_n - \frac{1}{\beta} \nabla J\left(\boldsymbol{w}_n\right) \\
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\end{aligned}
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## Where, we use the following constants

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\lambda_0 &= 0 \\
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**Theorem (Nesterov 1983)**

- Let $f$ be a convex and $\beta$-smooth function ($\nabla f$ is $\beta$-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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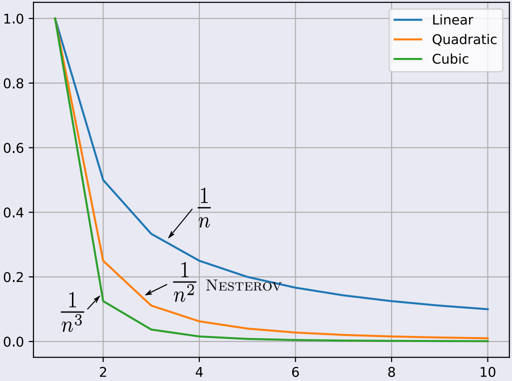
# Example

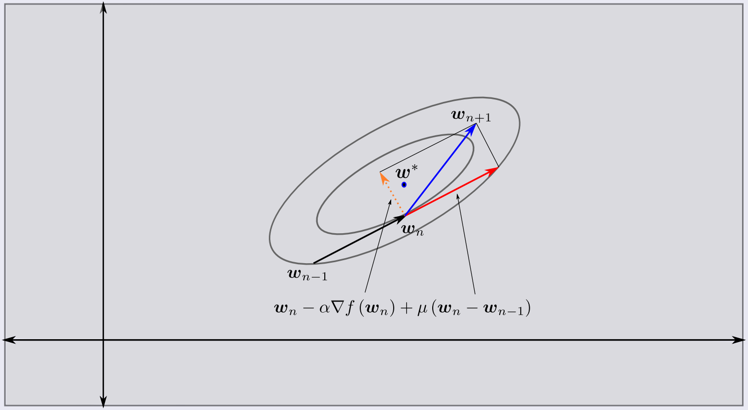
## As you can see Nesterov is faster...



# 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

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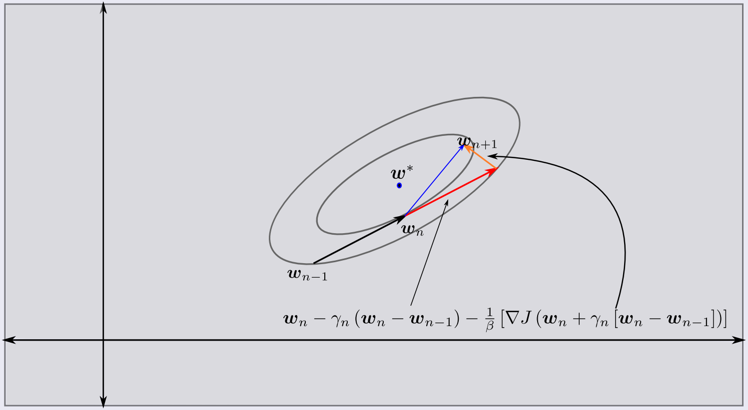

# There is a dependence with respect with different properties of $f$

In this table, we can see upper bounds for the convergences $D = \left\| \boldsymbol{x}_1 - \boldsymbol{x}^* \right\|_2$ and $\lambda$ 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 $\beta$-smooth | $\frac{\beta D_1^2}{n}$ |
| $\alpha$-strongly convex and $L$-Lipschitz | $\frac{L^2}{\alpha n}$ |
| $\alpha$-strongly convex and $\beta$-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.

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## Zeroth Order Methods

- These methods only require the value of function $f$ at the current guess $x$.
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- These methods can inquire the value of the function $f$ and its first derivative.
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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.

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# Finally, but not less important

## Lower Bounds

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## 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**

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

# 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**

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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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  - Accelerating Gradient Decent Using Stochastic Gradient Descent!!!
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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**

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

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

$$MSE = \underbrace{Var_D\left(\widehat{y}|\boldsymbol{x} \in D\right)}_{Variance} + \underbrace{\left(E_D\left[\widehat{y} - y|\boldsymbol{x} \in D\right]\right)^2}_{BIAS}$$

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**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 $MSE_t$ evolves over time**

- $Var_D^{(t)}(\widehat{y}|x \in D) \to V > 0$ 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**

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

**We can see that the optimal $w^*$ as the root of the function $\nabla L$ the minimal possible for $L$**

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

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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 $(\boldsymbol{x}, y) \in \mathbb{R}^d \times \mathbb{R}$ joint distributed random variables of zero mean values

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

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## 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

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

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# Then, we can simply use $\nabla J(\boldsymbol{w}) = 0$

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\nabla J(\boldsymbol{w}) =& \nabla E\left[\left(y - \boldsymbol{w}^T \boldsymbol{x}\right)^2\right] \\
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\boldsymbol{p} = \left[E\left[yx_1\right], E\left[yx_2\right], \ldots, E\left[yx_d\right]\right] = E\left[\boldsymbol{x}y\right]
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# 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**

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

- This is the first step in the idea of Stochastic Gradient Descent (SGD)
  - Given that SGD depends on specifics $\mu$

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**Therefore, we have**

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# Outline

# How can we do this?

**We can use our error to measure the convergence by $\mu$**

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

**Thus, we obtain**

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

**Then**

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

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# Therefore

**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**

$$\Sigma_x = Q \Lambda Q^T \text{ with } QQ^T = I$$

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

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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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**We have that**

$$\begin{aligned} -1 <& 1-\mu\lambda_{max} < 1 \\ -1 <& -\mu\lambda_{max} < 0 \\ 0 <& \mu\lambda_{max} < 2 \end{aligned}$$

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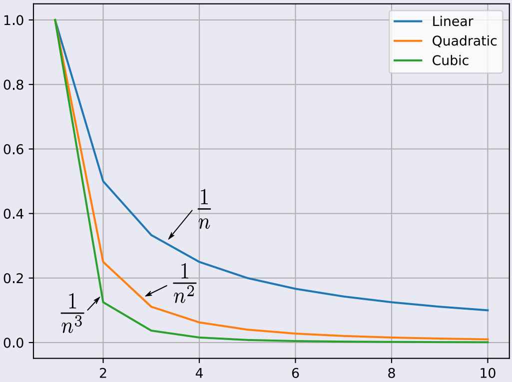
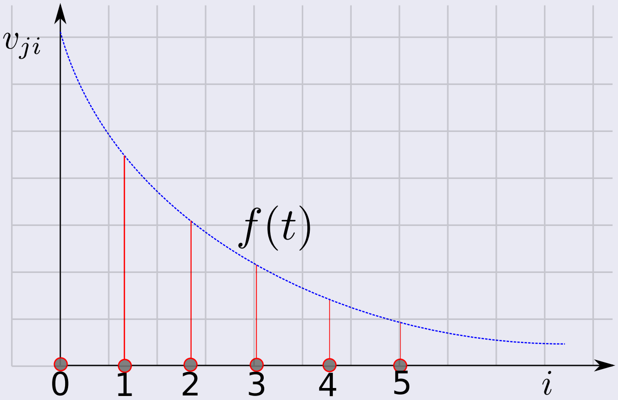
# What about the Rate of Convergence?

## 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 $f(t) = \exp\left\{-{}^{t}/_{\tau_j}\right\}$**

- We can try to guess the rate of convergence $\tau_i$.

**Then we have $t = iT$ and $t = (i-1)T$**

- Assuming a step size of $T$

**Then, using $v_{ji} = [1-\mu\lambda_j] v_{ji-1}$**

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

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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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# However

**However, this is only true for small enough values of $\mu$**

- Therefore, we need to consider something different

# Therefore, we take two extreme vases

**Let us consider as an example the case of $\mu$ taking a value**

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

**The value of $|1 - \mu\lambda_j|$ 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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# Now, we have

**On the other hand, when using the minimum eigenvalue in the previous formula**

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

**In such a case**

- The maximum eigenvalue exhibits slower convergence.

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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**

$$\mu_0 = \frac{2}{\lambda_{max} + \lambda_{min}}$$

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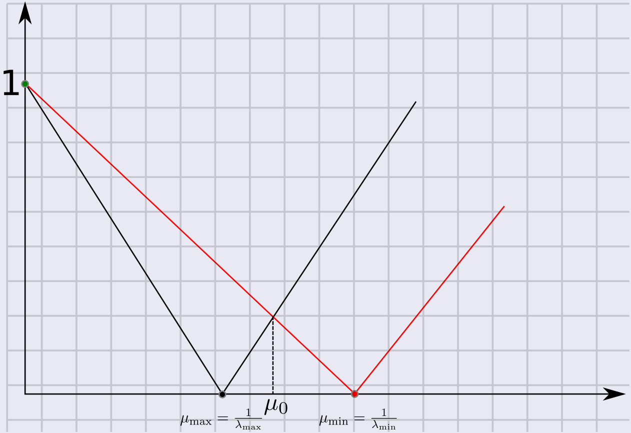
# Graphically

## We have the following situation



# The solution

### 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**

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} J(\boldsymbol{w}) \text{ and } \Sigma_x\boldsymbol{w}^* = \boldsymbol{p}$$

**Therefore, we have**

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

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

# 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

**Taking in account that $\Sigma_x$ is a diagonal matrix**

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

# 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 $J\left(\boldsymbol{w}^{*}\right)$ asymptotically**

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

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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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# Outline

# 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 $\Sigma_x$

$$\Sigma_x w^* = p$$

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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 $\alpha$ such that the equation

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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 $\boldsymbol{w}_1, \boldsymbol{w}_2, ..., \boldsymbol{w}_{n-1}$ thus, we generate $\boldsymbol{w}_n$ from**

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

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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**

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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 $\alpha$ 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 $\{\boldsymbol{w}_n\}$

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

## Where $y_n$ is a random variable such that

$$Pr[y_n \leq y | \boldsymbol{w}_n] = H(y | \boldsymbol{w}_n)$$

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

$$d_n \geq 0$$

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# Additionally

**Now, assuming that exist $C$ such that**

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

**We can prove that**

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

**Now, given**

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**Then, summing over $i$ we obtain**

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

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

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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...**

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

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

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

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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

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

**We have the following Expected Risk**

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**If we additionally have that**

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

# Then under the following constraints

**For some $\delta > 0$**

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

**Or Else**

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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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**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**

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

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

- The following iterative procedure (Robbins-Monro Scheme)

$$\boldsymbol{w}_n = \boldsymbol{w}_{n-1} - \mu_n \phi(\boldsymbol{w}_{n-1}, \boldsymbol{x}_n)$$

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# Robbins-Monro Proposal

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

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

**Under some general conditions about the step size**

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

$$\sum_{i=0}^{\infty} \mu_i \rightarrow \infty$$

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# Outline

# Mean-Square Error [2]

## 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.

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# Mean-Square Error [2]

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## We can get the Gradient of the Expected Cost Function

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

## Therefore, everything depends on the form of the Loss function

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

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

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# Then

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

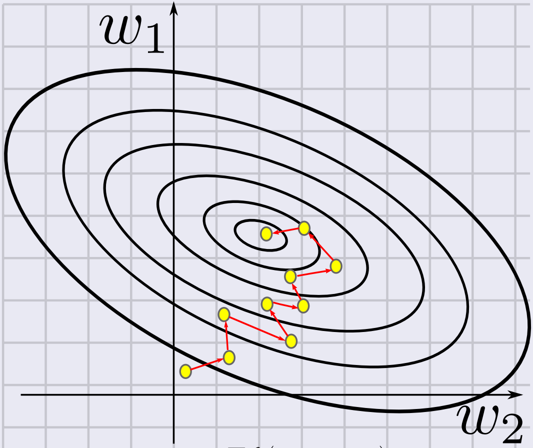
- We have that the iterative procedure becomes:

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

  - The Well known Vanilla Stochastic Gradient Descent (SGD)

# Geometrically

## We have the following

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# 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.

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**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**

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

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

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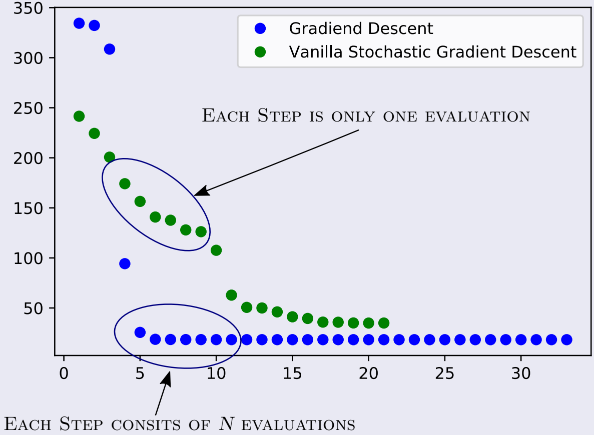
# Outline

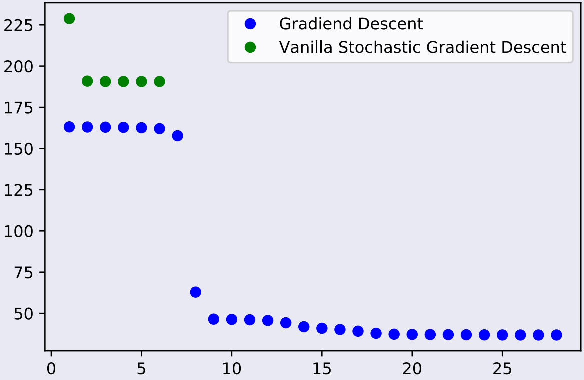
# Example of SGD for, $\frac{1}{2}\sum_{i=1}^{N}\left(\boldsymbol{w}^T\boldsymbol{x}-\boldsymbol{y}\right)^2$

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



# Problems

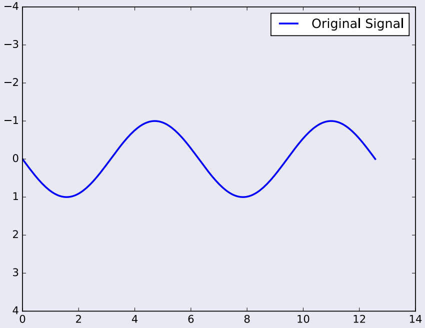
## However, we need to improve such Vanilla Stochastic Gradient Descent

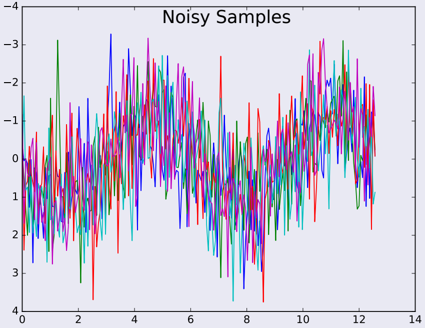


# Outline

# 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**

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

**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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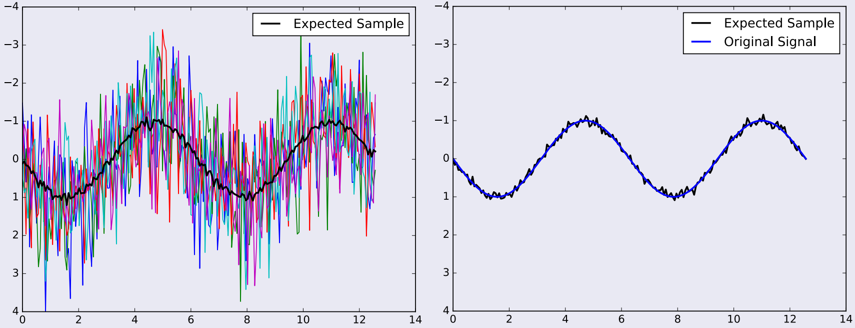
# In our example

## We have a nice result



# Thus

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

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

- 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 $k$

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

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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 $\alpha$

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) - \dots \\
& \alpha \nabla J\left(\boldsymbol{w}_{k-1}, \boldsymbol{x}_{i+1}, y_{i+1}\right) - \dots \\
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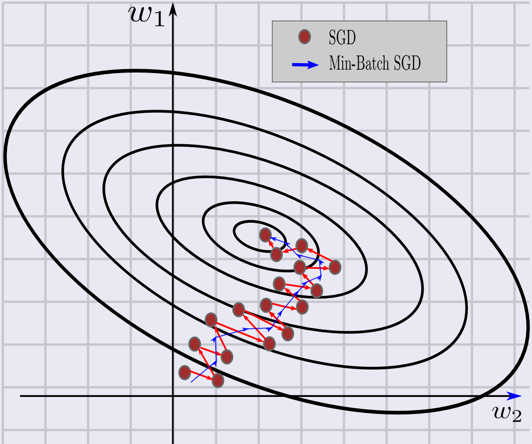
# Notes

## 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

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# 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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# Observations

**Using Traditional Methods used in Gradient Descent**

- Golden Ratio
- Bisection Method
- etc

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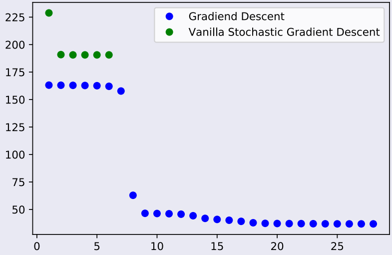

# Adaptive Rate Speeds in SGD [10]

## Structure of SGD with an adaptive learning rate

$$\boldsymbol{w}(t+1) = \boldsymbol{w}(t) - \eta(t)\, g(t)$$
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# First Order Methods

## Gradient descent on the learning rate

- Introducing the following function:

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f :& \mathbb{R}^n \to \mathbb{R} \\
& \eta \to L\left(\boldsymbol{w}\left(t\right) - \eta g\left(t\right)\right)
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## 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:
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**If we continue in a similar direction**

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

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- The algorithm is not scale invariant anymore:

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

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## In order to avoid such problems

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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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# Finally

**We have an approximation to the $\eta$ hyper-parameter**

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

**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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## 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 $f(\eta + 2\epsilon) + f(\eta - 2\epsilon) - 2f(\eta) \approx 0$
2. $$\eta(t+1) = \eta(t) - 2\epsilon \frac{f(\eta+\epsilon) - f(\eta-\epsilon)}{f(\eta+2\epsilon) + f(\eta-2\epsilon) - 2f(\eta) + \delta^{-6}}$$

**A typical value for $\delta$ 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**

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

- With an appropriate smoothing $\delta$ 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

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

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

**Your task**

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

**Clearly, you have looses**

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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 $X \sim N\left(\mu, \sigma^2\right)$
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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?**

**A simple function**

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## A simple function

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# 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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**The player instead of picking highest cost**

- The player pick a distribution over the actions $\{1, ..., n\}$

**Then, the player pays $E\left[l_t\left(I\right)\right]$ observes $l_t$**

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

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

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# Furthermore

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

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

**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 $t$.

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# Randomized Weighted-Majority($n$ experts)

## Algorithm

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

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# Then

## Theorem

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

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

- with $\mathcal{L}_T = \sum_{t=1}^{T} p_t l_t$, $\mathcal{L}_T^{\min} = \min_{i \in \{1,\ldots,N\}} \sum_{t=1}^{T} l_t(i)$
- For $\beta = 1 - \frac{\sqrt{\log n}}{T}$ when $1 - \frac{\sqrt{\log n}}{T} \geq \frac{1}{2}$,

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# 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

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

## Then by using $p_t(i) = \frac{w_t(i)}{W_t}$ and assuming that

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## 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

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

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

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

**Then, we have by using the inequality $\forall x < 1, \log(1-x) \leq -x$**

$$\mathcal{L}_T^{\min} \log \beta \leq \log n - (1-\beta) \sum_{t=1}^{T} L_T$$

# Finally, we have that

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**After a small math manipulation we have**

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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**

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

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# Therefore

## We know

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

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

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

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# The Least-Mean Squares Adaptive Algorithm

### The stochastic gradient algorithm for MSE

- It converges to the optimal mean-square error solution provided that $\mu_n$ 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 $\mu_n$**

- To a preselected fixed value, $\mu$.

**The celebrated Least-Mean-Squares Algorithms**

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

### Given that $\mu$ has a constant value

- The algorithm has now the "agility" to update the estimates
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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

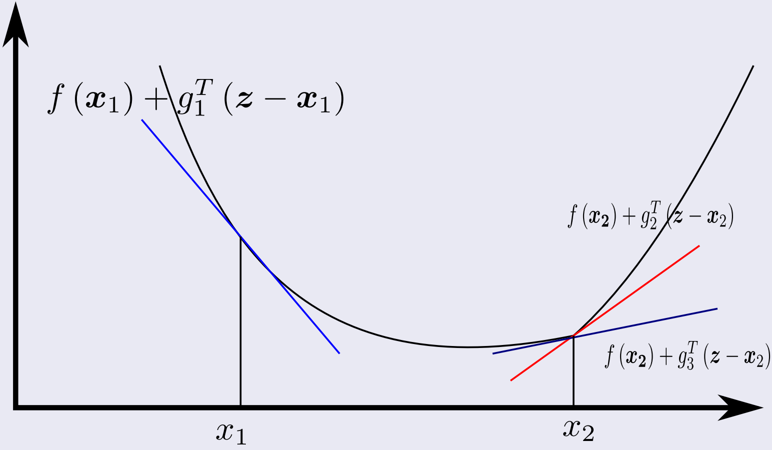
## Definition (Subgradient) [12]

- 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



# Standard Subgradient Algorithms

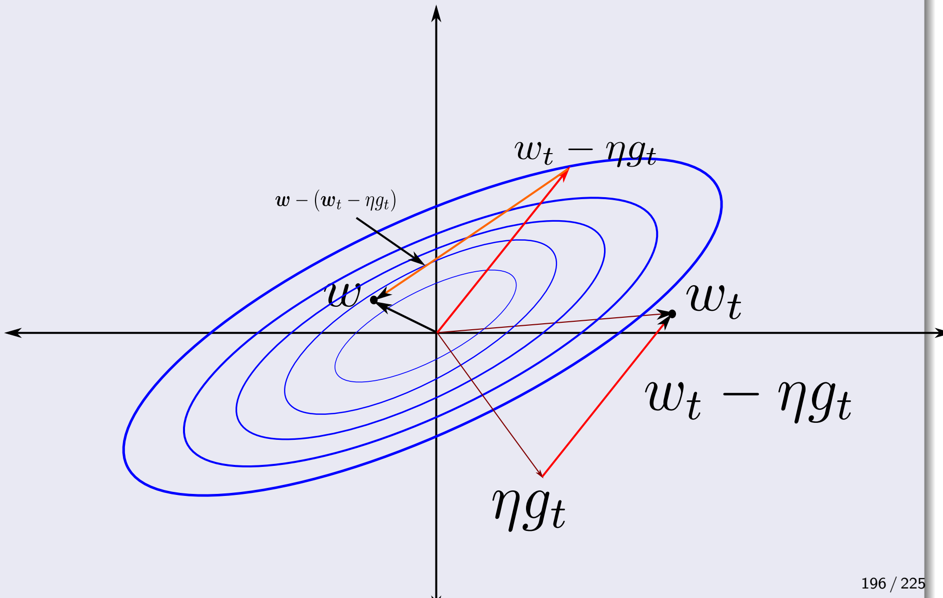
**At Every Timestamp $t$, the learner gets the subgradient information $g_t \in \partial f_t(\boldsymbol{w}_t)$**

- They move the predictor $x_t$ in the opposite direction of $g_t$ while projecting the gradient update

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

# Graphically

**As we can see the traditional setup does not get a faster convergence**



# 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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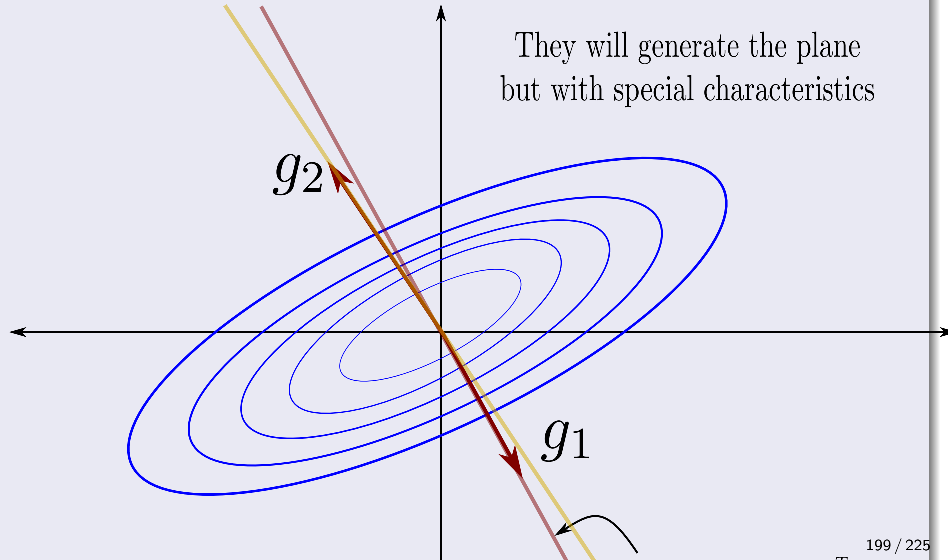
# Graphically

**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 $A$

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

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# Using this, we define

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

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

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

# Remarks

**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 $O\left(d\right)$:

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

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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.

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# As in MSE [13]

**We are interested in minimizing the expected value of $f$**

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

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

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

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

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**You could thing on the following concepts**

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

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

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- This value becomes zero when reaching to the optimal.

## Leading to smaller effective steps in parameter space

- A form of automatic annealing.

# Finally, ADAM Algorithm

## Adam Algorithm

**Input:** $\alpha$ 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. $\quad g_t = \nabla f(w_{t-1}) \leftarrow$ Get gradients w.r.t. stochastic objective at timestep $t$
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# Regret in ADAM

**The adaptive method ADAM achieves**

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

**Compared with the Online Gradient Descent**

- Hazan, Elad, Alexander Rakhlin, and Peter L. Bartlett. "Adaptive online gradient descent." Advances in Neural Information Processing Systems. 2008.

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# Outline

# Looking into the past

## If we look at the following equations

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1)\, g_t$$
$$v_t = \beta_2 v_{t-1} + (1 - \beta_2)\, g_t^2$$

## with the update

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

## Now, we have

$$w_t = w_{t-1} - \alpha \frac{\widehat{m}_t}{\left(\sqrt{\widehat{v}_t} + \epsilon\right)}$$

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# Then, if we apply the recursion to it

## We have

$$\boldsymbol{w}_t = \boldsymbol{w}_{t-2} - \alpha\left[\frac{\widehat{m}_{t-1}}{\left(\sqrt{\widehat{v}_{t-1}}+\epsilon\right)} + \frac{\widehat{m}_t}{\left(\sqrt{\widehat{v}_t}+\epsilon\right)}\right]$$

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

- It works as a variance that if $\nabla f(w_{t-1}) \longrightarrow 0$ 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 $\epsilon = 0$**

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

**Clearly**

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

**But the first one faster than the second one**

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# 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!!!

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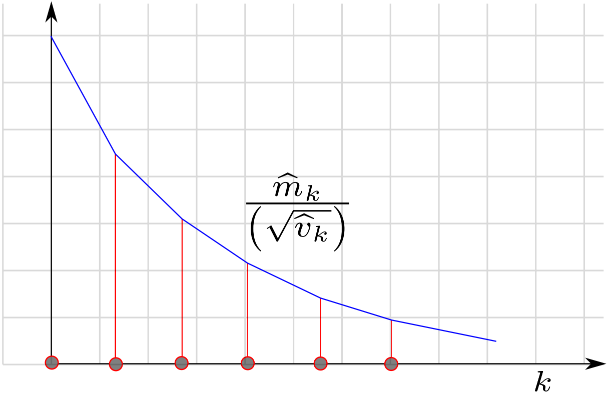
# Actually we need to analyze the convergence

## We could have



# 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

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## Question

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I could result in something heavier, but more effective to obtain better performance

A naive idea would be to substitute the term $\frac{\alpha}{\left(\sqrt{\widehat{v}_t}+\epsilon\right)}$ by the Fisher Information matrix [14]

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

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# Final Remarks

## 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.
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# Outline

# 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

- It is clear that optimization for Big Data is one of the hottest trends in Machine Learning

## Take a look to

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