CMPSC 448: Machine Learning

Lecture 4. Basic Convex Optimization

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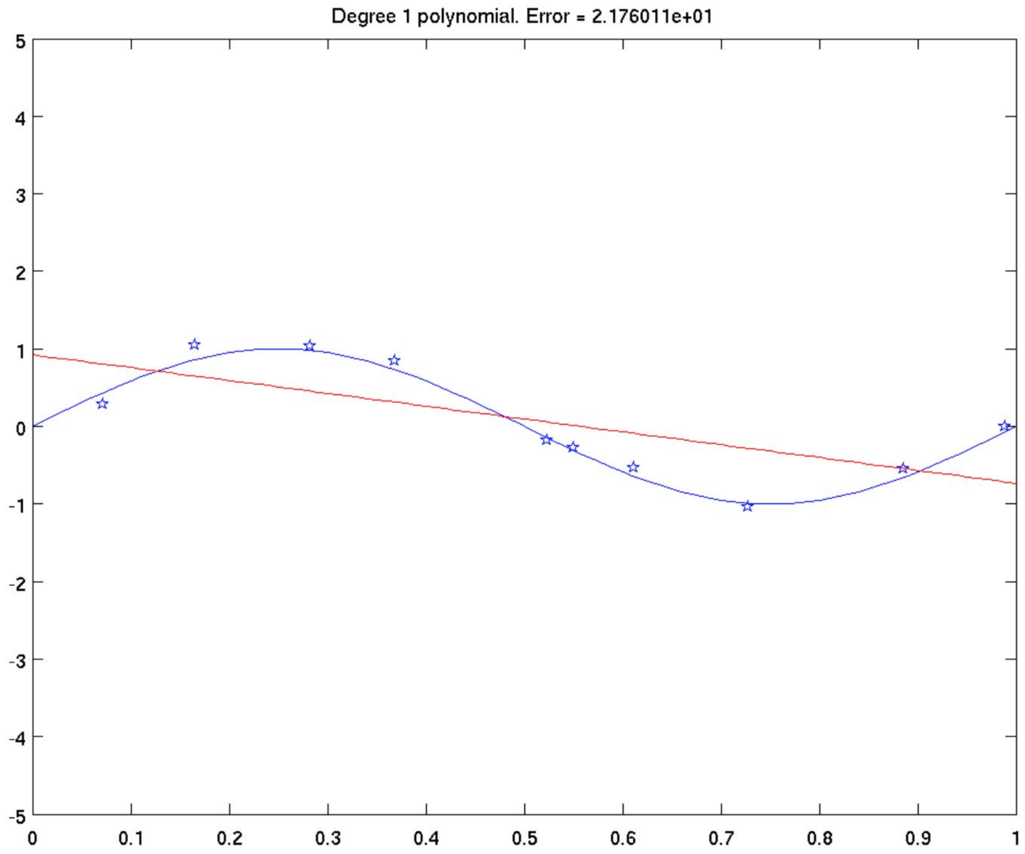
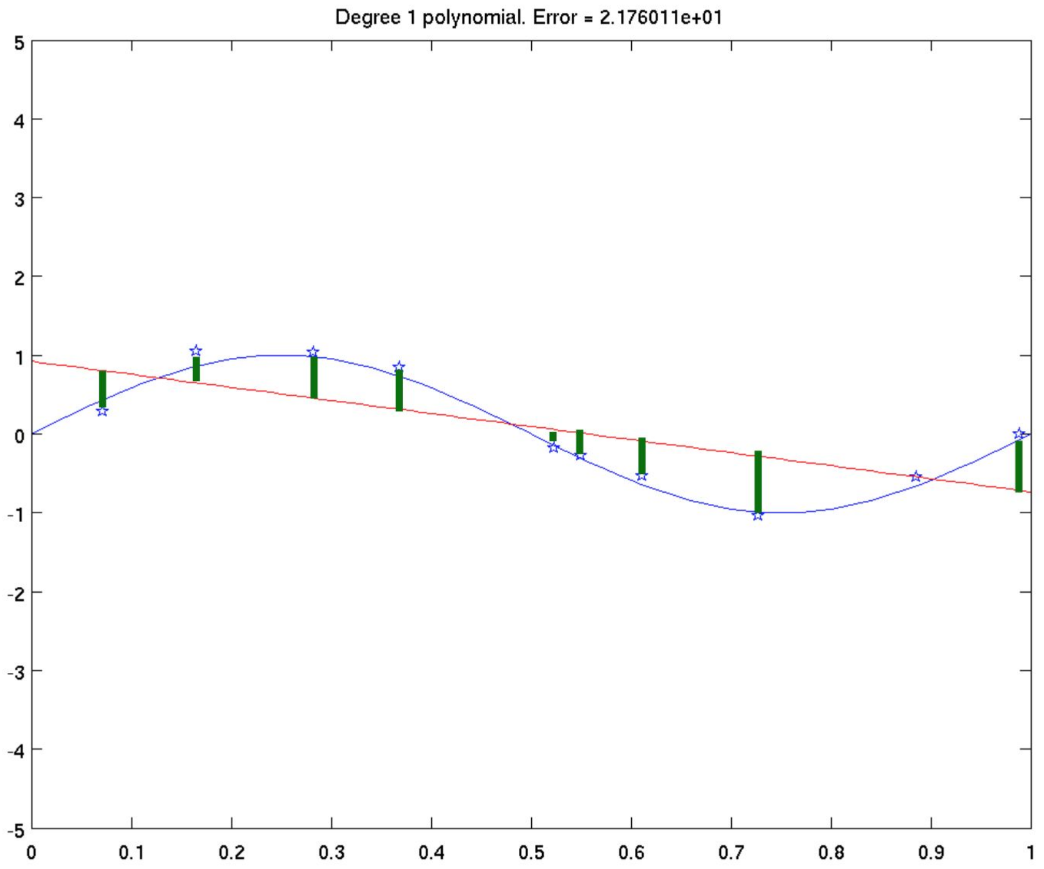
Fall 2021

PennState

Why optimization?



Why optimization?



Why optimization?

For a given training data:

$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$$

$$\left(\begin{array}{c}\text{difference between } \textbf{true} \\ \textbf{value } \; y_i \; \text{ and } \textbf{what} \\ \textbf{model predicts for } x_i\end{array}\right) + \begin{array}{c}\textbf{some regularization} \\ \textbf{of model parameters}\end{array}$$

Why optimization?

For a given training data:

$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$$

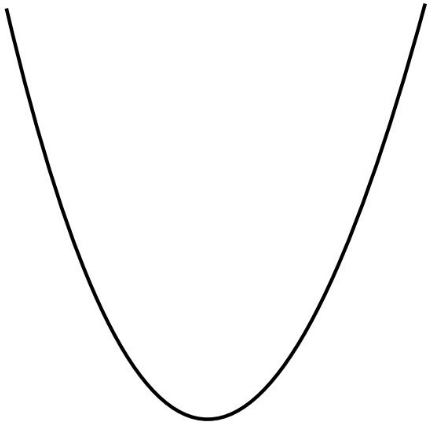
minimize

all possible values of model parameters

$$\sum_{i=1}^{n} \left(\text{difference between } \textbf{true value } y_i \text{ and } \textbf{what model predicts for } x_i \right) + \textbf{some regularization of model parameters}$$

One minute calculus

Find the minimum x_* of $f(x)$?

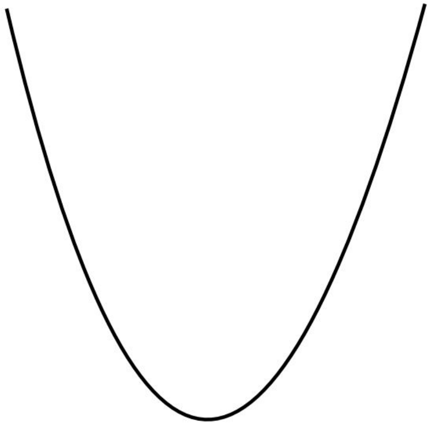


$$f(x) = (x-2)^2$$

One minute calculus

Find the minimum x_* of $f(x)$?

Easy: set the derivative to zero!



$$f(x) = (x-2)^2$$

$$f'(x) = 2(x-2) = 0$$

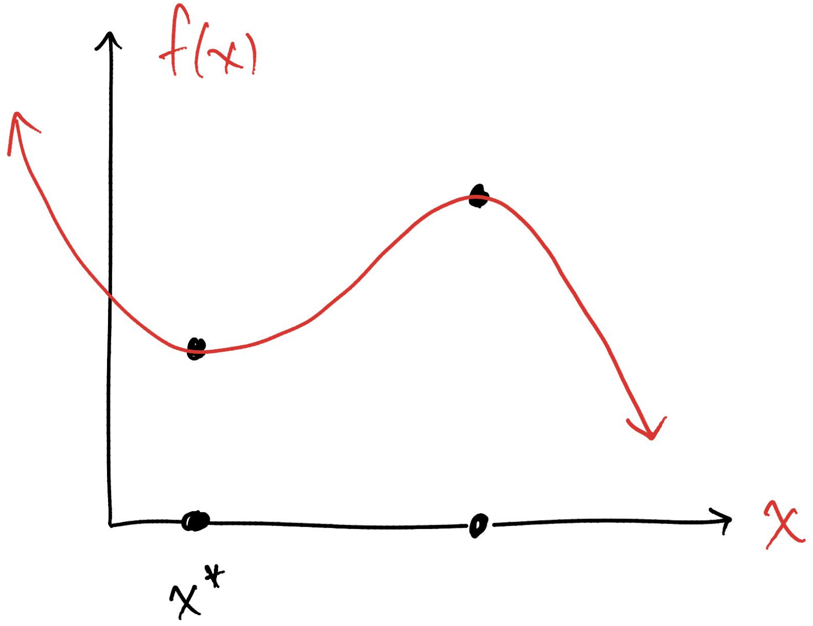
$$\Rightarrow \quad x_* = 2$$

Property 1

Theorem. Given a function $f : \mathbb{R}^d \mapsto \mathbb{R}$, if $f(\boldsymbol{x})$ is differentiable and and $\boldsymbol{x}^*$ is a local minimum, then $\nabla f(\boldsymbol{x}^*) = \mathbf{0}$.

Property 1

Theorem. Given a function $f : \mathbb{R}^d \mapsto \mathbb{R}$, if $f(\boldsymbol{x})$ is differentiable and and $\boldsymbol{x}^*$ is a local minimum, then $\nabla f(\boldsymbol{x}^*) = \mathbf{0}$.



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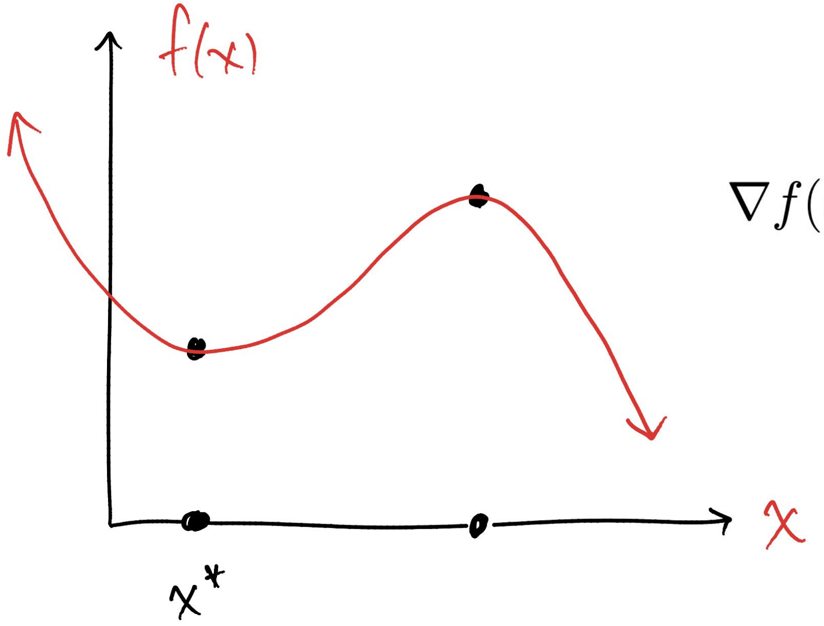

$\nabla f(\boldsymbol{x}^*) = \mathbf{0}$ is necessary but not sufficient

One minute calculus

How about this function?

$$\min_{x \in \mathbb{R}} \quad x^4 - 3x^3 + x^2 + \frac{3}{2}x$$

$$f'(x) = \frac{df}{dx} = 4x^3 - 9x^2 + 2x + \frac{3}{2}$$

One minute calculus

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(1) There might not be a closed form solution for $f'(x) = 0$!

One minute calculus

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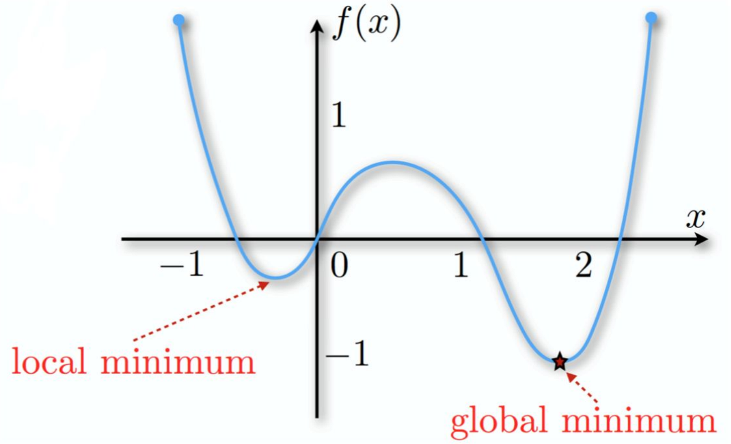


(1) There might not be a closed form solution for $f'(x) = 0$!

(2) Having derivative equals zero is NOT sufficient for optimality!

Property 2

Theorem. If $f(\boldsymbol{x})$ is twice continuously differentiable and $\boldsymbol{x}^*$ is a local minimum, then $\nabla^2 f(\boldsymbol{x}^*)$ is positive semidefinite (i.e., $z^\intercal \nabla^2 f(\boldsymbol{x}^*) z \geq 0, \quad \forall z \in \mathbb{R}^d$).

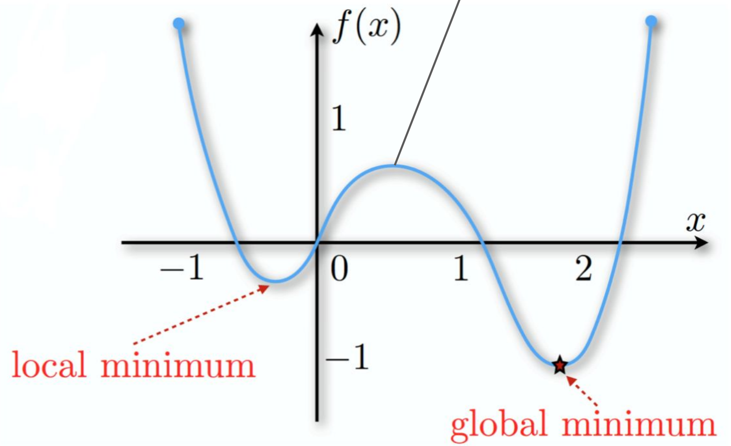
Property 2

Theorem. If $f(\boldsymbol{x})$ is twice continuously differentiable and $\boldsymbol{x}^*$ is a local minimum, then $\nabla^2 f(\boldsymbol{x}^*)$ is positive semidefinite (i.e., $z^\intercal \nabla^2 f(\boldsymbol{x}^*) z \geq 0, \quad \forall z \in \mathbb{R}^d$).

This can't be a local minimum because second order derivative <0

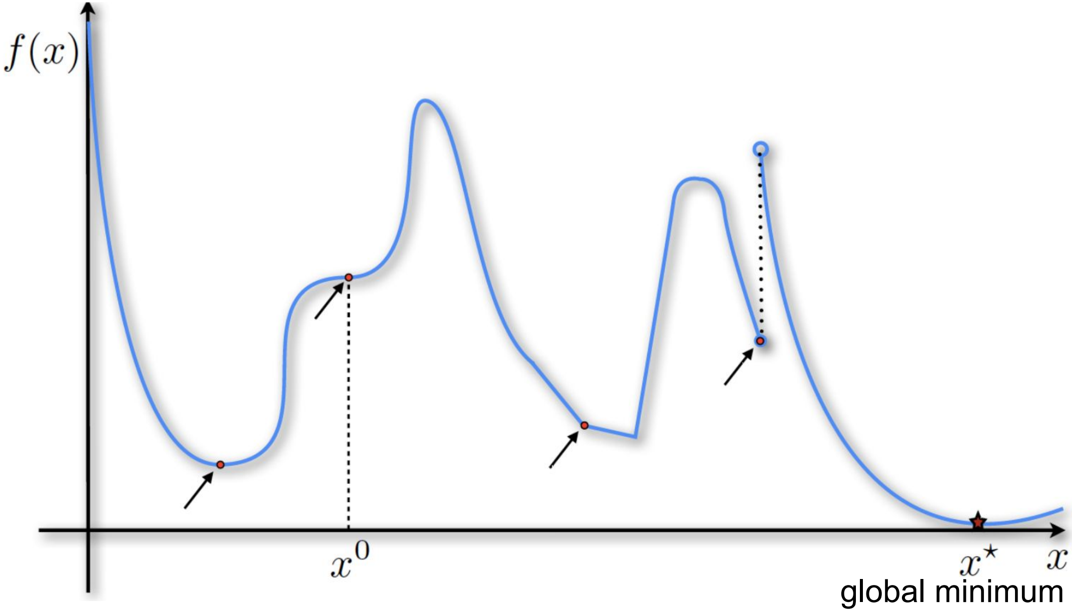
$$\min_{x \in \mathbb{R}} \; x^4 - 3x^3 + x^2 + \frac{3}{2}x$$

$$f'(x) = \frac{df}{dx} = 4x^3 - 9x^2 + 2x + \frac{3}{2}$$



Iterative optimization

Fog of war



Iterative optimization

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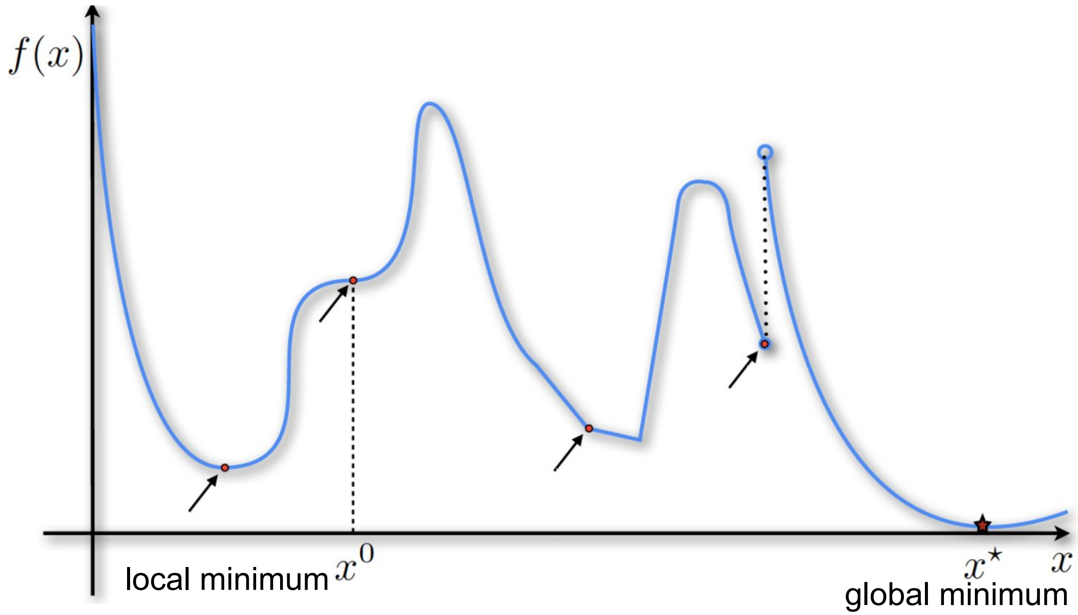

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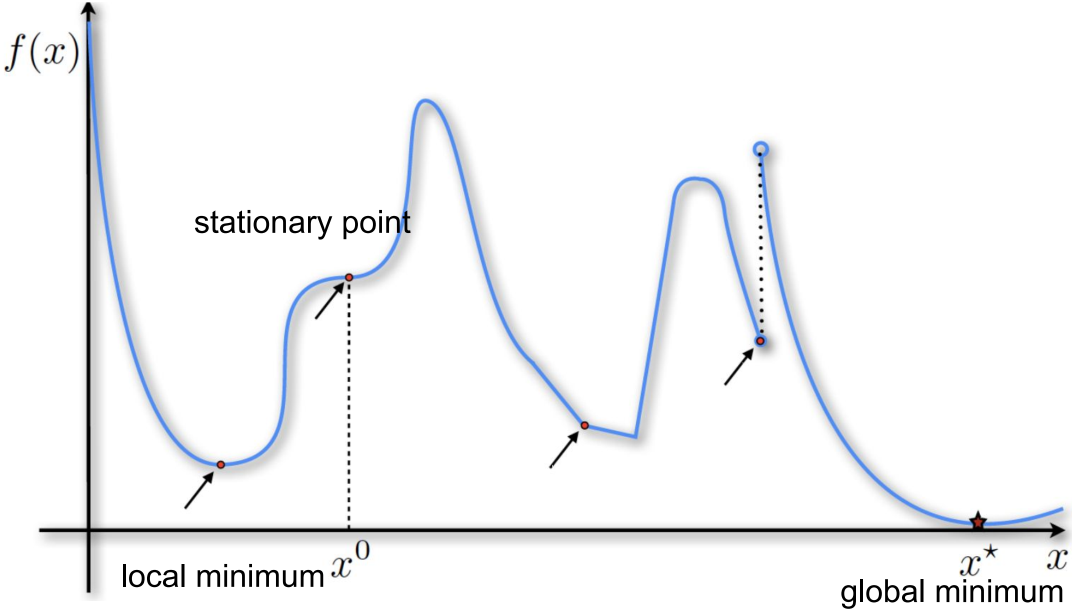

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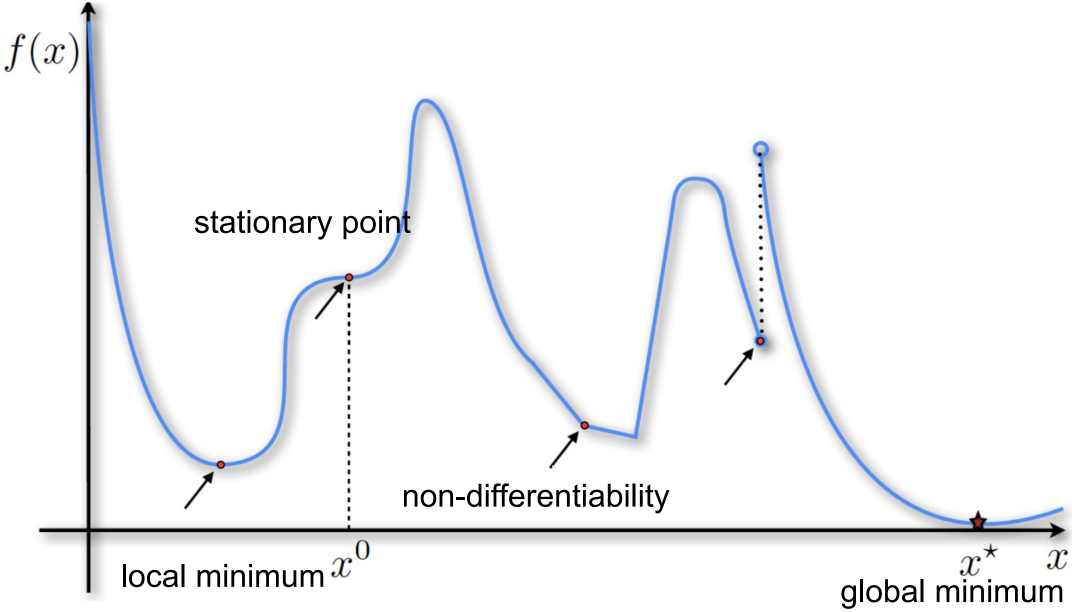

Iterative optimization

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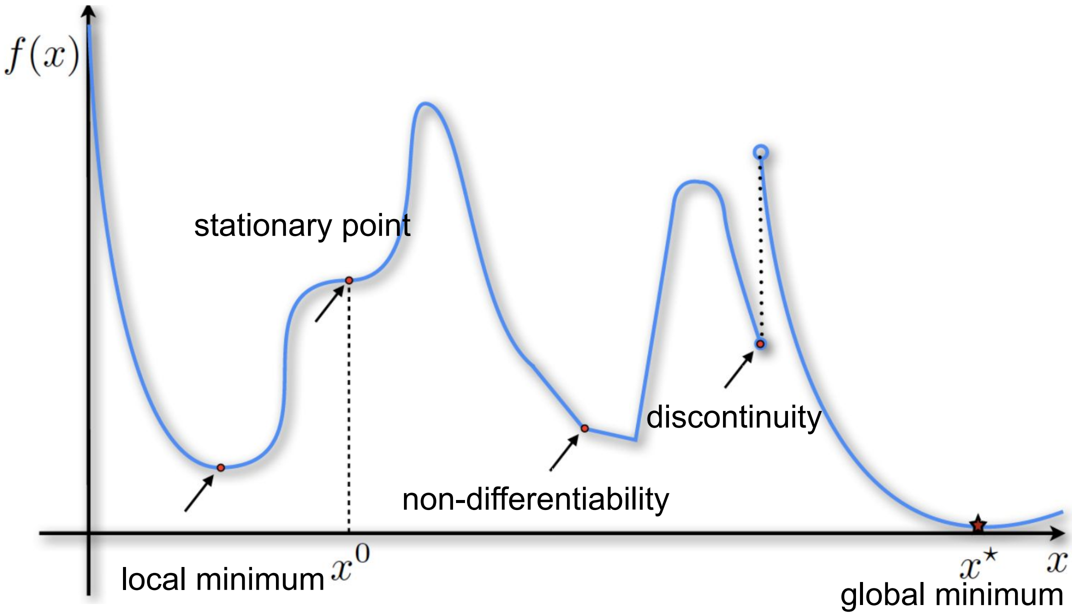

Iterative optimization

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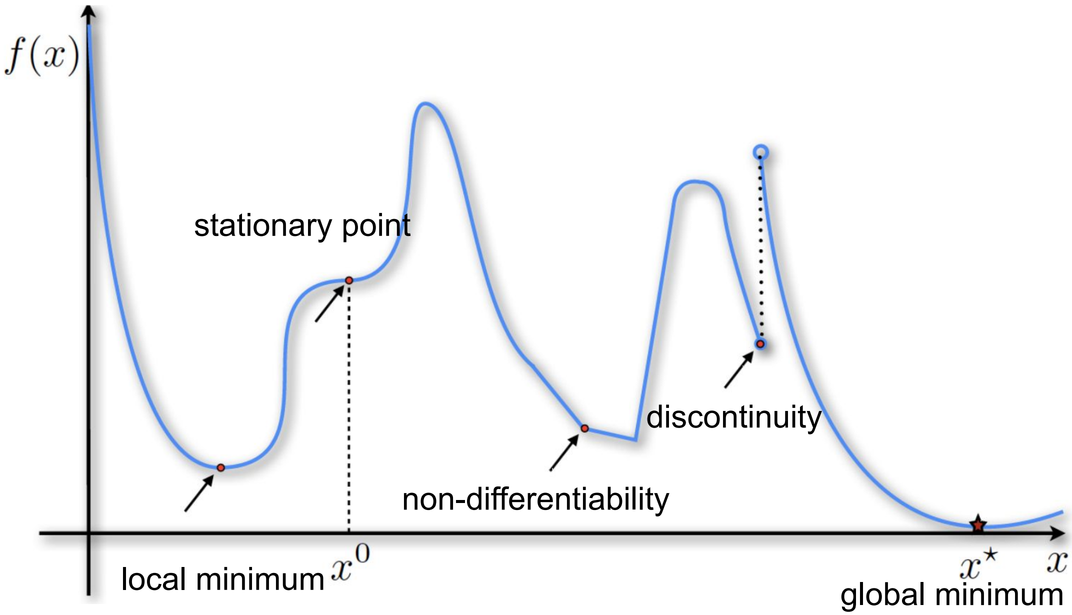

We need a key structure on the function local minima: Convexity.

Convex set

Definition

A set $\mathcal{C} \subseteq \mathbb{R}^d$ is convex if for any $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{C}$ and any $\lambda \in [0, 1]$, we have:

$$\lambda \boldsymbol{x} + (1 - \lambda)\boldsymbol{y} \in \mathcal{C}$$

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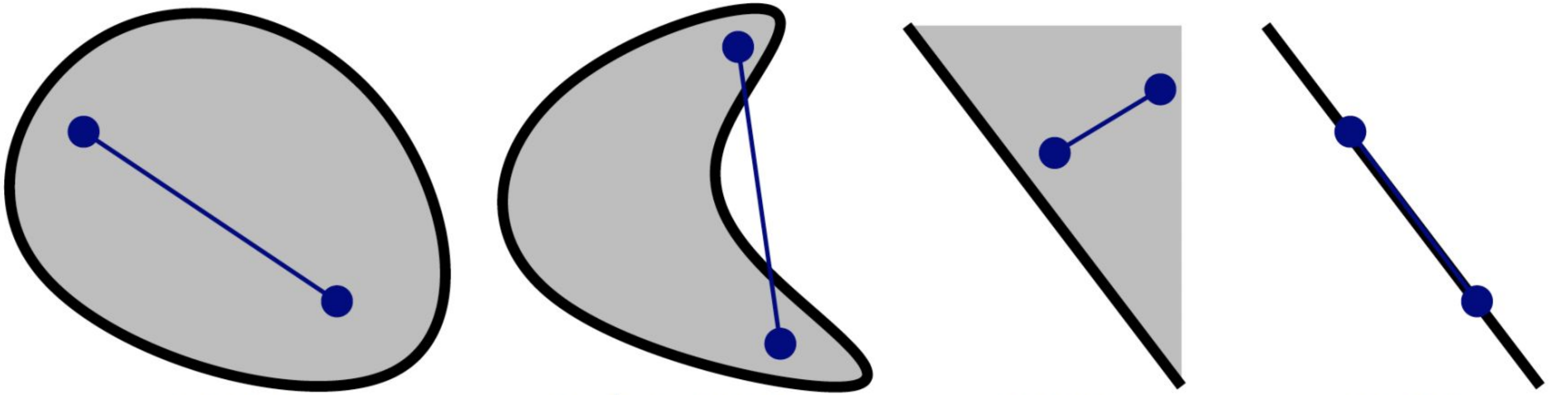

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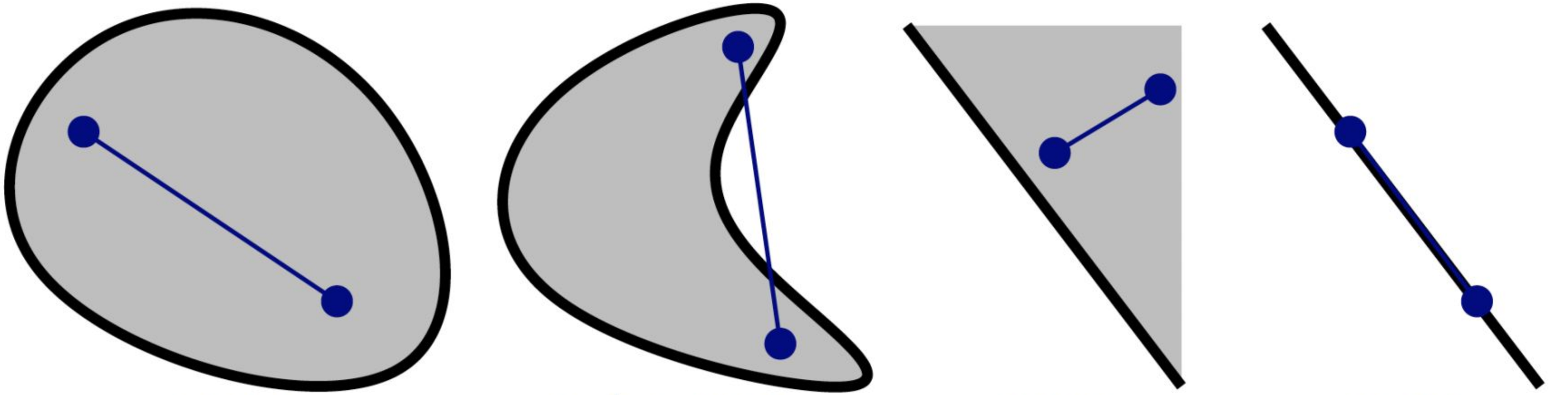


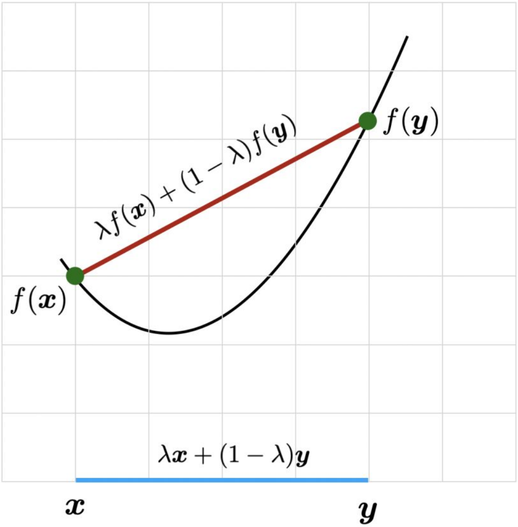
convex not convex convex convex

Convex function

Definition

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

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



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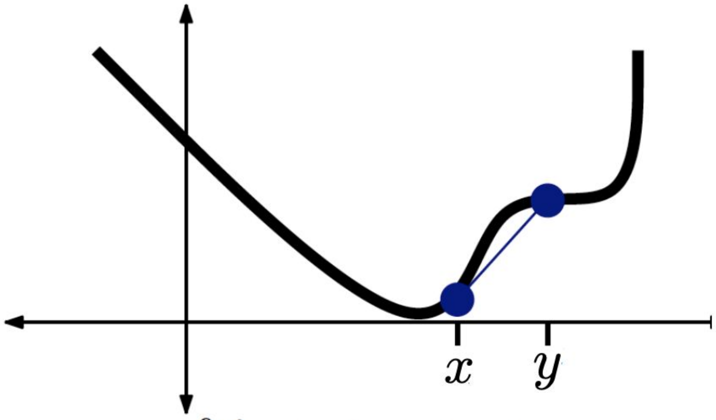
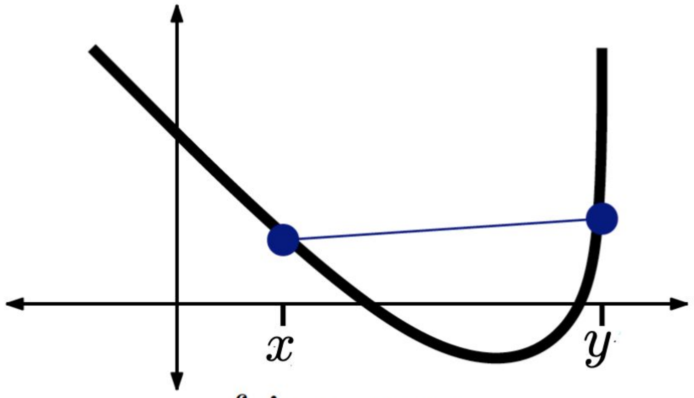


f is not convex

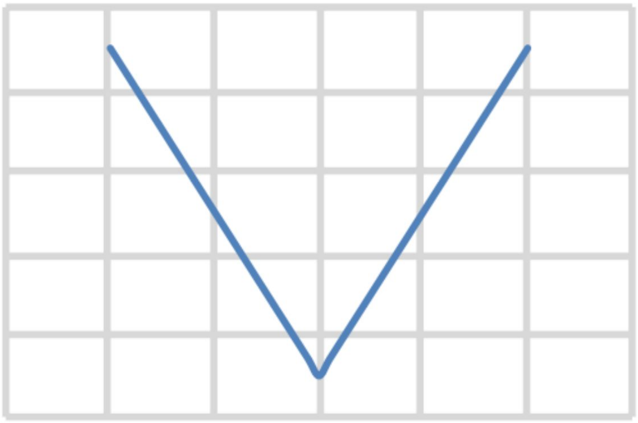


f is convex

Property 3

Theorem. If $f(\boldsymbol{x})$ is convex, then every local minimum is a global minimum.

Example: absolute



$f(x) = |x|$

$$\begin{aligned} f(\lambda x + (1-\lambda)y) &= |\lambda x + (1-\lambda)y| \\ &\leq |\lambda x| + |(1-\lambda)y| \\ &= \lambda|x| + (1-\lambda)|y| \\ &= \lambda f(x) + (1-\lambda)f(y) \end{aligned}$$

Example: norm

Is $f(\boldsymbol{x}) = \|\boldsymbol{x}\|_2$ convex for $\boldsymbol{x} \in \mathbb{R}^d$?

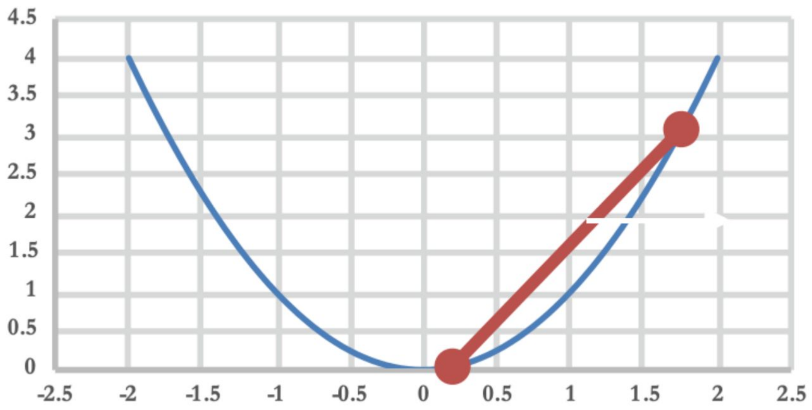
Example: norm

Is $f(\boldsymbol{x}) = \|\boldsymbol{x}\|_2$ convex for $\boldsymbol{x} \in \mathbb{R}^d$?

$$
\begin{aligned}
f(\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}) &= \|\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}\|_2 \\
&\leq \|\lambda \boldsymbol{x}\|_2 + \|(1-\lambda)\boldsymbol{y}\|_2 \quad \textbf{(triangle inequality)} \\
&= \lambda \|\boldsymbol{x}\|_2 + (1-\lambda)\|\boldsymbol{y}\|_2 \quad \textbf{(homogeneity)} \\
&= \lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y})
\end{aligned}
$$

Yes, the norm of a vector is a convex function.

Example: quadratic

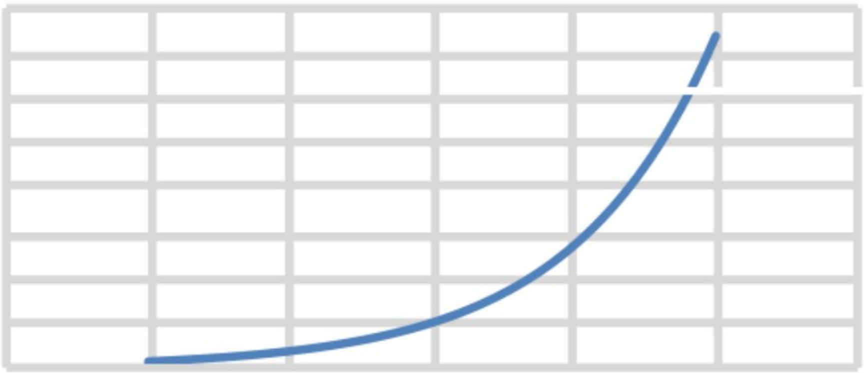


$f(x) = x^2$

$$
\begin{aligned}
\lambda f(x) + (1-\lambda) f(y) - f(\lambda x + (1-\lambda) y) &= \lambda x^2 + (1-\lambda) y^2 - (\lambda x + (1-\lambda) y)^2 \\
&= \lambda x^2 + (1-\lambda) y^2 - \lambda^2 x^2 - 2\lambda(1-\lambda) xy - (1-\lambda)^2 y^2 \\
&= \lambda(1-\lambda) x^2 + \lambda(1-\lambda) y^2 - 2\lambda(1-\lambda) xy \\
&= \lambda(1-\lambda)(x^2 + y^2 - 2xy) \\
&= \lambda(1-\lambda)(x-y)^2 \geq 0
\end{aligned}
$$

Example: exponential

$$f(x) = \exp(x) = e^x$$



- Show that above function is convex using basic definition of convexity?
- While it is obviously convex, You will find it's a bit hard to prove…
- but we can use second order derivative to show this very easy, which will be discussed later

Property 4: Alternate Definition of Convex Functions

Theorem

Let f be a differentiable function. Then, f is convex if and only if its domain is convex and the following inequalities hold:

$$\forall \boldsymbol{x}, \boldsymbol{y} \in \mathtt{dom}(f), \quad f(\boldsymbol{y}) - f(\boldsymbol{x}) \geq \langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle$$

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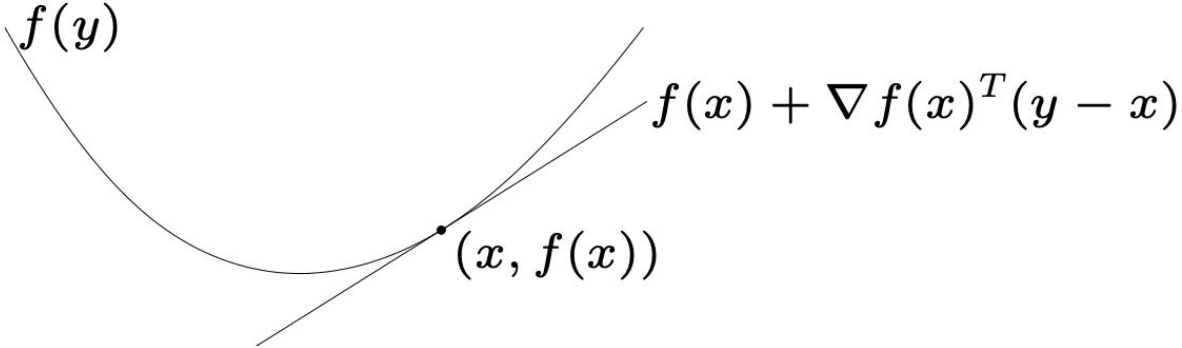

Property 4: Alternate Definition of Convex Functions

Is $f(\boldsymbol{x}) = e^{\boldsymbol{x}^\top \boldsymbol{a}}$ convex ?

$$
\begin{aligned}
f(\boldsymbol{y}) - (f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle) &= e^{\langle \boldsymbol{y}, \boldsymbol{a} \rangle} - \left(e^{\langle \boldsymbol{x}, \boldsymbol{a} \rangle} + e^{\langle \boldsymbol{x}, \boldsymbol{a} \rangle} \langle \boldsymbol{y} - \boldsymbol{x}, \boldsymbol{a} \rangle \right) \\
&= e^{\langle \boldsymbol{x}, \boldsymbol{a} \rangle} \left(e^{\langle \boldsymbol{y} - \boldsymbol{x}, \boldsymbol{a} \rangle} - (1 + \langle \boldsymbol{a}, \boldsymbol{y} - \boldsymbol{x} \rangle) \right) \\
&\geq 0 \quad (\text{because} \quad 1 + z \leq e^z \quad \text{for all} \quad z \in \mathbb{R})
\end{aligned}
$$

Yes, it is!

Property 5: Optimality condition for Convex function

Theorem. If $f(\boldsymbol{x})$ is convex and continuously differentiable, then $\boldsymbol{x}^*$ is a global minimum if and only if $\nabla f(\boldsymbol{x}^*) = \mathbf{0}$.

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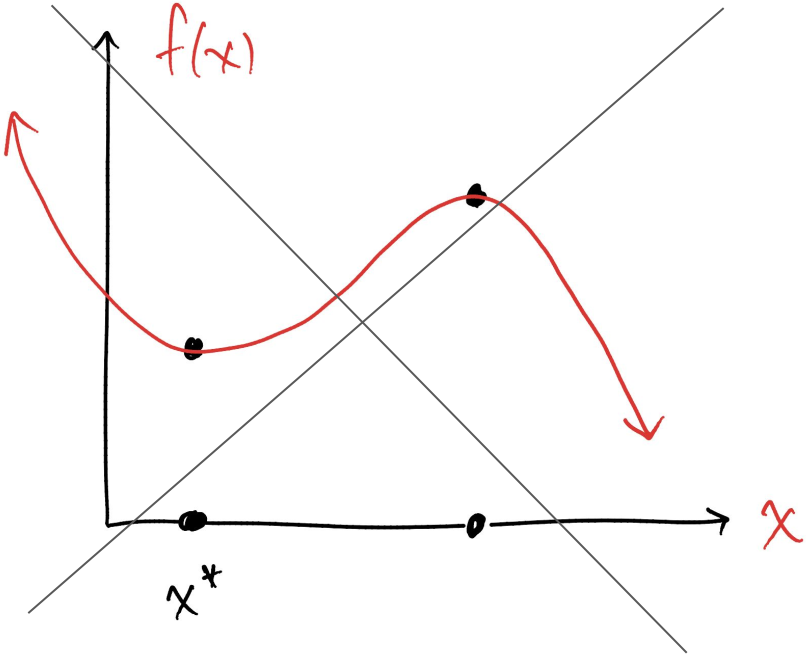

When convex, $\nabla f(\boldsymbol{x}^*) = \mathbf{0}$ is necessary and sufficient

Property 5: Optimality condition for Convex function

Theorem. If $f(\boldsymbol{x})$ is convex and continuously differentiable, then $\boldsymbol{x}^*$ is a global minimum if and only if $\nabla f(\boldsymbol{x}^*) = \mathbf{0}$.

Why?

From Property 4 we have:

$$f(\boldsymbol{y}) \geq f(\boldsymbol{x}_*) + \langle \nabla f(\boldsymbol{x}_*), \boldsymbol{y} - \boldsymbol{x}_* \rangle$$

When $\nabla f(\boldsymbol{x}^*) = \mathbf{0}$

$$f(\boldsymbol{y}) \geq f(\boldsymbol{x}_*)$$

Property 6: twice continuously differentiable functions

- If the function $f : \mathbb{R} \to \mathbb{R}$ is twice-differentiable, then it is convex if and only if:

$$f''(x) \geq 0$$

Property 6: twice continuously differentiable functions

Is $f(x) = x^4$ convex ?

$$f''(x) = 12x^2 \geq 0$$

Yes, it is!

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Is $f(x) = x^4$ convex ?

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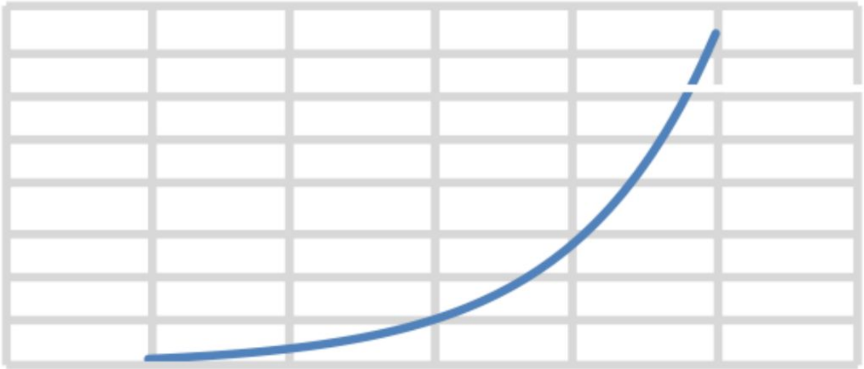
$$f(x) = \exp(x) = e^x$$



Property 6: twice continuously differentiable functions

- If the function $f : \mathbb{R} \rightarrow \mathbb{R}$ is twice-differentiable, then it is convex if and only if:

$$f''(x) \geq 0$$

- If the function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is twice-differentiable, then it is convex if and only if:

$$\nabla^2 f(\boldsymbol{x}) \succeq 0$$

for all $\boldsymbol{x} \in \mathbb{R}^d$

- the Hessian matrix is positive semidefinite
- all the eigenvalues of its Hessian matrix are non-negative

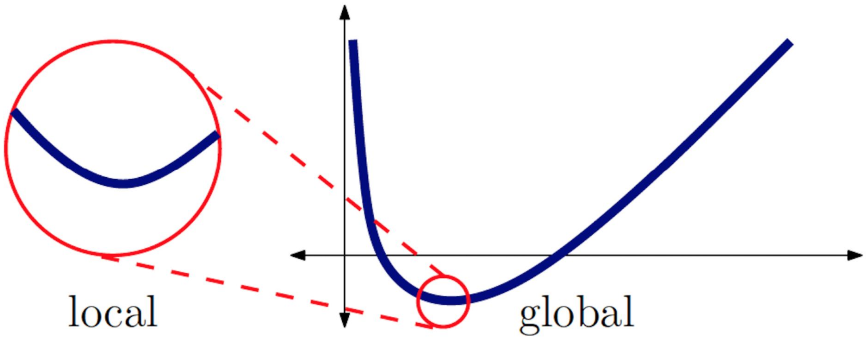
Convex Optimization

Problem:

Find the minimum of x_* of $f(x)$, when the function is convex!

From Property 3:

Every local minimum is a global minimum for convex functions!

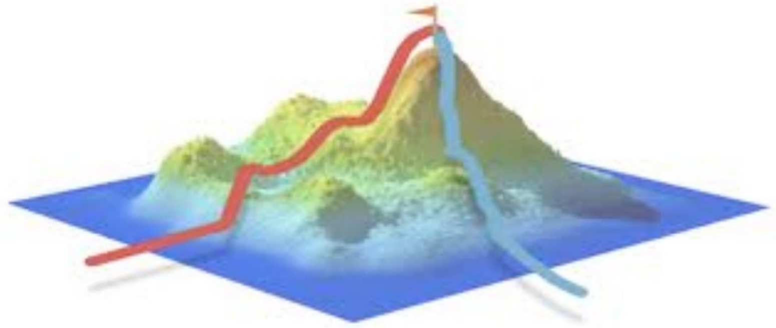


Convex functions are EASY to solve!

It suffices to find a local minimum, because we know it will be global

Descent direction

Let assume at iteration t the algorithms is at point $\boldsymbol{x}_t$ and got local information from oracle such as $f(\boldsymbol{x}_t)$ and $\nabla f(\boldsymbol{x}_t)$



I would like to move to a new point $\boldsymbol{x}_{t+1}$

such that

$$f(\boldsymbol{x}_{t+1}) \leq f(\boldsymbol{x}_t)$$

Descent direction

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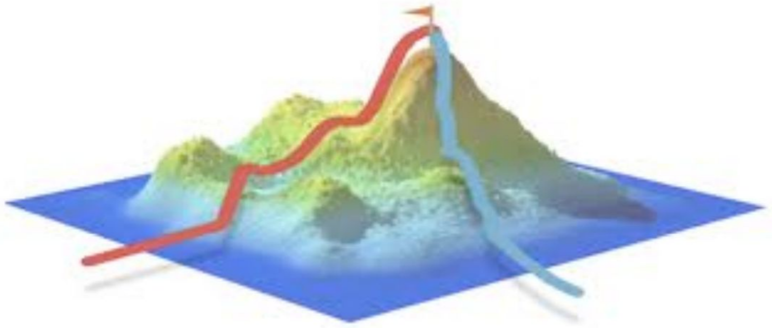


I would like to move to a new point $\boldsymbol{x}_{t+1}$

such that

$$f(\boldsymbol{x}_{t+1}) \leq f(\boldsymbol{x}_t)$$

Answer? negative gradient at current point $-\nabla f(\boldsymbol{x}_t)$

Gradient Descent (GD) algorithm

The simplest algorithm in the world (almost)

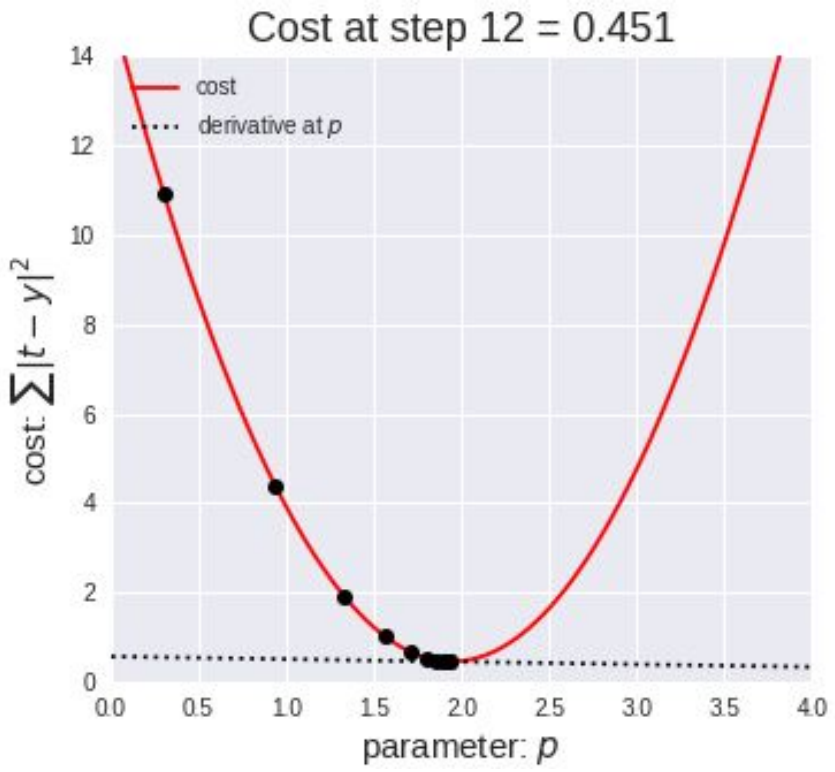
Initialize $\quad \boldsymbol{x}_0$

Iterate $\quad t = 1, 2, \ldots, T$

$$\boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \eta_t \nabla f(\boldsymbol{x}_t)$$

Step size

Example



Cost at step 12 = 0.451
cost
derivative at p
cost: $\sum|t-y|^2$
parameter: p
14
12
10
8
6
4
2
0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0

Step size selection

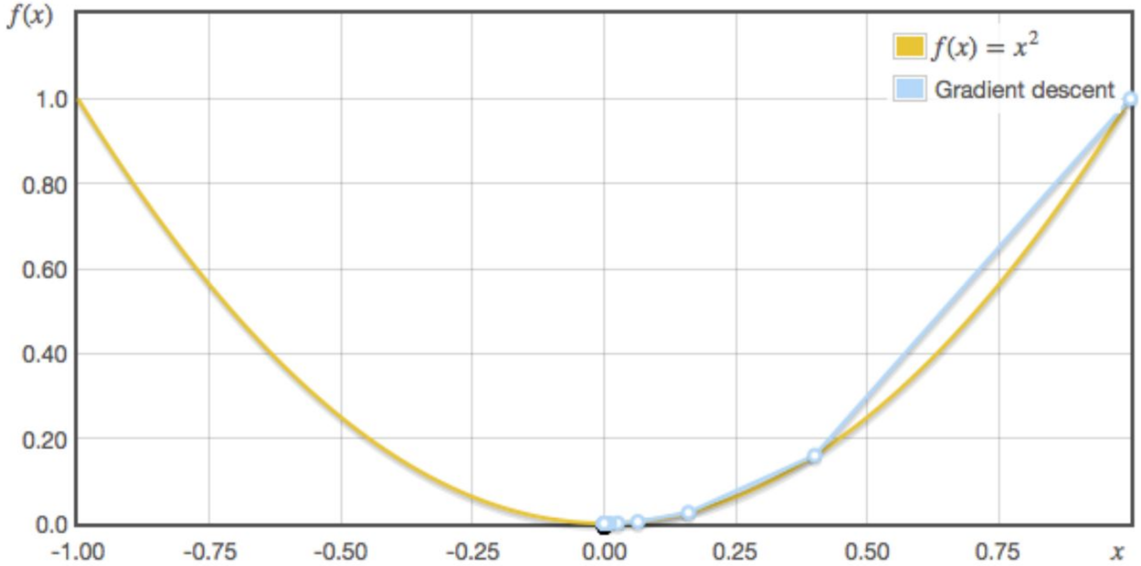
How do I choose the step size?

- Exact line search (usually expensive)
- Heuristics (practical)
- Fixed
- Adaptive based on iteration # [smaller steps at end]

Example Step size selection

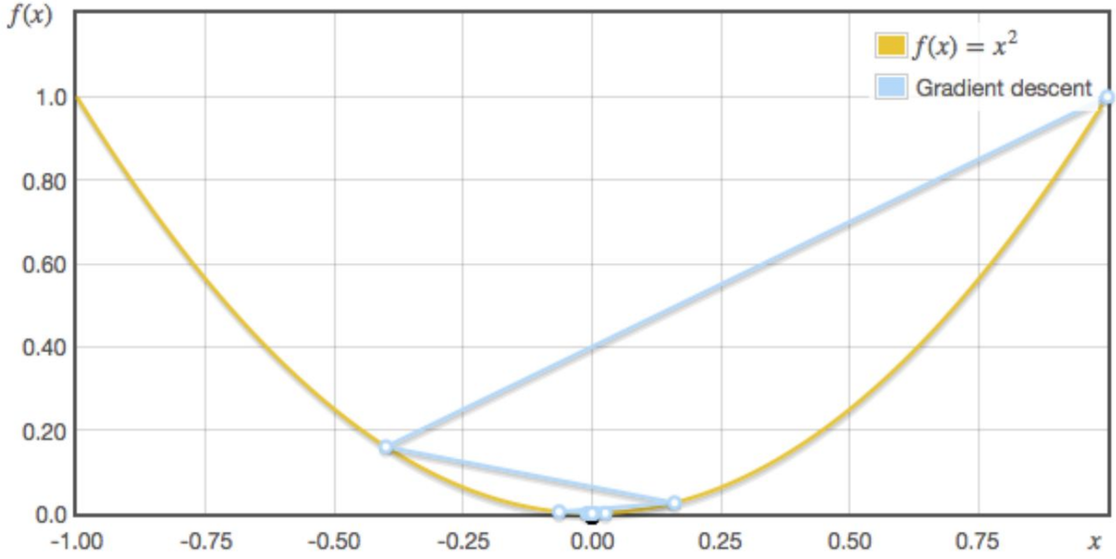
$$f(x) = x^2$$

$$\eta = 0.3$$



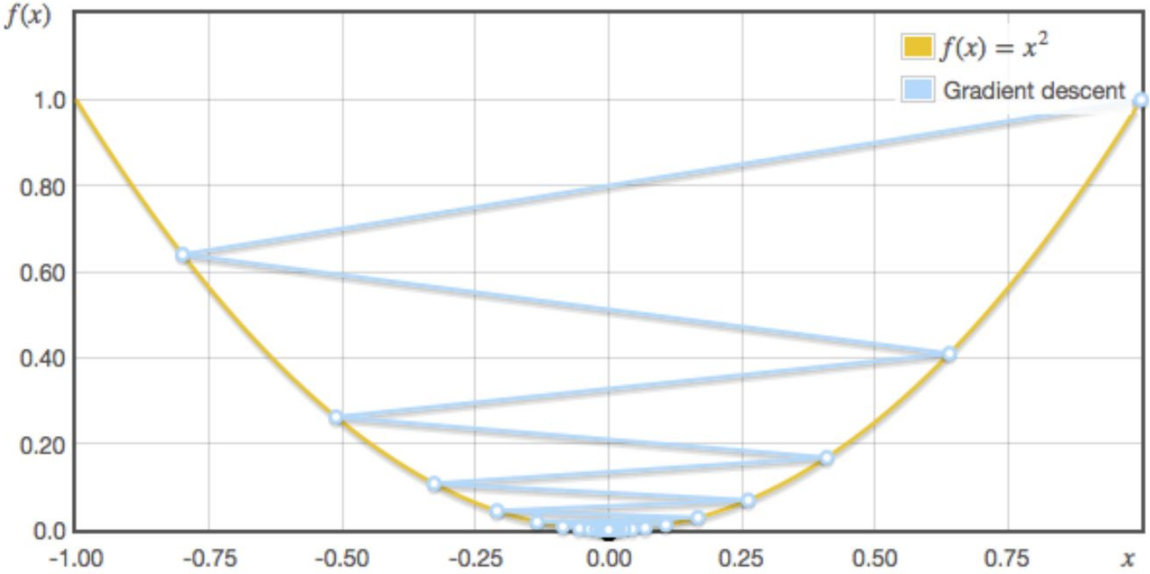
Example Step size selection

$$f(x) = x^2$$
$$\eta = 0.7$$



Example Step size selection

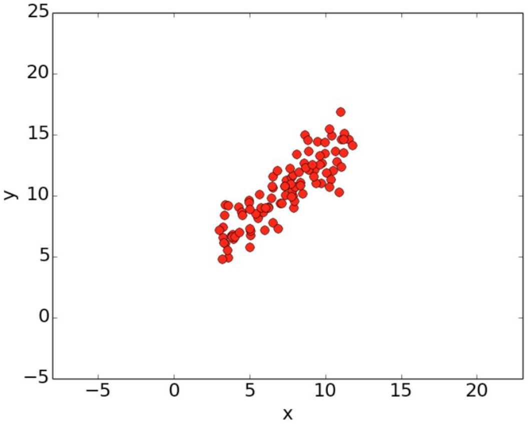
$$f(x) = x^2$$
$$\eta = 0.9$$



Polynomial degree 1

Given: a set of points on the plane

Goal: find the best line that approximates the points



$$(x_1, y_1)$$
$$(x_2, y_2)$$
$$\vdots$$
$$(x_n, y_n)$$

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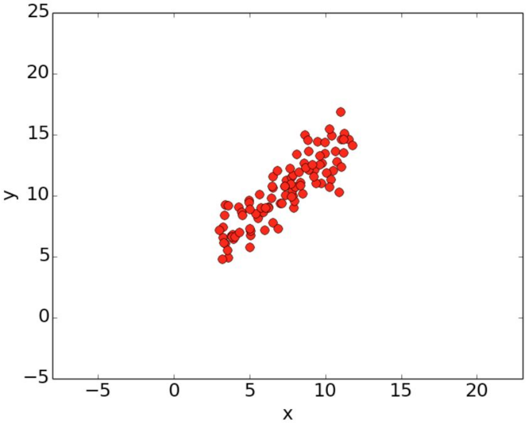
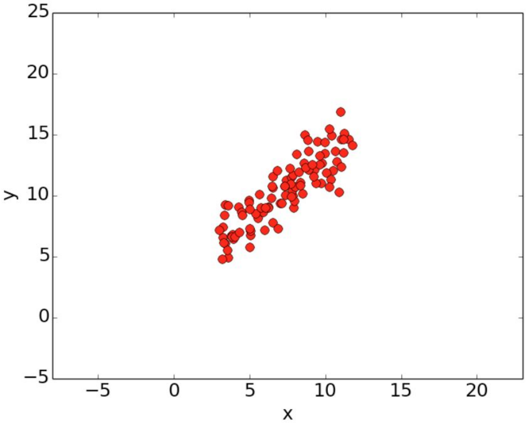


$$(x_1, y_1)$$
$$(x_2, y_2)$$
$$\vdots$$
$$(x_n, y_n)$$

Error of a line:

$$f(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} (w_0 + w_1 x_i - y_i)^2$$

Polynomial degree 1



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$$\vdots$$
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Error of a line:

$$f(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}(w_0 + w_1 x_i - y_i)^2$$

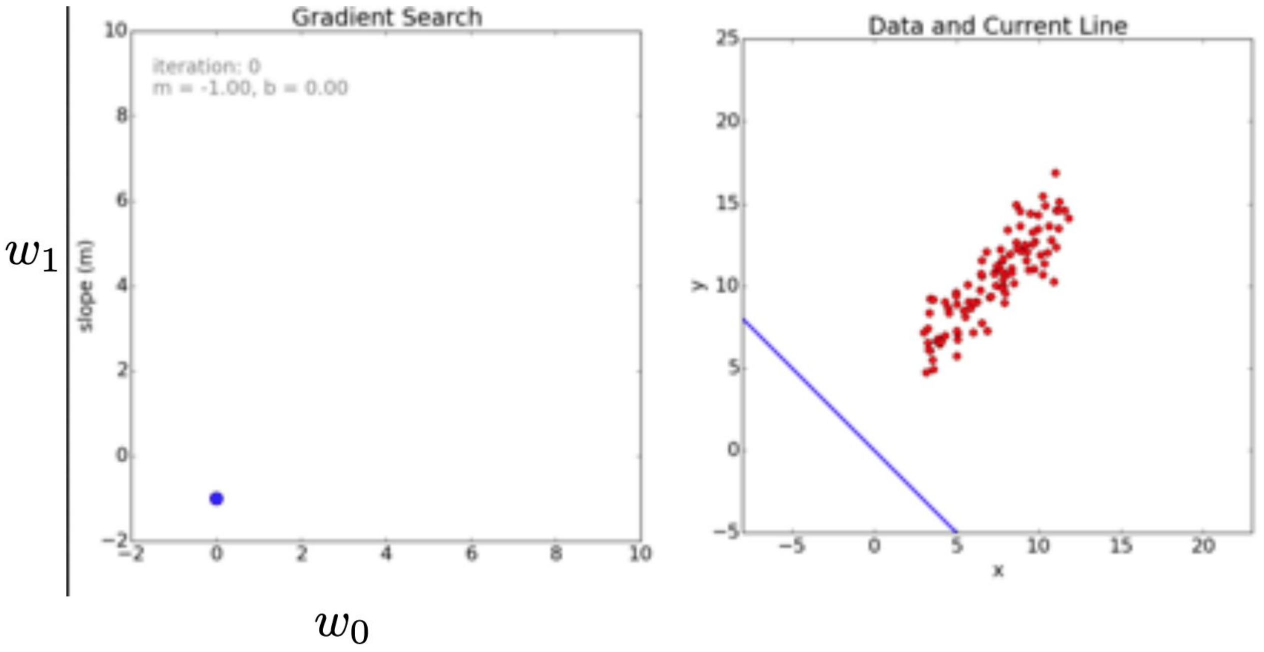
Gradient at a point:

$$\frac{\partial f(w_0, w_1)}{\partial w_0} = \frac{2}{n}\sum_{i=1}^{n} w_0 + w_1 x_i - y_i$$

$$\frac{\partial f(w_0, w_1)}{\partial w_1} = \frac{2}{n}\sum_{i=1}^{n}(w_0 + w_1 x_i - y_i)x_i$$

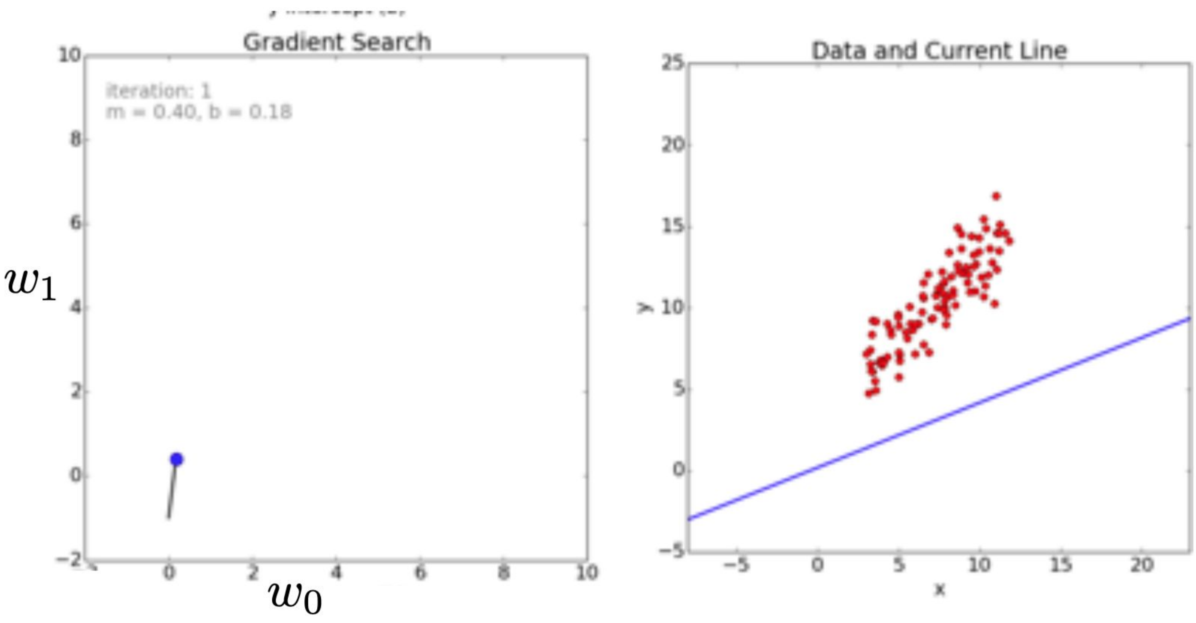
Polynomial degree 1

Iteration = 0



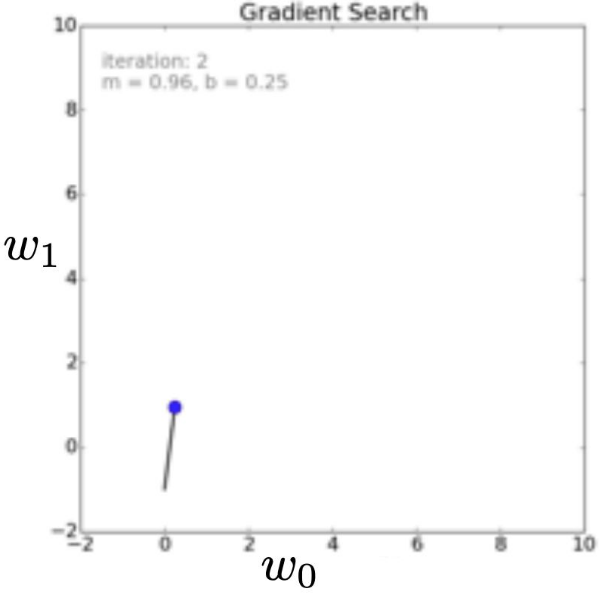
Polynomial degree 1

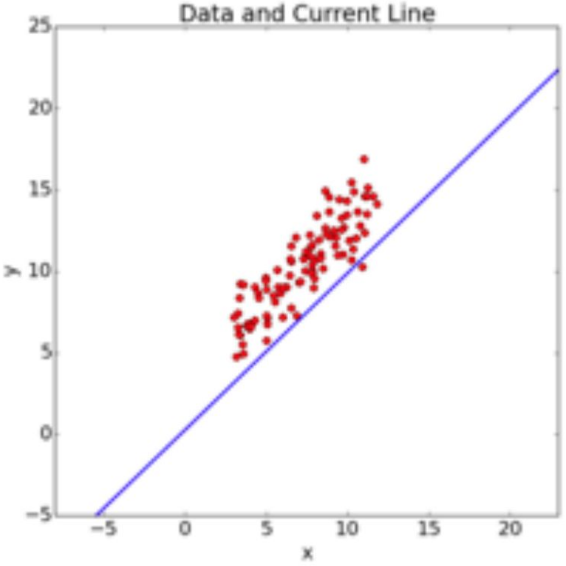
Iteration = 1



Polynomial degree 1

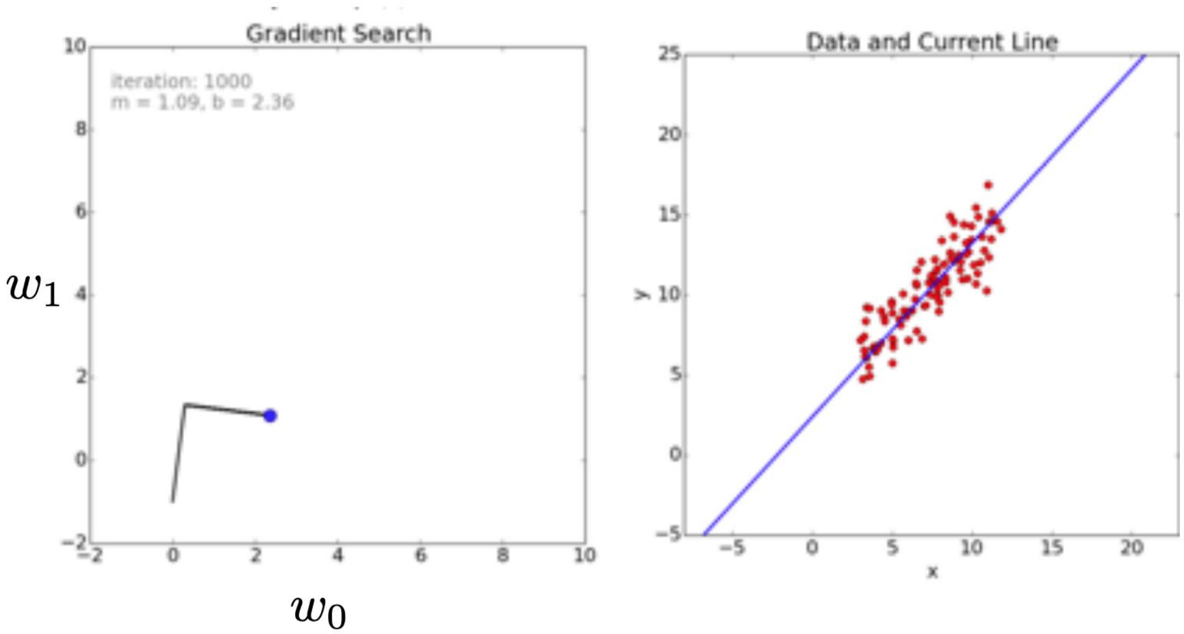
Iteration = 2





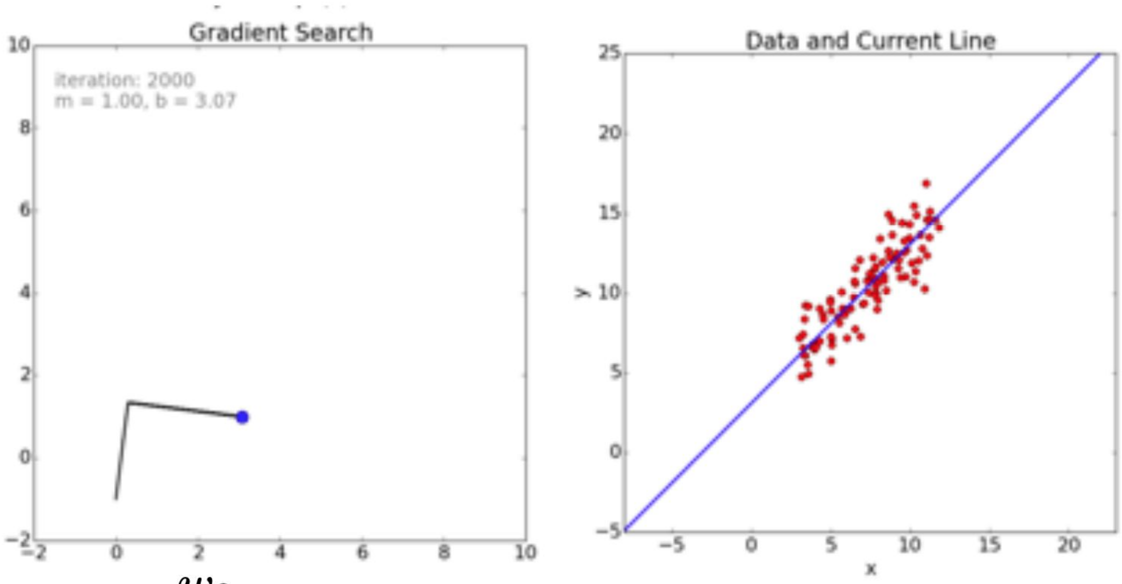
Polynomial degree 1

Iteration = 1000



Polynomial degree 1

Iteration = 2000

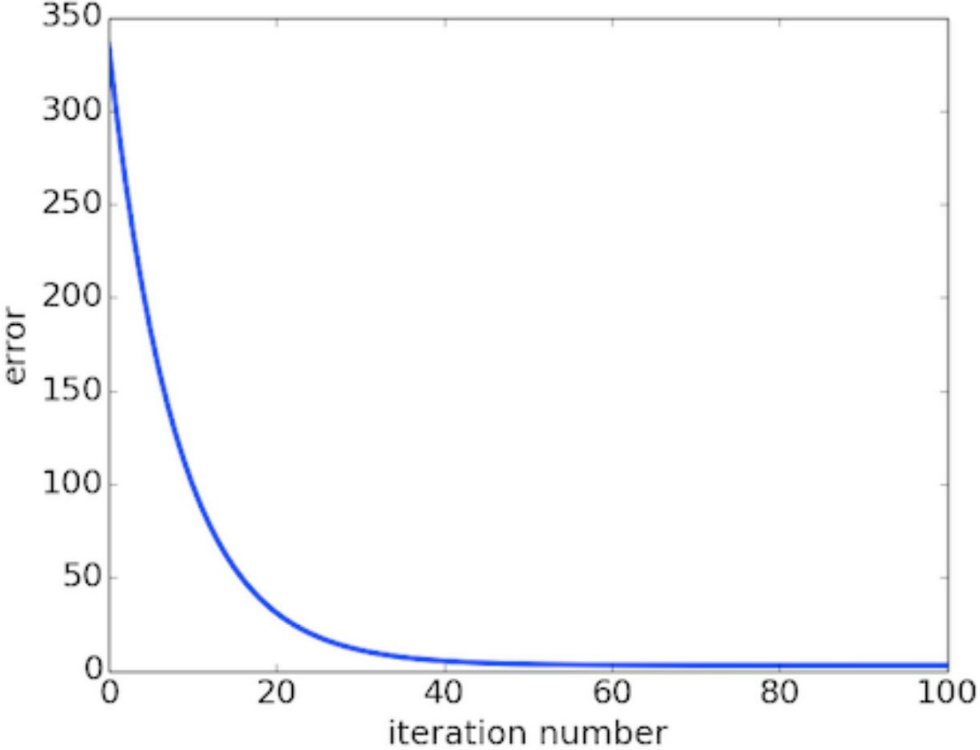


w_1

w_0

Polynomial degree 1

How error decreases



Stochastic gradient descent

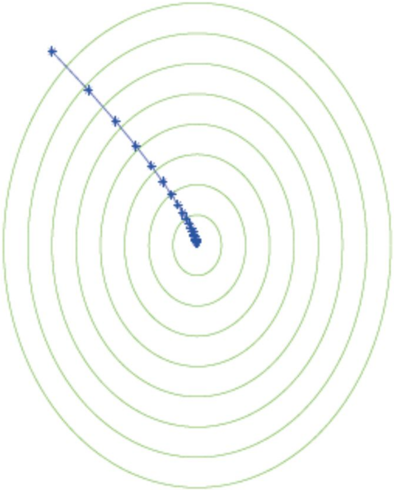
GD is not practical for large-scale data!

Consider a learning problem with millions of images?

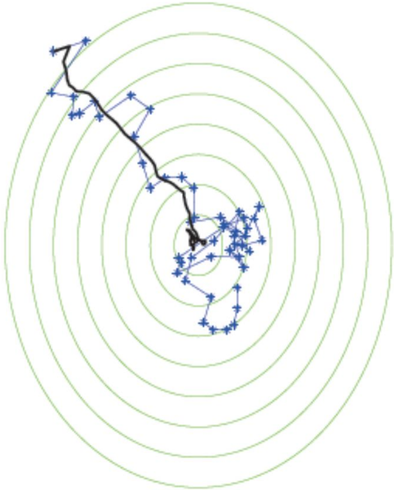
n gradient computations for n training samples per iteration!

GD versus SGD

Stochastic Gradient Descent (SGD): At each iteration, compute the gradient over a small fixed-size subset of data (min-batch)!



GD

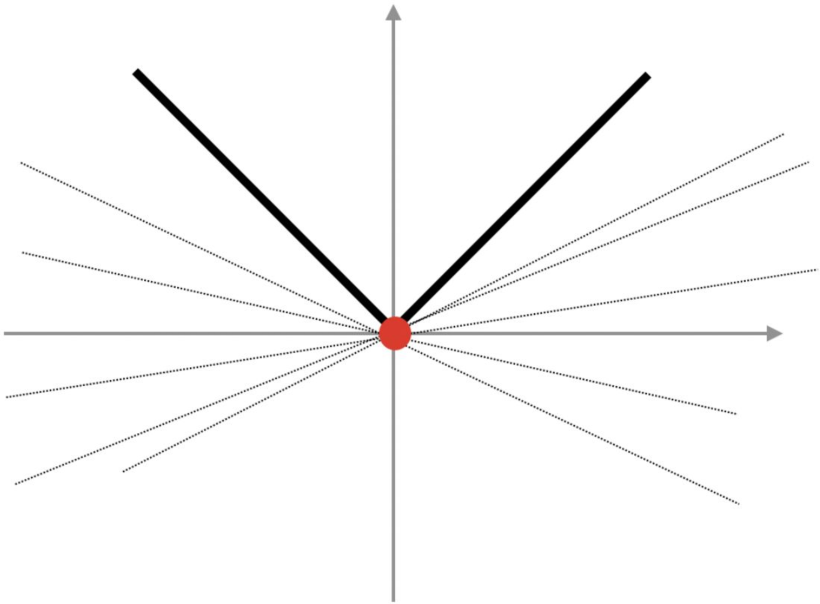


SGD

Stay tuned! We will talk about SGD in future lectures!

What if the function is not differentiable?

$$f(x) = |x|$$



To many tangent vectors at non-differentiable a point! Which direction should I take?

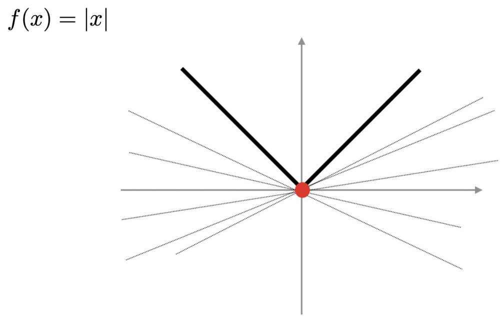
Subgradients

Definition

Let $f : \mathcal{C} \to \mathbb{R}$ be a proper function and let $\boldsymbol{x} \in \mathrm{dom}(f)$. A vector $\boldsymbol{g}$ is called a subgradient of f at $\boldsymbol{x}$ if

$$f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \langle \boldsymbol{g}, \boldsymbol{y} - \boldsymbol{x} \rangle \text{ for all } \boldsymbol{y} \in \mathrm{dom}(f)$$

We denote the set of all subgradients at point $\boldsymbol{x}$ by $\partial f(\boldsymbol{x})$ which is $\partial f(\boldsymbol{x}) = \{\nabla f(\boldsymbol{x})\}$ if the function is differentiable at $\boldsymbol{x}$.



Later in the course, we will introduce Subgrdient Descent algorithm!