CMPSC 448: Machine Learning

Lecture 3. Basic Convex Optimization

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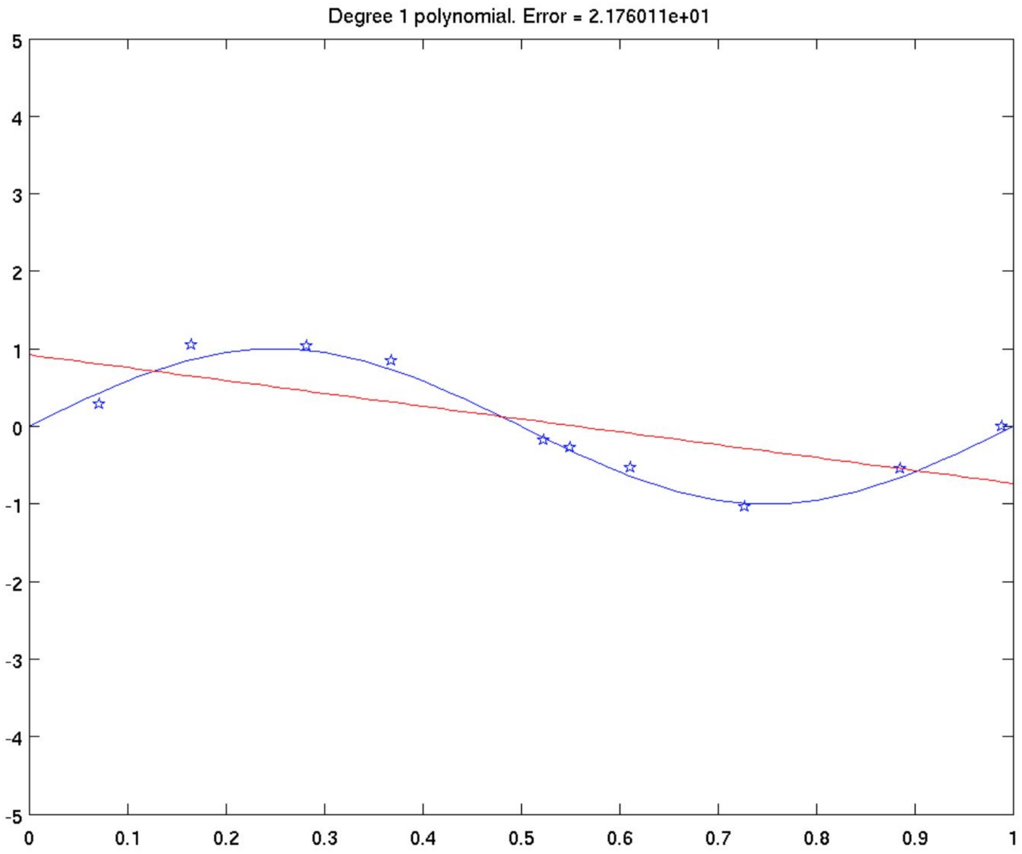
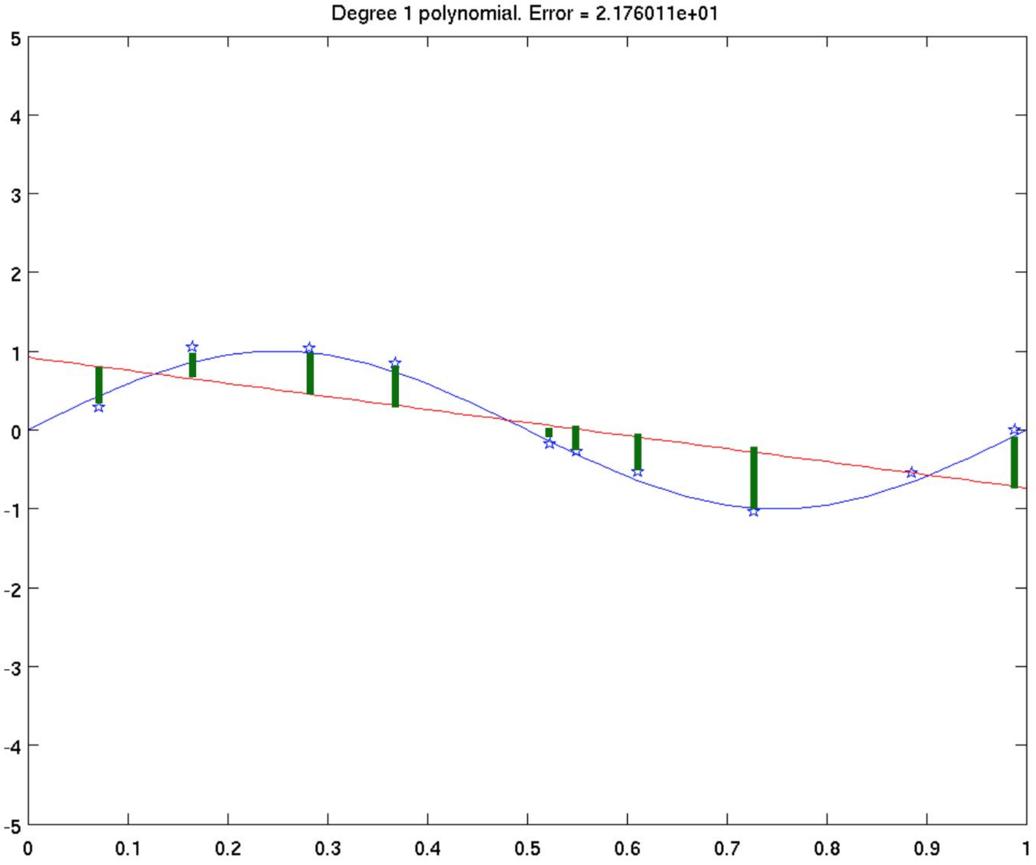
Fall 2022

Why optimization?



Why optimization?



Why optimization?

For a given training data:

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

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

Why optimization?

For a given training data:

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

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

Scalar valued functions of scalars

We are all familiar with basic calculus, and functions of the form $f : \mathbb{R} \to \mathbb{R}$ and their derivatives:

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}.$$

The derivative of a function of a real variable measures the sensitivity to change of the function value (output value) with respect to a change in its argument (input value).

- $f(x) = x^r$, then $f'(x) = rx^{r-1}$,
- $\frac{d}{dx} e^x = e^x$.
- Sums rule: $(\alpha f + \beta g)' = \alpha f' + \beta g'$ for all functions f and g and all real numbers α and β
- Product rule: $(fg)' = f'g + fg'$ for all functions f and g.
- Chain rule: If $f(x) = h(g(x))$, then

$$f'(x) = h'(g(x)) \cdot g'(x).$$

Scalar valued functions of vectors

Multivariable calculus (also known as multivariate calculus) is the extension of calculus in one variable to calculus with functions of several variables, $f : \mathbb{R}^d \to \mathbb{R}$, e.g.,

$$f(x, y) = \frac{x^2 y}{x^4 + y^2}$$

In many machine learning applications, our model can be modeled as a function f that takes d features as inputs and maps it to a real number (regression) or binary variable (classification), e.g.,

- Linear regressions: let's $\boldsymbol{x} \in \mathbb{R}^d$ be d features of a samples and $\boldsymbol{w} \in \mathbb{R}^d$ be parameter vector of of a linear model f, then the prediction is:

$$f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} = \sum_{i=1}^{d} w_i x_i$$

So, we need to have a basic understanding of multivariable calculus.

Gradient (first order)

Definition

Let $f : \mathcal{C} \subseteq \mathbb{R}^d \to \mathbb{R}$ be a differentiable function. Then, the gradient of f at $\boldsymbol{x} \in \mathcal{C}$ is the vector in $\mathbb{R}^d$ denoted by $\nabla f(\boldsymbol{x})$ and defined by

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\boldsymbol{x}) \\ \vdots \\ \frac{\partial f}{\partial x_d}(\boldsymbol{x}) \end{bmatrix}$$

An an example, let's consider the function $f(\boldsymbol{x}) = \langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^\top \boldsymbol{y} = \sum_{i=1}^d x_i y_i$, then

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial \sum_{i=1}^d x_i y_i}{\partial x_1} \\ \vdots \\ \frac{\partial \sum_{i=1}^d x_i y_i}{\partial x_d} \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_d \end{bmatrix} = \boldsymbol{y}$$

Hessian (second order)

Definition

Let $f : \mathcal{C} \subseteq \mathbb{R}^d \to \mathbb{R}$ be a twice differentiable function. Then, the Hessian of f at $\boldsymbol{x} \in \mathcal{C}$ is the vector in $\mathbb{R}^d$ denoted by $\nabla^2 f(\boldsymbol{x})$ and defined by

$$\nabla^2 f(\boldsymbol{x}) = \left[\frac{\partial^2 f}{\partial x_i x_j}(\boldsymbol{x})\right]_{1\le i,j\le d} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2}(\boldsymbol{x}) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(\boldsymbol{x}) & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1}(\boldsymbol{x}) & \frac{\partial^2 f}{\partial x_2^2}(\boldsymbol{x}) & \dots & \vdots \\ \vdots & \vdots & \dots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1}(\boldsymbol{x}) & \frac{\partial^2 f}{\partial x_d \partial x_2}(\boldsymbol{x}) & \dots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix}$$

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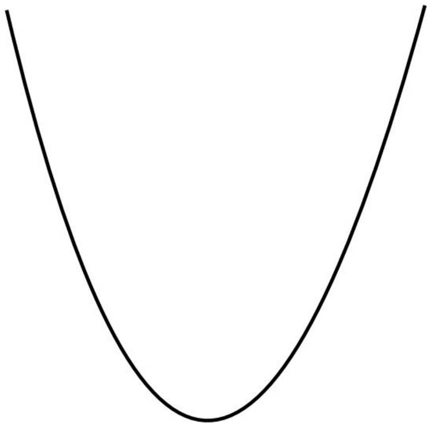
$$f(x, y) = x^3 - 2xy - y^6 \xrightarrow{\textbf{Hessian}} \begin{bmatrix} 6x & -2 \\ -2 & -30y^4 \end{bmatrix}$$

One minute calculus

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

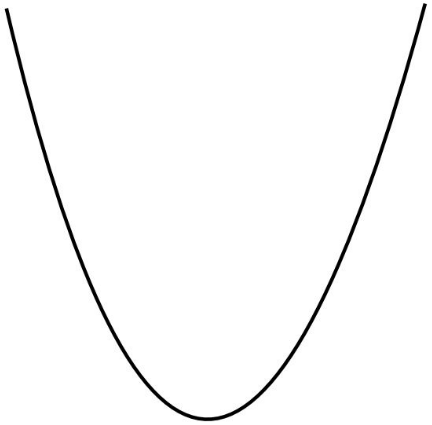


$$f(x) = (x-2)^2$$

One minute calculus

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

Easy: set the derivative to zero!



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

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

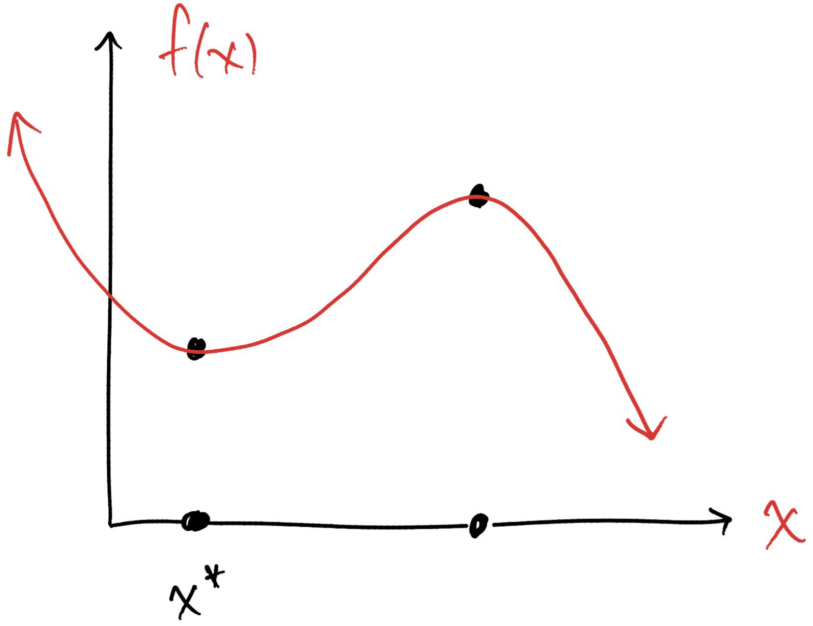
$$\Rightarrow \quad x_* = 2$$

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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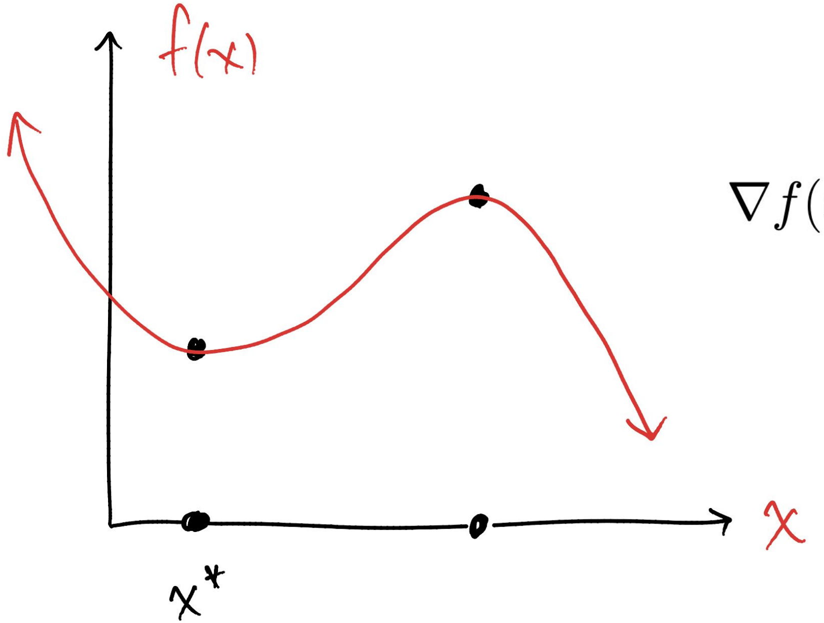

$\nabla f(\boldsymbol{x}^*) = \mathbf{0}$ is necessary but not sufficient

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 $f'(x) = 0$!

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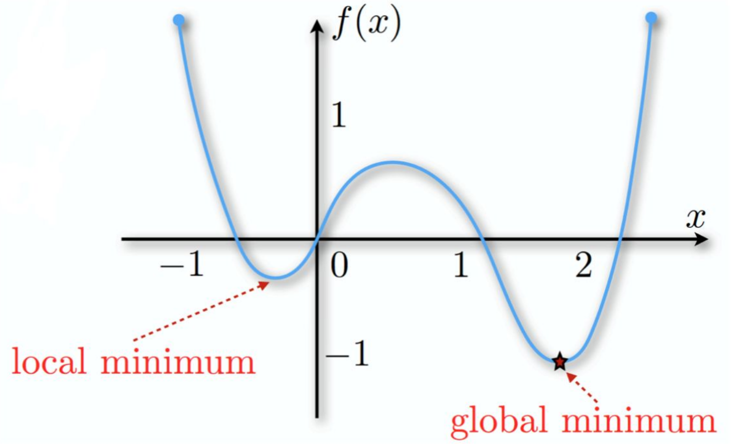


(1) There might not be a closed form solution for $f'(x) = 0$!

(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., $z^\intercal \nabla^2 f(\boldsymbol{x}^*) z \geq 0, \quad \forall z \in \mathbb{R}^d$).

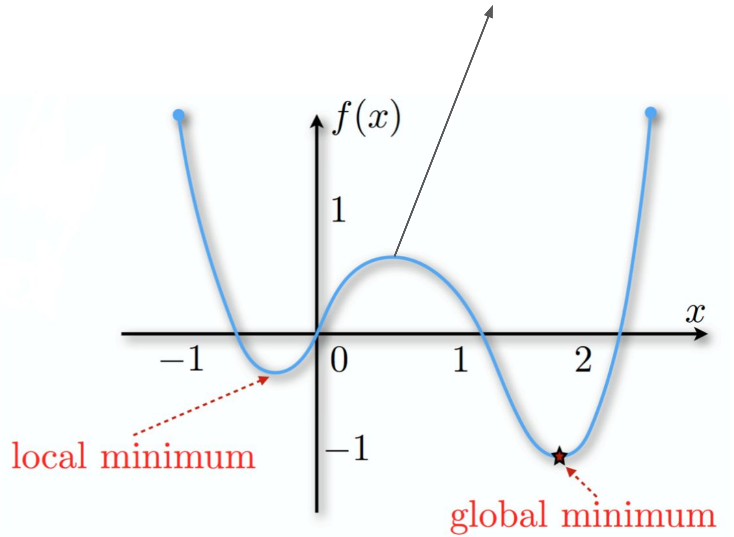
Property 2

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

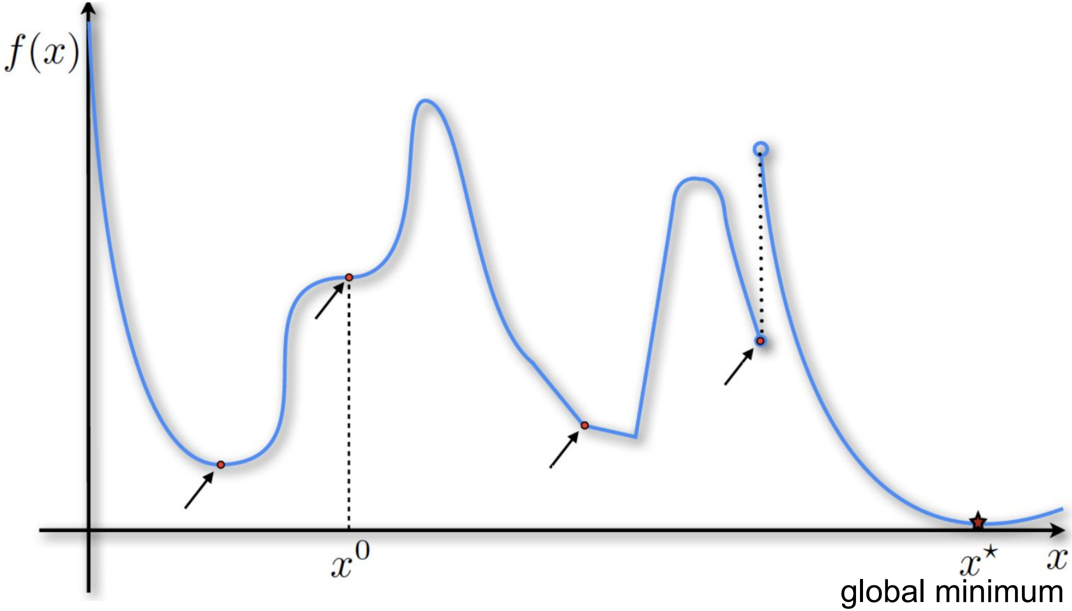
$$\min_{x \in \mathbb{R}} \quad x^4 - 3x^3 + x^2 + \frac{3}{2}x$$

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



Iterative optimization

Fog of war



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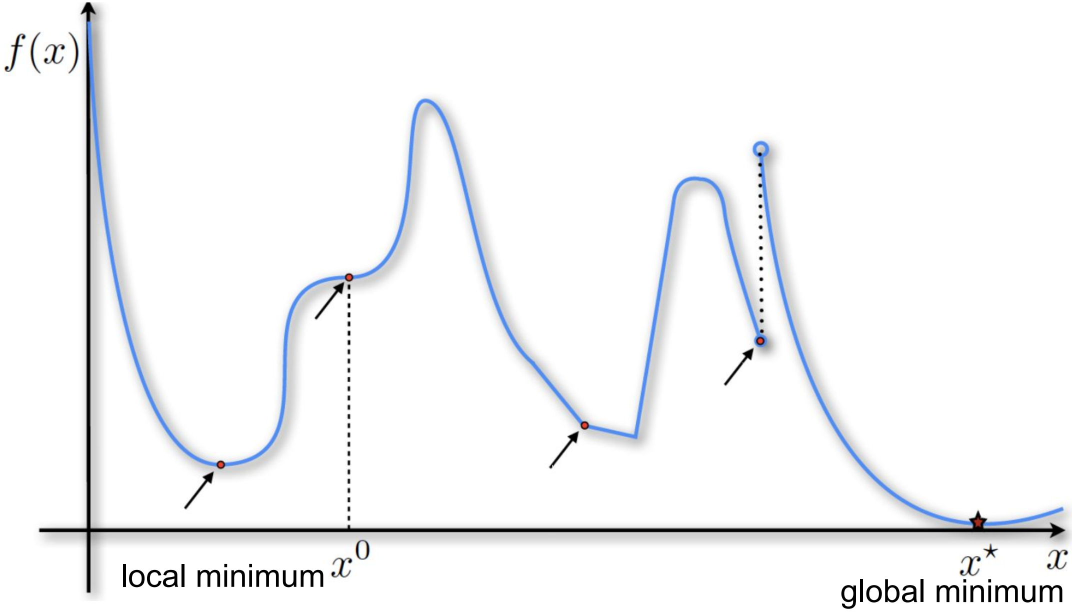

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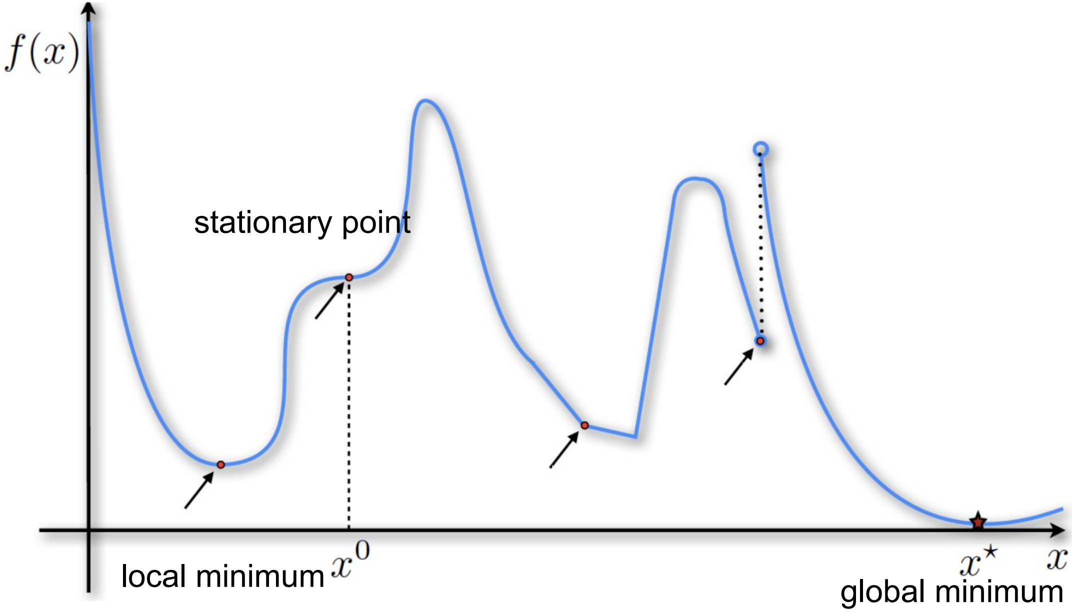

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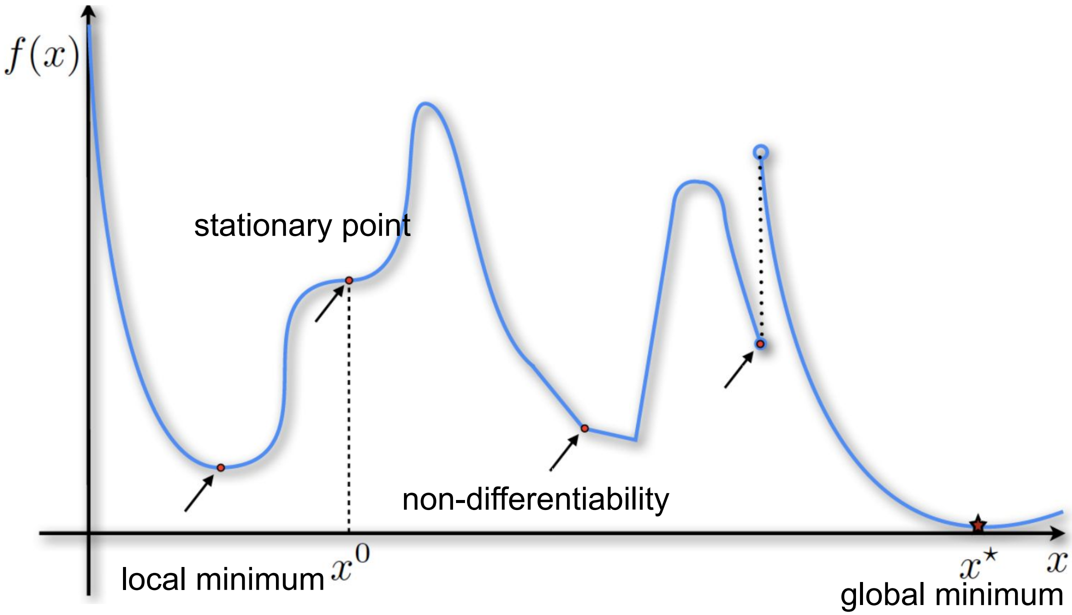

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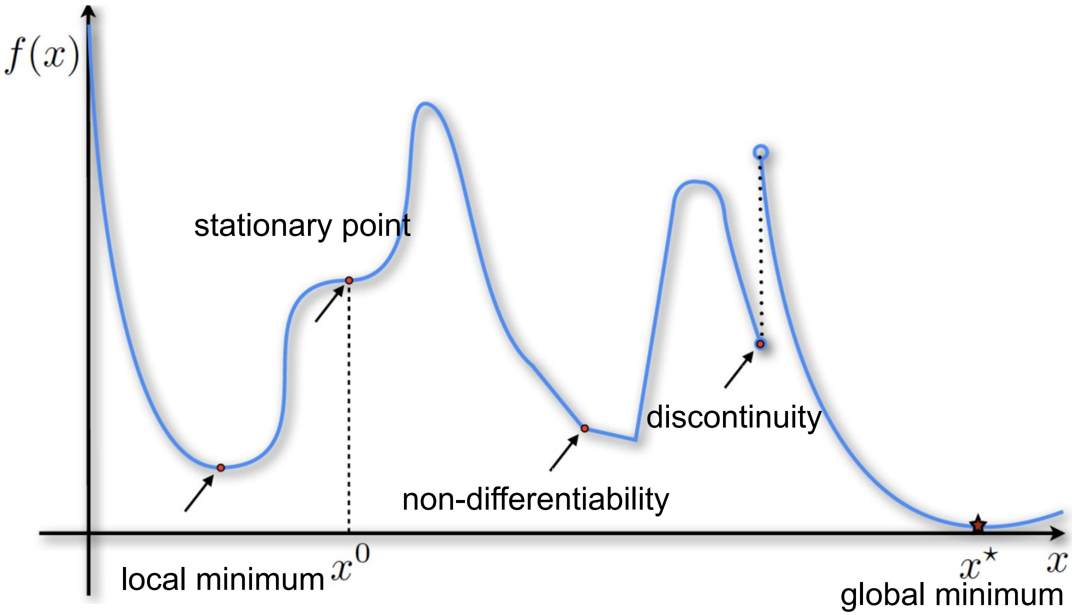

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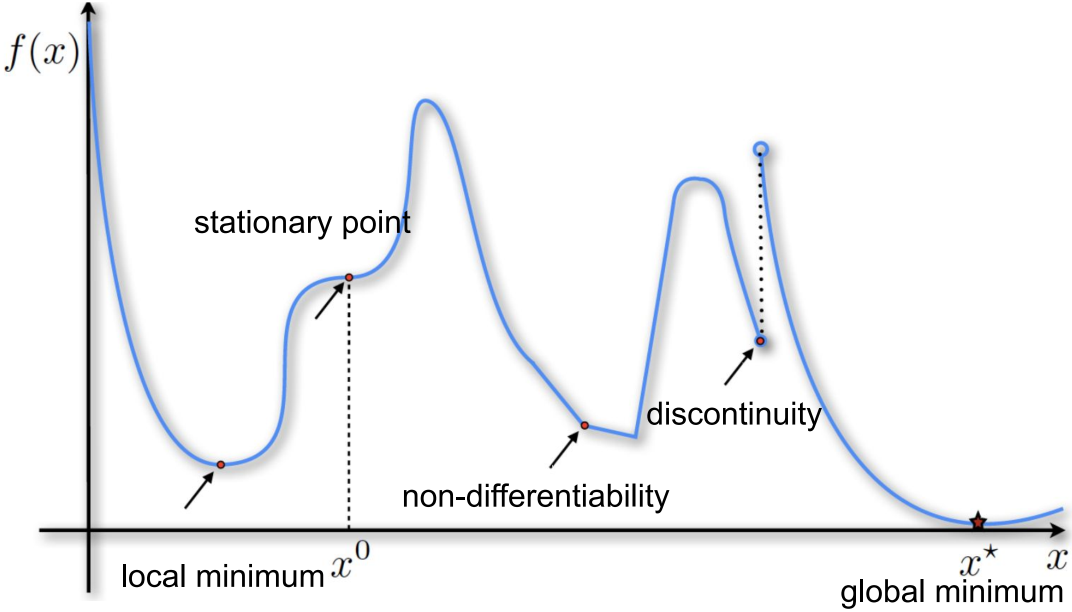

We need a key structure on the function: Convexity.

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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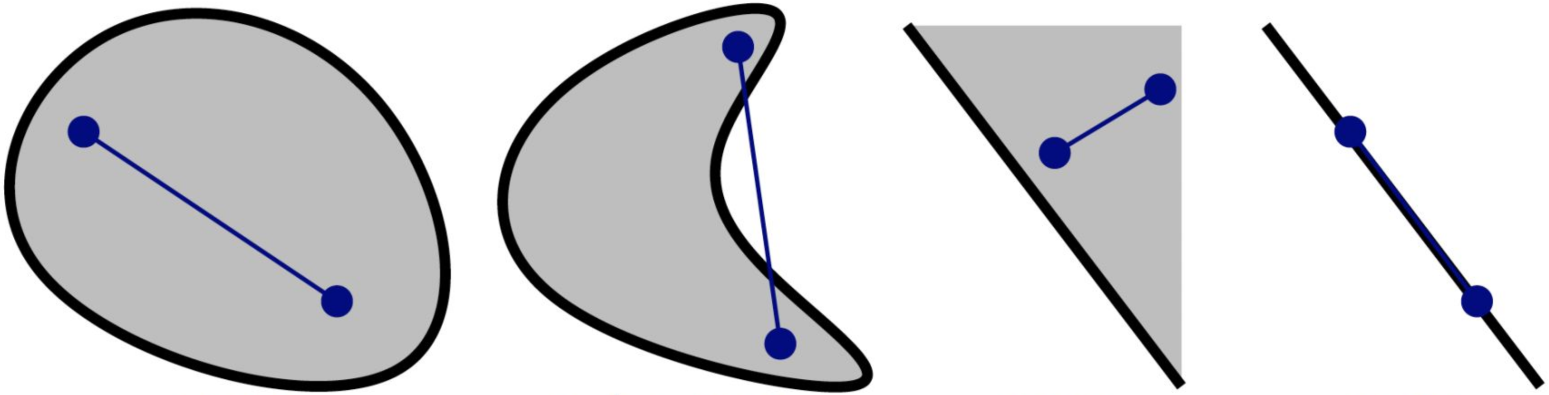

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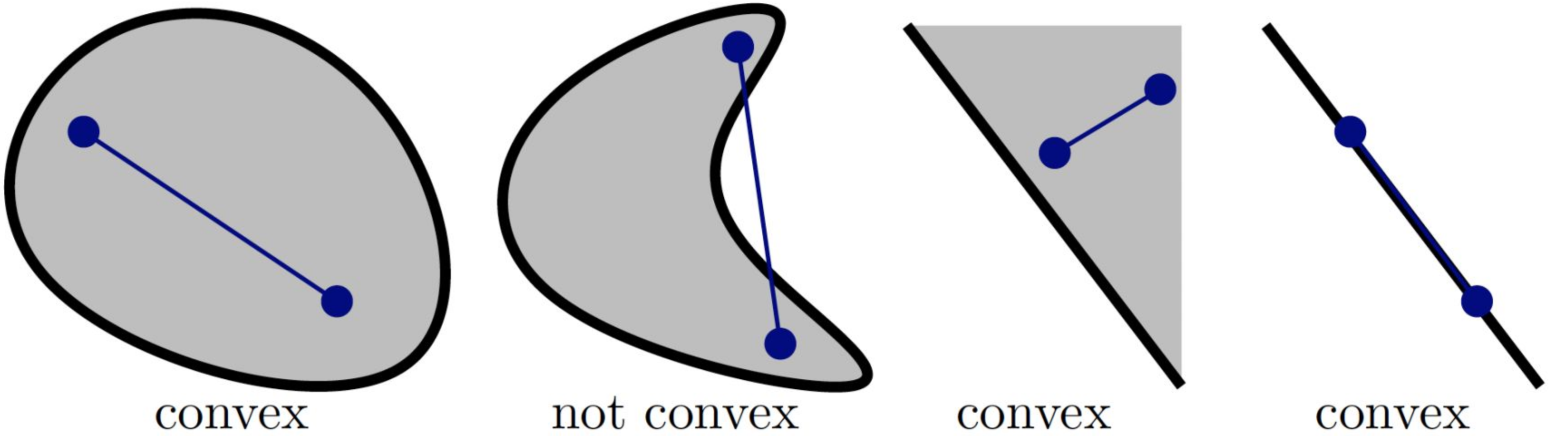
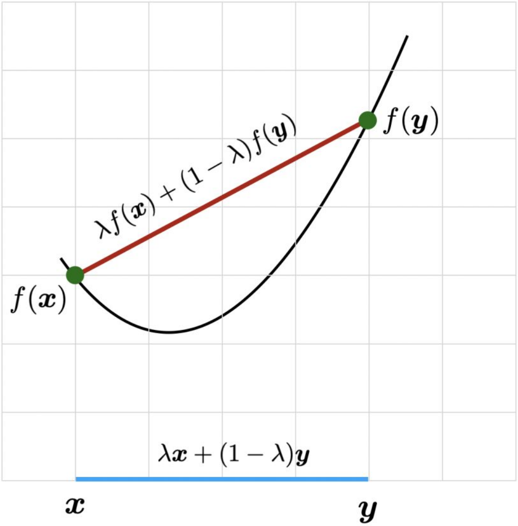


Convex function

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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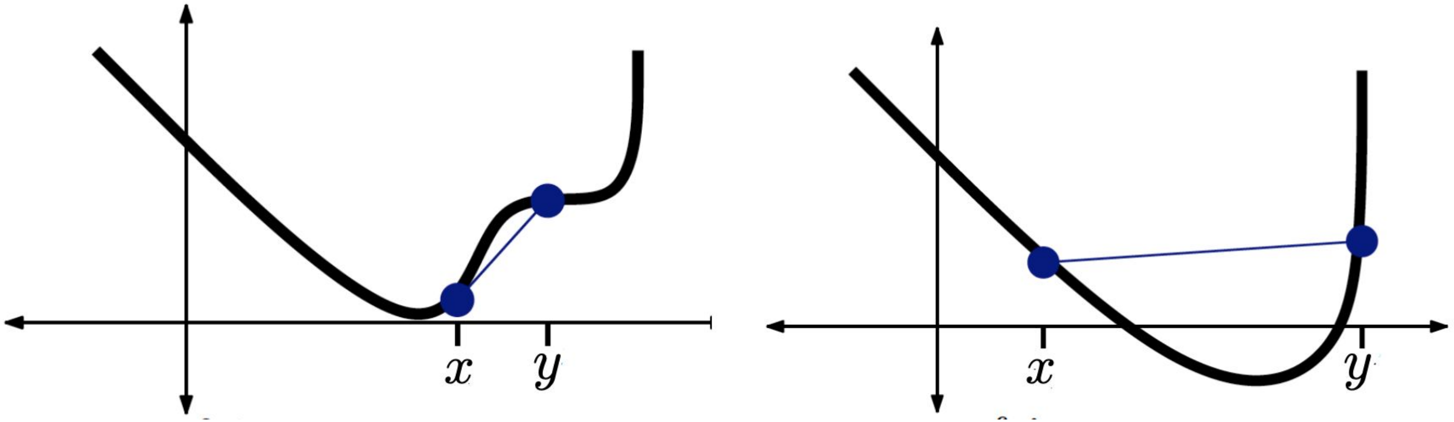

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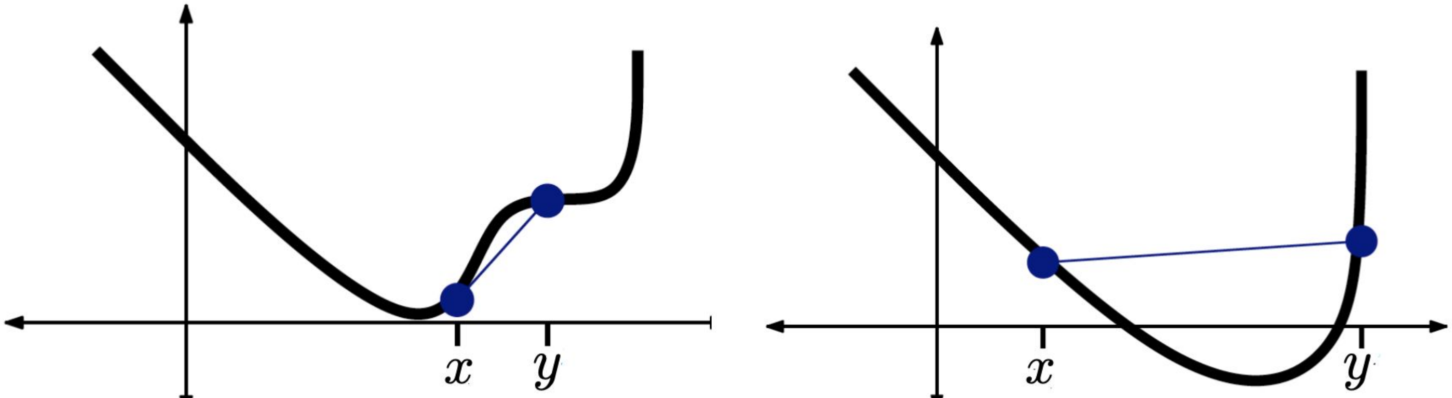


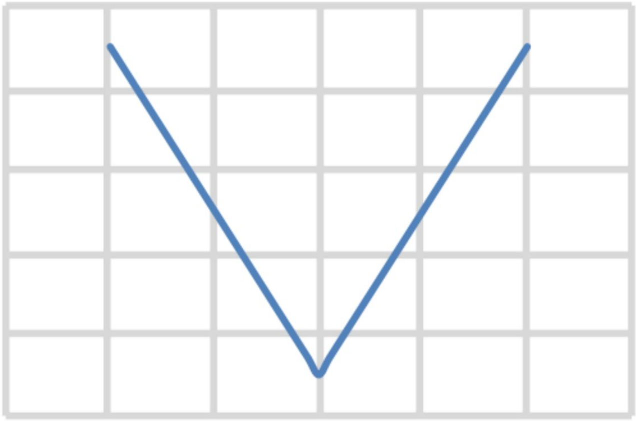
f is not convex

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 $\boldsymbol{x} \in \mathbb{R}^d$?

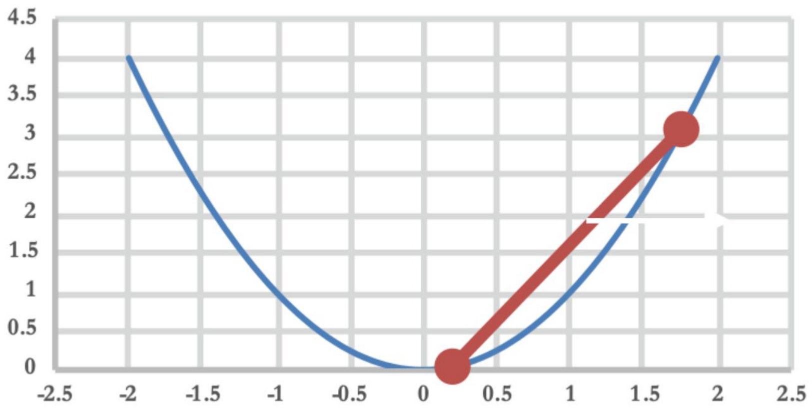
Example: norm

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

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

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

Example: quadratic

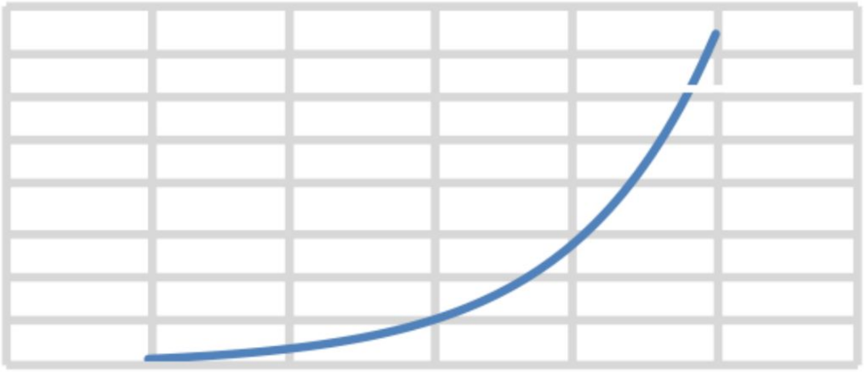


$f(x) = x^2$

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

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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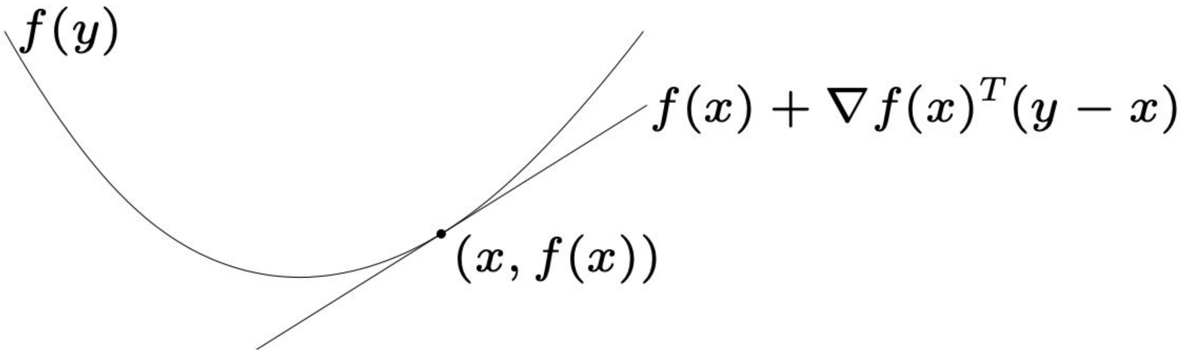

Property 4: Alternate Definition of Convex Functions

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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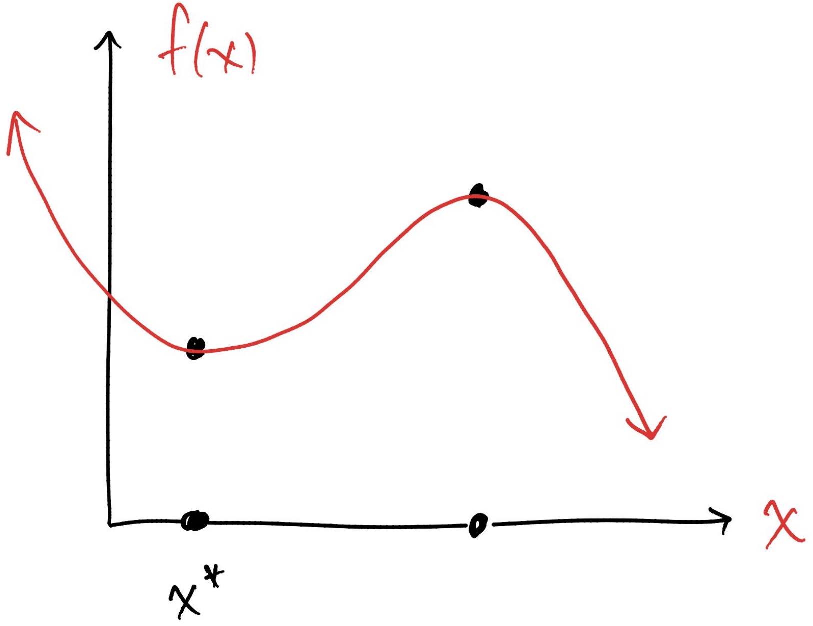

When convex, $\nabla f(\boldsymbol{x}^*) = \mathbf{0}$ is necessary and sufficient

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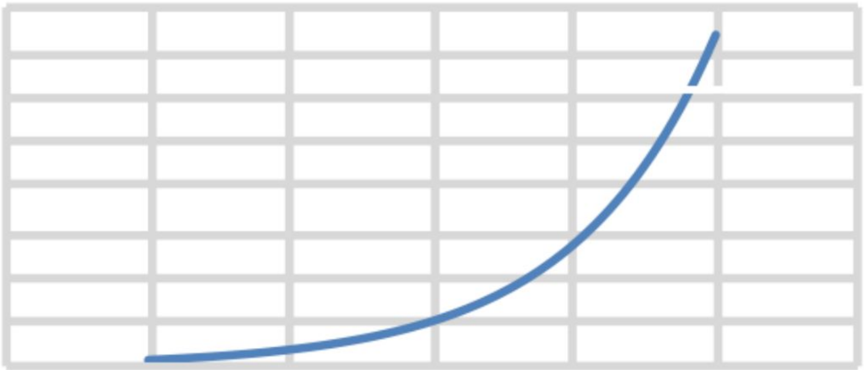
$$f(x) = \exp(x) = e^x$$



Property 6: twice continuously differentiable functions

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

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

- If the function $f : \mathbb{R}^d \to \mathbb{R}$ 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

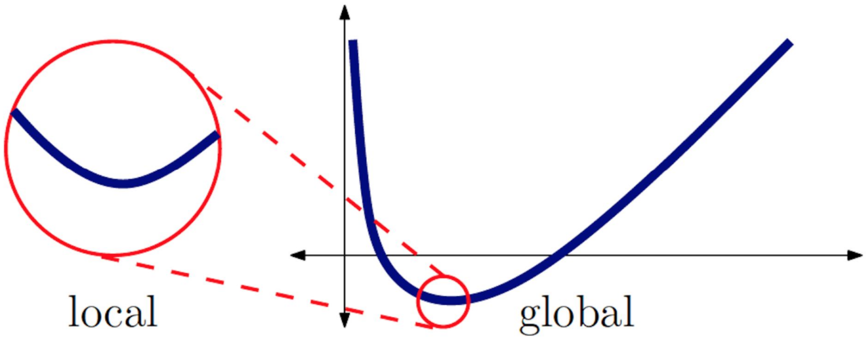
Convex Optimization

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!



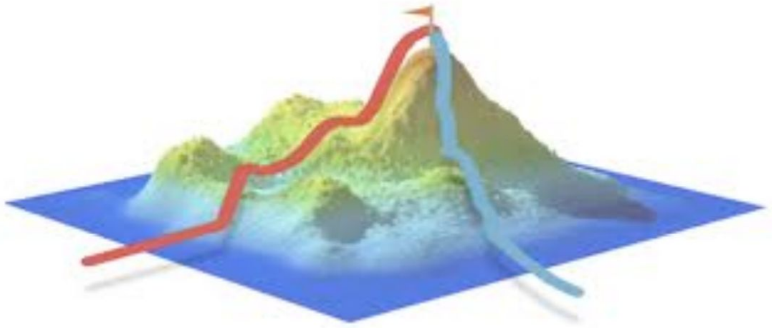
Convex functions are EASY to solve!

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 $\boldsymbol{x}_{t+1}$

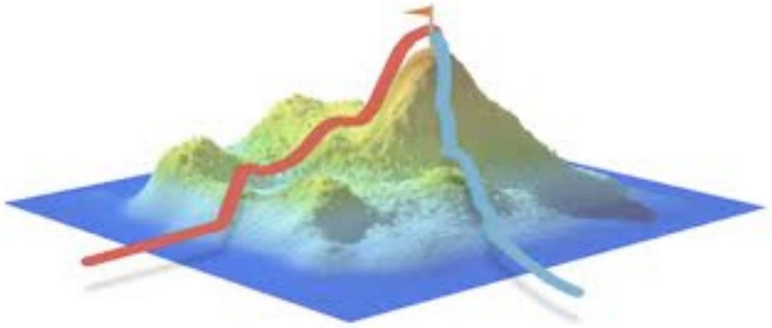


such that

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

Descent direction

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

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

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

Gradient Descent (GD) algorithm

The simplest algorithm in the world (almost)

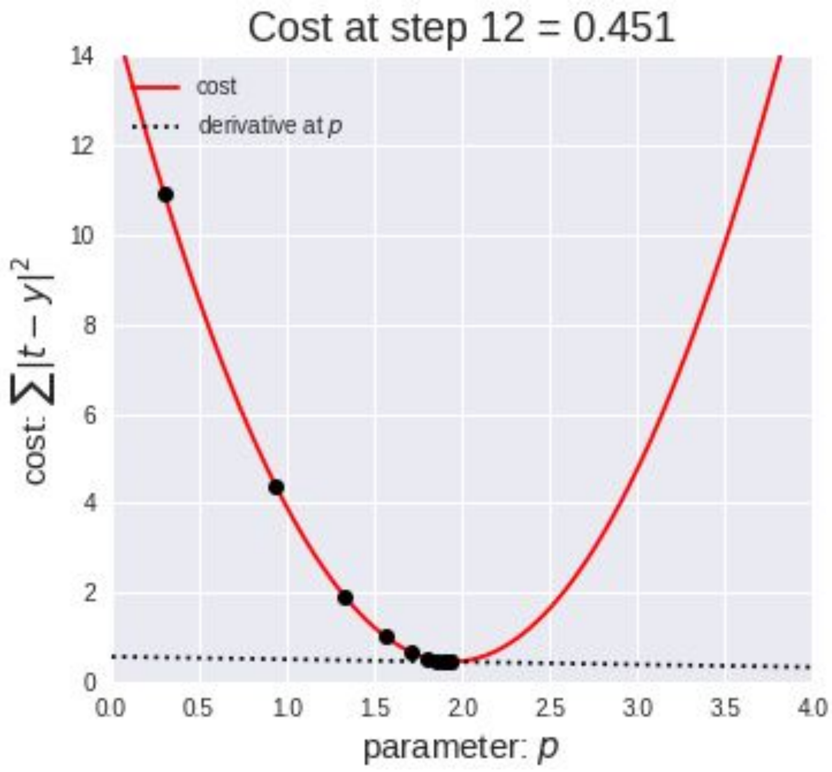
Initialize $\boldsymbol{x}_0$

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

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

Step size

Example



Cost at step 12 = 0.451
cost
derivative at p
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
cost: $\sum |t-y|^2$
parameter: p

Step size selection

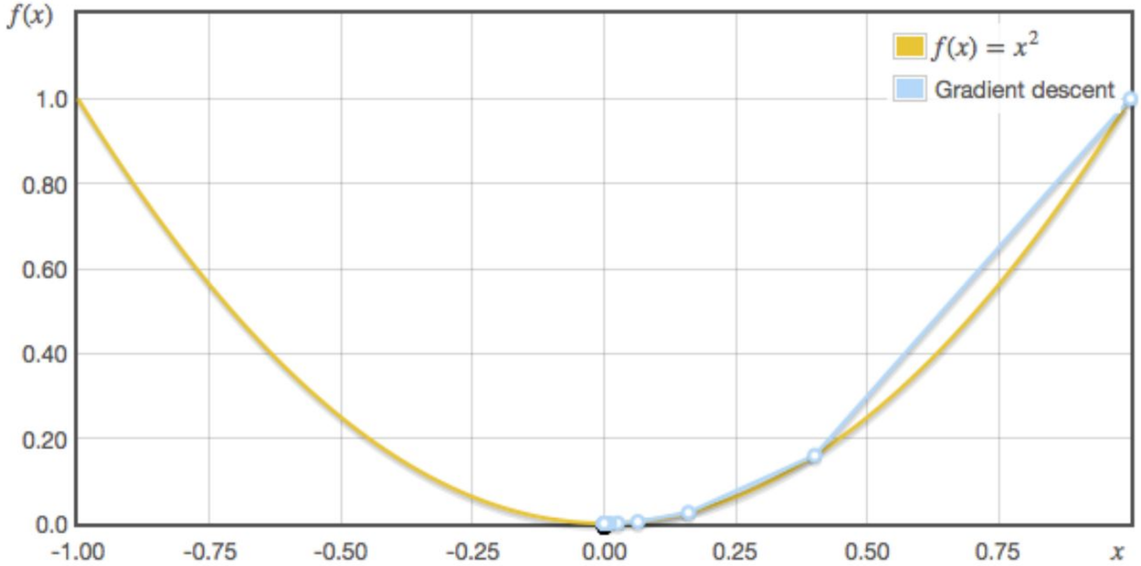
How do I choose the step size?

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

Example Step size selection

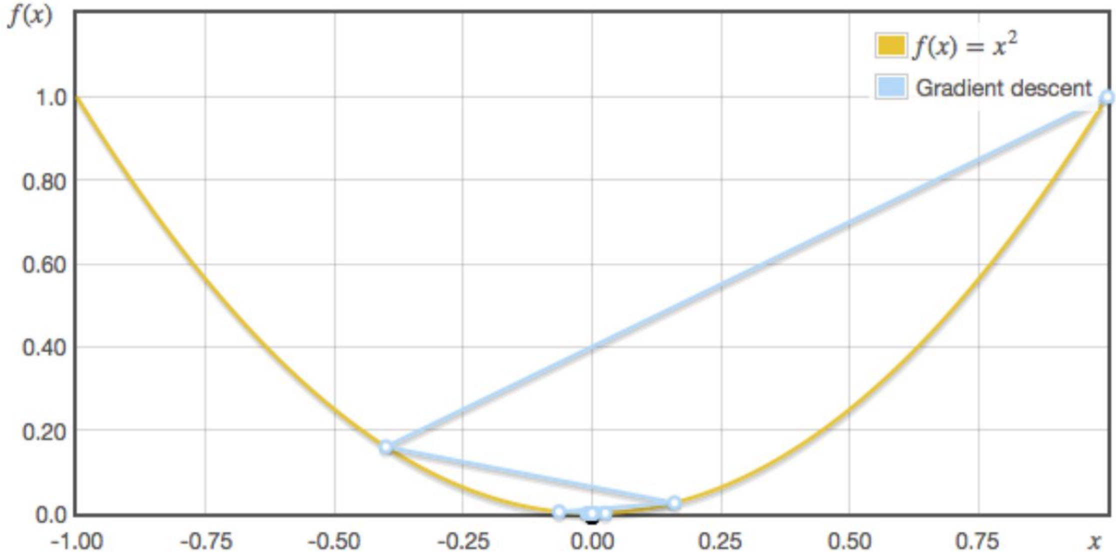
$$f(x) = x^2$$

$$\eta = 0.3$$



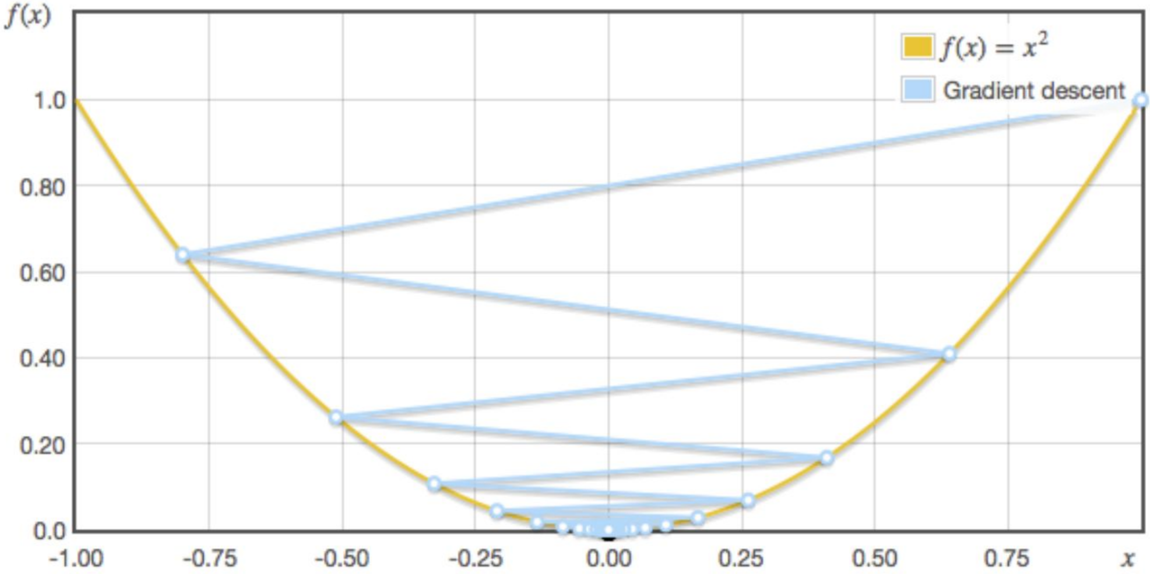
Example Step size selection

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



Example Step size selection

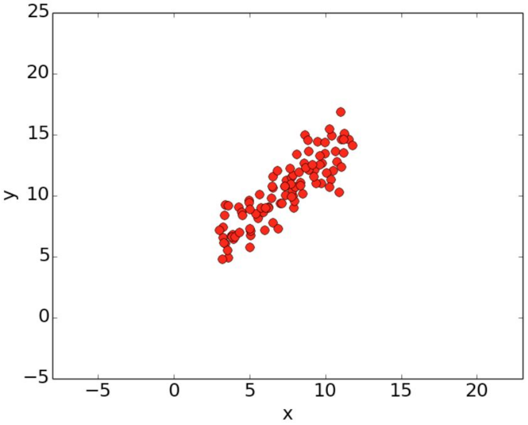
$$f(x) = x^2$$
$$\eta = 0.9$$



Polynomial degree 1

Given: a set of points on the plane

Goal: find the best line that approximates the points



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

Polynomial degree 1

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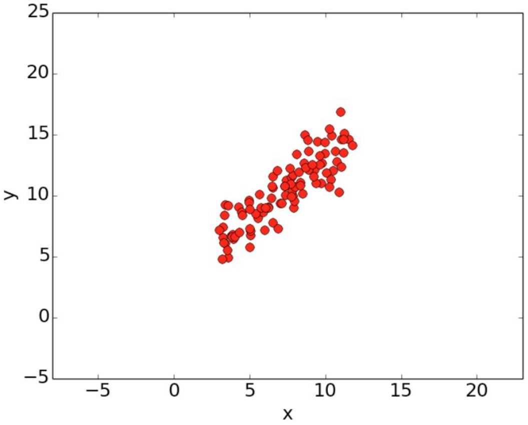

$$(x_1, y_1)$$
$$(x_2, y_2)$$
$$\vdots$$
$$(x_n, y_n)$$

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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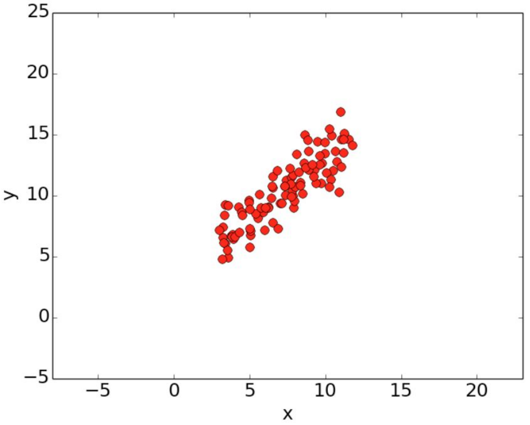

$$(x_1, y_1)$$
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$$(x_n, y_n)$$

Error of a line:

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

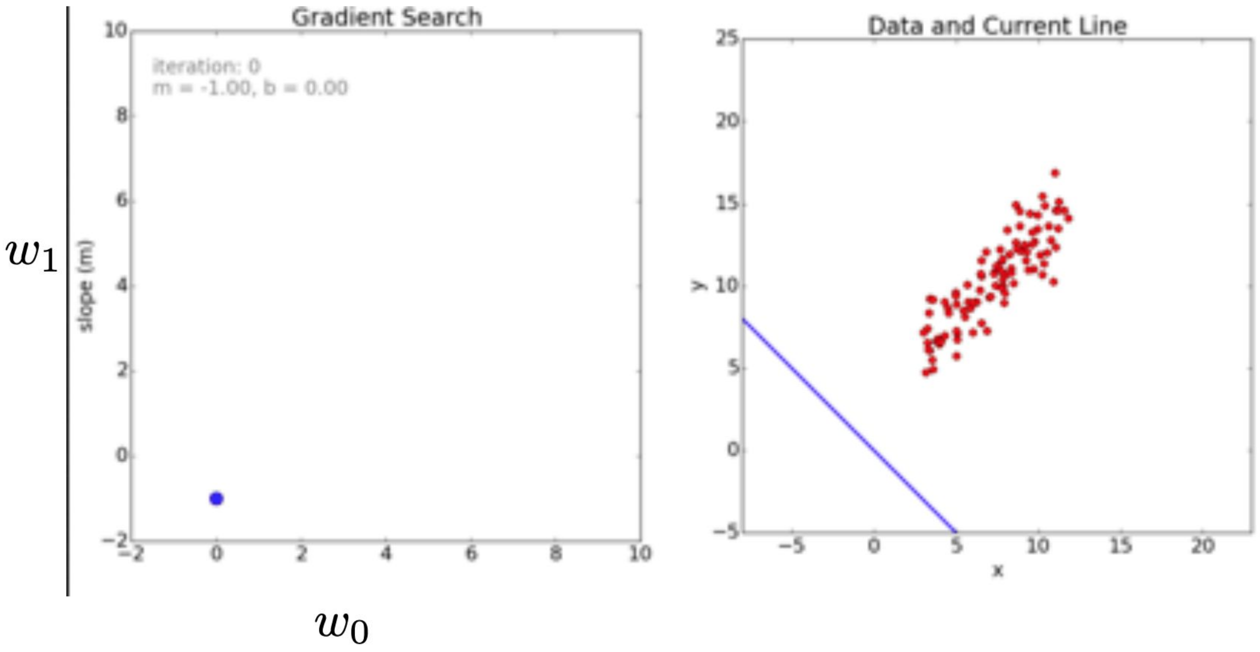
Gradient at a point:

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

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

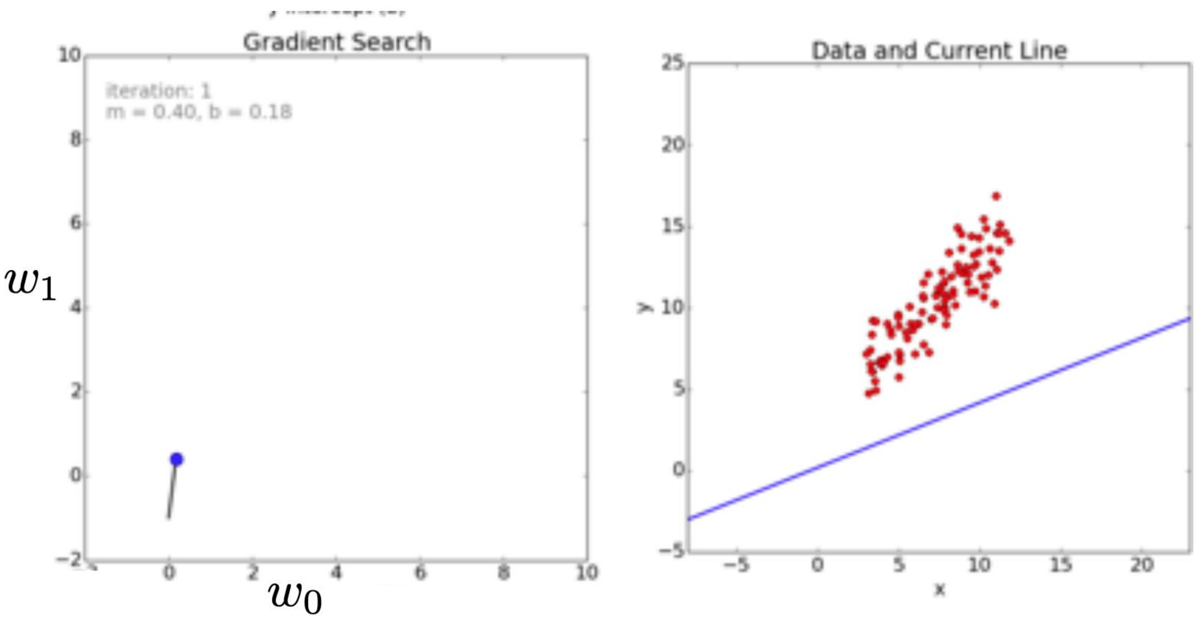
Polynomial degree 1

Iteration = 0



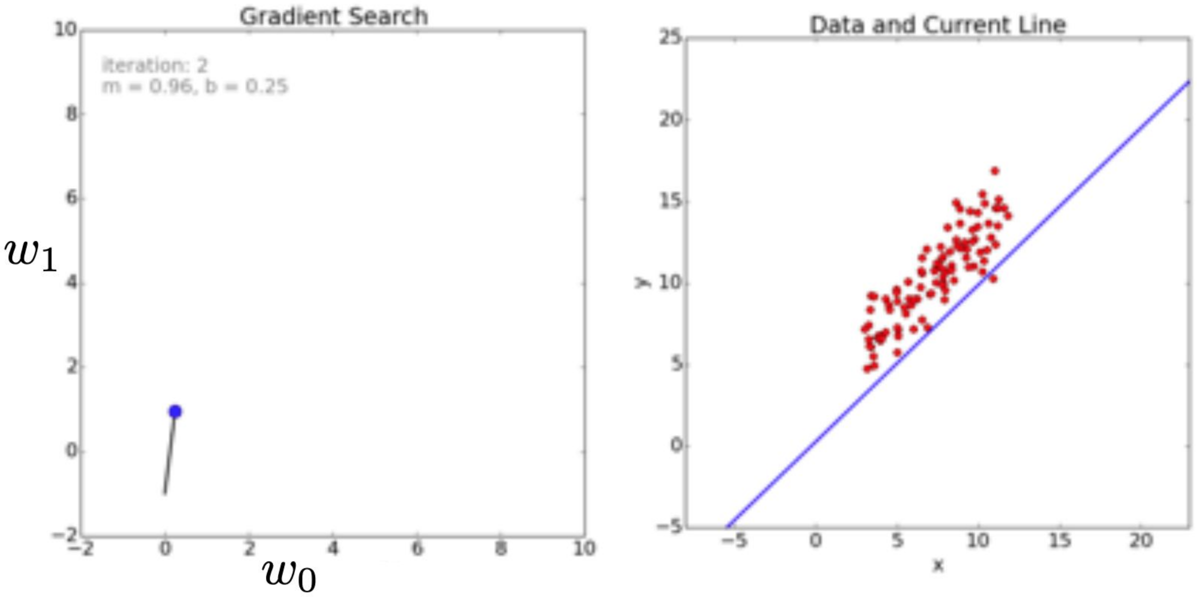
Polynomial degree 1

Iteration = 1



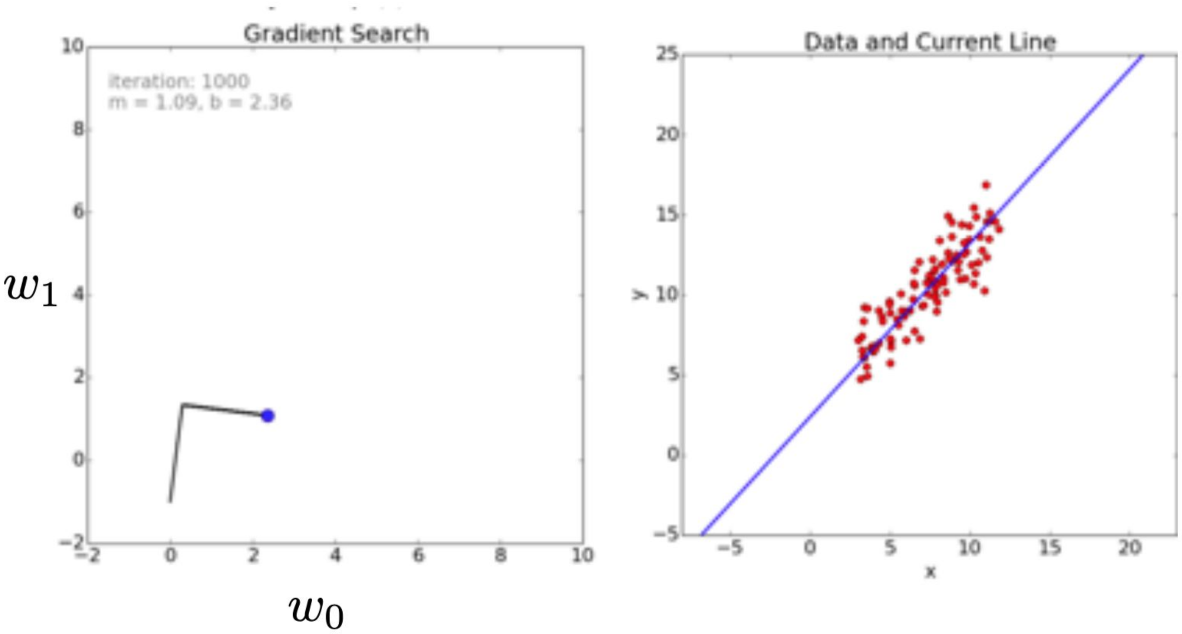
Polynomial degree 1

Iteration = 2



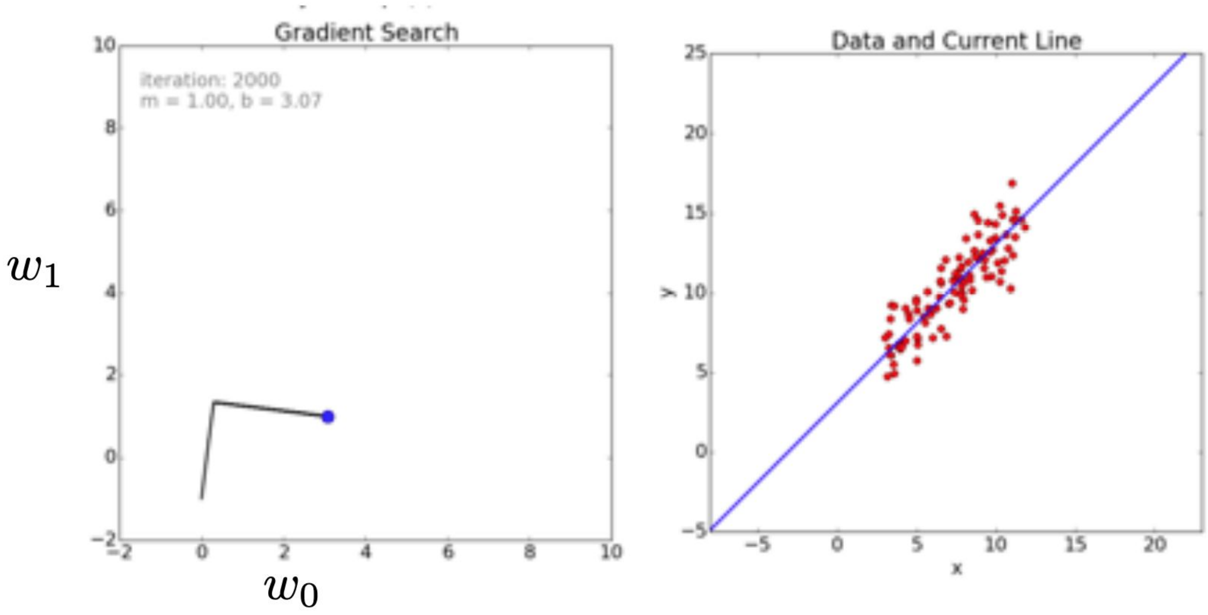
Polynomial degree 1

Iteration = 1000



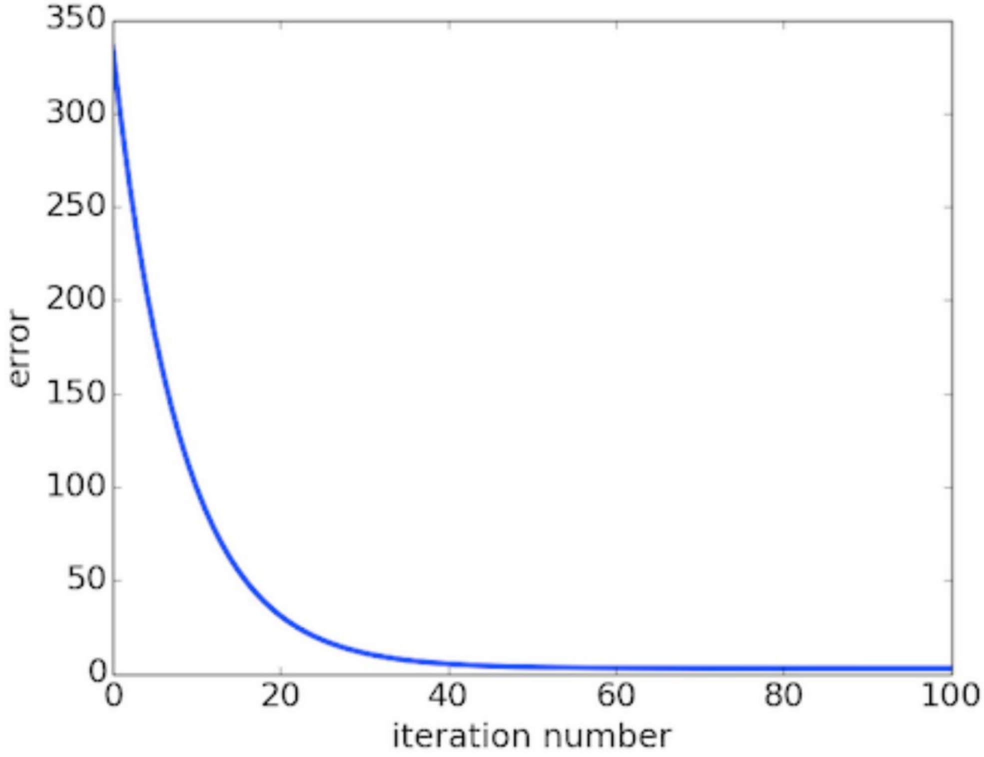
Polynomial degree 1

Iteration = 2000



Polynomial degree 1

How error decreases



Stochastic gradient descent

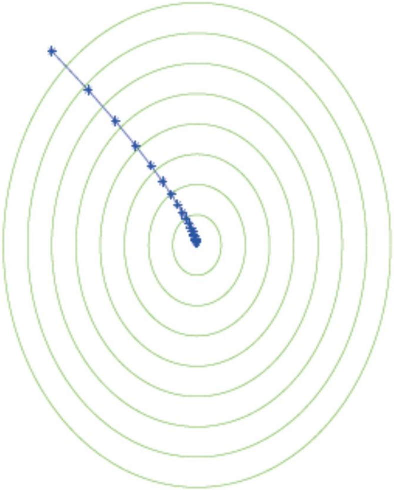
GD is not practical for large-scale data!

Consider a learning problem with millions of images?

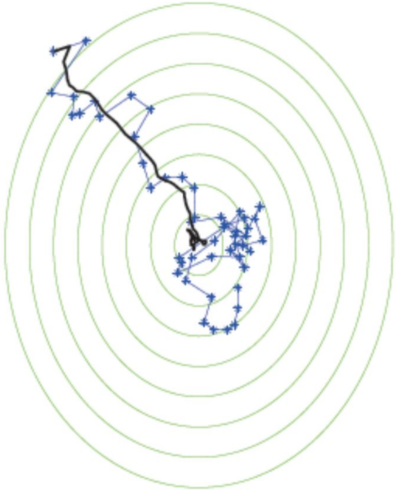
n gradient computations for n training samples per iteration!

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!