# Optimization for Data Science

Unconstrained nonlinear optimization
Constrained nonlinear optimization
Connections to data science





## Three pillars of data science


## Fundamentals of optimization

What is optimization ?

"An optimization problem consists of maximizing or minimizing a real function by systematically choosing input values from within an allowed set and computing the value of the function."*

*"http://en.wikipedia.org/wiki/Mathematical_optimization"





## What is optimization?

- … the use of specific methods to determine the "best" solution to a problem
  - Find the best functional representation for data
  - Find the best hyperplane to classify data

Minimize / maximize $f(X)$

$X$ = Decision variables on $X$

min error → $\sum_{i=1}^{m} e_i^2$

$e_1 = y_1 - a_0 - a_1 x_1$

$e_n = y_n - a_0 - a_1 x_n$

$y_1 = a_0 + a_1 x_1$

$y_n = a_0 + a_1 x_n$

$\sum_{i=1}^{n} e_i^2$

| $y$ | $x$ |
|---|---|
| $y_1$ | $x_1$ |
| $y_2$ | $x_2$ |
| $y_n$ | $x_n$ |

$y = a_0 + a_1 x$

## Why optimization for machine learning

- (Almost) All machine learning (ML) algorithms can be viewed as solutions to optimization problems
  - Even in cases where, the original machine learning technique has a basis derived from other fields
- A basic understanding of optimization approaches help in
  - More deeply understand the working of the ML algorithm
  - Rationalize the workings of the algorithm
  - And (may be !!!), develop new algorithms ourselves





## Components of an optimization problem

- Objective function $f$ $\quad f \quad -f$
  - We look at minimization problem
- Decision variables $\min f(x)$
- Constraints $x \in \Omega$

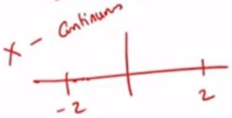
# Types of optimization problems

- Depending on the type of objective function, constraints and decision variables
  - Linear programming problem ✓
  - Nonlinear programming problem ✓
    - Convex vs Non-convex
  - Integer programming problem (linear and nonlinear)
  - Mixed integer linear programming problem
  - Mixed integer nonlinear programming problem

$f(x)$

S.t Constraints → line

$x$ – Continuous variables




$f(x_1, x_2)$

$x_1 \in [0,1,2,3]$

$x_2$ is Continuous

min $f(x_1, x_2)$

$x_1 \in [0,1,2,3]$

$x_2 \in [0,1,2,3]$

Constraints on $x_1$ and $x_2$

$x_1 \in [0,1]$

$x_2 \in [0,1]$



Nonlinear Optimization

# UNCONSTRAINED CASE

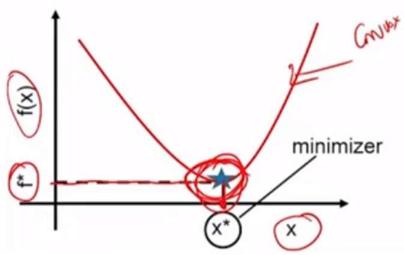
# Univariate Optimization – Local and Global Optimum

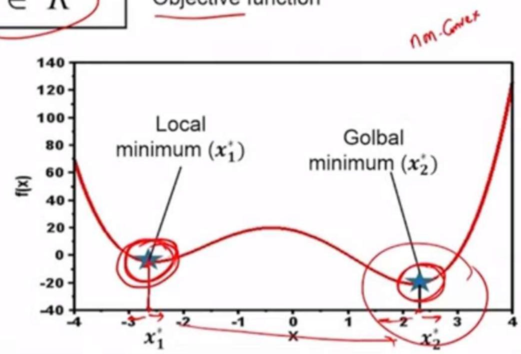
Univariate optimization

$$\min_{x} f(x)$$
$$x \in R$$

Decision variable

Objective function



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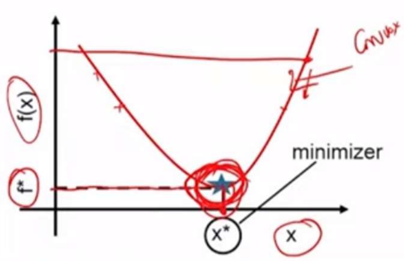
# Univariate Optimization – Local and Global Optimum

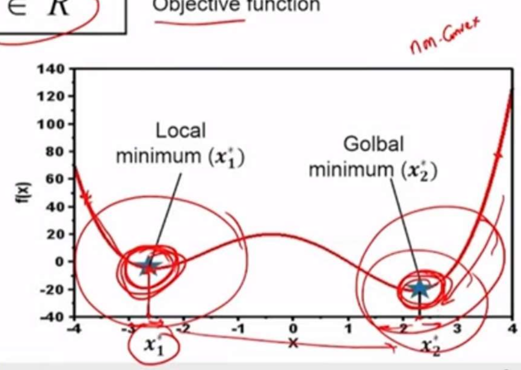
Univariate optimization

$$\min_{x} f(x)$$
$$x \in R$$

Decision variable

Objective function

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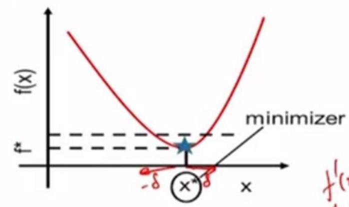
## Univariate Optimization – Conditions for Local Optimum

Univariate optimization

$$\begin{array}{|c|}\hline \min\limits_{x} \quad f(x) \\ x \in R \\ \hline\end{array}$$




$f'(x) = 0$
$f''(x^*) > 0$

Approximate $f(x)$ as a quadratic function using Taylor series at a point $x^k$

$$f(x) \approx f(x^k) + \frac{1}{1!}f'(x^k)(x - x^k) + \frac{1}{2!}f''(x^k)(x - x^k)^2$$

When $x^k = x^*$,

$$f(x) \approx f(x^*) + \frac{1}{1!}\underbrace{f'(x^*)}_{0}(x - x^*) + \frac{1}{2!}f''(x^*)(x - x^*)^2$$

$$\underbrace{f(x) - f(x^*)}_{\text{Positive}} \approx \frac{1}{2!}\underbrace{f''(x^*)}_{\text{Has to be positive}}\underbrace{(x - x^*)^2}_{\text{Always positive}}$$





## Univariate Optimization – Summary

Univariate optimization

$$\begin{array}{|c|}\hline \min\limits_{x} \quad f(x) \\ x \in R \\ \hline\end{array}$$

Necessary and sufficient conditions for $x^*$ to be the minimizer of the function $f(x)$

First order necessary conditon: $f'(x^*) = 0$ ✓

Second order sufficiency condition: $f''(x^*) > 0$ ✓

# Univariate Optimization – Numerical Example

$$\min_{x} \; f(x)$$

$$f(x) = 3x^4 - 4x^3 - 12x^2 + 3$$

| First order condition | Second order condition |
|---|---|
| $f'(x) = 12x^3 - 12x^2 - 24x = 0$<br>$= 12x(x^2 - x - 2x) = 0$<br>$= 12x(x+1)(x-2) = 0$<br>$x = 0, x = -1, x = 2$ | $f''(x) = 36x^2 - 24x - 24$<br>$f''(x)\big\rvert_{x=0} = -24$<br>$f''(x)\big\rvert_{x=-1} = 36 > 0$<br>$f''(x)\big\rvert_{x=2} = 72 > 0$ |
| $f(-1) = -2$ | $f(2) = -29$ |
| $x^* = -1$, is a local minimizer of $f(x)$ | $x^* = 2$, is a global minimizer of $f(x)$ |

$x = -1, 2$
$f'(x) = 0$
$f''(x^*) > 0$