Numerical Optimization

Unconstrained Optimization (I)

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NPTEL Course on Numerical Optimization

Global Minimum

Let $X \subseteq \mathbb{R}^n$ and $f : X \to \mathbb{R}$
Consider the problem,

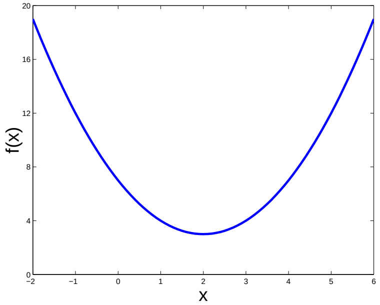
Constrained optimization problem

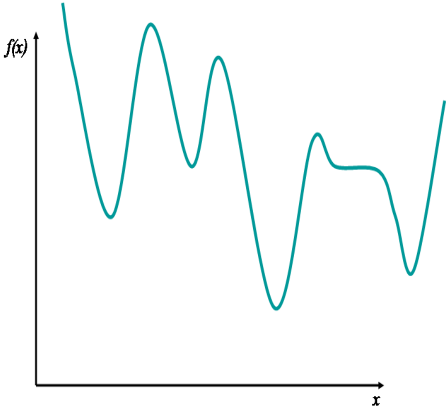
$$\begin{array}{cc} \min\limits_{\boldsymbol{x}} & f(\boldsymbol{x}) \\ \text{s.t.} & \boldsymbol{x} \in X \end{array}$$

Definition

$\boldsymbol{x}^* \in X$ is is said to be a *global minimum* of f over X if
$f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \quad \forall\, \boldsymbol{x} \in X$.

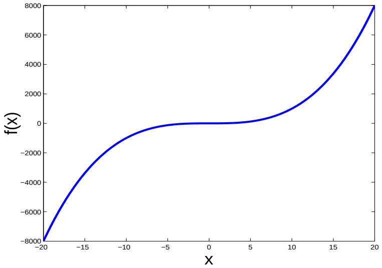
Question: Under what conditions on f and X does the function f attain its maximum and/or minimum in the set X?


20
16
12
8
4
0
f(x)
−2
−1
0
1
2
3
4
5
6
x


f(x)
x

Global Minimum

- $X = \mathbb{R}, f : X \rightarrow \mathbb{R}$ defined as $f(x) = x^3$.

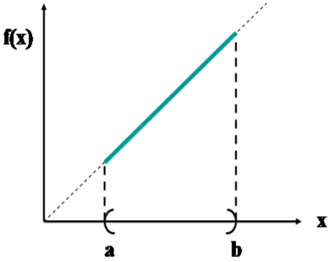


f attains neither a minimum nor a maximum on X

Note: X is closed, but not bounded; that is, X is not a compact set

Constrained Optimization

- $X = (a, b), f : X \to \mathbb{R}$ defined as $f(x) = x$.

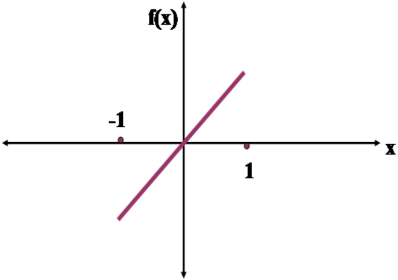


f attains neither a minimum nor a maximum on X

Note:

- X is bounded, but not closed; that is, X is not a compact set
- f does attain infimum at a and supremum at b

- $X = [-1, 1], f : X \to \mathbb{R}$ defined as $f(x) = x$ if $-1 < x < 1$ and 0 otherwise.



f attains neither a minimum nor a maximum on X

Note:

- X is closed and bounded; X is compact
- f is not continuous on X

Weierstrass' Theorem

Theorem

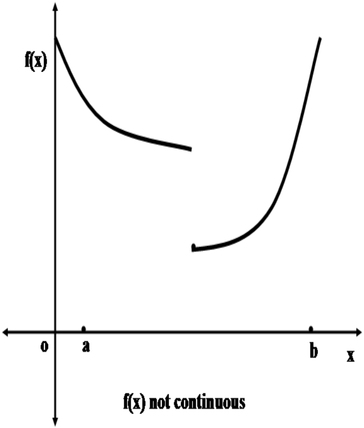
Let $X \subset \mathbb{R}^n$ be a nonempty compact set and $f : X \to \mathbb{R}$ be a continuous function on X. Then, f attains a maximum and a minimum on X; that is, there exist $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ in X such that

$$f(\boldsymbol{x}_1) \geq f(\boldsymbol{x}) \geq f(\boldsymbol{x}_2) \quad \forall \boldsymbol{x} \in X.$$

Note: Weierstrass' Theorem provides only *sufficient* conditions for the existence of optima.

Constrained Optimization

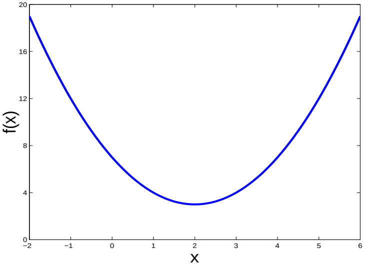
- $X = [a, b], f : X \to \mathbb{R}$



- $f(x)$ not continuous; but f attains a minimum

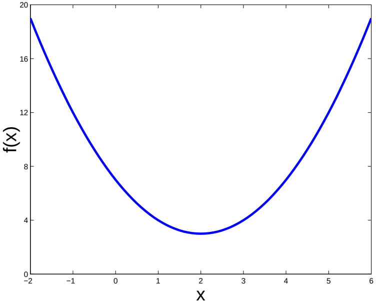
Constrained Optimization

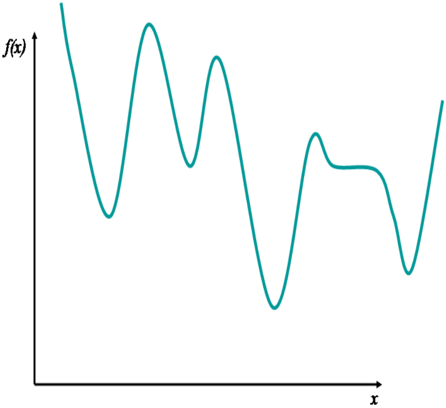
- $X = \mathbb{R}, f : X \to \mathbb{R}$ defined as $f(x) = (x-2)^2$.



- $f(x)$ continuous, X not compact; but f attains a minimum

Unconstrained Optimization





Global Minimum

Let $X \subseteq \mathbb{R}^n$ and $f : X \to \mathbb{R}$
Consider the problem,

Constrained optimization problem

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{s.t.} \quad & x \in X \end{aligned}$$

Definition

$\boldsymbol{x}^* \in X$ is is said to be a *global minimum* of f over X if
$f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \quad \forall\, \boldsymbol{x} \in X.$

- Global minimum is difficult to find or characterize for a general nonlinear function

Local Minimum

Let $X \subseteq \mathbb{R}^n$ and $f : X \to \mathbb{R}$
Consider the problem,

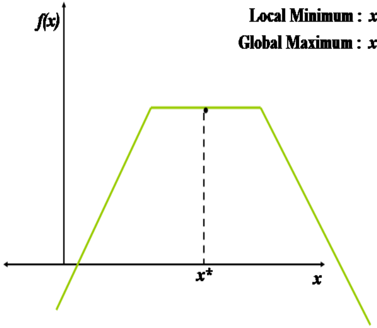
Constrained optimization problem

$$\begin{array}{ll} \min\limits_{x} & f(x) \\ \text{s.t.} & x \in X \end{array}$$

Definition

$\boldsymbol{x}^* \in X$ is is said to be a *local minimum* of f if there is a $\delta > 0$ such that $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \quad \forall\, \boldsymbol{x} \in X \cap B(\boldsymbol{x}^*, \delta)$.

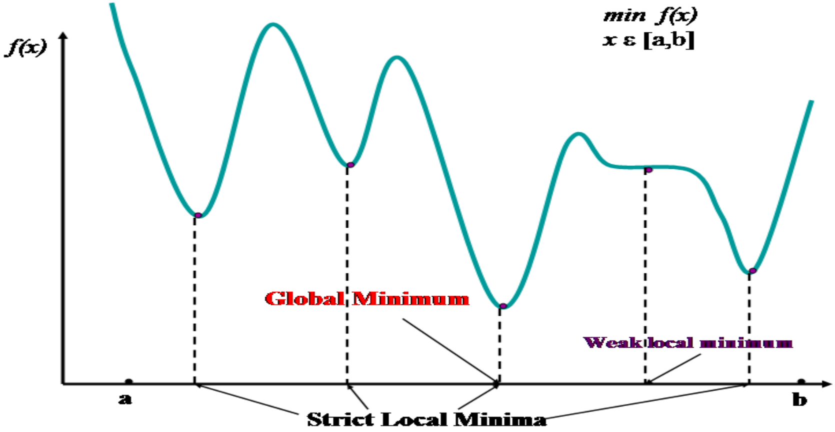
Strict Local Minimum



Definition

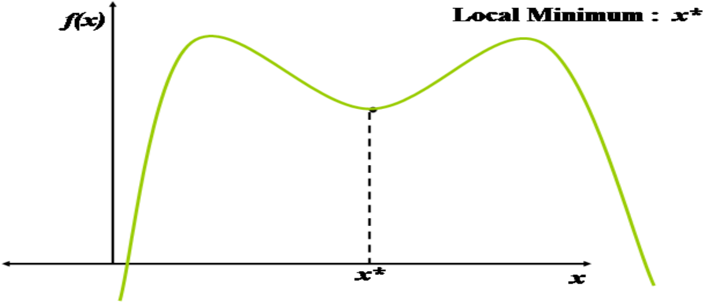
$\boldsymbol{x}^* \in X$ is is said to be a *strict local minimum* of f if
$f(\boldsymbol{x}^*) < f(\boldsymbol{x}) \quad \forall\, \boldsymbol{x} \in X \cap B(\boldsymbol{x}^*, \delta), \boldsymbol{x} \neq \boldsymbol{x}^*$.

Different Types of Minima



Global Minimum and Local Minimum

- Every global minimum is also a local minimum.
- It may not be possible to identify a global min by finding all local minima



- f does not have a global minimum

Optimization Problems

Let $X \subseteq \mathbb{R}^n$ and $f : X \to \mathbb{R}$

- Constrained optimization problem:

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{s.t.} \quad & x \in X \end{aligned}$$

- Unconstrained optimization problem:

$$\min_{x \in \mathbb{R}^n} \quad f(x)$$

Now, consider $f : \mathbb{R} \to \mathbb{R}$

- Unconstrained one-dimensional optimization problem:

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

Unconstrained Optimization

Let $f : \mathbb{R} \to \mathbb{R}$

Unconstrained problem

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

- What are *necessary and sufficient conditions* for a local minimum?
  - Necessary conditions: Conditions satisfied by every local minimum
  - Sufficient conditions: Conditions which guarantee a local minimum
- Easy to characterize a local minimum if f is *sufficiently* smooth

First Order Necessary Condition

Let $f : \mathbb{R} \to \mathbb{R}$, $f \in \mathcal{C}^1$.
Consider the problem, $\min_{x\in\mathbb{R}} \quad f(x)$

Result (First Order Necessary Condition)

If x^* is a local minimum of f, then $f'(x^*) = 0$.

Proof.

Suppose $f'(x^*) > 0$. $f \in \mathcal{C}^1 \Rightarrow f' \in \mathcal{C}^0$.
Let $D = (x^* - \delta, x^* + \delta)$ be chosen such that $f'(x) > 0 \quad \forall\, x \in D$.
Therefore, for any $x \in D$, using first order truncated Taylor series,

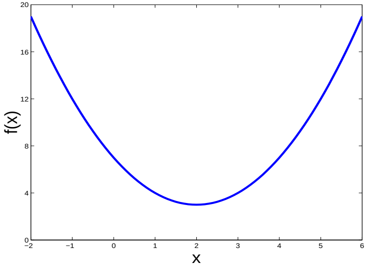
$$f(x) = f(x^*) + f'(\bar{x})(x - x^*) \quad \text{where } \bar{x} \in (x^*, x).$$

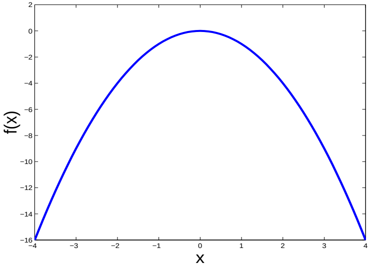
Choosing $x \in (x^* - \delta, x^*)$ we get,

$$f(x) < f(x^*), \quad \text{a contradiction.}$$

Similarly, one can show, $f(x) < f(x^*)$ if $f'(x^*) < 0$. □

First Order Necessary Condition



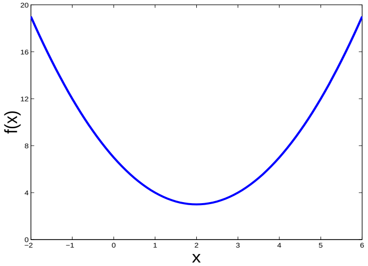


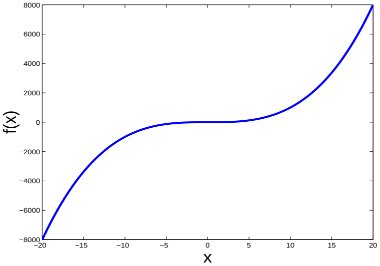
$$f(x) = (x-2)^2$$
$$f'(2) = 0$$

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

Slope of the function is zero at local minimum and also at local maximum

First Order Necessary Condition





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

$$f(x) = x^3$$
$$f'(0) = 0$$

Slope of the function is zero at a saddle point

Stationary Points

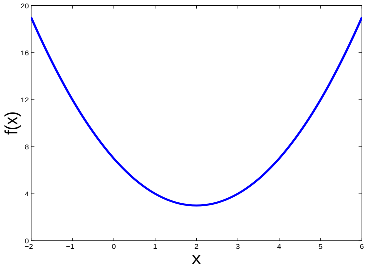
Let $f : \mathbb{R} \to \mathbb{R}, f \in \mathcal{C}^1$.
Consider the problem, $\min_{x \in \mathbb{R}} \ f(x)$.

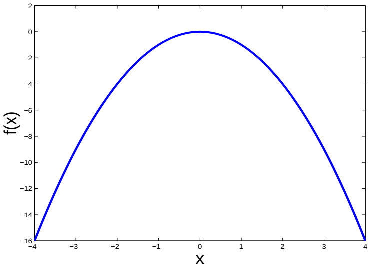
Definition

x^* is called a *stationary point* if $f'(x^*) = 0$.

$f'(x^*) = 0$ is a *necessary* but not sufficient condition for a local minimum.

Question: How do we ensure that a stationary point is a local minimum?





$$f(x) = (x-2)^2, f'(2) = 0$$
$$f''(2) = 4$$

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

Second Order Necessary Conditions

Let $f : \mathbb{R} \to \mathbb{R}, f \in \mathcal{C}^2$.
Consider the problem, $\min_{x \in \mathbb{R}} f(x)$

Result (Second Order Necessary Conditions)

If x^* is a local minimum of f, then $f'(x^*) = 0$ and $f''(x^*) \geq 0$.

Proof.

By the first order necessary conditions, $f'(x^*) = 0$.
Suppose $f''(x^*) < 0$. Now, $f \in \mathcal{C}^2 \Rightarrow f'' \in \mathcal{C}^0$.
Let $D = (x^* - \delta, x^* + \delta)$ be chosen such that $f''(x) < 0 \quad \forall\, x \in D$.
Therefore, for any $x \in D$, using second order truncated Taylor series,

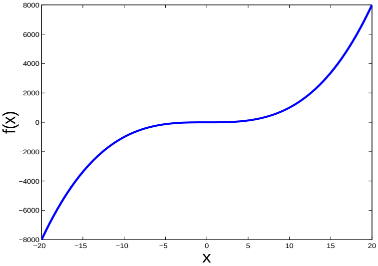
$$f(x) = f(x^*) + f'(x^*)(x - x^*) + \frac{1}{2} f''(\bar{x})(x - x^*)^2 \quad \text{where } \bar{x} \in (x^*, x).$$

Using $f'(x^*) = 0$ and $f''(\bar{x}) < 0 \quad \forall\, x \in D$, we get,

$$f(x) < f(x^*), \quad \text{a contradiction.}$$

Second Order Sufficient Conditions

- Are the second order necessary conditions also sufficient?
  - No
  - Example: min x^3 subject to $x \in \mathbb{R}$
  - At $x^* = 0, f'(x^*) = f''(x^*) = 0$; but x^* is a saddle point!



$$f(x) = x^3$$
$$f'(0) = f''(0) = 0$$

Second Order Sufficient Conditions

Let $f:\mathbb{R}\to\mathbb{R}, f\in\mathcal{C}^2$.
Consider the problem, $\min_{x\in\mathbb{R}} \ f(x)$

Result (Second Order Sufficient Conditions)

If $x^*\in\mathbb{R}$ such that $f'(x^*)=0$ and $f''(x^*)>0$, then x^* is a *strict* local minimum of f over $\mathbb{R}$.

Proof.

$f\in\mathcal{C}^2\Rightarrow f''\in\mathcal{C}^0$.
Let $D=(x^*-\delta,x^*+\delta)$ be chosen such that $f''(x)>0 \quad \forall\, x\in D$.
Therefore, for any $x\in D$, using second order truncated Taylor series,

$$f(x)=f(x^*)+f'(x^*)(x-x^*)+\frac{1}{2}f''(\bar{x})(x-x^*)^2 \quad \text{where } \bar{x}\in(x^*,x).$$

Therefore, $f'(x^*)=0\Rightarrow f(x)-f(x^*)=\frac{1}{2}f''(\bar{x})(x-x^*)^2>0$.
That is, $f(x)>f(x^*) \quad \forall\, x\in D \quad \Rightarrow \quad x^*$ is a strict local minimum.

□

Second Order Sufficient Conditions

Note: Second order sufficient conditions

- guarantee that the local minimum is strict, and
- are *not necessary*. (For $f(x) = x^4$, $x^* = 0$ is a strict local minimum; but $f'(x^*) = f''(x^*) = 0$.)

Sufficient Optimality Conditions

- Let $f : \mathbb{R} \to \mathbb{R}, f \in \mathcal{C}^\infty$.
- Let us assume that f is not a constant function.
- Let the k-th derivative of f at x be denoted by $f^{(k)}(x)$.
- Consider the problem, $\min_{x\in\mathbb{R}} \quad f(x)$.

Result

x^* is a local minimum if and only if the first non-zero element of the sequence $\{f^{(k)}(x^*)\}$ is positive and occurs at even positive k.

Result

Consider the problem, $\max_{x\in\mathbb{R}} \quad f(x)$. x^* is a local maximum if and only if the first non-zero element of the sequence $\{f^{(k)}(x^*)\}$ is negative and occurs at even positive k.

Example 1

- Consider the problem,

$$\min_{x \in \mathbb{R}} \quad (x^2 - 1)^2$$

- Find the stationary points of $f(x) = (x^2 - 1)^2$

$$f'(x) = 0 \Rightarrow 4x(x^2 - 1) = 0 \Rightarrow f'(0) = f'(1) = f'(-1) = 0$$

- Second Derivatives
  - $f''(1) = f''(-1) = 8 > 0 \Rightarrow 1$ and -1 are strict local minima
  - $f''(0) = -4 < 0 \Rightarrow 0$ is a strict local maximum

Example 2

- Consider the problem,

$$\min_{x \in \mathbb{R}} \quad (x^2 - 1)^3$$

- Find the stationary points of $f(x) = (x^2 - 1)^3$

$$f'(x) = 0 \Rightarrow 6x(x^2 - 1)^2 = 0 \Rightarrow f'(0) = f'(1) = f'(-1) = 0$$

- Second Derivative: $f''(x) = 6(x^2 - 1)(5x^2 - 1)$
    - $f''(0) = 6 > 0 \Rightarrow 0$ is a strict local minimum
    - $f''(1) = f''(-1) = 0 \Rightarrow$ Higher order derivatives need to be considered

- Third derivative: $f'''(x) = 12(4x + 1)(x^2 - 1) + 48x^3$

$$\left.\begin{array}{l} f'''(1) = 48 > 0 \\ f'''(-1) = -48 < 0 \end{array}\right\} \Rightarrow 1 \text{ and } -1 \text{ are saddle points}$$

Example 3

- Consider the problem, $\min_{x\in\mathbb{R}} \quad x^4$
- Find the stationary points of $f(x) = x^4$

$$f'(x) = 0 \Rightarrow 4x^3 = 0 \Rightarrow f'(0) = 0$$

- Second Derivative: $f''(x) = 12x^2$
  - $f''(0) = 0$
- Third Derivative: $f'''(x) = 24x$
  - $f'''(0) = 0$
- Fourth Derivative: $f''''(x) = 24$
  - $f''''(0) = 24$
- $f'(0) = f''(0) = f'''(0) = 0, f''''(0) = 24 > 0$
  $\Rightarrow$ 0 is a strict local minimum

Necessity of an Algorithm

- Consider the problem

$$\min_{x \in \mathbb{R}} \ (x-2)^2$$

- We first find the stationary points (which satisfy $f'(x) = 0$).

$$f'(x) = 0 \Rightarrow 2(x-2) = 0 \Rightarrow x^* = 2.$$

- $f''(2) = 2 > 0 \Rightarrow \ x^*$ is a strict local minimum.
- Stationary points are found by solving a nonlinear equation,

$$g(x) \equiv f'(x) = 0.$$

- Finding the real roots of $g(x)$ may not be always easy.
  - Consider the problem to minimize $f(x) = x^2 + e^x$.
  - $g(x) = 2x + e^x$
  - Need an algorithm to find x which satisfies $g(x) = 0$.