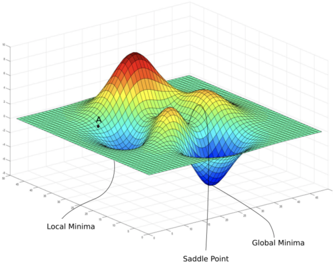
Optimization in Machine Learning

Mathematical Concepts:
Conditions for optimality



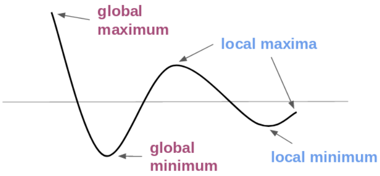
Learning goals

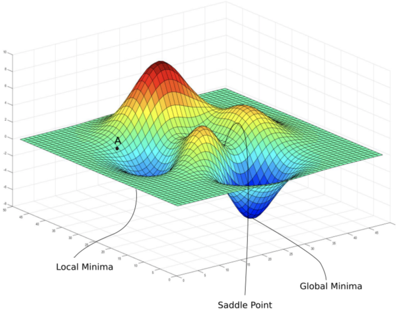
- Local and global optima
- First & second order conditions

DEFINITION LOCAL AND GLOBAL MINIMUM

Given $\mathcal{S} \subseteq \mathbb{R}^d$, $f : \mathcal{S} \to \mathbb{R}$:

- f has **global minimum** in $\mathbf{x}^* \in \mathcal{S}$, if $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{S}$
- f has a **local minimum** in $\mathbf{x}^* \in \mathcal{S}$, if $\epsilon > 0$ exists s.t. $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in B_\epsilon(\mathbf{x}^*)$ ("ϵ"-ball around $\mathbf{x}^*$).





Source (**left**): `https://en.wikipedia.org/wiki/Maxima_and_minima`.

Source (**right**): `https://wngaw.github.io/linear-regression/`.

EXISTENCE OF OPTIMA

We regard the two main cases of $f : \mathcal{S} \to \mathbb{R}$:

- f **continuous**: If $\mathcal{S}$ is **compact**, f attains a minimum and a maximum (extreme value theorem).
- f **discontinuous**: **No general** statement possible about existence of optima.

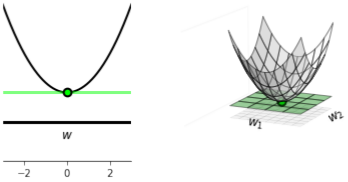
Example: $\mathcal{S} = [0, 1]$ compact, f discontinuous with

$$f(x) = \begin{cases} 1/x & \text{if } x > 0, \\ 0 & \text{if } x = 0. \end{cases}$$

FIRST ORDER CONDITION FOR OPTIMALITY

Observation: At an interior local optimum of $f \in \mathcal{C}^1$, first order Taylor approximation is flat, i.e., first order derivatives are zero.

This condition is therefore **necessary** and called **first order**.



Strictly convex functions (**left:** univariate, **right:** multivariate) with unique local minimum, which is the global one. Tangent (hyperplane) is perfectly flat at the optimum. (Source: Watt, *Machine Learning Refined*, 2020)

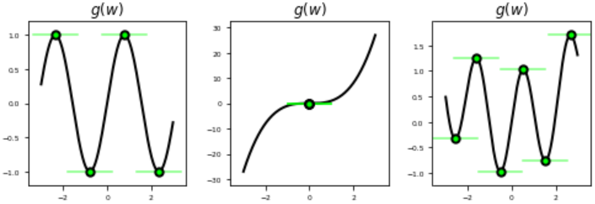
FIRST ORDER CONDITION FOR OPTIMALITY

First order condition: Gradient of f at local optimum $\mathbf{x}^* \in \mathcal{S}$ is zero:

$$\nabla f(\mathbf{x}^*) = (0, \ldots, 0)^T$$

Points with zero first order derivative are called **stationary**.

Condition is **not sufficient**: Not all stationary points are local optima.



Left: Four points fulfill the necessary condition and are indeed optima.
Middle: One point fulfills the necessary condition but is not a local optimum.
Right: Multiple local minima and maxima.
(Source: Watt, 2020, Machine Learning Refined)

SECOND ORDER CONDITION FOR OPTIMALITY

Second order condition: Hessian of $f \in \mathcal{C}^2$ at stationary point $\mathbf{x}^* \in \mathcal{S}$ is positive or negative definite:

$$H(\mathbf{x}^*) \succ 0 \text{ or } H(\mathbf{x}^*) \prec 0$$

Interpretation: Curvature of f at local optimum is either positive in all directions or negative in all directions.

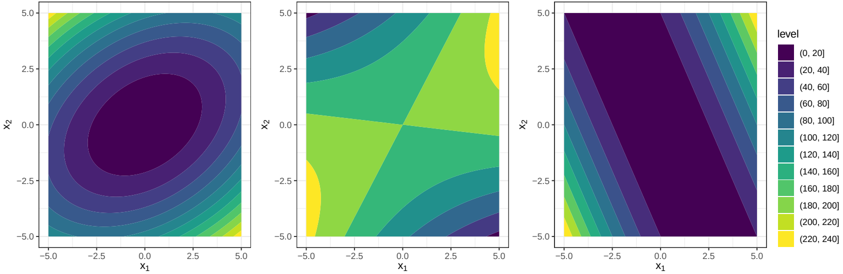
The second order condition is **sufficient** for a stationary point.

Proof: Later.

CONDITIONS FOR OPTIMALITY AND CONVEXITY

Let $f : \mathcal{S} \to \mathbb{R}$ be **convex**. Then:

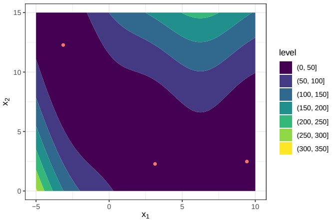
- Any local minimum is **also global** minimum
- If f **strictly convex**, f has **at most one** local minimum which would also be unique global minimum on $\mathcal{S}$

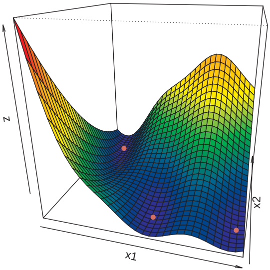


Three quadratic forms. **Left:** $H(\mathbf{x}^*)$ has two positive eigenvalues. **Middle:** $H(\mathbf{x}^*)$ has positive and negative eigenvalue. **Right:** $H(\mathbf{x}^*)$ has positive and a zero eigenvalue.

CONDITIONS FOR OPTIMALITY AND CONVEXITY

Example: Branin function





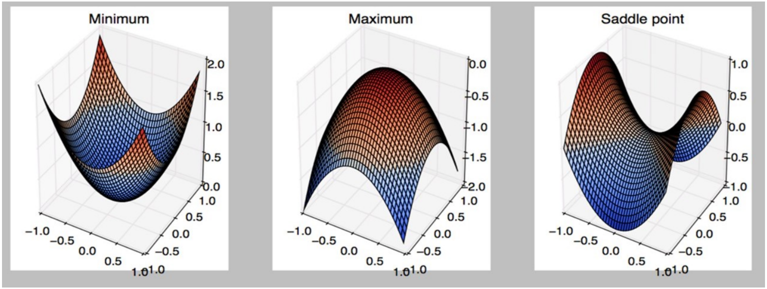
Spectra of Hessians (numerically computed):

	λ_1	λ_2
Left	22.29	0.96
Middle	11.07	1.73
Right	11.33	1.69

CONDITIONS FOR OPTIMALITY AND CONVEXITY

Definition: **Saddle point** at $\mathbf{x}$

- $\mathbf{x}$ stationary (necessary)
- $H(\mathbf{x})$ indefinite, i.e., positive and negative eigenvalues (sufficient)



CONDITIONS FOR OPTIMALITY AND CONVEXITY

Examples:

- $f(x,y) = x^2 - y^2$, $\nabla f(x,y) = (2x, -2y)^T$,
  $H_f(x,y) = \begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix}$
  $\implies$ Saddle point at $(0,0)$ (sufficient condition met)

- $g(x,y) = x^4 - y^4$, $\nabla g(x,y) = (4x^3, -4y^3)^T$,
  $H_g(x,y) = \begin{pmatrix} 12x^2 & 0 \\ 0 & -12y^2 \end{pmatrix}$
  $\implies$ Saddle point at $(0,0)$ (sufficient condition **not** met)