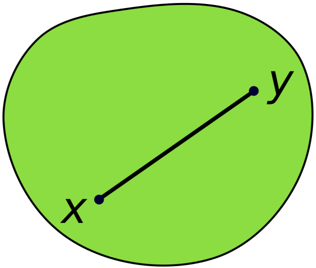
# Optimization in Machine Learning

## Mathematical Concepts
## Convexity

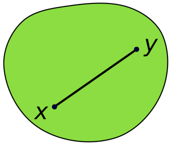


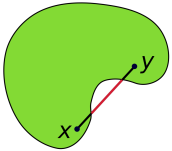

**Learning goals**

- Convex sets
- Convex functions

# CONVEX SETS

- Set $\mathcal{S} \subseteq \mathbb{R}^d$ is convex, if $\forall \boldsymbol{x}, \boldsymbol{y} \in \mathcal{S}$ and $\forall t \in [0, 1]$:
  $\boldsymbol{x} + t(\boldsymbol{y} - \boldsymbol{x}) \in \mathcal{S}$
- Intuition: Line between any $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{S}$ lies entirely in $\mathcal{S}$
- Left: convex set; Right: not convex. (Source: Wikipedia)



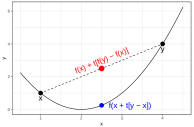



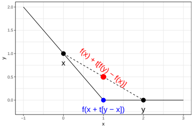
# CONVEX FUNCTIONS

- Let $f : \mathcal{S} \to \mathbb{R}$, $\mathcal{S}$ convex
- $f$ is convex if $\forall \boldsymbol{x}, \boldsymbol{y} \in \mathcal{S}$ and $\forall t \in [0, 1]$:

$$f(\boldsymbol{x} + t(\boldsymbol{y} - \boldsymbol{x})) \leq f(\boldsymbol{x}) + t(f(\mathbf{y}) - f(\boldsymbol{x}))$$

- Intuition: Connecting line for any $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{S}$ above function $f$




Left: Strictly convex function; Right: Convex, but not strictly

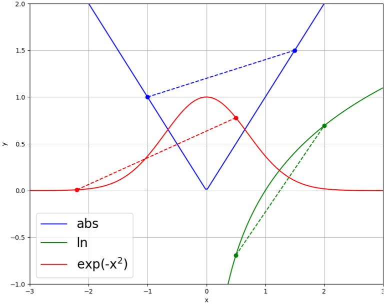
- Strictly convex if $<$ instead of $\leq$
- Concave (strictly) if inequality holds with $\geq$ $(>)$
- NB: $f$ (strictly) concave $\Leftrightarrow -f$ (strictly) convex

# SOME EXAMPLES

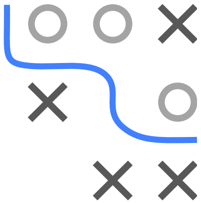
- Convex: $f(x) = |x|$

$$\begin{aligned} f\left(x + t(y - x)\right) &= |x + t(y - x)| = |(1 - t)x + t \cdot y| \\ &\leq |(1 - t)x| + |t \cdot y| = (1 - t)|x| + t|y| \\ &= |x| + t \cdot (|y| - |x|) = f(x) + t \cdot (f(y) - f(x)) \end{aligned}$$

- Concave: $f(x) = \log(x)$
- Neither: $f(x) = \exp(-x^2)$ (but log-concave)



# OPERATIONS PRESERVING CONVEXITY

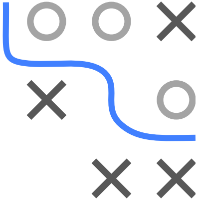


- Nonnegatively weighted summation:
  For $w_1, \dots, w_n \geq 0$ and convex $f_1, \dots, f_n$:
  $w_1 f_1 + \dots + w_n f_n$ is convex
  So: Sum of convex functions is also convex
- Composition: $g$ convex, $f$ linear: $h = g \circ f$ is also convex:

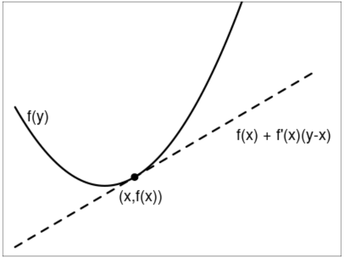
$$
\begin{aligned}
h(\boldsymbol{x} + t(\boldsymbol{y} - \boldsymbol{x})) &= g(f(\boldsymbol{x} + t(\boldsymbol{y} - \boldsymbol{x}))) \\
&= g(f(\boldsymbol{x}) + t(f(\boldsymbol{y}) - f(\boldsymbol{x}))) \\
&\leq g(f(\boldsymbol{x})) + t(g(f(\boldsymbol{y})) - g(f(\boldsymbol{x}))) \\
&= h(\boldsymbol{x}) + t(h(\boldsymbol{y}) - h(\boldsymbol{x}))
\end{aligned}
$$

- Element-wise maximization: $f_1, \dots, f_n$ convex functions:
  $g(\boldsymbol{x}) = \max\{f_1(\boldsymbol{x}), \dots, f_n(\boldsymbol{x})\}$ is also convex

# FIRST ORDER CONDITION



- For differentiable $f$, useful characterisation via gradient
- $f$ convex
  $\Longleftrightarrow$
  $f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})(\boldsymbol{y} - \boldsymbol{x})$ for all $\boldsymbol{x} \neq \boldsymbol{y} \in \mathcal{S}$




- Strictly convex if $>$ instead of $\geq$

# SECOND ORDER CONDITION

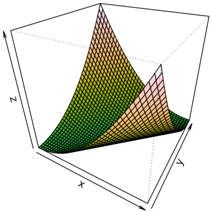
- For $f \in \mathcal{C}^2$: can characterize convexity via Hessian
- $f$ convex $\iff H(\boldsymbol{x})$ psd for $\boldsymbol{x} \in \mathcal{S}\ \forall \boldsymbol{x} \in \mathcal{S}$
- $f$ strictly convex if $H(\boldsymbol{x})$ pd $\forall \boldsymbol{x} \in \mathcal{S}$

- To check global convexity, either verify the direct definition of psd by showing that $\boldsymbol{v}^T H(\boldsymbol{x}) \boldsymbol{v} \geq 0$ for all $\boldsymbol{v} \in \mathbb{R}^d$ and all $\boldsymbol{x}$, or, equivalently, check that all eigenvalues $\lambda_i$ of all $H(\boldsymbol{x})$ satisfy $\lambda_i \geq 0$ for all $\boldsymbol{x} \in \mathcal{S}$

# SECOND ORDER CONDITION

- Example:

$$f(\boldsymbol{x}) = x_1^2 + x_2^2 - 2x_1x_2; \quad \nabla f(\boldsymbol{x}) = \begin{pmatrix} 2x_1 - 2x_2 \\ 2x_2 - 2x_1 \end{pmatrix}^T; \quad H(\boldsymbol{x}) = \begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix}$$




- $f$ is convex since $H(\boldsymbol{x})$ is p.s.d. for all $\boldsymbol{x} \in \mathcal{S}$:

$$\mathbf{v}^T \begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix} \mathbf{v} = 2v_1^2 - 2v_1v_2 - 2v_1v_2 + 2v_2^2$$
$$= 2v_1^2 - 4v_1v_2 + 2v_2^2 = 2(v_1 - v_2)^2 \geq 0$$

# CONVEX FUNCTIONS IN OPTIMIZATION

- Will see later:
- For a convex function, every local optimum is also a global one
  $\Rightarrow$ No need for involved global optimizers, local ones are enough
- A strictly convex function has at most one optimal point
- "... in fact, the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity."
  – R. Tyrrell Rockafellar. *SIAM Review*, 1993

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**LAGRANGE MULTIPLIERS AND OPTIMALITY***

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**Abstract.** Lagrange multipliers used to be viewed as auxiliary variables introduced in a problem of constrained minimization in order to write first-order optimality conditions formally as a system of equations. Modern applications, with their emphasis on numerical methods and more complicated side conditions than equations, have demanded deeper understanding of the concept and how it fits into a larger theoretical picture.

A major line of research has been the nonsmooth geometry of one-sided tangent and normal vectors to the set of points satisfying the given constraints. Another has been the game-theoretic role of multiplier vectors as solutions to a dual problem. Interpretations as generalized derivatives of the optimal value with respect to problem parameters have also been explored. Lagrange multipliers are now being seen as arising from a general rule for the subdifferentiation of a nonsmooth objective function which allows black-and-white constraints to be replaced by penalty expressions. This paper traces such themes in the current theory of Lagrange multipliers, providing along the way a free-standing exposition of basic nonsmooth analysis as motivated by and applied to this subject.

**Key words.** Lagrange multipliers, optimization, saddle points, dual problems, augmented Lagrangian, constraint qualifications, normal cones, subgradients, nonsmooth analysis

**AMS subject classifications.** 49K99, 58C20, 90C99, 49M29