DSC 190

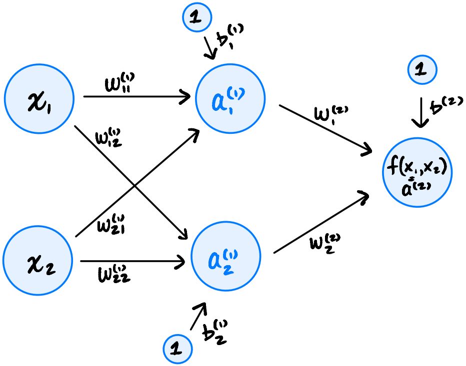
Machine Learning: Representations

Lecture 13 | Part 1

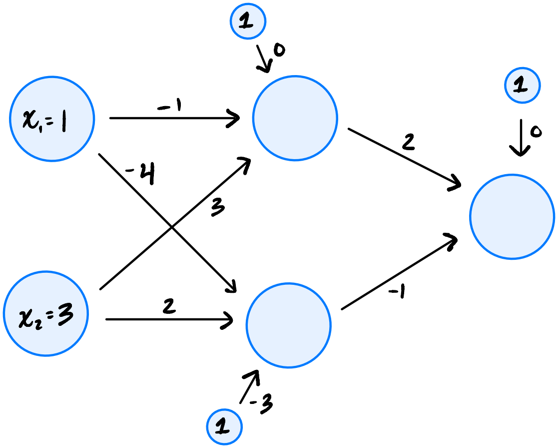
Convexity in 1-d

Neural Networks

A NN is just a function: $f(\vec{x}; \vec{w})$



Example



Learning

- **Given**: a data set $(\vec{x}^{(i)}, y_i)$
- **Find**: weights $\vec{w}$ minimizing some cost function (e.g., expected square loss):

$$C(\vec{w}) = \frac{1}{n}\sum_{i=1}^{n}\left(f(\vec{x}^{(i)};\vec{w}) - y_i\right)^2$$

- **Problem**: there is no closed-form solution

Gradient Descent

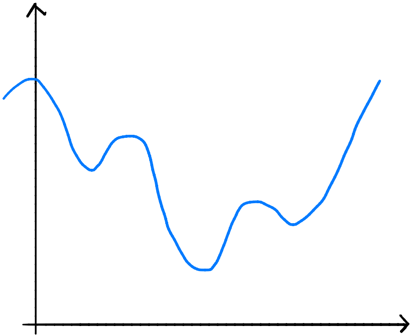
- **Idea**: start at arbitrary $\vec{w}^{(0)}$, walk in direction of gradient:

$$\nabla C = \begin{pmatrix} \frac{\partial C}{\partial w_0} \\ \frac{\partial C}{\partial w_1} \\ \vdots \\ \frac{\partial C}{\partial w_k} \end{pmatrix}$$

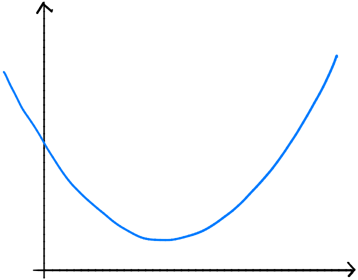
Question

When is gradient descent guaranteed to work?

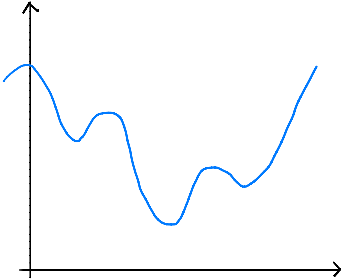
Not here...



Convex Functions



Convex



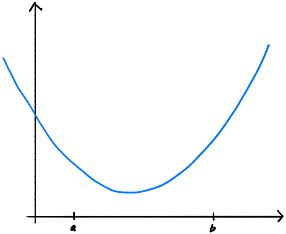
Non-convex

Convexity: Definition

- f is **convex** if for **every** a, b the line segment between

$$(a, f(a)) \qquad \text{and} \qquad (b, f(b))$$

does not go below the plot of f.



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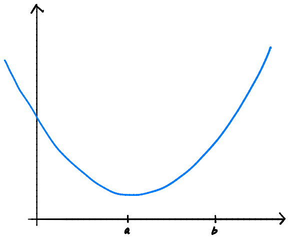

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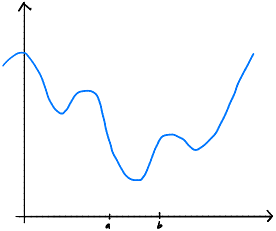

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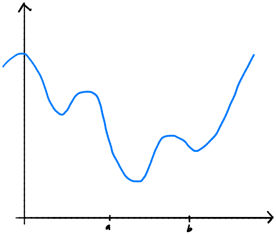


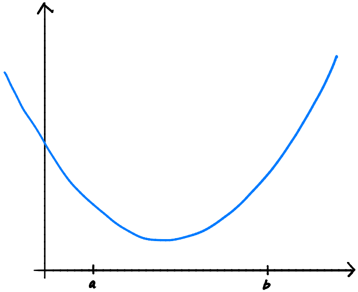
Other Terms

- If a function is not convex, it is **non-convex**.
- **Strictly convex**: the line lies strictly above curve.
- **Concave**: the line lines on or below curve.

Convexity: Formal Definition

- A function $f : \mathbb{R} \to \mathbb{R}$ is **convex** if for every choice of $a, b \in \mathbb{R}$ and $t \in [0, 1]$:

$$(1-t)f(a) + tf(b) \geq f((1-t)a + tb).$$

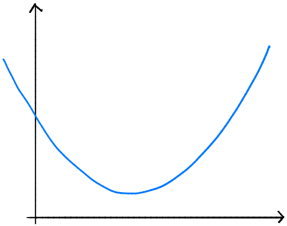


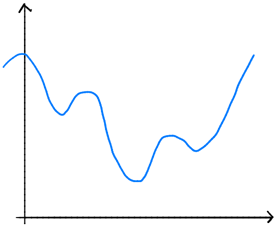
Example

Is $f(x) = |x|$ convex?

Another View: Second Derivatives

- If $\frac{d^2 f}{dx^2}(x) \geq 0$ for all x, then f is convex.
- Example: $f(x) = x^4$ is convex.
- **Warning!** Only works if f is twice differentiable!





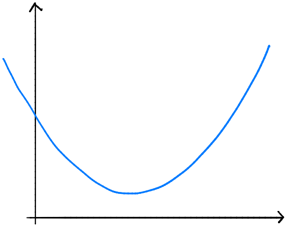
Another View: Second Derivatives

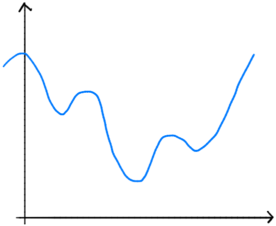
- "Best" straight line at x_0:
  - $h_1(z) = f'(x_0) \cdot z + b$

- "Best" parabola at x_0:
  - At x_0, f looks likes $h_2(z) = \frac{1}{2} f''(x_0) \cdot z^2 + f'(x_0) z + c$
  - Possibilities: upward-facing, downward-facing.

Convexity and Parabolas

- Convex if for **every** x_0, parabola is upward-facing.
  - That is, $f''(x_0) \geq 0$.





Convexity and Gradient Descent

- Convex functions are (relatively) easy to optimize.
- **Theorem**: if $R(x)$ is convex and differentiable[1][2] then gradient descent converges to a **global optimum** of R *provided* that the step size is small enough[3].

[1] and its derivative is not too wild
[2] actually, a modified GD works on non-differentiable functions
[3] step size related to steepness.

Nonconvexity and Gradient Descent

- Nonconvex functions are (relatively) hard to optimize.
- Gradient descent can still be useful.
- But not guaranteed to converge to a global minimum.

DSC 190

Machine Learning: Representations

Lecture 13 | Part 2

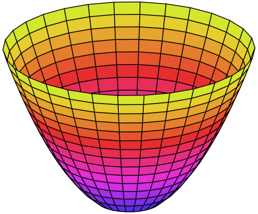
Convexity in Many Dimensions

Convexity: Definition

- $f(\vec{x})$ is **convex** if for **every** $\vec{a}, \vec{b}$ the line segment between

$$(\vec{a}, f(\vec{a})) \qquad \text{and} \qquad (\vec{b}, f(\vec{b}))$$

does not go below the plot of f.



Convexity: Formal Definition

- A function $f : \mathbb{R}^d \to \mathbb{R}$ is **convex** if for every choice of $\vec{a}, \vec{b} \in \mathbb{R}^d$ and $t \in [0, 1]$:

$$(1 - t)f(\vec{a}) + tf(\vec{b}) \geq f((1 - t)\vec{a} + t\vec{b}).$$

The Second Derivative Test

- For 1-d functions, convex if second derivative ≥ 0.
- For 2-d functions, convex if ???

The Hessian Matrix

- Create the **Hessian** matrix of second derivatives:

$$H(\vec{x}) = \begin{pmatrix} \frac{\partial f^2}{\partial x_1^2}(\vec{x}) & \frac{\partial f^2}{\partial x_1 x_2}(\vec{x}) \\ \frac{\partial f^2}{\partial x_2 x_1}(\vec{x}) & \frac{\partial f^2}{\partial x_2^2}(\vec{x}) \end{pmatrix}$$

In General

- If $f : \mathbb{R}^d \to \mathbb{R}$, the **Hessian** at $\vec{x}$ is:

$$H(\vec{x}) = \begin{pmatrix} \frac{\partial f^2}{\partial x_1^2}(\vec{x}) & \frac{\partial f^2}{\partial x_1 x_2}(\vec{x}) & \cdots & \frac{\partial f^2}{\partial x_1 x_d}(\vec{x}) \\ \frac{\partial f^2}{\partial x_2 x_1}(\vec{x}) & \frac{\partial f^2}{\partial x_2^2}(\vec{x}) & \cdots & \frac{\partial f^2}{\partial x_2 x_d}(\vec{x}) \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial f^2}{\partial x_d x_1}(\vec{x}) & \frac{\partial f^2}{\partial x_d^2}(\vec{x}) & \cdots & \frac{\partial f^2}{\partial x_d^2}(\vec{x}) \end{pmatrix}$$

The Second Derivative Test

- A function $f : \mathbb{R}^d \to \mathbb{R}$ is **convex** if for any $\vec{x} \in \mathbb{R}^d$, the Hessian matrix $H(\vec{x})$ is **positive semi-definite**.
- That is, all eigenvalues are ≥ 0