Lecture 8. Function convexity and Gradient descent

COMP 551 Applied machine learning

Yue Li
Assistant Professor
School of Computer Science
McGill University

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Outline

Learning objectives

Understanding the basic ideas of

- Function convexity
- Gradient descent as general algorithm
- Stochastic gradient descent method of momentum
- Adaptive learning rate

Numerical optimization is the workhorse of machine learning algorithms

In this lecture we consider:

- Continuous variables
- Unconstrained
- Convexity testing
- Local optima
- Analytic gradient
- Stochastic
- Smooth error surface

In this lecture we do **not** consider:

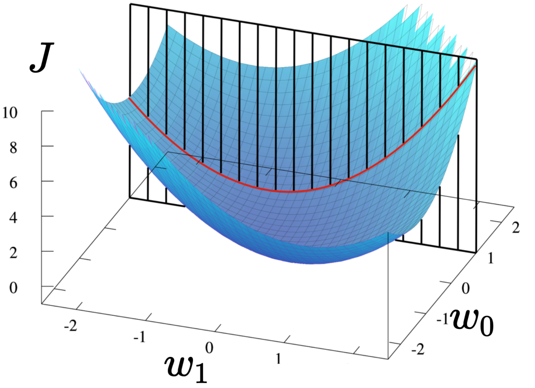
- Discrete variables
- Constrained (next lecture)
- Global optima
- Proximal gradient
- Analytic Hessian
- Non-smooth error surface

Gradients

For a cost function involving multiple variables, gradient is the partial derivative of the function w.r.t. each variable while fixing other variable.

For example, in a two-variable regression, the gradient of the coefficient w_1 is:

$$\frac{\partial}{\partial w_1} J(w_0, w_1) = \lim_{\epsilon \to 0} \frac{J(w_0, w_1 + \epsilon) - J(w_0, w_1 - \epsilon)}{2\epsilon}$$



Gradients

In a more generally of D variables setting, we have

$$\frac{\partial}{\partial w_d} J(w_0, w_1, \ldots, w_{D-1}) = \lim_{\epsilon \to 0} \frac{J(w_d + \epsilon, \mathbf{w}_{\setminus d}) - J(w_d - \epsilon, \mathbf{w}_{\setminus d})}{2\epsilon}$$

where $\mathbf{w}_{\setminus d}$ denotes all coefficients except for coefficient w_d.
Gradients in matrix notation:

$$\nabla J(\mathbf{w}) = \begin{bmatrix} \frac{\partial}{\partial w_0} J(\mathbf{w}) \\ \frac{\partial}{\partial w_1} J(\mathbf{w}) \\ \vdots \\ \frac{\partial}{\partial w_{D-1}} J(\mathbf{w}) \end{bmatrix}$$

General gradient descent algorithm

Gradient descent is an iterative algorithm for optimization.

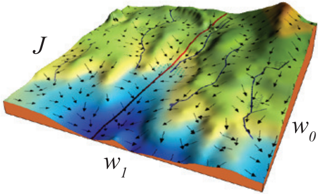
Algorithm 1 GradientDecent($\alpha = 0.005$, Convergence Criteria)

1: Initialize coefficients $\mathbf{w}^{(0)}$
2: **while** convergence criterion is not met **do**
3: $\quad \mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \alpha \nabla J(\mathbf{w})$ // *update using gradient*
4: **end while**

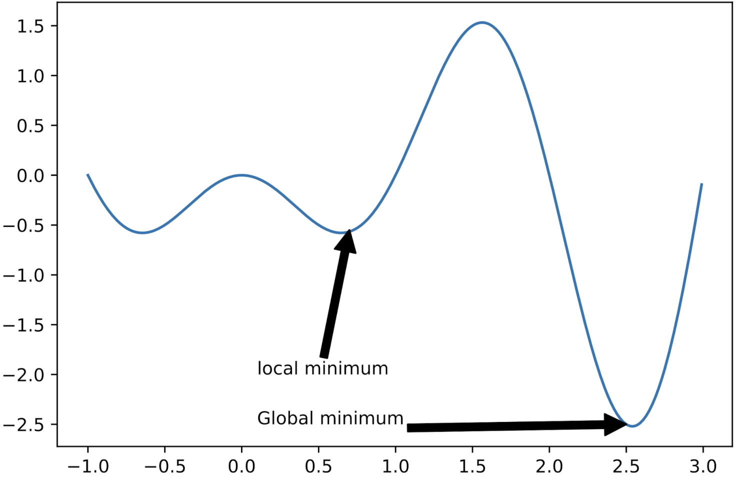
where

- $\mathbf{w}^{(t)}$: weights at the t^{th} iteration
- α: learning rate
- $\nabla J(\mathbf{w}) = \left[\frac{\partial}{\partial w_0} J(\mathbf{w}), \frac{\partial}{\partial w_1} J(\mathbf{w}), \ldots \frac{\partial}{\partial w_{D-1}} J(\mathbf{w})\right]^\top$ are the gradients

Steepest decent into a *global or local optimum* of the error surface



How to determine if we can always find *the global optimum* not local optimum given a loss function?

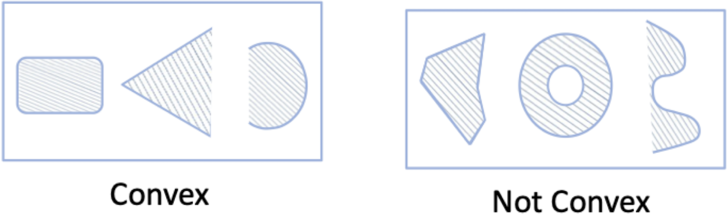


Convex sets

$\mathcal{S}$ is a **convex sets** if, for any $\mathbf{x}, \mathbf{x}' \in \mathcal{S}$, we have

$$\lambda \mathbf{x} + (1-\lambda)\mathbf{x}' \in \mathcal{S}, \forall \lambda \in [0,1]$$

In English: if we draw a line from $\mathbf{x}$ to $\mathbf{x}'$, all points on the line lie inside the set.

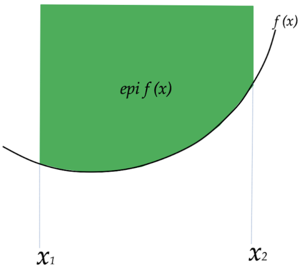


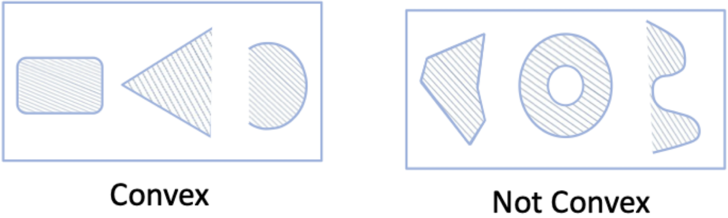
Convex functions

- *epigraph* is defined by a set of points above the function
- A function $f(\mathbf{x})$ is *convex* if its epigraph is a convex set
- Equivalently, a function $f(\mathbf{x})$ is convex if

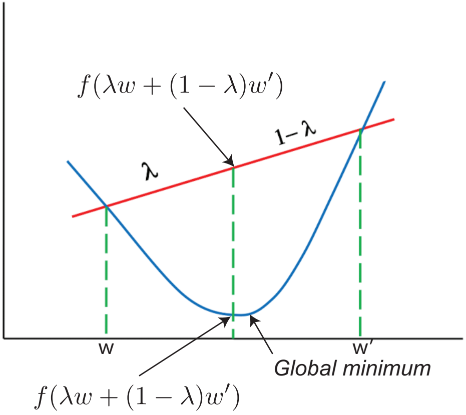
$$f(\lambda w + (1-\lambda)w') \leq \lambda f(w) + (1-\lambda) f(w')$$

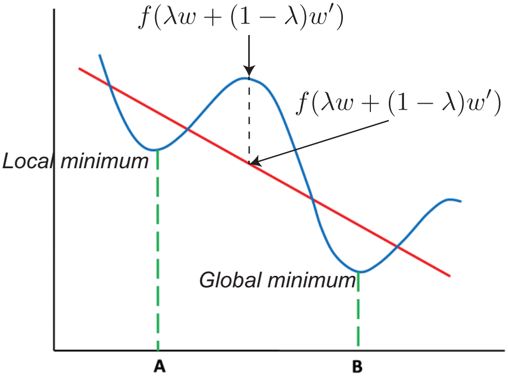
where $f(\lambda w + (1-\lambda)w')$ are points on the curve and $\lambda f(w) + (1-\lambda) f(w')$ are points on the red line



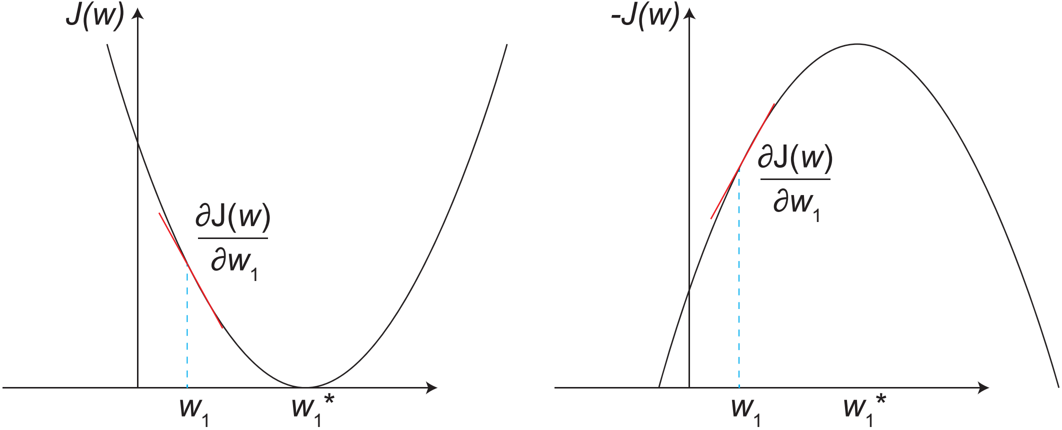


Examples of a convex and a non-convex function





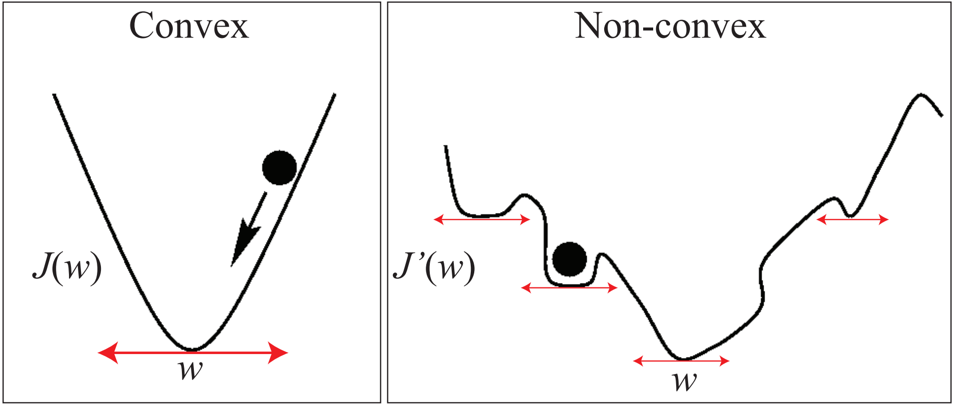
Negative of a convex function is a concave function



For example, minimizing sum of squared error is a convex function and its negative is a concave function and is equivalent to the log likelihood of a Gaussian (Lec 5).

Why do we care about convexity?

- Gradient descent (GD) can find the global minimum on a convex function.
- GD on a non-convex function may find local minimum (i.e., ultimately resulting in low prediction accuracy)



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Recognizing convex functions

The principled way to test whether a function $f(x)$ is convex is by taking the second order derivative of the function:

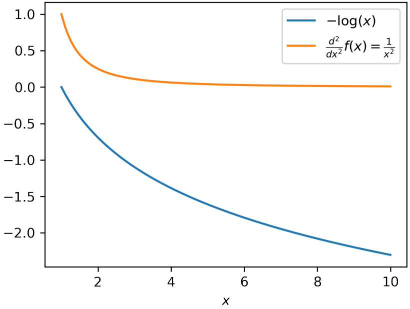
$$\frac{\partial}{\partial x}\frac{\partial f(x)}{\partial x} = \frac{\partial^2 f(x)}{\partial x^2} \equiv \nabla^2 f(x)$$

For example, the first-order derivative of the negative natural log function $f(x) = -\log(x)$ is:

$$\frac{\partial f(x)}{dx} = -\frac{1}{x}$$

and its second-order derivative is:

$$\frac{d^2 f(x)}{dx^2} = \frac{1}{x^2}$$



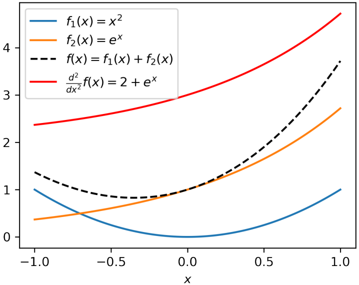
which is *always positive* for $\forall x \in \mathbb{R}$.

Some more examples of 1d convex functions $f(x)$: $-\sqrt{x}$, x^2, e^x, $x\log(x)$

Sum and max of convex functions are still convex functions

Sum of convex functions is convex.

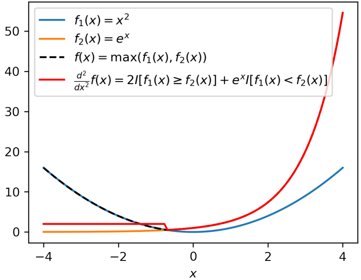
- Example 1. $f_1(x) = x^2$ and $f_2(x) = e^x$ are both convex and $f(x) = f_1(x) + f_2(x)$ is also convex.



- Example 2. sum of squared errors is a convex function: $J(\mathbf{w}) = ||\mathbf{X}\mathbf{w} - y||_2^2 = \sum_n (\mathbf{x}^{(n)}\mathbf{w} - y^{(n)})^2$

Maximum of convex functions is convex.

- Example 1. $f_1(x) = x^2$ and $f_2(x) = e^x$ are convex, $f(x) = \max(f_1(x), f_2(x))$ is also convex.



- Example 2. $f_1(y) = y^4$ is convex and maximum of $f_1(y)$ is also convex:

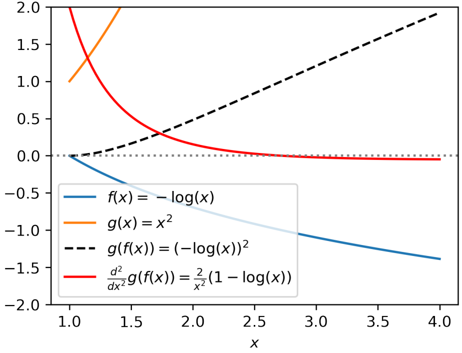
$$f(y) = \max_{x \in [0,2]} x^3 y^4 = 8y^4$$

Composition of convex functions may or may not be convex

For example, $f(x) = -\log(x)$ and $g(x) = x^2$ are convex but not:

$$g(f(x)) = (-\log(x))^2$$

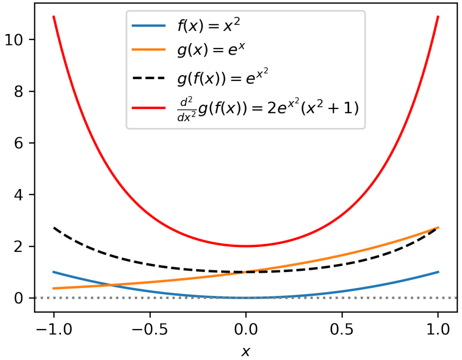
$$\nabla^2 g(f(x)) = \frac{2}{x^2}(1 - \log(x)) < 0 \text{ if } x > e$$



If $f(x)$, $g(x)$ are convex, and $g(x)$ is **non-decreasing**, then $g(f(x))$ is convex. e.g.,

$$f(x) = x^2, g(x) = e^x, g(f(x)) = e^{x^2}$$

$$\nabla^2 g(f(x)) = 2e^{x^2}(x^2 + 1) > 0 \, \forall x \in \mathbb{R}$$



Verify if cross-entropy is a convex functions

Coming soon . . .

Summary

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